Inhaltsverzeichnis • Contents

Kapitel 1

Wissenschaftliche Arbeit und ihre Organisation am Institut- ein Überblick

1.1 Institutsgeschichte und -entwicklung

1992-1994 • Das Max-Planck-Institut für Physik komplexer Systeme wurde auf Beschluss des Senats der Max-Planck-Gesellschaft im November 1992 gegründet und *Prof. Fulde* (Stuttgart) als Gründungsdirektor berufen. Das Gründungskonzept sah für das Institut drei wissenschaftliche Abteilungen sowie ein großes Gästeprogramm vor, mit dessen Hilfe ein Seminar- und Workshop-Programm wesentlicher Teil der Institutsarbeit werden sollte. Das Programm soll es möglich machen, neue weltweite Entwicklungen auf dem breiten Gebiet der Physik komplexer Systeme aufzugreifen, und den Nachwuchs der Hochschulen früher als bisher mit diesen Entwicklungen bekannt zu machen. Hierdurch erfährt die Entwicklung der theoretischen Physik in wichtigen Teilbereichen eine besondere Förderung.
Aufgrund des günstigen wissenschaftlichen Umfelds und der guten Verkehrsanbindung wurde Dresden als Standort für das neue Institut ausgewählt. Da dort anfangs keine entsprechenden Räumlichkeiten zur Verfügung standen, erfolgte der Arbeitsbeginn am 1. Juli 1993 in Stuttgart. Im Januar 1994 konnte die Arbeit in Dresden aufgenommen werden, wofür die TU Dresden trotz eigener Raumnot in dankenswerter Weise eine Baracke in der Bayreuther Straße in unmittelbarer Nähe der Universität zur Verfügung stellte. Das Institut wurde am 2. Mai 1994 von Prof. Dr. H. Zacher, dem Präsidenten der Max-Planck-Gesellschaft, eingeweiht. Sowohl das Land Sachsen als auch die Stadt Dresden haben durch ihre Hilfe und Unterstützung den zügigen Aufbau des Instituts sehr erleichtert. So stellte die Stadt Dresden unentgeltlich eine Villa mit ungeklärten Eigentumsverhältnissen zwischenzeitlich zur Verfügung. Zusätzlich wurden verschiedene Räumlichkeiten in unmittelbarer Nachbarschaft in Ergänzung zu den nur begrenzt vorhandenen Arbeitsräumen angemietet. Die Verwaltung unter Leitung von *Frau I. Auguszt* konnte mit der Arbeit beginnen, Gäste wurden eingeladen und der erste Workshop fand im März 1994 statt.
Mit nachdrücklicher Unterstützung von Präsident Zacher konnten zur Verbreiterung der wissenschaftlichen Basis in kürzester Zeit Nachwuchsgruppen gegründet werden. 1995 wurde die erste selbständige Nachwuchsgruppe *Nichtlineare Zeitreihenanalyse* un-

ter der Leitung von *Dr. H. Kantz* ins Leben gerufen. Im gleichen Jahr nahm *Dr. M. Bär* als Leiter der Nachwuchsgruppe *Strukturbildung* seine Arbeit auf. Im Januar 1996 begann *Dr. K. Richter* mit dem Aufbau einer Gruppe auf dem Gebiet *Mesoskopische Systeme*. Dem folgte die Gruppe *Quantenchemie* unter der Leitung von *Dr. M. Dolg*.
1995-1998 • Als Sieger eines eingeladenen Architekturwettbewerbes für den Institutsneubau mit Gästehäusern ging das Architekturbüro Brenner und Partner (J. Wittfoht, Stuttgart) hervor, dessen Entwurf ab September 1995 am Standort Nöthnitzer Straße realisiert wurde. Nach knapp zweijähriger Bauzeit wurden das neue Institutsgebäude und die drei Gästehäuser am 23./24.9.1997 im Zusammenhang mit dem gleichzeitig stattfindenden Symposium *Complexity in Physics* feierlich eingeweiht. Zu dieser Zeit war das Seminar- und Gästeprogramm bereits auf gutem Weg, seine vorgesehene Größe zu erreichen. Mehrere hundert Wissenschaftler waren bis dahin bereits am Institut zu Gast.
1999-2000 • *Dr. J. M. Rost* (Freiburg) wurde im Dezember 1998 zum Direktor der zweiten Abteilung des Instituts berufen und begann im Mai 1999 mit dem Aufbau seiner Abteilung *Endliche Systeme*. *Dr. A. Buchleitner* (Garching) konnte als Leiter der Arbeitsgruppe *Nichtlineare Dynamik in Quantensystemen* gewonnen werden. Nachdem *Dr. Dolg* im Jahr 2000 an die Universität Bonn berufen wurde, nahm *Dr. U. Birkenheuer* (TU München) als Nachfolger im März 2000 die Arbeit auf. *Dr. K. Richter* nahm einen Ruf an die Universität Regensburg an, woraufhin die Arbeit der Nachwuchsgruppe *Mesoskopische Systeme* endete. Dieses Fachgebiet wurde in modifizierter Form von *Dr. H. Schomerus* (Leiden) weiter gepflegt, der im November 2000 mit dem Aufbau einer Nachwuchsgruppe *Wellen in komplexen Medien* begann.
2001-2002 • Um am Institut den immer wichtiger werdenden Bereich zwischen Physik und Biologie anzusiedeln, wurde im Jahr 2001 *Dr. F. Jülicher* (Paris) an das Institut berufen, so dass im Dezember 2001 mit dem Aufbau der dritten Abteilung *Biologische Physik* begonnen wurde. In der zweiten Jahreshälfte 2002 erfuhr die Abteilung *Biologische Physik* mit den neuen Arbeitsgruppen *Physik biologischer und weicher Materie* unter Leitung von *Dr. R. Everaers* (Mainz) sowie *Biologische Physik des Geruchsinns*, geleitet von *Dr. M. Zapotocky* (New York), eine weitere inhaltliche wie organisatorische Akzentuierung. Auch die Abteilung *Endliche Systeme* gewann mit *Dr. A. Becker* (Bielefeld) einen weiteren Gruppenleiter, dessen Gruppe auf dem Gebiet *Nichtlineare Prozesse in starken Laserfeldern* forscht.
2003-2004 • Im darauffolgenden Jahr 2003 begann *Dr. S. Kümmel* (New Orleans) mit dem Aufbau einer Emmy Noether-Gruppe auf dem Gebiet der *Elektronischen Struktur endlicher Systeme*. Im Oktober 2004 gründete *Dr. K. Kruse* (Dresden) eine Nachwuchsgruppe *Physik der Zellteilung*. Dies war die erste von drei Nachwuchsgruppen im Rahmen eines Forschungsprogramms *Physik biologischer Systeme*, das gemeinsam mit dem Max-Planck-Institut für molekulare Zellbiologie und Genetik initiiert wurde. Eine zweite Nachwuchsgruppe dieses gemeinsamen Forschungsprogramms *Mechanik der Zellteilung* wurde Ende 2004 von *Dr. I.M. Tolic-Norrelykke* (Firenze) gegründet. Frau Tolic-Norrelykke arbeitet experimentell am MPI-CBG. *Dr. M. Bär* wechselte im Oktober 2004 zur Physikalisch-Technischen Bundesanstalt nach Berlin als Abteilungsleiter. Im Jahr 2004 begann die Arbeit an einer Erweiterung des Institutsgebäudes, das wegen des Wachstums des Instituts nötig geworden war.
2005-2006 • *Dr. S. Kümmel* und *Dr. H. Schomerus* nahmen Rufe an die Universität Bayreuth bzw. an die Lancaster University im Jahr 2005 an. *Dr. M. Hentschel* (Re-

gensburg) begann mit dem Aufbau einer Emmy Noether-Gruppe *Vielteilcheneffekte in mesoskopischen Systemen*. *Dr. S. Grill* (Berkeley) vervollständigte das gemeinsame Forschungsprogramm des mpipks und des MPI-CBG als Leiter einer aufzubauenden Nachwuchsgruppe *Motor Systeme*. Seine Gruppe ist an beiden Instituten beheimatet und betreibt sowohl theoretische als auch experimentelle Forschungsarbeiten. Die Internationale Max Planck Research School *Dynamical Processes in Atoms, Molecules and Solids* begann ihre Arbeit im Jahr 2005. Dieses Programm bringt Doktoranden aus vielen Ländern nach Dresden und wird vom mpipks in Zusammenarbeit mit der Technischen Universität Dresden, dem Max-Planck-Institut für Chemische Physik fester Stoffe, dem Leibnitz-Institut für Festkörper- und Materialforschung Dresden, dem Forschungszentrum Rossendorf, sowie dem Institut für Tieftemperatur- und Strukturforschung der polnischen Akademie der Wissenschaften in Wrocław geleitet. Der Institutsanbau wurde Ende 2005 fertiggestellt. Dem Institut stehen seitdem 35 neue Arbeitsplätze sowie Seminar- und Besprechungsräume und Kommunikationsbereiche zur Verfügung. Im Jahr 2006 nahmen *Dr. K. Kruse* und *Dr. R. Everaers* Rufe auf Professuren an der Universität Saarbrücken bzw. an der Ecole normale Superieure in Lyon an.
Ständig forschen etwa 50-100 Langzeitgäste am Institut, neben jährlich 1200-1500 Gästen, die an verschiedenen Seminaren und Workshops teilnehmen.
Ein seit 1995 bestehendes Kuratorium pflegt die Beziehungen zum Land Sachsen, zur Stadt Dresden und zahlreichen wissenschaftlichen Einrichtungen. Die Entwicklung des Instituts wird seit Juni 1996 von einem wissenschaftlichen Beirat begleitet.

1.2 Forschungsschwerpunkte und Organisation

Das Institut vertritt die Physik komplexer Systeme von der klassischen Physik bis zur Quantenphysik in drei Schwerpunkten, geformt durch die Forschung der drei permanenten Abteilungen:

- In der Quantenphysik forscht die Abteilung *Elektronische Korrelationen* von *Prof. Fulde* auf dem Gebiet der kondensierten Materie.
- Mit Hilfe semiklassischer Methoden studiert die Abteilung *Endliche Systeme* von *Prof. Rost* nichtlineare Phänomene in der Dynamik von Atomen, Molekülen und Clustern.
- In der klassischen Physik widmet sich die Abteilung *Biologische Physik* von *Prof. Jülicher* biologischen Themen mit Mitteln der statistischen Physik.

Darüber hinaus verstärken vier Arbeitsgruppen die Forschungsarbeit in den Abteilungen. Zwei weitere Gruppen interpolieren und ergänzen die Schwerpunkte:

- Die Emmy Noether-Gruppe *Vielteicheneffekte in mesoskopischen Systemen* von *Dr. M. Hentschel* ist ein Bindeglied zwischen den Abteilungen *Elektronische Korrelationen* und *Endliche Systeme*.
- Die einzige permanente Arbeitsgruppe am Institut unter Leitung von *Prof. Kantz* vertritt die *Zeitreihenanalyse*. Oft kommen hierbei Methoden des klassischen Chaos zum Einsatz, welche auch in anderer Weise für semiklassische Fragestellungen eine wichtige Rolle spielen.

Ein gemeinsames Programm der Max-Planck-Institute für Physik komplexer Systeme und für molekulare Zellbiologie und Genetik zum Thema *Physik biologischer Systeme* besteht aus drei interagierenden Nachwuchsgruppen, die in enger Zusammenarbeit verschiedene Aspekte zellulärer Systeme untersuchen und dabei die Kompetenzen beider Institute zusammenführen:

- Die von *Dr. K. Kruse* geleitete Theorie-Nachwuchsgruppe *Physik der Zellteilung* bestand bis zum Sommer 2006 am mpi**pks**.
- Die Nachwuchsgruppe *Motor Systeme* unter der Leitung von *Dr. S. Grill* ist an beiden Instituten beheimatet und betreibt sowohl theoretische als auch experimentelle Forschung.
- Eine dritte experimentelle Gruppe *Inneres Design der Zelle* unter der Leitung von Dr. I. M. Tolic-Norrelykke befindet sich am MPI-CBG.

1.3 Workshop- und Gästeprogramm

Eine zentrale Aufgabe des Instituts ist die Durchführung von internationalen *Workshops und Seminaren* (S. 168). Hinsichtlich dieser Funktion nimmt das mpi**pks** eine Sonderstellung innerhalb der MPG ein. Ein kleiner, aber effizienter Mitarbeiterstab unter der Leitung von *Dr. S. Flach* übernimmt die logistische Organisation der Veranstaltungen und berät die in der Regel externen wissenschaftlichen Organisatoren bei der Planung und Durchführung ihrer Veranstaltung.

Das *Gästeprogramm* (S. 158) bietet Forschungsaufenthalte am Institut, die von wenigen Wochen bis zu zwei Jahren reichen können. Die Wissenschaftler haben mannigfache Möglichkeiten der Zusammenarbeit, indem sie sich einer der bestehenden Gruppen am Institut anschließen, mit anderen Gästen gemeinsam forschen, oder Forschungspartner bei einem der zahlreichen Workshops/Seminare finden. Darüber hinaus besteht auch die Möglichkeit, mit Partnern lokal an der TU Dresden oder einer der vielen anderen Forschungseinrichtungen in Dresden zu kooperieren. Von dieser Möglichkeit wird auch rege Gebrauch gemacht, wie die Veröffentlichungen dokumentieren (S. 217).
Vorschläge für Workshops/Seminare sowie die Bewerbungen für Gastaufenthalte werden von je einem Komitee evaluiert. Beide Komitees sind mit externen Wissenschaftlern und Vertretern des Instituts besetzt.
Zur weiteren Strukturierung des Gästeprogramms vergibt das mpi**pks** seit 2000 das *Martin-Gutzwiller-Fellowship* jährlich an einen international angesehenen erfahrenen Wissenschaftler. Mit ihm forschten *Prof. L. S. Schulman* (Potsdam, NY) 2005 und *Prof. S. L. Tomsovic* (Pullman) 2006 jeweils bis zu einem akademischen Jahr am Institut (S. 163).
Ferner schreibt das mpi**pks** jedes Jahr ein *PKS-Distinguished Postdoctoral-Fellowship* aus. Hiermit sollen hervorragende Nachwuchswissenschaftler mit einiger Forschungserfahrung angesprochen werden (S. 159).
Im Jahr 2006 beschloss das Institut, jedes Jahr eine *Advanced Study Group* zu etablieren. Im Rahmen dieser Aktivität werden 3-5 erfahrene Wissenschaftler gemeinsam während eines Jahres ein Forschungsprogramm auf dem Gebiet der Physik komplexer Systeme am mpi**pks** umsetzen. Die erste *Advanced Study Group 2007* wird ihre Arbeit voraussichtlich im März 2007 aufnehmen.

1.4 Lehre und Ausbildung

Das Institut strebt eine umfassende Weiterbildung junger Wissenschaftler an. Dies gilt selbstverständlich für die Forschung, aber auch für Lehre und Forschungsorganisation.
Lehre • Hierbei handelt es sich nicht nur um traditionelle Vorlesungen, die sowohl an der TU Dresden als auch an anderen Universitäten von Institutsmitarbeitern gehalten werden (S. 201). Vielmehr bietet sich im Rahmen der Öffentlichkeitsarbeit die Möglichkeit, Lehrerfahrung in Veranstaltungen für Lehrer und Schüler, sowohl am Institut als auch an den Schulen (S. 204), zu sammeln.
International Max-Planck Research School • Seit 2005 betreibt unser Institut die IMPRS *Dynamical Processes in Atoms, Molecules and Solids* in Zusammenarbeit mit der TU Dresden, dem Max-Planck-Institut für Chemische Physik fester Stoffe, dem Forschungszentrum Rossendorf, dem Leibniz-Institut für Festkörper und Werkstoffforschung sowie dem Institut für Tieftemperaturphysik in Wrocław, Polen. Die IMPRS zieht Doktoranden aus vielen Ländern an und bietet eine strukturierte Doktorandenausbildung mit einem umfangreichen Kursprogramm. Desweiteren ist unser Institut als externer Knoten an die IMPRS *Molecular Cell Biology and Bioengineering* angeschlossen, die vom MPI für Molekulare Zellbiologie und Genetik organisiert wird.
Forschungsorganisation • Durch unser großes Workshop-/Seminarprogramm haben wir die einmalige Chance, auch Training im Organisieren von Tagungen bieten zu können. Von 34 Veranstaltungen in den Jahren 2005-2006 (S. 168) waren bei einem Sechstel (6)

junge Wissenschaftler des mpipks Mitorganisatoren. Das hat für unsere Nachwuchswissenschaftler einen Ausbildungs- und Profilierungseffekt und erleichtert den externen Organisatoren die Arbeit, da sie einen Wissenschaftler als direkten Ansprechpartner am Institut haben.

1.5 Öffentlichkeitsarbeit

Das Institut sieht sich als eine Plattform für das Entstehen, den Austausch und die Weiterentwicklung kreativer Ideen in der Forschung. Dies betrifft in erster Linie die Wissenschaftler, schließt aber auch insbesondere potentielle zukünftige Wissenschaftler, also Schüler, sowie die wissenschaftlich interessierte Bevölkerung mit ein. Im Rahmen unseres Schul-Kontakt-Programms bieten wir von Workshops für Lehrer über mehrtägige Winterschulen für Schüler bis hin zu Vorträgen an den Schulen vielfältige Möglichkeiten, die Faszination aktueller Forschung hautnah zu erleben. Für die interessierte Bevölkerung organisiert das Institut in Zusammenarbeit mit der Universität und der Stadt seit 1999 die Vortragsreihe *Wissenschaft im Rathaus*, in der prominente Wissenschaftler aktuelle Forschung bürgernah erläutern (S. 204). Außerdem ermutigen wir die Organisatoren von Workshops, einen öffentlichen Abendvortrag im mpipks anzubieten. 2006 wurde Dresden zur "Stadt der Wissenschaft" gekürt. Diese Ehrung wird vom Stifterverband der Wirtschaft vergeben. Das Institut beteiligte sich an dieser Gemeinschaftsaktion der Dresdner Forschungslandschaft mit zahlreichen Veranstaltungen.

1.6 Vernetzung der Forschung

Lokal • Das mpipks befindet sich inmitten vielfältiger Forschungsaktivitäten, die von der Technischen Universität Dresden und zahlreichen außeruniversitären Forschungseinrichtungen getragen werden. Mit der Fachrichtung Physik der TU Dresden gibt es einen wissenschaftlichen Dialog, der sich in zwei gemeinsamen Seminaren (*Quantum Dynamics* mit Prof. Schmidt und *Complex Systems* mit Prof. Ketzmerick) niederschlägt sowie einer Zusammenarbeit mit Frau Prof. Schwille. Das mpipks kooperiert besonders eng mit dem Institut für Theoretische Physik sowie mit dem Institut für Biophysik im Fachbereich Physik. Außerdem sind Wissenschaftler des Instituts an zwei Sonderforschungsbereichen beteiligt (S. 199). Eine Zusammenarbeit besteht weiterhin durch die Abteilung *Elektronische Korrelationen* mit dem IFW und dem benachbarten MPI für Chemische Physik fester Stoffe. Über die Abteilung Biologische Physik ist das Institut an einem gemeinsamen Forschungsprogramm mit dem MPI für Molekulare Zellbiologie und Genetik beteiligt. Desweiteren bestehen enge Verbindungen zum Biotechnologischen Zentrum und zum Center for Regenerative Therapies, der im Jahr 2006 gegründet wurde. Die Abteilungen *Endliche Systeme* und *Elektronische Korrelationen* arbeiten eng mit dem Forschungszentrum Rossendorf zusammen.
National und International • Die Auflistung der vielfachen internationalen und nationalen Kontakte findet sich in den folgenden Darstellungen der Arbeitsgruppen. Weiterhin verfügt das Institut über ein kleines Budget, aus dem Zusammenarbeit mit experimentellen Gruppen gefördert wird (S. 166).

1.7 Kurzdarstellung der Arbeitsgruppen

Abteilung: Elektronische Korrelationen
(Leiter: Prof. Dr. P. Fulde)

Das Hauptarbeitsgebiet in der Abteilung sind elektronische Korrelationen im weitesten Sinn in Festkörpern und Molekülen. Hinzu kommen ultrakalte Gläser, Spintransport etc.
Die Berechnung von Grundzustandswellenfunktionen von Festkörpern unter quantitativer Berücksichtigung elektronischer Korrelationen sowie derer Energiebänder nehmen nach wie vor einen angemessenen Platz ein. Das geschieht mit Hilfe lokaler quantenchemischer Methoden. Diese ab initio Verfahren sind bezüglich der verwendeten Näherungen vollkommen kontrolliert und willkürfrei. Es ist deshalb lohnend, diese Methoden weiter zu entwickeln, als Alternative zu Dichtefunktionalsrechnungen - trotz deren großer Erfolge und starker Dominanz. Denn insbesondere bei stark korrelierten Elektronensystemen wird man von diesem, auf Wellenfunktionen beruhenden, Weg viel lernen können. Ein schönes Beispiel dafür ist das erfolgreich entwickelte Duale Modell zur Beschreibung von $5f$ Elektronen.
Bisher wurden große Teile dieser Arbeiten in der Arbeitsgruppe Quantenchemie betrieben. Nach Ablauf der vorgesehenen 5 Jahre wurde die Gruppe aufgelöst. Ein Teil der Aktivitäten, die zuvor in der Abteilung angesiedelt waren, wurden dabei zurückverlegt. Was die Berechnung von Grundzustandswellenfunktionen betrifft, so wurden von B. Paulus in Zusammenarbeit mit N. Gaston und K. Rosciszewski hauptsächlich Metalle untersucht (Hg, Cd, Zn). Diese sind viel schwieriger zu behandeln als Isolatoren oder Halbleiter. Sehr zufriedenstellende Resultate für die Bindungsenergie, Gitterkonstante und Elastizitätsmodul wurden erhalten. Daneben wurde mit CeO_2 auch ein technisch interessanter Festkörper (Katalysator) untersucht (E. Voloshina). Die Gruppe ist am Schwerpunktprogramm der DFG über ab initio Methodenentwicklungen für Mehrelektronensysteme in Chemie und Physik beteiligt und wird auch von diesem finanziell gefördert.
Bei der Berechnung von Energiebändern und Energiegaps liegen jetzt Ergebnisse für MgO vor, die sich relativ leicht auf weitere Systeme erweitern lassen (L. Hozoi). Statt vom Programmpaket CRYSTAL zu starten und dann aus dessen Lösungen lokalisierte Orbitale zu konstruieren, sind wir in Zusammenarbeit mit A. Shukla dabei, die Rechnungen auf das von ihm entwickelte Programmpaket WANNIER umzustellen. Dazu muss noch eine Schnittstelle zum Paket MOLPRO geschaffen werden, welche es erlaubt Korrelationen quantitativ zu berücksichtigen. Solch eine Schnittstelle gibt es bereits für CRYSTAL.
Wir haben auch weiterhin die Möglichkeit verfolgt, Korrelationen mit der LSDA und LDA+U Methode zu berechnen. Diese sind zwar in ihren Näherungen nicht voll kontrolliert, ergeben aber dennoch oft sehr wichtige und nützliche Resultate. Zum Beispiel wurden die effektiven Kopplungskonstanten für die magnetischen Momente von Cr Ionen in den Spinellen ACr_2X_4 (A = Zn, Cd; X = O, S, Se) bestimmt. Diese Konstanten finden Eingang in einen effektiven Heisenberg Hamiltonoperator. So konnte gezeigt werden, dass die Kopplungskonstante für nächste Nachbarn Cr Ionen zwischen antiferromagnetisch in den O Spinellen bis ferromagnetisch in den S und Se Spinellen variiert (A. Yaresko).

Ein stark expandierender Teil der Arbeiten der Abteilung betrifft die Eigenschaften von Fermionen in frustrierten Gittern. Für spinlose Fermionen auf halbgefüllten Checkerboard Gittern konnte gezeigt werden, dass es eine Reihe von Ähnlichkeiten zur Theorie der Elementarteilchen gibt. Zum Beispiel gibt es Anregungen mit der Ladung $\pm e/2$, die ähnlich wie quarks mit einer abstandsunabhängigen Kraft gebunden sind (asympt. freedom). Zieht man diese Ladungen zu weit auseinander, so kommt es zur Erzeugung neuer Teilchen-Antiteilchenpaare mit der Ladung $\pm e/2$ - ähnlich wie bei μ Mesonen. Der Vakuumzustand besteht aus Schleifen (loops), welche das Checkerboard Gitter ausfüllen und deren Dynamik zu einer einfachen Form einer Stringtheorie führt. Auch wurde gezeigt, dass die entsprechende Feldtheorie eine U(1) Eichtheorie ist. Dieses Arbeitsgebiet stellt sich als außerordentlich lohnend dar und wird uns noch länger beschäftigen. Ein großer Teil der Ergebnisse geht auf eine Doktorarbeit von F. Pollmann zurück sowie auch Zusammenarbeiten mit K. Shtengel, E. Runge und J. Betouras (s. Beitrag von F. Pollmann, S. 71).
Eine Reihe von gelösten Problemen betraf ganz spezifische Marerialien. Als Beispiel sei UPd_2Al_3 genannt. Hier wurde gezeigt, wie der Übergang zur Supraleitung die kollektiven magnetischen Anregungen des Systems beeinflussen. Die Theorie konnte die vorhandenen Experimente inelastischer Neutronenstreuung sehr schön erklären (s. Beitrag von I. Eremin, der auch Arbeiten über hoch-T_c Supraleiter beschreibt, die damit im Zusammenhang stehen, S. 75). Die in den letzten Jahren gewonnenen Erkenntnisse wurden in einem sehr umfangreichen Beitrag "Strongly correlated electrons" zur Serie *Solid State Sciences* Bd. 60 (P. Fulde, P. Thalmeier und G. Zwicknagl) dokumentiert. Die Arbeiten zum Verständnis ultrakalter Gläser ($T < 100$ mK) in Magnetfeldern, deren außergewöhnliche Eigenschaften viele experimentelle und theoretische Gruppen beschäftigt, wurden auf der Basis quadrupolarer Kernmomente und deren Wechselwirkung mit den 2-Niveau Systemen vorangetrieben. Einige Experimente konnten erklärt werden (D. Bodea, A. Burin, I. Polishchuk). Die Kooperation mit P. Mohanty über Spintransport wurde fortgesetzt. Die Experimente, welche von der National Science Foundation unterstützt werden, brauchen aber noch einige Zeit.

Kooperationen:
Quantenchemische Verfahren: H. Stoll (Univ. Stuttgart), A. Shukla (IIT, Bombay), K. Rosciszewski (Univ. Krakow), K. Doll, M. Jansen (MPI-FKF, Stuttgart)

Stark korrelierte Elektronen: P. Thalmeier (MPI-CPfS), verschiedene Mitarbeiter (CPfS), G. Zwicknagl (Univ. Braunschweig)

Frustrierte Gitter: K. Shtengel (UC Riverside), K. Penc (Univ. Budapest), N. Shannon (Univ. Bristol), E. Runge (TU Ilmenau), G. Hotta (Aoyama Gakuin Univ.), J. Betouras (Univ. of St. Andrews, Schottland)

Ultracold glasses: A. Burin (Tulane, Univ., Los Angeles), I. Polishchuk (Kurtschatow-Inst., Moskau)

GdI_2: A. Taraphder (IIT, Kharagpur)

Spintransport: P. Mohanty (Boston Univ.)

Arbeitsgruppe: Quantenchemie
(Leiter: Dr. U. Birkenheuer bis (12/05))

In den vergangenen Jahren sind in der Quantenchemiegruppe eine Reihe von lokalen wellenfunktionsbasierten Verfahren zur Bestimmung der elektronischen Struktur von Festkörpern und Polymeren entwickelt worden. Neben dem Inkrementenschema für Grundzustandseigenschaften, welches nun schon seit mehr als einem Jahrzehnt mit Erfolg eingesetzt wird, sind hier vor allem die lokale Hamilton-Operator-Methode für Einteilchenanregungen (Quasiteilchenbandstruktur) und die periodische Variante des auf der Lösung der Dyson-Gleichung basierenden ADC-Formalismus (algebraisch-diagrammatische Konstruktion) zu erwähnen.
Mit Beendigung der Doktorarbeit von Christian Buth im November 2005 hat die letztgenannte Methode ihren Höhepunkt erreicht. Es konnte gezeigt werden, dass sich mit der CO-ADC-Methode (Kristallorbital-ADC) sowohl die Bandstrukturen von linearen Systemen (hier HF-Zickzackketten) als auch Volumenbandstrukturen (hier LiF mit Kochsalzstruktur) zuverlässig und mit vertretbarem Rechenaufwand berechnen lassen. Ein im Sommer 2005 angelaufenes Projekt zur Berechnung der Bandstruktur von MgO mit dem fertig gestellten CO-ADC-Programm als ein System mit einer deutlich größeren Anzahl an Valenzelektronen und tiefliegenden unbesetzten Leitungsbändern konnte aus Personalgründen nicht mehr zu Ende geführt werden.
Die lokale Hamilton-Operator-Methode ist das andere bisher eingesetzte Verfahren zur Bestimmung der elektronischen Anregungen in Festkörpern. Ursprünglich zur Beschreibung von Einteilchenanregungen (Valenz- und Leitungsbändern) entwickelt, hat sich der lokale Ansatz, der diesem Verfahren zu Grunde liegt, als so tragfähig herausgestellt, dass das Verfahren sogar auf die Berechnung kristallimpulsaufgelöster *exzitonischer* Anregungen von stark gebundenen Elektronenlochpaaren (Frenkel-Exzitonen) erweitert werden konnte.
Dennoch ist der Aufwand zur Erstellung, Verwaltung und Weiterverarbeitung der vielen Einzelergebnisse, die zur inkrementellen Aufsummierung des Gesamtkorrelationseffektes notwendig sind, recht groß, weshalb das Hauptaugenmerk in der letzen Phase der Quantenchemiegruppe auf der Entwicklung eines *vereinfachten* Ansatzes zur Bestimmung der Bandstruktur korrelierter Elektronen lag. Einer Pionierarbeit aus dem Sommer 2004, in der die neue Methode erstmals in einer Anwendung an Diamant und Silizium vorgestellt wurde, folgte eine systematische Untersuchung der Qualität der zur Vereinfachung der lokalen Hamilton-Operator-Methode eingeführten "frozen local hole"-Approximation, einer Art adiabatischen Näherung für die Gestalt des von den beweglichen Elektronen mitgeführten Korrelationslochs. Der Beweis der Leistungsfähigkeit des neuen Verfahrens für nicht-triviale 3-dimensional periodische Systeme wurde am Beispiel des Magnesiumoxids erbracht. So konnten die Korrelationseffekte sowohl in den Valenz- als auch in den *Leitungs*bändern von MgO erfolgreich quantifiziert werden.
Durch die Auflösung der Quantenchemiegruppe Ende 2005 und die beruflichen Veränderungen bei vielen der ursprünglichen Mitarbeitern und Kollaborationspartnern sind die Aktivitäten auf dem Gebiet der wellenfunktionsbasierten Korrelationsmethoden für Festkörper und Polymere inzwischen stark zurückgegangen, und es bestehen auch keine aktuellen Kooperationen mit anderen Arbeitsgruppen auf diesem Gebiet mehr.

Arbeitsgruppe: Nichtlineare Zeitreihenanalyse
(Leiter: Prof. Dr. H. Kantz)

Komplexe Dynamik bleibt eine Herausforderung sowohl an die Theorie wie auch die Praxis. Unsere Arbeitsgruppe konzentriert sich auf Aspekte von komplexem Verhalten in klassischen (d.h., nicht-quantenmechanischen) Systemen, wobei wir uns sowohl für grundlegende Eigenschaften wie auch für spezifische Phänomene interessieren. Die Rolle von schnellen chaotischen Freiheitsgraden in Hamiltonschen Systemen als Wärmebäder mit endlicher Energie wurde sowohl theoretisch als auch in Modellsystemen weiter untersucht. Damit konnten wir beispielsweise das folgende System verstehen: Hüpft ein Teilchen auf einer periodisch bewegten Platte mit Sägezahnprofil, so beobachten wir eine Diffisionsbewegung in horizontaler Richtung, wenn die Hüpfbewegung chaotisch ist, während das Teilchen lokalisert ist oder ballistisch wegläuft, wenn die Hüpfbewegung periodisch ist. Reguläre Bahnen erzeugen Strukturen in Hamiltonischen Systemen mit gemischten Phasenräumen, die Transporteigenschaften und den Korrelationszerfall massiv beeinflussen. In einer Doktorarbeit konnten hier neue Erkenntnisse gewonnen werden, insbesondere die Existenz von einparametrigen Familien von marginal instabilen Bahnen in lokal gestörten integrablen Systemen stellt sich als relevant heraus. Im Rahmen eines BMBF-geförderten Verbundes studieren wir die Eigenschaften von Oberflächenwind, um eine verbesserte Modellierung von Windfeldern zu erzielen. Ein weiteres durch die Anwendung motiviertes Projekt ist die stochastische Modellierung von Autobahnverkehr. Fokker-Planck-Gleichungen mit zeitperiodischen Koeffizienten in zwei Dimensionen wurden aus Daten rekonstruiert.
Ein besonderes Merkmal komplexer deterministischer wie auch stochastischer Systeme ist ihre Fähigkeit, extreme Ereignisse zu generieren. Damit bezeichnen wir kurzzeitige große Abweichungen eines Systems von seinem mittleren Verhalten. Wir studieren dynamische Mechanismen zur Erzeugung von Extremereignissen, wir versuchen die Rolle von Vorläuferstrukturen zu verstehen, und wir betrachten statistische Aspekte der Detektion und Charakterisierung von Extremereignissen. Zwei Ergebnisse unserer Arbeit sind besonders erwähnenswert: In einem Modell zur Rückkopplung der Reaktion eines Systems auf extreme Ereignisse finden wir in bestimmten Parameterbereichen Relaxationsoszillationen. Die Kombination von zufälligen Ereignissen und Systemantwort führt zu annähernd periodischen Sequenzen von Schwellwertüberschreitungen. Bei Vorhersagen von Extremereignissen durch die Beobachtung von Vorläuferstrukturen sehen wir für bestimmte Prozessklassen, dass Ereignisse umso besser vorhersagbar sind, je stärker sie sind. Im Oktober 2006 konnten wir zum Thema „Extreme events in complex dynamics" am mpi**pks** eine internationale Konferenz organisieren.
In der Zukunft wird das Studium extremer Ereignisse noch stärker in das Zentrum unserer Arbeit rücken. Zum besseren Verständnis von Mechanismen werden wir verstärkt Modelle studieren. Im Hinblick auf Management und Prävention wollen wir dabei exemplarisch aus physikalischen Wirkungen auf die Wahrnehmung der Menschen extrapolieren, also eine Ankopplung an Modelle der Soziophysik vornehmen, wobei wir uns der Unsicherheiten solcher Ansätze bewusst sind.

Kooperationen

- W. Just, University of London; G. Radons, TU Chemnitz: Modellierung schneller Freiheitsgrade durch stochastische Prozesse.
- J. Peinke, Universität Oldenburg; im Konsortium mit R. Friedrich, Uni. Münster, A. Schaffarczyk, FH Kiel, C. Wagner, DLR Göttingen: Bodenwind, Turbulenz und Windkraftanlagen.
- S. Albeverio, Uni. Bonn: zeitabhängige Fokker-Planck-Gleichungen zur Modellierung von Autobahnverkehr.
- Prof. C. Grebogi, University of Aberdeen: Einfluß von Rauschen auf deterministische Dynamik.
- N. Vitanov, IMB Sofia: Datenanalyse von Windgeschwindigkeiten, Turbulenz.

Abteilung: Endliche Systeme
(Leiter: Prof. Dr. J.-M. Rost)

Die Gruppe interessiert sich für nicht lineare Dynamik angeregter Quantensysteme, die aus einer endlichen Anzahl von Teilchen bestehen, mit einer Betonung auf Atomen und Clustern. Wir haben die Arbeit der letzten Jahre auf diesen beiden Schwerpunkten – ultrakalte Plasmen und Wechselwirkung von Edelgasclustern mit intensiven Laserpulsen – in zwei Übersichtsartikeln (Physics Reports und Topical Review for J Phys B) zusammengefasst.

Forschungsthemen
Auf dem Gebiet der ultrakalten Gase verlagert sich unser Interesse hin zu Korrelationsphänomenen in der Rydbergdynamik. Ein ultrakaltes Gas bietet die ideale Umgebung, um die langsamen Zeitskalen und die geringen Energiedifferenzen von Rydbergatomen zu studieren, die man als eingebettet in ein Gas kalter Grundzustandsatome betrachten kann (S. 99).
Einbettung ist auch ein leitendes Motiv für unsere gegenwärtige Arbeit an Clustern: Edelgascluster dotiert mit Fremdatomen oder -molekülen, ebenso wie Cluster umgeben von superfluiden Heliumtropfen, zeigen Eigenschaften, die sich überraschend deutlich von denen reiner Cluster unterscheiden. Dies wurde in verschiedenen, wenig verstandenen Experimenten, gezeigt. Dabei war die Dotierung zu Anfang eher ein Zufall aufgrund des unrein präparierten Clustertargets. In ähnlicher Weise ergab sich der Einschluss in ein Heliumtröpfchen daraus, dass man auf diese Art elegant mit einem Atomstrahl Cluster erzeugen kann und man der Meinung war, dass der Heliumtropfen die Clustereigenschaften wenig beeinflusst.
Wir haben eine neue Forschungsaktivität zur Untersuchung der Antwort kleiner Quantensysteme auf die Kombination eines Laserpulses und externen Rauschens begonnen. Wenn das Rauschen von vergleichbarer Stärke ist wie der Laserpuls – beide im nichtstörungstheoretischen Wechselwirkungsregime – dann reagiert das Quantensystem sehr empfindlich. Darüber hinaus kann man mit einer Zeitstruktur, die dem Rauschen aufgeprägt wird, selektiv an veschiedene Bewegungsmoden, z.B. Kern- oder Elektronendynamik in einem Molekül, ankoppeln. Diese Art von Rauschen kann mit Hilfe von geformten Laserpulsen erzeugt werden.

Angelegt über einen längeren Zeitraum sind unsere Bemühungen, Vielfachionisation in Atomen mit Hilfe von klassischer Mechanik zu verstehen. Diese Arbeit hat zwei Ziele: Zum einen soll eine quantitative Beschreibung von Wenig-Teilchen Coulombsystemen erreicht werden, die bereits zu viele Freiheitsgrade haben, um exakt quantenmechanisch erfasst werden zu können. Zum anderen streben wir ein Verständnis der komplizierten Dynamik mit Hilfe klassischer Trajektorien an (S. 102). Die bisherigen Resultate führten zu der überraschenden Hypothese, dass nicht das Zwei-Körper-Coulombproblem der fundamentale Baustein von Viele-Elektronen Atomen ist, sondern das Helium-ähnliche Drei-Körper-Coulombproblem.
Schließlich sei noch erwähnt, dass wir unsere Zusammenarbeit mit experimentellen Gruppen (Ron Phaneuf, Reno and Nora Berrah, Kalamazoo) zum Verständnis der kollektiven Dynamik in Fullerenen und Fullerenionen fortgesetzt haben.

Methoden
Unsere Techniken reichen von quantenmechanichen Zugängen einschließlich zeitabhängiger Dichtefunktionaltheorie über semiklassische Näherungen bis hin zu vollständig klassischen Ansätzen für mikroskopische Phänomene. Dies schließt hochentwickelte numerische Techniken, wie Tree-Codes oder Particle-in-cell Codes ein.

Zukunftsperspektiven
Phänomene langreichweitiger Wechselwirkung in ultrakalten Gasen stellen auf Grund ihres Vielteilchencharakters eine Herausforderung für die Theorie dar. Für den Fall dominanter Coulombwechselwirkung in ultrakalten Plasmen haben wir einen komplementär quasi-analytischen und numerischen Zugang entwickelt, der ein gutes Verständnis der Phänomene ermöglicht. Wir haben auch eine Beschreibung gefunden, die geeignet ist bei speziellen Laseranregungen Korrelationseffekte von Rydbergatomen aufgrund dipolarer und van der Waals Wechselwirkung in ultrakalten Gasen zu verstehen. Global kohärente Vielteilchendynamik in kalten Gasen bleibt aber ein schwieriges Thema. Wir werden uns zunächst auf die zeitliche Entwicklung von Verunreinigungen in Bose-Einstein-Kondensaten und deren experimentelle Verifizierung konzentrieren. Dabei können Korrelationseffekte gezielt zusätzlich zu einer *mean field* Näherung für das Kondensat beschrieben werden.

Die Arbeit zur Wechselwirkung von Clustern und Atomen mit Laserpulsen wird stark geprägt werden von den neuen Lichtquellen, die nach und nach verfügbar werden. Dies sind die Freien Elektronen Laser im Röntgenbereich (XFELs) in Hamburg und Stanford und Attosekundenlaserpulse, erzeugt in mehreren Labors weltweit. Attosekundenpulse erlauben es, Elektronendynamik in Atomen und ausgedehnten Systemen zu verfolgen (die Periode des Elektrons im Wasserstoffgrundzustand beträgt 24 Attosekunden). XFELs ermöglichen, Dynamik auf der Femtosekundenskala zeitlich aufzulösen und zugleich eine Ortsgenauigkeit von atomaren Dimensionen mit Hilfe der kurzen Wellenlänge des Lichtes zu erreichen, also im Prinzip Ionendynamik wirklich als Film aufzuzeichnen.
Wir haben begonnen Alternativen zum gewöhnlichen diffraktiven Abbilden mikroskopischer Obkjekte zu suchen, da die Standardtechnik aller Wahrscheinlichkeit nach nicht zum Ziel führen wird: Da im relevanten Parameterregime der Photoionisationsquer-

schnitt größer als der Streuquerschnitt ist, werden die Targets zerstört, bevor sie abgebildet werden können.
Im Bereich der Attosekundenphysik planen wir das pump-probe Schema, wohl bekannt aus der Femtosekundenchemie, zu mikroskopischen Flugzeitmessungen zu nutzen. So sollte es möglich sein, dass der erste Attosekundenpuls (pump) ein Photoelektron erzeugt, z.B. an der Kante eines Metallclusters, während der zweite Attosekundenpuls (probe) den Wiedereinfang des Elektrons an einer anderen Clusterkante stimuliert. Aus der Zeitverzögerung τ zwischen Erzeugung und Wiedereinfang des Elektrons lässt sich unter idealen Bedingungen die Wegstrecke berechnen, die es zurückgelegt hat, was einer Messung mikroskopischer Distanzen entspricht. Die Verwendung ähnlicher pump-probe Schemata bietet sich auch im Kontext unserer quasiklassischen Studien in der Wenig-Elektronen-Dynamik von Atomen an.
Wir teilen das Interesse an Attosekundenphänomenen mit Andreas Beckers Gruppe im Department. Mit unserer jeweils komplementären Expertise sind wir gut auf dieses wachsende Feld atomarer Attosekundenphänomene vorbereitet.

Schließlich werden wir das Konzept der Einbettung von Quantensystemen weiter verfolgen, auf der einen Seite mit Zwei-Komponenten Clustern wie bereits beschrieben, auf der anderen Seite durch die Einbettung kleiner Quantensysteme in Rauschen. Letzteres kann entweder direkt erzeugt werden, oder kann die Konsequenz von Stößen mit einer nicht weiter spezifizierten Umgebung aus massiven Teilchen sein.

Kooperationen
Mit experimentellen Gruppen
Wir haben zusammengearbeitet mit den Gruppen von Prof. Müller (Uni Giessen) und Prof. Phaneuf (Univ. of Nevada, Reno, USA) zur kollektiven Anregung von Elektronen in komplexen Systemen durch Photonen. Eine neue Zusammenarbeit zu C_{60}^- hat mit Prof. Nora Berrah (Kalamazoo, USA) begonnen. Die Zusammenarbeit mit Prof. Kaindl (FU Berlin) und Prof. Dörner (Uni Frankfurt) zur Photoanregung von Helium wurde mit gemeinsamen Publikationen fortgesetzt. Desweiteren waren wir in engem Kontakt mit den Gruppen von Prof. Weidemüller (Freiburg), Prof. Pillet (Orsay, France) und Prof. Raithel (Ann Harbor, USA) hinsichtlich der Wechselwirkung von Rydbergatomen in ultrakalten Gasen und mit Prof. Killian (Rice, USA) zu ultrakalten Plasmen.

Mit theoretischen Gruppen (einige Beispiele):
– zur klassischen Dynamik von Quantensystemen mit A. Emmanouilidou (Eugene, USA)
– zu semiklassischer Theorie mit A. Ozorio de Almeida (Rio, Brazil)
– zu Transport durch einzelne Cluster und Clusterreihen mit M. Garcia (Kassel).

Lokale Kooperationen
Der Austausch mit Prof. Rüdiger Schmidts Gruppe an der TU Dresden wurde fortgesetzt - die Grundlage ist das gemeinsame Seminar *Quantum Dynamics*. Es findet am mpi**pks** mit externen Sprechern, eingeladen von beiden Gruppen, statt. Gemeinsame wissenschaftliche Aktivitäten betreffen *semiklassische Propagationstechniken* und die Wirkung externen Rauschens mit F. Großmann von der TU Dresden. Eine neue Verbindung mit der TU wie auch mit anderen Instituten in der Nachbarschaft besteht

durch die *International Max Planck Research School* und ihr monatliches Seminar, das am mpi**pks** stattfindet.

Arbeitsgruppe: Nichtlineare Prozesse in starken Feldern
(Leiter: Dr. Andreas Becker)

Die Gruppe besteht zur Zeit aus drei Postdoktoranden und zwei Doktoranden und ist an dem Verständnis von ultraschnellen, nichtlinearen Prozessen interessiert. Unsere Aktivitäten umfassen die Dynamik von einzelnen Atomen, Molekülen und Clustern in starken Feldern, die Erzeugung und Anwendung von ultrakurzen und Attosekunden-Pulsen und die Propagation von intensiven Laserpulsen in der Luft. Wir analysieren diese Themen aus unterschiedlichen Perspektiven mit analytischen Ansätzen, S-Matrix Theorien und numerischen Simulationen.
Ein neuer Schwerpunkt unserer Arbeiten in den letzten Jahren lag in der Entwicklung von ab-initio Techniken zur direkten Integration der zeitabhängigen Schrödingergleichung für die Wechselwirkung eines intensiven Laserpulses mit Systemen mit wenigen Teilchen. In einem gemeinsamen Projekt der Gruppe ist ein virtuelles Labor entstanden, welches eine effiziente Analyse und Visualisierung von ultraschnellen atomaren und molekularen Prozessen ermöglicht. Wir haben dieses numerische Programmpaket genutzt, um zwei stark diskutierte Themenkomplexe zu untersuchen. Zum einen haben wir ein Modell zur Doppelionisation von Atomen und Molekülen vorgeschlagen, in dem die Korrelation zwischen den Elektronen vollständig einbezogen wird, welche in den bisherigen eindimensionalen Modellen so nicht berücksichtigt wurde (siehe Bericht *A virtual laboratory for ultrashort processes in strong fields*, S. 107). Zum anderen untersuchen wir Kontrollmechanismen zur Anregung und Lokalisierung von Elektronen in einem Atom oder Molekül im Rahmen der Möglichkeiten heutiger Lasertechnologie. Dazu haben wir Techniken wie Pulsformung oder die Kombination zweier Pulse in den numerischen Simulationen genutzt.
Desweiteren haben wir uns für das Verhalten von großen Molekülen in intensiven Laserfeldern interessiert. Da die numerischen Integrationstechniken in Praxis auf Systeme mit wenigen Teilchen beschränkt sind, haben wir als Alternative die S-Matrix Theorie genutzt. Diesen Ansatz, den wir bereits früher bezüglich der Ionisation von diatomaren Molekülen angewandt haben, haben wir jetzt durch die Einbeziehung von Vibrationsanregungen und die Anwendung auf polyatomare Moleküle erweitert. Es war uns dadurch möglich, Erklärungen für zwei unerwartete Phänomene zu finden, das sind die Abweichung der Verteilung in den Vibrationsleveln eines Ions von der Franck-Condon Verteilung und die Unterdrückung der Ionisationswahrscheinlichkeit von Fullerenen im Vergleich zu jener eines Atoms mit dem gleichen Ionisationspotential (siehe Bericht *Molecules in intense laser pulses: S-matrix analysis of ionization and high harmonic generation*, S. 104).
Neue Modelle zur Erzeugung von Pulsen mit wenigen Feldzyklen und Attosekundenpulsen wurden ebenfalls untersucht. Dazu haben wir unsere Arbeiten zur Hoch Harmonischen Erzeugung in dichten Medien fortgesetzt. Daneben haben wir in Zusammenarbeit mit der experimentellen Gruppe von S.L. Chin (Québec, Kanada) gezeigt, dass sich abstimmbare Laserpulse mit wenigen Zyklen durch Vier-Wellen-Mischung in einem Laserfilament mit hoher Effizienz erzeugen lassen.
Das Wechselspiel von Selbstfokussierung durch den Kerr-Effekt und Defokussierung

durch ein selbsterzeugtes Plasma lässt einen ultrakurzen Puls über weite Strecken propagieren. Viele theoretische Studien beschränken sich dabei auf die Analyse der Pulsdynamik im Kern des Filaments. Unsere Resultate aus numerischen Rechnungen und einem Variationsansatz zeigen dagegen, dass ein Hintergrundreservoir niedriger Intensität um den Filamentkern eine entscheidene Rolle spielt.
Neben den wissenschaftlichen Aktivitäten waren wir an der Organisation von zwei internationalen Workshops, dem Internationalen Seminar und Workshop *Intense laser-matter interaction and pulse propagation* (mpi**pks** Dresden, 1.-24. August 2005) und dem *International Symposium on Ultrafast Intense Laser Science 4* (Hawaii, 12.-14. Dezember 2005), als auch der *International Wilhelm und Else Heraeus Summerschool: Few-body dynamics in atomic and molecular systems* (Wittenberg, 10.-23. September 2006) beteiligt. Sowohl das Seminar als auch die Sommerschule wurden von einer großen Anzahl von jungen Postdoktoranden und Doktoranden besucht, denen dadurch die Gelegenheit gegeben wurde, Stand und Perspektiven der Forschung mit internationalen Experten zu diskutieren.

Zukunftsperspektiven
Die Erzeugung von Laserpulsen mit wenigen Feldzyklen und einer kontrollierten Phase zwischen Feld und Einhüllender sowie von Attosekundenpulse sind wichtige neue Technologien. Unser virtuelles Labor ermöglicht uns inzwischen, die Dynamik von Atomen und Molekülen in solchen Pulsen zu untersuchen. Dies wird ein Schwerpunkt unserer Arbeiten in der nächsten Zeit sein.
Desweiteren planen wir das virtuelle Labor durch die Einbeziehung von Ionenstößen zu erweitern. Experimente am atomaren Wasserstoff werden dazu am MPI-K in Heidelberg vorbereitet.
Letztlich werden wir unsere S-Matrix Analysen fortsetzen, um zu sehen, wie sich die geometrische Struktur und Orbitalsymmetrie eines polyatomaren Moleküls in den Spektren des Photoelektrons und der Hoch Harmonischen widerspiegeln. Dies würde eine Methode zur Beobachtung von Veränderungen von Molekülen auf einer ultraschnellen Zeitskala ermöglichen.

Kooperationen
Wir sind an zwei internationalen Kooperationen beteiligt, die im Jahr 2004 initiiert wurden, einem Center of Advanced Science and Technology (COAST) *Ultrafast Intense Laser Science* (Koordination: K. Yamanouchi, Tokio, Japan) und einem Special Research Opportunity Programm *Controlled electron rescattering: sub-A, sub-fs imaging of single molecules* (Koordination: M.Yu. Ivanov, Ottawa, Kanada). Unsere Kooperation mit der Gruppe von Luis Plaja (Universidad Salamanca, Spanien) wird durch ein DAAD-Austauschprogramm gefördert.

Mit experimentellen Gruppen:
• mit S.L. Chin (Québec, Kanada) (a) zur Propagation von Femtosekunden-Pulsen und (b) zur Erzeugung von abstimmbaren ultrakurzen Pulsen.
• mit P. Agostini (z.Zt., Ohio State Universität, USA) und S.L. Chin (Québec, Kanada) zur Fragmentation von Molekülen in intensiven Laserfeldern
• mit R. Dörner (Frankfurt) und P.B. Corkum (Ottawa, Kanada) zu Rückstreudynamik

in der Doppelionisation in intensiven Feldern

Theoretische Gruppen:
• mit N. Aközbek (Huntsville, USA) zur Zwei-Farben Filamentation und zur Erzeugung von abstimmbaren ultrakurzen Laserpulsen
• mit F.H.M. Faisal (Bielefeld) und A. Jaroń-Becker (Dresden) zur Ionisation von Molekülen in Laserfeldern
• mit O. Kosareva und V.P. Kandidov (Moskau, Russland) zur Fragmentation von Molekülen
• mit J. Moloney (Tucson, USA) zur Erzeugung Dritter Harmonischer in Laserfilamenten
• mit L. Plaja und L. Roso (Salamanca, Spanien) zur korrelierten Elektronendynamik in Laserpulsen mit wenigen Feldzyklen.

Arbeitsgruppe: Nichtlineare Dynamik in Quantensystemen
(Leiter: Dr. A. Buchleitner)

Die Gruppe widmet sich der komplexen Dynamik auf den ersten Blick einfacher Quantensysteme. "Komplexität" erwächst aus der Zerstörung von Symmetrien infolge der starken Kopplung weniger Freiheitsgrade, aus den vielen Freiheitsgraden eines wechselwirkenden Vielteilchensystems, aus Unordnung oder stochastischer Aktivierung, und schließlich – spezifisch quantenmechanisch – aus Interferenz, Dekohärenz und Verschränkung. Schwerpunkte unserer Arbeit während der letzten Jahre waren

- die Darstellung quantenmechanischer Verschränkungsmaße durch geeignete experimentelle Observable (F. Mintert, L. Aolita)
- die Dynamik quantenmechanischer Verschränkung unter dem Einfluss von Rauschen (M. Busse, C. Viviescas, I. García-Mata, O. Brodier, T. Gorin, A. Aragão, B.V. Fine, A.R. Ribeiro de Carvalho, F. Mintert)
- Ericson-Fluktuationen, dynamische Lokalisierung und resonanz-assistiertes Tunneln in zerfallenden Ein- und Zweielektronen-Rydbergsystemen (J. Madroñero, A. Krug, S. Wimberger, C. Eltschka, A. Dudarev, P. Schlagheck)
- kohärente Rückstreuung von Licht an kalten Atomen (V. Shatokhin, C.A. Müller)
- Dynamik und Dekohärenz ultrakalter (wechselwirkender und nichtwechselwirkender) Atome in periodischen Lichtgittern (A. Ponomarev, J. Madroñero, A. Kolovsky, S. Wimberger)

mit sehr engem Bezug zu aktuellen Experimenten in Quantenoptik und Atomphysik. Neben tiefliegenden mathematischen Methoden aus Operatoranalysis und Quantenwahrscheinlichkeitstheorie kommen hier auch modernste Methoden der rechnergestützten Physik auf einem der derzeit weltweit leistungsfähigsten Parallelgroßrechner, der IBM p690 des Rechenzentrums Garching der Max-Planck-Gesellschaft, zum Einsatz.
Im Mai und August 2006 schlossen Marc Busse und Alexej Schelle (beide LMU München) ihre Diplomarbeiten ab. Herrn Busse zog es zur Promotion wieder zurück nach München, während Herr Schelle der Gruppe im Rahmen einer binationalen Promotion an den

Universitäten Paris 6 (dort verantwortlich: Dominique Delande) und München erhalten bleibt. Des weiteren konnten wir im Herbst 2006 zwei neue Doktoranden – Markus Tiersch (Dresden) und Hannah Venzl (Ulm) – gewinnen, ebenso wie die neuen Post-Docs Ming-Chiang Chung (Aachen), Fernando de Melo (Rio de Janeiro) und Sangchul Oh (Seoul). Carlos Viviescas, Artëm Dudarev, Thomas Gorin, Olivier Brodier und Andrey Kolovsky haben die Gruppe nach Ablauf ihrer Gaststipendien verlassen – Herr Viviescas erhielt an seiner Heimatuniversität in Bogotá eine Professur, Herr Brodier trat eine permanente Stelle als Maître de Conférence an der Université de Tours an, Herr Dudarev beendete seine wissenschaftliche Laufbahn, Herr Gorin wechselte nach Mexico, und Herr Kolovsky kehrte zurück nach Krasnoyarsk.
Die engen Kontakte zu Arbeitsgruppen in Brasilien, Polen, Frankreich, Italien und Israel, in den ersten drei Fällen gefördert durch bilaterale Forschungsmittel des DAAD bzw. der VolkswagenStiftung, waren wissenschaftlich außerordentlich fruchtbar und werden durch den intensiven Austausch von Nachwuchswissenschaftlern getragen. Insbesondere seien mehrwöchige Gastaufenthalte von Herrn Busse und Herrn Viviescas in Warschau bzw. Krakau, mehrmonatige Gastaufenthalte von Herrn L. Aolita und Herrn A. Aragão, zweier Doktoranden unserer Partnergruppe in Rio de Janeiro, hier in Dresden, sowie ein mehrwöchiger Aufenthalt von Herrn Schelle in Paris genannt.
Das Gästeprogramm des Instituts ermöglichte erneut Gastaufenthalte etablierter (K. Dietz, S. Fishman, I. Guarneri, M. Kuś, H. Narnhofer) wie auch vielversprechender jüngerer Kollegen (F. Mintert, T. Wellens, S. Wimberger, K. Hornberger, P. Schlagheck, V. Shatokhin, T. Paul, M. Hartung, J. Bae, T. Barthel, D. Burgharth, B. Hiesmayr).
Eine am mpi**pks** im September 2005 zusammen mit Richard Gill (Utrecht) und Rainer Blatt (Innsbruck) veranstaltete, einmonatige Sommerschule zum Thema "Quanteninformation" war didaktisch und wissenschaftlich höchst erfolgreich und hat vielfache, inzwischen bereits dokumentierte, neue wissenschaftliche Kontakte und Zusammenarbeiten angeregt. Ein Teil der Vorlesungen wird derzeit in einem Buch zusammengefasst.
Spezialvorlesungen über "Quantenchaos" und "Quanteninformation" wurden von A. Buchleitner im Rahmen von Gastprofessuren bzw. Sommerschulen an der Université Catholique de Louvain (Belgien), am ICTP Trieste (Italien), sowie am National Center for Theoretical Sciences, Hsinchu (Taiwan), gehalten.
Die Forschungsaktivitäten der nächsten Jahre werden durch folgende Schwerpunkte unserer aktuellen Arbeit definiert:

I die quantenmechanisch möglichst näherungsfreie Beschreibung von Helium bzw. Helium-artiger Atome unter dem Einfluss statischer oder oszillierender elektrischer Felder;

II die dynamische Charakterisierung von Verschränkung in zusammengesetzten Quantensystemen unter dem Einfluss von Rauschen;

III der Transport von Photonen oder wechselwirkender Materiewellen in ungeordneten Streumedien bzw. in optischen Potentialen.

Während wir unter (I) die näherungsfreie Beschreibung der Fragmentationsdynamik des periodisch getriebenen Dreikörper-Coulombproblems – realisiert in aktuellen Experimenten zur Laserionisation von Helium – ins Auge fassen, zielt (II) auf eine allgemeine Theorie der Zeitentwicklung quantenmechanischer Verschränkung unter Lindblad-

oder allgemeinerer inkohärenter Dynamik – mit dem besonderen Anliegen, auch experimentell direkt umsetzbare Messstrategien anzugeben. Unter (III) werden wir uns in nächster Zeit insbesondere mit Dekohärenzphänomenen in der Theorie wechselwirkender ultrakalter atomarer Gase bzw. schwacher (und womöglich starker) Lokalisierung von Licht in Streumedien mit Quantenstruktur widmen.

Abteilung: Biologische Physik
(Leiter: Prof. Dr. F. Jülicher)

Kernthemen unserer Forschungsprojekte sind aktive und dynamische Phänomene in lebenden Zellen. Ausgehend von dem physikalischen Verständnis molekularer Prozesse (z.B. Motorproteine) ist es unser Ziel, grundlegende Mechanismen und Funktionsprinzipien in komplexen zellulären Systeme (z.B. Zellbewegung, Zellteilung) zu charakterisieren. Dabei stehen raumzeitliche Vorgänge im Zentrum des Interesses und es wird eine grundlegende theoretische und quantitative Beschreibung dynamischer Prozesse in biologischen Systemen angestrebt. Methoden und Konzepte der Statistischen Physik, und Nichtgleichgewichtsphysik und nichtlinearer Dynamik spielen eine wichtige Rolle, um kollektives Verhalten vieler Komponenten, Selbstorganisationsphänomene und den Einfluss von Fluktuationen zu untersuchen und theoretisch zu beschreiben. Projekte reichen von den aktiven physikalischen Eigenschaften von Zellen und deren Komponenten bis zur Kommunikation zwischen Zellen und deren raumzeitlichen Organisation in Zellverbänden. Beispiele aktueller Forschungsaktivitäten sind:

Aktive molekulare Prozesse: Motorproteine sind die Prototypen aktiver Prozesse auf molekularer Ebene, die in tierischen und pflanzlichen Zellen für Bewegungserzeugung, Materialtransport und Zellteilung eine herausragende Bedeutung haben. Verwandte aktive Prozesse finden statt, wenn die Zelle ihr genetisches Material (DNA) dupliziert, kopiert und korrigiert. Wir untersuchen die physikalischen Grundlagen dieser Vorgänge auf molekularer Ebene sowie das kollektive Verhalten einer großen Zahl aktiver Moleküle.

Dynamik von Zellen und zellulären Strukturen: Zellen sind ausgesprochen dynamische Systeme, die sich in ständiger Bewegung befinden. Beispiele sind Zellteilung, Zellbewegung auf Unterlagen und die schwimmende Fortbewegung vieler Zellen. Wir untersuchen die von Motorproteinen getriebene Dynamik zellulärer Strukturen wie z.B. der mitotischen Spindel, von Geißeln und von Mechanosensoriellen Haarbündeln. Die mitotische Spindel ist eine räumliche Struktur des Zytoskeletts, die für die Trennung der duplizierten Chromosomen während der Zellteilung eine entscheidende Rolle spielt. In bestimmten Situationen wird eine komplexe Dynamik beobachtet, die Symmetriebrechung und spontane Oszillationen beinhaltet. Diese Phänomene können quantitativ beschrieben werden. Geißeln sind haarartige Zellfortsätze, die zur schwimmenden Fortbewegung eingesetzt werden. Komplexe nichtlineare Biegewellen enstehen durch die Selbstorganisation vieler Motoren mit elastischen Proteinfilamenten.

Aktive weiche Materialien: Das Zytoskelett ist ein polymerisches Material, das inhärent aktiv ist und durch molekulare Prozesse ins Nichtgleichgewicht getrieben wird. Als Konsequenz besitzt es ungewöhnliche Materialeigenschaften. Es kann spontane Bewegungen

und komplexe Dynamik hervorrufen. Ausgehend von mikroskopischen Beschreibungen auf der Ebene von Filamenten, entwickeln wir eine allgemeingültige hydrodynamische Beschreibung aktiver weicher Materialien, die die Physik viskoelastischer Fluide ins Nichtgleichgewicht verallgemeinert. Ausgehend von aktiven Materialgleichungen kann, unter Verwendung geeigneter Randbedingungen die Adhäsion und die Polymerisation von Filamenten berücksichtigen, z.B. die Physik der Bewegung von Zellen auf Unterlagen beschrieben werden.

Organisation von Zellen in Zellverbänden: Ein wichtiges Modellsystem für Zellverbände sind Epithelien, d.h. zweidimensionale Zellschichten in denen während der Embryonalentwicklung komplexe Musterbildungsvorgänge ablaufen. Ein Epithelium wächst durch Zellteilung. Dabei ändert es seine Form und bestimmte Zellen ändern in genau festgelegter Weise ihre Zelleigenschaften um neue Strukturen zu bilden. Wir untersuchen die Physik von Zellverbänden als weiche Materialien. Diese Materialien sind aktiv, da durch Krafterzeugung in Zellen sowie durch Zellteilung innere Kräfte auftreten und Bewegungen erzeugt werden. Zellverbände sind visko-elastisch und können Eigenschaften sowohl von Flüssigkeiten als auch von Festkörpern zeigen. Die Strukturbildung im Zellverband entsteht aus dem Zusammenspiel dieser aktiven Materialeigenschaften mit zellulären Kommunikationssystemen. Wir entwicklen theoretische Methoden, um die Prinzipien, die dabei wichtige Rollen spielen, zu identifizieren und zu untersuchen.

Kommunikation zwischen Zellen durch Morphogene: Morphogene sind Signalmoleküle, die von bestimmten Zellen im Zellverband erzeugt werden und viele Zellabstände weiter detektiert werden und Signale auslösen. Typischerweise bilden sie graduell abfalende Konzentrationsprofile aus, welche Positionsinformationen and Zellen vermitteln können. Unsere Gruppe untersucht die Transportprozesse die für die Ausbreitung dieser Moleküle verantwortlich sind. Dabei konnten wir in Zusammenarbeit mit experimentellen Gruppen zeigen, dass aktiver Transport durch das Zellinnere eine wichtige Rolle spielt. Ausgehend von den Eigenschaften zelulärer Transportprozesse können effektive nichtlineare Transportgleichungen hergeleitet werden, die die Dynamik der Gradientenbildung beschreiben können. Die Präzision der im Gradienten übertragenen Information kann quantitativ untersucht und mit theoretischen Vorhersagen verglichen werden. Diese Ansätze erlauben uns in Zusammenarbeit mit experimentellen Gruppen die Rolle unterschiedlicher Transportmechanismen für die Entstehung von Morphogengradienten zu untersuchen und Fragen der Robustheit und Präzision des Gesamtsystems zu diskutieren.

Physik von Sinneszellen und des Gehörs: Haarzellen sind mechanisch empfindliche Sinneszellen, die in unserem Innenohr Schallsignale aufnehmen und in Nervensignale umsetzen. Unser Gehör ist mithilfe dieser Zellen in der Lage, über einen dynamischen Bereich von 12 Größenordnungen der Schallintensität zu arbeiten und extrem schwache Schallsignale wahrzunehmen. Dabei werden aktive und nichtlineare Verstärkungsmechanismen verwendet. Nichtlineare Oszillatoren und universelle Eigenschaften solcher Systeme in der Nähe eines kritischen Punktes bilden eine wichtige konzeptuelle Grundlage zum Verständnis aktiver Prozesse des Gehörs. Unsere Gruppe untersucht aktive molekulare Prozesse, die im Haarbündel zu Oszillationen führen sowie die Rolle von Fluktuationen, die aufgrund aktiver und passiver molekularer Prozesse entstehen. Das

universelle Verhalten kritischer Oszillatoren wird mithilfe feldtheoretischer und Renormierungsgruppenmethoden untersucht. Als weiteres Besipiel ist die Physik nichtlinearer Wellen zu nennen die, von aktiven zellulären Prozessen angetrieben, sich auf der Basilarmembran in der Schnecke des Innenohrs ausbreiten.

Diese Arbeiten erfolgen in enger Zusammenarbeit mit experimentellen Gruppen. Hervorzuheben ist dabei die Zusammenarbeit mit dem Institut Curie in Paris und dem AMOLF in Amsterdam im Rahmen eines European Associate Laboratory, sowie die Vernetzung mit dem MPI für molekulare Zellbiologie und Genetik (MPI-CBG) in Dresden. Unsere Gruppe unterhält auch einen Laborraum mit Mikroskopieaustattung im Gebäude des MPI-CBG. In enger Anbindung an theoretische Arbeiten werden dort insbesondere oszillierende Verteilungen von Min-Proteinen in Bakterien untersucht (Karsten Kruse), sowie physikalische Eigenschaften von Zellbewegung auf festen Substraten. Von besonderer Bedeutung ist die enge Zusammenarbeit mit dem MPI-CBG. Neben vielen gemeinsamen Projekten besteht ein gemeinsames Forschungsprogramm welches aus drei gemeinsamen Nachwuchsgruppen besteht. Unsere Abteilung ist auch an das internationale PhD Programm "Cell Biology, Bioengineering, Biophysics" angeschlossen, welches vom MPI-CBG initiert wurde.

Zukunftsperspektiven
Biologische Physik durchläuft eine sehr dynamische Entwicklung. Wegen der schnellen Weiterentwicklung der Grundlagen von Molekularer- und Zellbiologie nimmt das Themenspektrum der Forschung in biologischer Physik laufend in Tiefe und Breite zu. Das Max-Planck-Institut für Physik komplexer Systeme bietet ein besonderes Umfeld für theoretische Arbeiten in biologischer Physik. Das breite Spektrum an Forschungskompetenz im Bereich komplexer Phänomene erlaubt den Austausch und die Zusammenarbeit mit anderen Gruppen, die sich z.B. mit nichtlinearer Dynamik beschäftigen. Die Nähe zum Max-Planck-Institut für molekulare Zellbiologie und Genetik (MPI-CBG), dem Biotechnologiezentrum, sowie der TU, ermöglichen eine Vernetzung mit vielfältigen verwandten Forschungsaktivitäten.
Von besonderer Bedeutung für die Zukunft ist die sehr fruchtbare Zusammenarbeit mit dem MPI-CBG. Das gemeinsame Forschungsprogramm mit drei gemeinsamen Nachwuchsgruppen erlaubt es, aktuelle Probleme der Zell- und Entwicklungsbiologie theoretischen Zugängen zu eröffnen. Dies führt zur Entwicklung neuer theoretischer Methoden und regt auch neue Entwicklungen in der Theorie biologischer Systeme an. Gleichzeitig bring es neue Impulse in die biologische Forschung. Schwerpunkt des gemeinsamen Forschungsprogramms sind integrierte zelluläre Prozesse, deren Funktion aus dem Wechselspiel vieler verschiedener Komponenten hervorgeht. Derartige komplexe Systeme treten im Rahmen der sich schnell entwickelnden Systembiologie zunehmend ins Zentrum des Interesses der Biologie. Eine Vielzahl wichtiger biologischer Prozesse, wie zum Beispiel das Studium der Signalwege in der Zelle und die Regulierung zellulärer Prozesse durch Genexpression, werden in Zukunft in den Blickpunkt einer physikalischen Beschreibung treten. Dabei wird es von besonderer Bedeutung sein, zu verstehen, wie Materialeigenschaften und bewegungserzeugende Prozesse in der Zelle von Signalsystemen reguliert werden. Quantitative Methoden und Theorie werden in Zukunft eine zunehmend wichtige Rolle bei der Analyse komplexer biologischer Systeme spielen.

Kooperationen

- Max-Planck-Institut für molekulare Zellbiologie und Genetik, Dresden
  - Zusammenarbeit mit den Gruppen von Jonathon Howard und Anthony Hyman zur Dynamik des Zytoskeletts, der Zellteilung und der Physik molekularer Motoren
  - Zusammenarbeit mit Marcos González-Gaitán zur Entstehung von Gradienten von Morphogenen in der Fruchtfliege Drosophila
  - Zusammenarbeit mit Suzanne Eaton zu den Morphologien von Zellverbänden in der Fruchtfliege
  - Zusammenarbeit mit Andy Oates zur Segmentierung von Wirbeltieren durch oszillierende und raumzeitliche Genexpressionsmuster
  - Zusammenarbeit mit Carl-Phillip Heisenberg zur Untersuchung von Zellbewegungen während der Embryonalentwicklung des Zebrafisches.
  - Zusammenarbeit mit Marino Zerial zur Analyse der Dynamik des Endosomalen Netzwerks in Zellen.
- Cavendish Laboratory, Cambridge, UK
  - Zusammenarbeit mit Thomas Duke zur Physik des Gehörs und aktiven Wellenphänomenen in der Schnecke
- Institute Curie, Paris
  Zusammenarbeiten im Rahmen eines European Associate Laboratory
  - Zusammenarbeit mit Jean-Francois Joanny und Jacques Prost zur Physik aktiver Gele, der Dynamik des Zytoskeletts sowie zur Zellbewegung.
  - Zusammenarbeit mit Pascal Martin zur Physik von mechanosensiblen Sinneszellen (Haarzellen).
  - Zusammenarbeit mit Michel Bornens zur Orientierung der mitotischen Spindel sowie zur Zytokinese (dem Trennen der Tochterzellen nach der Zellteilung)
- AMOLF, Amsterdam
  - Zusammenarbeit mit Marileen Dogterom und Bela Mulder zur Entstehung kontraktiler Ringe und zur Dynamik des Zytoskeletts in Pflanzenzellen
- Ben-Gurion University, Beer-Sheva
  - Zusammenarbeit mit Anne Bernheim-Groswasser zur Physik aktiver Gele

Arbeitsgruppe: Biologische Physik des Geruchsinns
(Leiter: Dr. M. Zapotocky)

Die Arbeitsgruppe besteht zur Zeit aus zwei Postdocs und einem Gastwissenschaftler. Wir benutzen Methoden der statistischen Physik, der nichtlinearen Dynamik und der Physik weicher kondensierter Materie um biologische Sinnessysteme zu untersuchen. Der Schwerpunkt liegt dabei auf dem olfaktorischen, d.h. Geruchssinn und dem mechanischen Sinn. Unser Interesse gilt in einem weiteren Sinne auch der Entwicklungsbiologie sowie der Theorie biochemischer Netzwerke. Wir haben uns in letzter Zeit auf drei spezielle Forschungsgebiete konzentriert:

1. Signaltransduktion in den Geruchszellen:

In den Zilien der Geruchszellen wird das äußere chemische (Eingangs-)Signal (die Art und Konzentration des Geruchsstoffs) in ein elektrisches Signal umgewandelt. Der entsprechende Signaltransduktionsweg ist biochemisch gut beschrieben und es ist bekannt, dass er einige durch intrazelluläres Kalzium vermittelte Rückkopplungsschleifen beinhaltet. In früheren Arbeiten haben wir mit Hilfe von deterministischen Ein-Kompartiment-Modellen die Rolle des Kalzium-Feedbacks in der Dynamik der Signaltransduktion untersucht. In letzter Zeit haben wir diese Untersuchung durch die Einbeziehung von Fluktuationen und Diffusionseffekten erweitert. Im Projekt "Response and fluctuations of a two-state signaling module with feedback" (Seite 128) untersuchen wir die Kinetik und Informationsübertragung in einem prototypischen Signalmodul, das aus einem stochastischen Zwei-Zustands-Punktprozess mit negativer Rückkopplung besteht. Mittelwerte, Autokorrelations- und Antwortfunktionen in erster Ordnung in der Rückkopplung konnten mit Hilfe einer Pfadintegralmethode explizit berechnet werden; das Regime starker Rückkopplung untersuchen wir mit Monte-Carlo-Simulationen. Eine überraschende Folgerung ist, dass die negative Rückkopplung das Signal-zu-Rauschverhältnis erhöhen oder verringern kann, abhängig von den genauen Werten der Parameter. Im Moment benutzen wir eine Erweiterung dieses Ansatzes auf eine eindimensionale Kette von diffusiv gekoppelten Schaltern, um die Genauigkeit der olfaktorischen Signalerzeugung bei sehr niedriger Geruchsstoffskonzentration zu untersuchen.

2. Kollektiveffekte in der axonalen Zielfindung:

Während der Entwicklung werden Verbindungen zwischen Hirnbereichen durch wachsende neuronale Fortsätze, die Axone, gebildet. In den derzeit vorherrschenden Erklärungsmodellen wird jedes wachsende Axon unabhängig voneinander zum richtigen Ziel geleitet, indem es einen räumlich verteilten chemischen Signalstoff detektiert. Wir entwickeln Modelle, in denen Axon-Axon Wechselwirkungen eine dominante Rolle spielen, wodurch die richtige Zielfindung ein Kollektiveffekt wird. Wir behandeln jedes wachsende Axon idealisiert als einen gerichteten random walk (Zufallslauf), der einer attraktiven Kontaktwechselwirkung mit anderen gleichzeitig wachsenden Axonen unterliegt. Die aus dem *Umsatz* von Axonen, wobei die voll ausgewachsenen Axone absterben und durch nachwachsende ersetzt werden, resultierende Dynamik wurde systematisch charakterisiert. Das entspricht der Situation im Geruchssystem der Säugetiere, wo der Umsatz von Sinneszellen bis ins Erwachsenenstadium anhält, und das Vernetzungsmuster zwischen dem nasalen Epithel und dem olfaktorischen Bulbus erst nach 3-5 Umsatzperioden einen stationären Zustand erreicht. Im stationären Zu-

stand unseres Modells findet man mit wachsendem Abstand zum Epithel immer dickere Axonbündel, und die Verteilung ihrer Dicke gehorcht einem Skalengesetz. Bei einer heterogenen Population von Axonen verschiedener Typen, mit typabhängiger Wechselwirkung untersuchen wir die Typenreinheit der resultierenden Bündel. Wir setzen unsere Resultate zu experimentellen Daten über Zielfindungseffekte im olfaktorischen Bulbus in der Maus in Beziehung.

3. Flugsteuerung von Drosophila durch mechanosensitive Rückkopplung:

Das Ziel dieses Projektes ist es zu verstehen, wie die Fruchtfliege mechanosensitive Information aus den Flügeln benutzt, um Flugstabilität und Manövrierbarkeit zu verbessern. Fliegen haben ungefähr 100 mechanosensitive Rezeptoren in jedem Fügel; das Verformungsmuster des Flügels ist somit in der zeitlichen Abfolge von durch die Sinneszellen erzeugten Aktionspotentialen kodiert. Den Flugapparat von Drosophila kann man sich vorstellen als einen Motor (ein Satz Flugmuskeln) und zwei Getriebe (Skleritgelenke mit daran angebrachten kleinen Kontrollmuskeln), welche die Flugmuskeln an den linken und rechten Flügel koppeln. Die Kontrollmuskeln werden durch die Aktivität der mechanosensitiven Neuronen in den Flügeln beeinflusst; jedes Getriebe wird daher von einer mechanosensitiven Rückkopplungsschleife dynamisch reguliert. In der theoretischen Beschreibung koppeln wir einen zentralen nichtlinearen Oszillator (die Flugmuskeln) an zwei lineare mechanische Systeme, deren Parameter durch die Aktivität der mechanosensitiven Neuronen kontrolliert werden. Unser erstes Ziel ist es, die Dynamik einer Sakkade, d.h. einer schnellen 90-Grad-Drehung um die Gierachse, zu beschreiben. In unserer Beschreibung wird die Sakkade von einer starken transienten Störung auf der rechten oder linken Seite eingeleitet, und sie setzt sich fort, bis rechter und linker Flügel wieder voll amplituden- und phasensynchronisiert sind. Wir analysieren den Einfluss der mechanosensitiven Rückkopplung auf die Synchronisation, und vergleichen die vorhergesagten Verläufe einer Sakkade mit experimentell gemessenen (Labor von S.N. Fry ETH Zürich). Unter Benutzung in der Gruppe von J. Howard (MPI-CBG Dresden) entwickelter genetischer und physiologischer Methoden werden wir dann die Aktivität der mechanosensitiven Neuronen systematisch stören und den Effekt auf die Flugsteuerung untersuchen. Dieses Projekt wird in Teilen von der VolkswagenStiftung finanziell gefördert (mit J. Howard und S.N. Fry).

Kooperationen

mit Biologen:
J. Howard, MPI for Cell Biology and Genetics, Dresden, and S. Frey, ETH Zurich
(Flugsteuerung durch mechanosensitive Rückkopplung)
P. Feinstein and P. Mombaerts, Rockefeller University, New York
(Kollektiveffekte in der axonalen Zielfindung)

mit Theoretikern:
F. Jülicher, mpi**pks**
P. Borowski, University of British Columbia, Canada
M. Gopalakrishnan, Harish-Chandra Research Institute, India
G. Sibona, Universidad Nacional de Cordoba, Argentina
P. K. Mohanty, Saha Institute of Nuclear Physics, India

Arbeitsgruppe: Physik biologischer und weicher Materie
(Leiter: Dr. Ralf Everaers bis (12/06))

Die Gruppe wurde im November 2002 gegründet und hat im Januar 2004 ihre typische Größe von zwei Doktoranden und vier Gastwissenschaftlern erreicht. In Folge der Berufung des Gruppenleiters an die École normale supérieur de Lyon im Jahre 2006, laufen die Aktivitäten in Dresden im Laufe des Jahres 2007 aus. Unsere Forschung bewegt sich im Grenzgebiet zwischen Materialwissenschaft und Biologischer Physik, wobei wir biologische Systeme als "lebende weiche Materie" betrachten. Wir nutzen Methoden der Statistischen Physik mit einem Schwerpunkt auf der Kombination von Computersimulationen mit analytischer und Skalentheorie.
Die theoretische Beschreibung des Wechselspiels von Lipiden, Proteinen und Nukleinsäuren in lebenden Zellen benötigt ähnliche Methoden wie die Analyse von Gelen und Lösungen bestehend aus kolloidalen Teilchen, Polymeren und oberflächenaktiven Molekülen. "Weiche" kondensierte Materie wird stark durch thermische Fluktuationen beeinflusst, verdankt ihren Namen ihrer großen Suszeptibilität für mechanische Spannungen und elektrische oder magnetische Felder und zeichnet sich oft durch ungewöhnlichen Fließeigenschaften aus. Typischerweise besitzen oder bilden die Systeme Strukturen weit oberhalb der atomaren Skala. Wir untersuchen den Zusammenhang zwischen mikroskopischen Wechselwirkungen, Struktur und Dynamik auf mesoskopischen Skalen und makroskopischen physikalischen Eigenschaften bzw. biologischer Funktion. Unsere Forschung konzentriert sich auf drei Themenbereiche:

Verhakungseffekte bei Polymeren: Polymere haben einzigartige viskoelastische Eigenschaften und bilden das Grundgerüst von so unterschiedlichen Systemen wie Autoreifen und dem Zytoskelett. Charakteristisch für lange Kettenmoleküle ist das Auftreten topologischer Verhakungen auf molekularen Skalen. Ähnlich zu verknoteten Schnüren können sich Polymerketten aneinander vorbeibewegen, aber nicht durchkreuzen. Das Standardmodell der Polymerdynamik, das Röhrenmodell, basiert auf der Vorstellung, dass die Verhakungen mit anderen Ketten die Fluktuationen jedes Polymers auf ein röhrenartiges Volumen um einen "primitiven Pfad" beschränken, der wiederum der geglätteten Kettenkonformation folgt. Nach Etablierung der mikroskopischen Grundlagen dieses erfolgreichen phänomenologischen Modells durch die Einführung einer "primitiven-Pfad-Analyse" (PPA) (s. den Institutsbericht 2003/04), haben wir uns auf Deformationseffekte in verhakten Polymernetzwerken konzentriert. Insbesondere ging es dabei um die Längenskalenabhängigkeit der mikroskopischen Deformationen, die Manifestation dieses Effektes in Kleinwinkel-Neutronstreuexperimenten teildeuterierter Systeme und um chemische Alterungseffekte in deformierten Systemen.

Polyelektrolyte: Polyelektrolyte sind Polymere mit ionisierbaren Seitengruppen. Beispiele sind Amino- und Nukleinsäuren ebenso wie Polyacrylsäure, das Material aus dem Babywindeln hergestellt werden. Dass viele Biopolymere in diese Klasse fallen, ist kein Zufall: irdisches Leben beruht auf einem Wechselspiel Kohlenstoff-basierter Makromoleküle in Wasser. Die Löslichkeit dieser typischerweise wenig polaren, organischen Moleküle beruht gerade auf dem Entropiegewinn der in wässriger Lösung dissoziierten Gegenionen. Die Behandlung der langreichweitigen elektrostatischen Wechselwirkungen ist besonders schwierig in der Umgebung unpolarer, hydrophober Elemente. Wir ent-

wickeln mit Unterstützung der Volkswagenstiftung neue Simulationsalgorithmen, die die Berechnung elektrostatischer Selbstenergien und -wechselwirkungen in dielektrisch inhomogenen Medien ermöglichen (s. S. 134).

DNA und Chromatin: Genetische Information ist in der komplementären Basensequenz der beiden Einzelstränge der DNA Doppelhelix gespeichert. Replikation und Transkription erfolgen durch lokale Dissoziation der Doppelhelix and Synthese komplementärer DNA- oder RNA-Stränge entlang der Einzelstränge. In eukaryotischen Zellen ist die DNA mit Proteinen komplexiert und hierarchisch in Chromatinfasern und Chromosomen organisiert. Die relevanten Längenskalen reichen von 1 nm (dem Durchmesser einzelner Basen) bis zur Gesamtkonturlänge der DNA von 2 m in jeder menschlichen Zelle. Unsere Arbeiten umfassen Theorien und Computersimulationen der Elastizität und thermischen Denaturierung von DNA auf Basenpaarebene (s. S. 136), der Struktur der 30 nm Chromatinfaser, elektrostatischer Wechselwirkungen in DNA und Chromatin und Effekte topologischer Einschränkungen bei der Dekondensation von Chromosomen in der Metaphase des Zellzyklus.

Kooperationen

- Dr. G. S. Grest (Sandia National Laboratories, Albuquerque, USA): Simulation von Polymerschmelzen und -netzwerken
- Prof. K. Kremer (Max-Planck-Institut für Polymerforschung, Mainz): Simulation von Verhakungseffekten in Polymersystemen
- Dr. A. C. Maggs (ESPCI, Paris, France): Elektrostatische Wechselwirkungen in weicher kondensierter Materie
- Prof. H. Schiessel (Lorentz Institut, Universität Leiden, Niederlande): Chromatin
- Prof. E. Straube (Universität Halle-Wittenberg): Analyse der Polymerdynamik in Röhrenmodellen
- Prof. N. Uchida (Tohoku Universität, Sendai, Japan): Simulation von Aktinlösungen

Nachwuchsgruppe: Wellen in komplexen Medien und mesoskopische Phänomene
(Leiter: Dr. H. Schomerus bis (3/05))

Die Nachwuchsgruppe bestand von November 2000 und beherbergte in diesem Zeitraum neben dem Gruppenleiter gut ein Dutzend junger Gastwissenschaftler für jeweils 1-3 Jahre währende Anstellungen. 2005 wechselte der ehemalige Gruppenleiter auf eine permanente Stelle als Reader in Condensed Matter Theory an der Universität Lancaster, UK. Die letzten verbliebenen Gruppenmitglieder verließen im Herbst 2006 das mpi**pks**. Bis auf ein Mitglied, welches nun in der Industrie tätig ist, sind alle ehemaligen Mitarbeiter weiterhin akademisch tätig, wobei eine Reihe von ihnen leitende Funktionen auf der Ebene von Nachwuchsgruppenleitern, Assistenten oder Assistenzprofessoren ausübt (M. Hentschel am mpi**pks**, J. Wiersig an der Uni Bremen, M. Titov an der Uni Konstanz, M. Zareyan am IASBS Zanjan, Iran).

Die Gruppe befasste sich mit dem elektronischen und photonischen Transport und der Dynamik in niederdimensionalen und mesoskopischen Quantensystemen. Dabei wurden das Wechselspiel von Unordnung, Geometrie, Wechselwirkungen, Phasenkohärenz, Chaos, und verschiedener Korrelationseffekte in normal- und supraleitenden sowie ferromagnetischen und photonischen Materialien untersucht.
Es entstanden 81 begutachtete Veröffentlichungen in internationalen Journalen, darunter 14 in Physical Review Letters.

Nachwuchsgruppe: Elektronische Struktur endlicher Systeme
(Leiter: Dr. S. Kümmel (bis 9/05))

Der Forschungsschwerpunkt der Emmy Noether-Nachwuchsgruppe "Elektronische Struktur endlicher Systeme" war die Untersuchung der Struktur, in zunehmendem Maße aber vor allem auch der Dynamik elektronischer Systeme. Insbesondere standen die Dichtefunktionaltheorie und ihre zeitabhängige Erweiterung im Zentrum unserer Arbeit. Das Ziel unserer Forschung war, eine zuverlässige Beschreibung nichtlinearnichtperturbativer Elektronendynamik zu erreichen. Typische Beispiele für die diese Arbeit motivierenden Fragestellungen finden sich in der Atomphysik. Dort werden Phänomene wie die Erzeugung hoher Harmonischer oder die nichtsequentielle Mehrfachionisation experimentell sehr erfolgreich untersucht. Auf theoretischer Seite steht den experimentellen Erfolgen die Schwierigkeit gegenüber, dass die Berechnung der zeitabhängigen korrelierten Vielteilchenwellenfunktion aus der zeitabhängigen Schrödingergleichung so aufwendig ist, dass sie bereits für ein scheinbar einfaches System wie das Helium Atom kaum ohne vereinfachende Annahmen möglich ist.
Hier kann die zeitabhängige Dichtefunktionaltheorie eine entscheidende Lücke schließen. Mit dem grundlegenden Ansatz, das quantenmechanische Vielteilchenproblem nicht mit der Wellenfunktion als grundlegender Variable zu lösen sondern mit der Dichte, ist sie rechnerisch wesentlich weniger aufwändig. Sie erlaubt daher die Vorhersage der korrelierten nichtperturbativen Elektronendynamik. Zudem führen Dichtefunktionalrechnungen meist zu einem klaren physikalischen Verständnis, da sie auf intuitiv interpretierbaren Größen wie der Teilchenzahldichte und lokalen Potentialen beruhen. Diesen positiven Seiten steht die zentrale Schwierigkeit der (zeitabhängigen) Dichtefunktionaltheorie gegenüber: Die Bestimmung der Funktionale, die die quantenmechanischen Austausch- und Korrelationseffekte beschreiben. In diesem Themenkreis haben wir uns v.a. damit beschäftigt zu zeigen, welche Eigenschaften das Austausch-Korrelationspotential haben muss, um Ionisationsdynamik korrekt zu beschreiben und entsprechende Näherungen wurden untersucht. Weitere Projekte beschäftigten sich mit der Strukturaufklärung metallischer Cluster mittels Photoelektronen-Spektroskopie und ihrer theoretischen Interpretation und mit den response-Eigenschaften ausgedehnter molekularer Systeme.
Die Projekte werden nun an der Universität Bayreuth fortgesetzt, an der Stephan Kümmel (Leiter der Emmy Noether-Gruppe) im Sommer 2005 eine Professur für Theoretische Physik übernommen hat. Damit endete die Emmy Noether-Nachwuchsgruppe "Elektronische Struktur endlicher Systeme". Die gemeinsamen Projekte und Kollaborationen, sowohl international als auch innerhalb des mpi**pks** fanden abschließend Niederschlag in der Ausrichtung der Focus Tage "Electronic correlation in atomic and

molecular dynamics" gemeinsam mit M. Lein und J.-M. Rost im Rahmen der Konferenz "Atomic Physics 2005".

Nachwuchsgruppe: Vielteilcheneffekte in mesoskopischen Systemen
(Leiter: Dr. M. Hentschel (ab 4/06))

Die Emmy Noether-Nachwuchsgruppe „Vielteilchenteilcheneffekte in mesoskopischen Systemen" hat im April 2006 die Arbeit am Institut aufgenommen. Derzeit beschäftigen sich neben der Gruppenleiterin zwei Doktoranden und zwei Postdoktoranden mit Auswirkungen von Andersons Orthogonalitätskatastrophe auf Photoabsorptionsspektren und Transportgrößen von realistischen mesoskopischen Systemen. Ein weiteres, praktisch disjunktes Arbeitsgebiet der Gruppe sind Aspekte des Quantenchaos in optischen Mikroresonatoren. Diese Forschung wird von der Gruppenleiterin zusammen mit (bisher einem) Postdoktoranden des Gästeprogramms des Instituts durchgeführt. Besonders erwähnenswert ist hier die aktive Einbindung der Gruppe in die (positiv bewertete, aber im April 2007 noch endgültig zu bestätigende) DFG-Forschergruppe 760 „Scattering Systems with Complex Dynamics". Seit Oktober 2006 führt die Arbeitsgruppe ein eigenes wöchentliches Seminar „Mesoscopic Systems" durch. Desweiteren ist die Gruppenleiterin Hauptorganisator der „Scientific Jam Session", einer Diskussionsrunde für die jungen Wissenschaftler (Postdoktoranden und fortgeschrittene Doktoranden) des Instituts am Freitagnachmittag, die seit Juni 2006 besteht.
Vielteilcheneffekte in Festkörpern haben von jeher das Interesse der Physiker geweckt und die Entwicklung neuer Theorien herausgefordert. Stellvertretend sei hier das Röntgenkantenproblem genannt, bei dem es um in Metallen beobachtete Abweichungen des Photoabsorptionssignals von der naiven Erwartung geht. Seit etwa 15 Jahren ist es nun möglich, sehr viel kleinere, nanoskalige Proben in Form von Quantenpunkten oder metallischen Nanoteilchen herzustellen und zu untersuchen. In solchen mesoskopisch-kohärenten Systemen werden die Eigenschaften der elektronischen Wellenfunktionen maßgeblich durch die Geometrie bestimmt. Das für Metalle gültige Bild der Bloch-Elektronen muss durch Überlegungen aus dem Gebiet des Quantenchaos ergänzt werden. Wird dies zusammen mit der im Vergleich zum metallischen Fall sehr viel geringeren Elektronenzahl Auswirkungen auf die Signaturen von Vielteilcheneffekten und Transportgrössen haben? Derartige Fragestellungen werden von der Emmy Noether-Gruppe untersucht.
Dass kleine Systeme tatsächlich andere Charakteristika aufweisen können als makroskopische, wurde von der Gruppenleiterin am Beispiel des Photoabsorptionsstreuquerschnitts generisch-chaotischer mesoskopischer Systeme gezeigt. Die Erweiterung dieser Arbeiten auf reguläre Systeme ist einer der aktuellen Forschungsschwerpunkte. Konkret geht es um Andersons Orthogonalitätskatastrophe in kreisrunden und rechteckigen Quantenpunkten sowie in Systemen mit parabolischen Potenzial. Für diesen letztgenannten, experimentell relevanten Fall beobachten wir charakteristische Schaleneffekte, deren Einfluss auf die Photoabsorptionssignatur sowie Transportgrößen wir untersuchen. Ein anderes System, das derzeit in der Arbeitsgruppe studiert wird, ist Graphen. Hier spiegeln sich die speziellen elektronischen Eigenschaften an den Dirac-Punkten im Verhalten des Anderson-Überlapps wider.
Die Arbeiten zum zweiten Forschungschwerpunkt der Gruppe, den optischen Mikroresonatoren, umfassen einerseits semiklassische Korrekturen zum Strahlenbild, anderer-

seits die Untersuchung des Einflusses eines aktiven Mediums (Laser) auf die Resonanzeigenschaften. Beispielsweise werden die Auswirkungen des Goos-Hänchen-Effekts auf die Fernfeldausstrahlung von Mikroresonatoren sowie Gemeinsamkeiten und mögliche Unterschiede zwischen Resonanzmoden in passiven und aktiven Kavitäten studiert. Die Beantwortung der dabei auftretenden Fragen ist für Anwendungen in Mikrolasern von enormer praktischer Bedeutung.

Zukunftsperspektiven
Ein weiteres Thema der Arbeiten zu mesoskopischen Vielteilcheneffekten wird in Zukunft der Kondo-Effekt in nanoskaligen Systemen sein, insbesondere die Überlagerung von Kondo- und Röntgenkantenphysik. In beiden Fällen wird die Zustandsdichte der Elektronen an der Fermikante verändert und resultiert in Fermikantensingularitäten. Mesoskopische Systeme erlauben es, beide Effekte in einer Weise zu koppeln, die in Metallen nicht realisierbar ist.
Im Bereich der optischen Mikroresonatoren wird ein zukünftger Problemkreis sein, inwieweit für geschlossene Billards gefundene Eigenschaften (beispielsweise hierarchische Zustände oder das Fluten regulärer Inseln durch chaotische Zustände) auch in offenen, optischen Billards relevant sind. Desweiteren soll die Bedeutung von spontaner Emission in Mikrolasern untersucht werden. Die derzeit benutzten Modelle vernachlässigen diesen Effekt bisher völlig. Seine Beschreibung im Rahmen des Schrödinger-Bloch-Modells ist nicht nur konzeptionell wünschenswert, sondern auch von praktischer Bedeutung.
Schließlich sei erwähnt, dass die Gruppenleiterin zusammen mit Mark Raizen (University of Texas at Austin, USA) und Jan Wiersig (Universität Bremen) Organisator der Konferenz „New Frontiers of Quantum Chaos in Mesoscopic Systems“ ist, die im Mai 2008 am Institut stattfinden wird.

Kooperationen
Die Anbindung der Nachwuchsgruppe an die nationale und internationale Forschungslandschaft ist vielfältig und umfasst sowohl theoretische als auch experimentelle Kooperationen. Im einzelnen sind, getrennt nach den beiden Hauptarbeitsrichtungen der Gruppe, zu nennen:

Vielteilcheneffekte in mesoskopischen Systemen:

- Fortsetzung der Zusammenarbeit mit Harold Baranger (Duke University, USA) und Denis Ullmo (Orsay, Frankreich), die seit der Postdoktorandenzeit der Gruppenleiterin an der Duke University besteht.

- Zusammenarbeit mit Francisco Guinea (Madrid, Spanien) zu Problemen von Andersons Orthogonalitätskatastrophe in Graphen.

Quantenchaos in optischen Mikroresonatoren

- Kooperationen im Rahmen der oben erwähnten DFG-Forschergruppe, insbesondere mit Jan Wiersig (Universität Bremen), mit Roland Ketzmerick und Arnd Bäcker (TU Dresden) sowie mit Henning Schomerus (Lancaster University, Großbritannien).

- Fortsetzung der erfolgreichen Zusammenarbeit mit den *experimentellen* Gruppen von Takahisa Harayama und Takehiro Fukushima (ATR Wave Engineering Laboratories, Kyoto, Japan und Okayama Prefectural University, Japan), mit denen u.a. Arbeiten zur Fernfeldcharakteristik von ovalen Mikrolasern durchgeführt wurden (Vergleich von Experiment und Strahlensimulationen).

- Zur *experimentellen* Gruppe von Achim Richter (Technische Universität Darmstadt) bestehen seit kurzem Kontakte, in denen es um die Messung des Goos-Hänchen-Effekts an gekümmten Grenzflächen geht. Desweiteren bestehen regelmässige Kontakte zu den Gruppen von Chil-Min Kim (Paichai University, Daejon, Korea) und Sang Wook Kim (Busan National University, Korea).

Gemeinsames Forschungsprogramm mpipks und MPI-CBG

Physik Biologischer Systeme

Das gemeinschaftliche Forschungsprogramm "Physik Biologischer Systeme" des Max-Planck-Instituts für Physik komplexer Systeme und des Max-Planck-Instituts für Molekulare Zellbiologie und Genetik intensiviert Kollaborationen zwischen diesen beiden Dresdner Instituten. Das Ziel des Programms ist das Entwickeln neuer physikalischer Methoden und Konzepte - experimenteller und theoretischer Natur - zum Analysieren biologischer Systeme. Drei Nachwuchsgruppen haben ihre Aktivitäten nach dem Start des Programms in 2004 aufgenommen. Die Gruppe von Dr. Karsten Kruse (Die Physik der Zellteilung) nahm im Oktober 2004 ihre Arbeit am mpipks auf, und studiert die Prinzipien der örtlichen und zeitlichen Organisation von Zellen während der Zellteilung. Die Gruppe von Dr. Iva Tolić-Nørrelykke (Inneres Design der Zelle) nahm im Dezember 2004 ihre Arbeit am Max-Planck-Institut für Molekulare Zellbiologie und Genetik auf, und untersucht, wie das Zellinnere sich während der Lebensdauer der Zelle organisiert. Die Gruppe von Dr. Stephan Grill (Motor Systeme) nahm im April 2006 ihre Arbeit an beiden Instituten auf und erforscht, wie molekulare Maschinen arbeiten und interagieren, um die Dynamiken innerhalb der Zelle zu erzeugen. Verschiedene Kollaborationen, gemeinsame Gruppentreffen und eine Seminarserie zur Physik biologischer Systeme garantieren ein hohes Niveau an Interaktion zwischen den drei Gruppen und anderen Gruppen an den beiden Instituten. Daraus ergibt sich ein einzigartiges wissenschaftliches Umfeld: theoretische Physik und experimentelle Biologie werden zusammengebracht mit dem Ziel, die physikalischen Prinzipien des Aufbaus und der Dynamik lebender Systeme zu untersuchen.

Nachwuchsgruppe: Physik der Zellteilung

(Leiter: Dr. K. Kruse (bis 8/06))

Das Arbeitsgebiet der von Oktober 2004 bis August 2006 bestehenden unabhängigen Nachwuchsgruppe war die Untersuchung physikalischer Aspekte der Zellteilung. Die Zellteilung illustriert in außerordentlicher Weise die Notwendigkeit einer zeitlichen und und räumlichen Kontrolle zellulärer Prozesse: z.B. muss die DNA so auf die zukünftigen Tochterzellen verteilt werden, dass jede einen vollständigen Satz genetischer Information erhält. Weiterhin muss die Mutterzelle im Anschluss daran an einer wohldefinierten Stelle zerteilt werden. Welche Mechanismen bewirken diese Organisa-

tion in Raum und Zeit? Es gibt deutliche Hinweise, daß Zellen modular organisiert sind. Die Forschung der Nachwuchsgruppe zielte darauf, bestimmte, an der Zellteilung beteiligte Module mit Mitteln der Theorie dynamischer Systeme sowie der Statistischen Physik von Systemen außerhalb des thermodynamischen Gleichgewichts zu analysieren. Die Leitidee war dabei, wesentliche Komponenten eines Moduls zu identifizieren, um so die Prinzipien, die der Funktion des Moduls zugrundeliegen, herauszuarbeiten. Dieses Vorgehen soll es insbesondere auch ermöglichen, Gemeinsamkeiten auf den ersten Blick unverwandter Module zu erkennen. Die Arbeit konzentrierte sich auf die beiden folgenden Module:

Das Zytoskelett. Das Zytoskelett ist eine wichtige zelluläre Substruktur, die nicht nur für die Zellteilung von Bedeutung ist, sondern z.B. auch für die Zellfortbewegung oder die Organisation des intrazellulären Transports. Das Zytoskelett ist ein Netzwerk fadenartiger Proteine, in eukaryotischen Zellen hauptsächlich Aktin Filamente und Mikrotubuli, die mit einer großen Zahl assoziierter Proteine wechselwirken. Darunter befinden sich insbesondere molekulare Motoren wie Myosine oder Kinesine, die die in ATP gespeicherte chemische Energie in mechanische Arbeit umwandeln und Spannungen in dem Netzwerk erzeugen können. Zellen verfügen über eine Reihe von Mechanismen zur Kontrolle und Regulation des Zytoskeletts. Experimente in vitro haben allerdings gezeigt, dass sich Motor-Filament-Systeme selbstorganisieren können. Wir haben verschiedene physikalische Beschreibungen der Dynamik des Zytoskeletts sowie der Spannungserzeugung in diesem aktiven polaren Gel entwickelt. Dabei haben wir mesoskopische wie auch makroskopische phänomenologische Ansätze verfolgt. Darüberhinaus haben wir diese Beschreibungen auf verschiedenen in vitro aber auch in vivo Situationen angewendet.

Die Min-Oszillationen. Eine wesentliche Aufgabe im Laufe einer Teilung besteht für eine Zelle darin, den Ort der Teilung zu bestimmen. In dem stäbchenförmigen Bakterium *Escherichia coli* erfolgt die Zellteilung mit hoher Präzision in der Mitte quer zur Längsachse. In der Folge entstehen zwei gleichgroße Tochterzellen. Die Bestimmung der Zellmitte beruht dabei wesentlich auf dem Min-System, welches aus den Proteinen MinC, MInD und MinE besteht. Von diesen ist MinC ein unspezifischer Inhibitor der Zellteilung. Durch Wechselwirkung mit MinD und MinE wechselt MinC zyklisch mit einer Periode von etwa 60s zwischen den beiden Zellenden, so daß die Teilung in der Nähe der Pole unterdrückt wird. Die Arbeit der Gruppe zielt auf die Identifikation möglicher Oszillationsmechanismen, wobei theoretische wie auch experimentelle Techniken eingesetzt werden.

Kooperationen

A. Bernheim-Groswasser (Ben Gurion University, Beer-Sheva), M. Dogterom (AMOLF, Amsterdam), Jonathon Howard (MPICBG, Dresden), Jean-Franç ois Joanny (Institut Curie, Paris), B. Mulder (AMOLF, Amsterdam), Jacques Prost (ESPCI, Paris), Petra Schwille (TU Dresden), Ken Sekimoto (Université Paris VII)
In der Zeit während ihres Bestehens wurden in der Gruppe eine Habilitation (K. Kruse) eine Doktorarbeit (G. Meacci) und eine Diplomarbeit (S. Günther) angefertigt. Drei weitere Doktorarbeiten wurden begonnen (K. Doubrovinski, E. Fischer-Friedrich, S.

Günther) und werden jetzt am MPIPKS (E. Fischer-Friedrich) bzw. der Universität des Saarlandes (K. Doubrovinski, S. Günther) fortgesetzt. K. Kruse ist inzwischen Professor (W3) an der Universität des Saarlandes, G. Meacci hat eine Postdocstelle am IBM Thomas J. Watson Center in Yorktown Heights, USA angetreten. Schließlich gehörten der Gruppe ein Gastwissenschaftler (A. Iomin), ein Postdoc (E. Nicola) und ein Gaststudent (R. Nguyen van yen, Ecole Normale Superieure, Paris) an. Mitglieder der Gruppe waren u.a. an der Publikation von vier Physical Review Letters und eines Artikels in Science beteiligt.

Nachwuchsgrupe: Motor Systeme
(Leiter: Dr. Stephan W. Grill)

Unsere Gruppe beschäftigt sich damit, wie molekulare Maschinen, die Arbeitspferde einer jeden Zelle, funktionieren und interagieren, um die komplexen Dynamiken eines lebenden Organismus erzeugen. Wir konzentrieren uns dabei auf die physikalischen Mechanismen der Koordination, Regulation und Erzeugung von Kraft und Bewegung in biologischen Systemen. Wir arbeiten sowohl experimentell als auch theoretisch an zwei Systemen, die vom einzelnen Makromolekül bis zur einzelnen Zelle reichen.
Transkriptions-Systeme. Wir untersuchen die Bewegung von einzelnen Molekülen von RNA Polymerase II (RNAP II) entlang der DNA. RNAP II liest den genetischen Code aus und kopiert ihn zu mRNA, welches später in eine Polypeptidkette übersetzt wird um ein Protein herzustellen. Alle Proteine werden auf diese Art erzeugt, daher repräsentiert RNAP II einen zentralen Kontrollpunkt für zelluläre Funktion. Wir konzentrieren uns in unseren Untersuchungen auf einem speziellen Zustand der Polymerase, der für das Korrigieren von Kopierfehlern verantwortlich ist. Während der Fehlerkorrektur, so glauben wir, unternimmt die Polymerase einen sogenannten "Random Walk" und diffundiert somit die DNA entlang. Wir untersuchen die Implikationen eines solchen diffusiven Zustandes sowohl auf die Kraftabhängigkeit der Transkription, der Lebensdauer dieses Korrekturzustandes, sowie der generellen Möglichkeit der Polymerase, Kopierfehler effizient zu entdecken und korrigieren. Dies beinhaltet das Erstellen eines mikromechanischen Modells der Transkription, welches den Vergleich der Fehlerkorrektur-Effizienz mit den Experimenten sowie der theoretisch zu erwartenden optimalen Effizienz, welche RNAP II wohl im Rahmen der Evolution erlangt hat, ermöglicht. Wir hoffen damit, die mikromechanischen Details der Transkription in allen höheren Lebewesen zu verstehen.
Zytoskelett-Systeme. Wir untersuchen die Mechanismen denen die Dynamik des Zytoskeletts während der frühen Embryogenese des Fadenwurmes *Caenorhabditis elegans* unterliegt. Im Zytoskelett verbirgt sich die gesamte aktive Mechanik der lebenden Zelle. *C. elegans* erlaubt das Anwenden eines perturbativen Ansatz auf einem "systembiologischen" Level: Für eine bestimmte Aktivität des Zytoskeletts erstellen wir zunächst eine theoretische Beschreibung. Um diese Beschreibung zu testen und zu verfeinern, stören wir das System auf eine kontrollierte Weise, sowohl mechanisch als auch genetisch, und schauen uns die Antwort des Systems an, sowohl in Theorie als auch in Experiment. Wir haben mit Hilfe dieses Ansatzes unser Verständnis der Positionierung und Oszillation der mitotischen Spindel während der Zellteilung erweitert, und widmen uns nun anderen Prozessen im Zytoskelett, insbesondere dem Actin-Myosin Netzwerk unterhalb der Zellmembran. Diese Filamente sind für eine Reihe lebensnotwendiger

Funktionen verantwortlich, unter anderem die Teilung einer Zelle in zwei Tochterzellen. Wir studieren den Mechanismus der Erzeugung zweier unterschiedlicher Domänen des Actin-Myosin Netzwerks im Rahme der asymmetrischen Zellteilung, die insbesondere für das Teilen von Stammzellen von Bedeutung ist. Nach dem Brechen der Symmetrie unterscheiden sich diese beiden Domänen, so wird vermutet, in ihren physikalischen Eigenschaften (Viskoelastizität und aktiv erzeugter Spannung), und diese Eigenschaften bestimmen die Größe, zu welcher die Domänen wachsen. Wir werden beide Domänen in Theorie und Experiment beschreiben, und hoffen damit die biophysikalischen Eigenschaften aller an der asymmetrischen Zellteilung beteiligten Komponenten zu verstehen.
Theorie und Experiment. Unsere Gruppe arbeitet sowohl am mpi**pks** als auch am MPI-CBG. Wir wenden Techniken der Physik von Nichtgleichgewichtssystemen und der nichtlinearen Dynamik an, um theoretische Modelle zu erstellen, die wir mittels einer hochauflösenden optischen Falle (für Einzelmolekülexperimente in minimalen Systemen), einem UV-Laserschneider (für mechanische Perturbationsexperimente an einzelnen Zellen) und titrierter RNA-Interferenz (für genetische Perturbationsexperimente an einzelnen Zellen) testen.

Kooperationen
C. Bustamante, Howard Hughes Medical Institute, University of California, Berkeley: Transkription mittels RNA Polymerase II
C. Müller, European Molecular Biology Laboratory, Grenoble Oustation, Grenoble: Transkription mittels RNA Polymerase III
A. A. Hyman, Max-Planck-Institut für Molekulare Zellbiologie und Genetik, Dresden: Die Mechanik der Actin-Mysoin Polarisation in *C. elegans*
J. Howard, Max-Planck-Institut für Molekulare Zellbiologie und Genetik, Dresden: Optische Fallen und Perturbationsexperimente mit einzelnen Zellen
E. Schäffer, Biotechnologiezentrum, TU Dresden: Hochpräzise Kalibration einer optischen Falle

Nachwuchsgruppe: Inneres Design der Zelle
(Leiter: Dr. Iva Tolić-Nørrelykke)

Wie ist das Innere einer Zelle organisiert? Räumliche und zeitliche Organisation ist entscheidend für das Leben in seiner ganzen Komplexität, von Makromolekülen zu Zellen, zu Organen und schliesslich zu Organismen. In Einzellern ist die Trennung des genetischen Materials und eine korrekte Teilung der Zelle abhängig von der Zellform und der Position von Organellen im Inneren der Zelle. Fehler beim Positionieren von Zellorganellen kann unter Umständen zum Tod oder zu Krankheiten wie z.B. Krebs führen.
Unsere Gruppe, bestehend aus Biologen und Physikern, untersucht die Dynamik der räumlichen Ordnung im Inneren der Zelle. Als Modellorganismus dient uns dabei die Spalthefe *Schizosaccharomyces pombe*, weil sie über eine einfache symmetrische Form, nur wenige Filamente des Zytoskletts sowie hoch entwickelte Genetik verfügt. Wir kombinieren experimentelle Methoden (Laser Scanning Mikroskopie, Laser-Ablation, Optische Pinzetten, Mutanten) mit erweiterter Bildanalyse und theroretischer Forschung an der Schnittstelle zwischen Physik und Biologie.

Mikrotubuli und der Zellkern spielen eine wichtige Rolle bei der Gestaltung des Zellinneren. Wir wollen verstehen, welche Mechanismen den Zellkern in der Interphase positionieren, welche Prozesse verantwortlich sind für die Bewegung des Zellkerns in der Meiose und der Mitose, und wie es der Zelle möglich ist zwischen verschieden Arten der Bewegung zu wechseln. Wir konzentrieren uns dabei auf folgende Themen:
Zentrieren. Wie bestimmt eine Zelle in der Interphase die Zellmitte? Die zylindrisch geformten Zellen der Spalthefe haben einen in der Mitte gelegenen Zellkern und teilen sich durch Spaltung in der Zellmitte. Ein direkter Weg, um herauszufinden wie die Zelle ihren Zellkern in der Mitte plaziert, besteht darin, die Position des Zellkerns mechanisch zu verändern. Wir haben eine Methode entwickelt, die es ermöglicht mit Hilfe optischer Pinzetten den Zellkern in der Zelle zu bewegen. Diese Art der Manipulation bietet einige Vorteile gegenüber bis dato genutzten Methoden (z.B. Zentrifugation), um Zellorganellen zu verschieben: Zellorganellen können selektiv verschoben werden; der Eingriff kann zu einem ganz bestimmten Zeitpunkt des Zellzyklus durchgeführt werden; und, geringste Veränderungen im Bereich von wenigen 100 nm werden registriert, weil das Bild der Zelle vor dem Eingriff direkt mit dem Bild danach verglichen werden kann. Unsere Experimente zeigen, dass, wenn der Zellkern mit Hilfe optischer Pinzetten von der Mitte der Zelle weg bewegt wird, die Pinzette dann entfernt wird, er zur Mitte der Zelle zurückkehrt. Die dafür benötigten Kräfte werden von Mikrotubuli bereitgestellt, indem sie gegen das Ende der Zelle drücken und dabei den Zellkern in Richtung Mitte bewegen.
Wie bestimmt eine Zelle die Stelle, an der sie sich teilt? Wir sind interessiert an der räumlichen und zeitlichen Koordination bestimmter Ereignisse im Zellkern (Trennung der Chromosomen) und am Zellkortex (Zytokinese). Ist der Hinweis darauf, wo genau sich die Zelle teilt, durch die Position des Zellkerns bestimmt? Sollte die Teilungsebene durch ein Signal des Zellkerns zu einem bestimmten Zeitpunkt des Zellzyklus bestimmt sein, müsste ein Verschieben des Zellkerns zu einem früheren Zeitpunkt zu einer entsprechenden Verschiebung der Teilungsebene führen, während das Verschieben zu einem späteren Zeitpunkt keinen Einfluss auf die Position der Teilungsebene in der Zellmitte hätte. Unsere Experimente in denen wir den Zellkern mit Hilfe optischer Pinzetten verschieben, deuten an, dass die Teilungsebene tatsächlich über die Position des Zellkerns bestimmt wird. Darüber hinaus fällt die Entscheidung der Zelle, wo genau sie sich teilt, bereits zu Beginn der Mitose. Warum so zeitig, wenn andere Zelltypen dies erst am Ende der Mitose entscheiden? Die Antwort ist wahrscheinlich in der Tatsache begründet, dass der Zellkern in Spalthefen während der Interphase durch Mikrotubuli in Position gehalten wird, jedoch nicht während der Mitose. Folglich kann das Anlegen der Teilungsebene zu Beginn der Mitose einen optimaler Mechanismus füer eine korrekte Teilung dieser Zellen darstellen.
Ausrichtung. Wie ordnet sich die mitotische Spindel innerhalb der Zelle richtig an? In allen eukaryotischen Zellen ist es wichtig, dass die Spindel in Bezug auf die Spaltebene positioniert wird damit die Chromosomen erfolgreich in die beiden Tochterzellen getrennt werden. In einigen Zellen bestimmt die Spindelachse die Spaltebene und damit Größe und Schicksal der Tochterzellen. Wann und wie richtet sich die Spindel richtig aus? Es gibt verschiedene komplementäre Mechanismen, mit denen die Spindel korrekt ausgerichtet wird. Mit Hilfe konfokaler Mikroskopie und hoch präzieser Verfolgung der Spindelpole haben wir drei Mechanismen identifiziert, mit denen die Spindel in Spalthefen ausgerichtet wird. Erstens, Interphasenmikrotubuli, welche zur Längsachse

der Zelle angeordnet sind, dienen als Vorlage für die werdende Spindel. Folglich ist die Spindel zur Zellachse ausgerichtet während sie sich formt. Zweitens, die zylindrische Form der Zelle zwingt die wachsende Spindel, sich zur Zellachse auszurichten. Der dritte Mechanismus beruht auf astralen Mikrotubuli, welche durch Drücken gegen die Zellmembran auf die Spindelpole Kräfte auswirken und damit helfen, die Spindel selber auszurichten.
Oszillation. Was treibt die Oszillation des Kerns während der meiotischen Prophase (Beginn der Zellteilung in der geschlechtlichen Fortpflanzung) an? Während dieser Phase bewegt sich der Zellkern in Spalthefen kontinuierlich zwischen beiden Enden der Zelle hin und her, bei einer Periodendauer von ungefähr 5 Minuten und einer Gesamtdauer von einigen Stunden. Warum sind Oszillationen des Kerns wichtig? Sie können die räumliche Anordnung homologer Chromosomen erleichtern, welches wiederum notwendig ist, um korrekte Chromosomenpaare in der meiotischen Prophase zu bilden. Wir wollen den Mechanismus, der der Oszillation zugrunde liegt, verstehen. Die periodische Bewegung des Kerns hängt von astralen Mikrotubuli ab, die strahlenförmig von den Spindelpolen wegführen und von zytoplasmatischem Dynein, einem Mikrotubulimotor. Gegenwärtig untersuchen wir mit Hilfe konfokaler Mikroskopie, Fluoreszenz-Recovery nach Photobleichen (FRAP) und Laser-Ablation von Mikrotubuli und Dyneinpunkten das Verhalten von Mikrotubuli und Dynein sowie deren Rolle in der Oszillation. In Zukunft sollen theoretische Modellierung und Computersimulationen mit einbezogen werden.

Kooperationen
F.S. Pavone, LENS - European Laboratory for Non-linear Spectroscopy, University of Florence, Italy: Laser-Ablation und Optische Pinzetten Technologie
K. Berg-Sørenesen und Lene Oddershede, Niels Bohr Institute, Copenhagen, Denmark: Diffusion in lebenden Zellen und Kalibration optischer Pinzetten
K. Kruse, mpi**pks** Dresden: Modellierung der Zellkern-Oszillationen
N. Pavin, University of Zagreb, Croatia: Modellierung der Zellkern-Oszillationen

Chapter 2

Scientific Work and its Organisation at the Institute- an Overview

2.1 History and Development of the Institute

1992-1994 • The Senate of the Max Planck Society decided to set up the Max Planck Institute for the Physics of Complex Systems in November 1992, with *Prof. Fulde* as the Founding Director. The concept for the institute included three scientific divisions and a large-scale guest program. The incorporation of a Seminar- and Workshop-Program within the guest program was expected to become a significant part of the institute activities. The program aims at promoting new developments in the field of the physics of complex systems. One important aspect is to provide a high-level platform for young scientists from universities to become acquainted with recent research developments much earlier than traditionally. At the same time, important new research areas in the field of theoretical physics are promoted efficiently. Dresden was chosen as the location for the institute due to its favorable scientific environment and good travel connections. The scientific activities started on July 1st, 1993, in Stuttgart, lacking proper office space in Dresden, which was supplied by January 1994 thanks to the support of the TU Dresden. The TU Dresden, itself lacking office space, generously offered a temporary location for the institute in a barrack in the Bayreuther Straße, close to the university campus. The institute was officially inaugurated by Prof. H. Zacher, President of the Max Planck Society, on May 2nd, 1994. Both the State of Saxony and the City of Dresden have contributed significantly to a smooth setting up of the activities of the institute, e.g., by the City of Dresden providing additional temporary office space in a villa with unsettled property claims, free of charge. The institute also had to rent several additional offices close to the barrack. An administration was installed, headed by Mrs.*I. Auguszt*. First guests were invited, and the first workshop took place in March 1994. An independent junior research group on *Nonlinear Time Series Analysis* was founded in 1995 and headed by *Dr. H. Kantz*. Strongly supported by President Zacher, the institute decided to considerably broaden its research spectrum by installing temporary junior research groups. *Dr. M. Bär* started his activities as head of the junior research group *Pattern Formation in Reaction-Diffusion-Systems* in 1995. *Dr. K. Richter* became head of the junior research group *Quantum Chaos*

and Mesoscopic Systems in January 1996, and *Dr. M. Dolg* of the group *Quantum Chemistry* shortly afterwards.
1995-1998 • At the same time, plans for the new institute building began to materialize. The architecture firm Brenner und Partner (Stuttgart) with J. Wittfoth won the competitive bidding, and constructions started in September 1995. After less than two years the institute took over the newly constructed main building, together with the three guest houses. The inauguration of the buildings was held during a simultaneous symposium on *Complexity in Physics*, September 23-24, 1997. In the meantime the Seminar- and Guest-Program were gaining momentum, with hundreds of scientists already having visited the institute.
1999-2001 • The next important step was the appointment of *Dr. J. M. Rost* (Freiburg) as head of the second division of the institute in December 1998. *Dr. Rost* started the activities on May 1st, 1999 by setting up the division *Finite Systems*. He appointed *Dr. A. Buchleitner* as head of a research group *Nonlinear Dynamics in Quantum Systems*. After *Dr. Dolg* accepted an offer for a professor position at the University of Bonn in 2000, *Dr. U. Birkenheuer* was appointed as his successor in March 2000. *Dr. K. Richter* soon afterwards also accepted the offer of a chair for Theoretical Physics at the University of Regensburg. This concluded the Junior Research Group *Quantum Chaos and Mesoscopic Systems*. To continue the successful work in this research field with modified premises, *Dr. H. Schomerus* (Leiden) was appointed as head of a new Junior Research Group *Waves in Complex Media and Mesoscopic Phenomena* in November 2000.
2001-2002 • To account for the increasing demand for bridging the field between physics and biology, *Dr. F. Jülicher* (Paris) was appointed as head of the third division *Biological Physics* in 2001. Shortly afterwards, two research groups on *Physics of Biological and Soft Matter* headed by *Dr. R. Everaers* (Mainz), and *Biological Physics of Olfaction: From Genes to Networks* headed by *Dr. M. Zapotocky* (New York) started their activities within the third division in 2002. The division *Finite Systems* also continued to broaden its research spectrum by appointing *Dr. A. Becker* (Bielefeld) as head of the new research group *Nonlinear Processes in Strong Fields* in 2002.
2003-2004 • In 2003 *Dr. S. Kümmel* (New Orleans) started the activities of an Emmy Noether-Group *Electronic Structure of Finite Systems*. It was followed in 2004 by setting up a Junior Research Group *Physics of Cell Division* headed by *Dr. K. Kruse* (Dresden). His group was the first of three research groups within a joint research program *Physics of Biological Systems* initiated together with the Max Planck Institute for Molecular Cell Biology and Genetics (MPI-CBG) in Dresden. A second Junior Research Group *Mechanics of Cell Division* of this joint research program was started at the end of 2004 by *I.M. Tolic-Norrelykke* (Firenze) who works experimentally at the MPI-CBG. The construction of an extension to the institute building was started in the year 2004. *Dr. M. Bär* took up a position of a department head at the Physikalisch-Technische Bundesanstalt in Berlin in the fall of 2004.
2005-2006 • In 2005 *Dr. S. Kümmel* accepted a Professor position at University of Bayreuth, and *Dr. H. Schomerus* accepted a faculty position at Lancaster University. Dr. *M. Hentschel* (Regensburg) started the activities of an Emmy Noether group *Many body effects in mesoscopic systems*. *Dr. S. Grill* (Berkeley) completed the joint research program of the **mpipks** and the MPI-CBG by starting the Junior Research Group *Motor Systems*. His group is affiliated with both institutes and does both theoretical

and experimental work. The International Max Planck Research School *Dynamical processes in Atoms, Molecules and Solids* started operation in 2005. It attracts PhD students from many countries and is operating jointly with the Technical University Dresden, the Max Planck Institute for Chemical Physics of Solids, the Leibnitz Institute for Solid State and Materials Research Dresden, the Forschungszentrum Rossendorf and the Institute for Low Temperature and Structure Research at the Polish Academy of Sciences Wroclaw. The new wing of the institute was completed at the end of 2005. It provides new office space and a new seminar room. In 2006, *Dr. K. Kruse* and *Dr. R. Everaers* accepted Professor positions at the University of Saarbrücken and the Ecole normale Superieure in Lyon.
The institute hosts approximately 50-100 long-term guest scientists at a given time, together with 1200-1500 short-term guests who annually participate in the workshop and seminar program.

The Board of Trustees has been supporting the work of the institute since 1995, thus providing important connections to the State, the City and the Academia. The research activities of the institute have been accompanied by a Scientific Advisory Board since June 1996.

2.2 Research Areas and Structure of the Institute

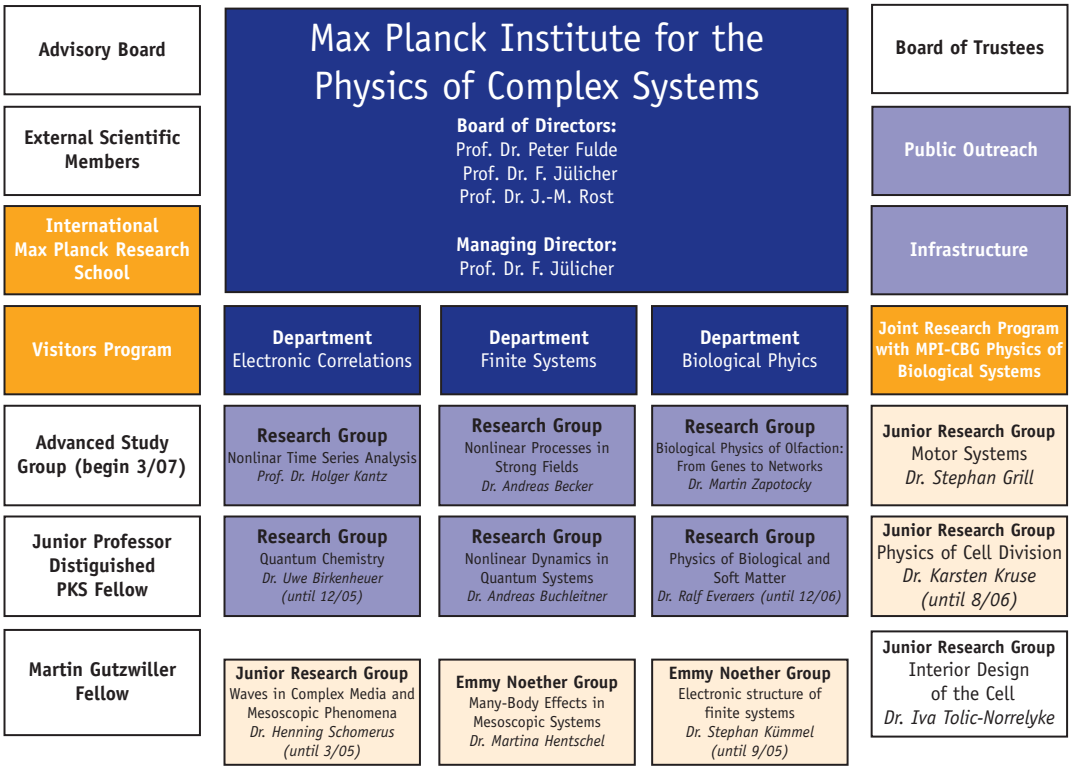
The research of the institute in the field of the physics of complex systems ranges from classical to quantum physics and focuses on three main areas, which correspond to the activities in the three divisions:

- The division *Electronic Correlations* headed by *Prof. Fulde* studies the quantum physics of condensed matter.
- With the help of semiclassical methods, the division *Finite Systems* headed by *Prof. Rost* focuses on the nonlinear dynamics of atoms, molecules and clusters.
- The division *Biological Physics* headed by *Prof. Jülicher* studies biological systems with tools of statistical physics and nonlinear dynamics.

Furthermore, four research groups are broadening and strengthening the work of the corresponding divisions. Additional groups interpolate with their research between and add to the above listed research topics:

- The Emmy Noether Group *Many Particle Physics in Mesoscopic Systems* is headed by *Dr. Martina Hentschel*. It bridges work between the divisions *Electronic Correlations* and *Finite Systems*.
- The only permanent research group, headed by *Dr. Kantz*, is working on *Nonlinear Time Series Analysis*. Here, methods are applied and developed, related to various aspects of classical chaos, which play an important role also for research on semiclassical topics.

Finally, a joint research program *Physics of Biological Systems* of the mpi**pks** and the Max Planck Institute of Molecular Cell Biology and Genetics (MPI-CBG) comprises three closely interacting Junior Research Groups. These joint research groups build



a close link between both institutes to promote collaborative work on the physics of cells:

- The theory group *Physics of Cell Division* headed by *Dr. Karsten Kruse* operated until Summer 2006 at the mpi**pks**.
- The Junior Research Group *Motor Systems* is headed by *Dr. Stephan Grill*. It is affiliated with both institutes and works both theoretically and experimentally.
- A third experimental Group *Interior Design of the Cell* headed by I.M. Tolic-Norrelykke is located at the MPI-CBG.

2.3 Workshop and Visitors Program

A central task of the institute is to conduct international *Workshops and Seminars* (p. 168), which makes mpi**pks** an almost unique institute within the Max Planck Society, only comparable with the mathematics institute in Bonn. A small but efficient group of staff headed by *Dr. S. Flach* is responsible for the logistics and the preparation of meetings, and gives advise to the (usually external) scientific coordinators on the various aspects of planning and conducting the corresponding event.
The *Visitors Program* (p. 158) offers research visits ranging from a few weeks to two years in duration. Guest scientists are using various ways of collaboration by joining research groups at the institute, by doing joint research with other guest scientists, or by starting collaborations with workshop and seminar participants. Further possibilities of collaboration include contacts with the TU Dresden or other local research

institutions, well documented, e.g., by common publications (see p. 217).
Proposals for workshops and seminars, as well as applications for guest scientist positions, are evaluated by two different committees. Members of each committee include external scientists and scientists of the institute.
In order to further strengthen and structure the Visitors Program, mpi**pks** started in 2000 to annually award the *Martin Gutzwiller Fellowship* to an internationally recognized and experienced scientist. The awardees *Prof. L. S. Schulman* (Potsdam, NY) 2005 and *Prof. S. L. Tomsovic* (Pullman) 2006 have spent up to one academic year at mpi**pks** (p. 163).
The mpi**pks** also offers one *Distinguished PKS Postdoctoral fellowship* annually. It aims at excellent young researchers, shortly before accepting a tenure track position (p. 159).
In 2006 the institute decided to install an *Advanced Study Group* each year at mpi**pks**. These groups will consist of 3-5 experienced researchers, who join forces to do cutting-edge research on a topic from the field of the physics of complex systems. The first *Advanced Study group 2007* will start its activities in March 2007.

2.4 Teaching and Training

The institute aims at a broad and far reaching education of young scientists in research, teaching and the organization of research.
Teaching • Standard lecture series are conducted by institute members, both at the TU Dresden and at other universities (p. 201). In addition, the public relations sector of our institute offers institute members possibilities to teach and lecture for high school teachers and high school students, both at mpi**pks** as well as at high schools (p. 204).
International Max Planck Research School • Since 2005 our institute is running the IMPRS *Dynamical Processes in Atoms, Molecules and Solids* together with the Technical University Dresden, the Max Planck Institute for Chemical Physics of Solids, the Leibniz Institute for Solid State and Materials Research Dresden, the Forschungszentrum Rossendorf and the Institute for Low Temperature and Structure Research at the Polish Academy of Sciences Wroclaw. It attracts PhD students from many countries and offers a well-structured PhD training with a large program of lecture courses. Finally mpi**pks** participates in the IMPRS *Molecular Cell Biology and Bioengineering* of the MPI for Cell Biology and Genetics.
Research Organization • The large-scale Workshop and Seminar Program at mpi**pks** offers the unique possibility for young scientists to take part in the organization of meetings. Out of the 34 events during 2005-2006, young scientists of the institute took part in the coordination of 6. This has a positive educational effect for young scientists, and helps the external coordinators through the permanent contact with a local scientific coordinator.

2.5 Public Relations

The institute consider itself as a platform for the emergence, exchange and development of creative ideas in research. While mainly focusing on scientists, this also includes potential future scientists, i.e., high school students, teachers, as well as the general public interested in science. Within our school-contact-program we offer workshops for high

school teachers, winter schools for high school students, and lectures at schools in order to spread the fascination of science as it happens.
Since 1999, mpi**pks** has been coordinating, together with the TU Dresden and the City of Dresden, the lecture series *Science in the City Hall*, aiming at a public interested in science. Well-known scientists are invited to give lectures for the broad public, which are intended to popularize modern research (p. 204). Furthermore, coordinators of workshops are encouraged to offer a public evening lecture at mpi**pks**, in the course of the workshop. Dresden was awarded the title "Stadt der Wissenschaft 2006". The mpi**pks** was participating in numerous activities, which were part of the full year program of the scientific community of Dresden.

2.6 Research Networking

Local • The mpi**pks** finds itself in the midst of a rich research environment, formed by the TU Dresden and many other research institutes. An intensive scientific dialogue with the Physics Department of the TU Dresden is taking place, e.g., with regular joint seminars (*Quantum Dynamics* with Prof. Schmidt and *Complex Systems* with Prof. Ketzmerick), and through a collaboration with Prof. Schwille. mpi**pks** has particular close contacts to the Institute of Theoretical Physics and the Institute of Biophysics at the Physics Department. Institute members are involved in two Collaborative Research Programs of the DFG (p. 199). It is also participating in the SFB 463. The division *Electronic Correlations* is cooperating with the IFW (Institut für Festkörper- und Werkstoffforschung) and with the neighbouring Max Planck Institute for Chemical Physics of the Solid State. The division *Biological Physics* established close contact to the Max Planck Institute of Molecular Cell Biology and Genetics. There are also intense collaborations with the Biotechnological Center and the newly founded Center for Regenerative Therapies. The divisions *Finite Systems* and *Electronic Correlations* cooperate closely with the Research Center Rossendorf.
National and International • The many different national and international collaborations and contacts are listed in the research group reports below. Furthermore, the institute has a small budget for collaborations with experimental groups (p. 166).

2.7 Brief Description of the Research Groups

Division: Electronic Correlations
(Head: Prof. Dr. P. Fulde)

The main focus of the scientific work of the Division is on the field of electron correlations in solids and molecules in the broadest sense. This is supplemented by work on ultracold glasses, spin transport etc.

Calculating the ground-state wavefunction for different solids, thereby including quantitatively electron correlations has been a challenging topic for a number of years. The same holds true for computations of energy bands. The wavefunction based calculations are using quantum chemical methods which involve well controlled approximations free of arbitrariness. We feel that it is very worthwhile to pursue that line of research as an

alternative to density functional theory despite of its great successes and dominance in electronic structure theory. But especially for strongly correlated electron systems one may learn a lot from a wavefunction based approach. A nice example is the previous development of the Dual Model for $5f$ electrons which has been very successful. Until recently a large part of the work had been done by the Research Group: Quantum Chemistry. But after the termination of the 5 years program, the group was dissolved and part of the program was moved back to the Division.

As regards ground-state wavefunction calculations B. Paulus in collaboration with N. Gaston and K. Rosciszewski concentrated on metals (Hg, Cd, Zn) which are more difficult than the hitherto treated insulators and semiconductors. Very satisfactory results were obtained for the binding energy, lattice constant and bulk modulus. In addition the technically important catalyst solid CeO_2 was treated (E. Voloshina). The group is participating in the special DFG program: "Development of ab initio methods for many-electron systems in chemistry and physics" which is also supporting it financially. As far as energy-band calculations are concerned results for MgO are now available which can be easily generalized to a number of other oxides (L. Hozoi). At present we start from the program package CRYSTAL and construct localized orbitals from the obtained Bloch orbitals with the help of which the correlation holes are constructed. In the future we want to start instead from the package WANNIER developed by A. Shukla. This will be done in cooperation with him. What is needed is the interface between WANNIER and the package MOLPRO, the latter serving for the inclusion of correlations.

Independent of the above we have also continued to treat correlations by LSDA and LDA+U within density functional theory. Although these approaches are not completely free of arbitrariness, they yield in many cases important and very useful results. For example, the effective coupling constants for the magnetic moments of Cr ions in the spinels ACr_2X_4 (A = Zn, Cd; X = O, S, Se) were calculated. They enter an effective Heisenberg Hamiltonian which can be used for describing those interactions. It was shown that the coupling constant for nearest-neighbor Cr interactions changes from antiferromagnetic in the O spinels to ferromagnetic in the S and Se spinels and the reason for that was unraveled (A. Yaresko).

A strongly expanding topic within our Division is the behavior of mobile fermions in geometrically frustrated lattices. For strongly correlated spinless fermions on a half-filled checkerboard lattice it was pointed out that some of the features of the system resemble phenomena in particle physics. For example, excitations do exist with fractional charges $\pm e/2$, similar to quarks. Like the latter they are confined by a *constant* force. If they are pulled too far apart, particle-antiparticle pairs are formed in analogy to μ meson production. The vacuum consists of a complete loop covering of the checkerboard lattice the dynamics of which leads to a simple version of string theory. We also showed that the theory of the low-lying excitations is a U(1) gauge theory. This research area is very interesting and rewarding and will keep us busy for the years to come. A large part of the results is contained in the PHD thesis of F. Pollmann (see contribution of F. Pollmann, p. 71) and was accomplished in cooperation with K. Shtengel, E. Runge and J. Betouras.

A number of problems solved concerned specific materials and their properties. The compound UPd_2Al_3 serves as an example here. It was demonstrated how the magnetic excitations of the system are modified by the appearance of a superconducting energy gap below T_c. The theory could nicely explain previous inelastic neutron scattering results (see contribution of I. Eremin, which also includes related work on high-T_c superconductors, p. 75). All the experiences and insights gained over the last few years on strongly correlated electron systems were documented in an extensive review which appeared in the series "Solid State Sciences" (P. Fulde, P. Thalmeier, G. Zwicknagl).

The work on the behavior of ultracold glasses in a magnetic field, a much discussed and investigated research topic, were extended on the basis of nuclear quadrupolar interactions with the 2-level tunneling systems. Some experiments could be explained this way (D. Bodea, A. Burin, I. Polishchuk). The cooperation with P. Mohanty on spin transport in nanostructures is continuing but the experiments need more time. They are supported by the National Science Foundation of the US.

Research Group: Quantum Chemistry
(Head: Dr. U. Birkenheuer (until 12/05))

In the last years the Quantum Chemistry Group has developed a couple of local wavefunction-based methods for the determination of the electronic structure of solids and polymers. Besides the incremental scheme for groundstate properties which is used with great success for more than a decade by now, there are, on the one hand, the local Hamiltonian approach for one-particle excitations (quasi-bandstructure) and, on the other hand, the periodic version of the ADC formalism (algebraic diagrammatic construction) which is based on solving the Dyson equation.
By the end of the Ph.D thesis of Christian Buth in November 2005 the latter approach reached its summit. It could be shown, that the CO-ADC method (crystal-orbital ADC) is capable to predict both, bandstructures of linear systems (HF zig-zag chains here) and bulk bandstructures (LiF with a rock salt structure) in a sound and computationally manageable way. A project on the determination of the bandstructure of MgO, a system with a much larger number of valence electrons and low-lying unoccupied conduction bands with the delivered CO-ADC program was launched in summer 2005, but could not be finished for human resource reasons.
The local Hamiltonian approach is the other method which has been used so far for the description of electronic excitations in solids. Originally designed for the determination of one-particle excitations (valence and conduction bands) the local ansatz underlying this approach turned out to be such sustainable, that it even allowed an extension to the description of crystal-momentum-resolved *excitonic* excitations of strongly bound electron hole pairs (Frenkel excitons).
Nevertheless, the effort for the compilation, handling and subsequent processing of the many individual results which are necessary for the ultimate incremental accumulation of the total correlation effects is quite large. For that reason, the main focus in the last period of the Quantum Chemistry Group was on the development of a *simplified* ansatz to the determination of the bandstructure of correlated electrons. After a pioneer study in summer 2004 in which the new method was first presented in application to diamond

and silicon, a systematic investigation was performed on the quality of the "frozen local hole" approximation, a sort of adiabatic approximation on the shape of the correlation hole carried along by the moving electrons, which had been introduced to simplify the local Hamiltonian approach. To demonstrate the ability of this new method to operate efficiently even on non-trivial 3-dimensionally periodic systems magnesium oxide was considered. The correlation effects in both, the valence and *conduction* bands of MgO could be quantified successfully.
With the closing of the Quantum Chemistry Group end of 2005 and due to the job-related changes of many of the former members and collaborators the activities in the area of wavefunction-based correlation methods for solids and polymers receded substantially in the meantime, and there are also no active cooperations with other working groups going on in this area anymore.

Research Group: Nonlinear Time Series Analysis
(Head: Prof. Dr. H. Kantz)

Complex dynamical behaviour remains to be a challenge to theory and to many applications. Our group concentrates on aspects of complexity in classical (i.e., non-quantum) systems, where we are both interested in basic properties and in specific phenomena. The rôle of fast chaotic degrees of freedom in Hamiltonian dynamics as heat baths with finite energy content was studied both theoretically and at hand of specific models. We could hence understand the following model system: A particle hopping on a oscillatory plate with a sawtooth profile undergoes diffusion in the horizontal direction, if the vertical motion is chaotic, whereas it is either localised or moves ballistically if the vertical motion is periodic. Regular orbits generate structures in Hamiltonian systems with mixed phase space which strongly influence transport properties and the decay of correlations. We gained some new insights in these long studied phenomena. One-parameter families of marginally unstable periodic orbits such as bouncing ball orbits known from the stadium occur generically in all billiards which are local perturbations of integrable billiards and have a strong influence on the chaotic motion. In a joint project with external funding we cooperate with experimentalists and engineers in a study of statistical properties of surface wind, aiming at better models for fluctuating wind fields. Also a project where we describe observed data from highway traffic by Fokker Planck Equations with time-periodic coefficients is motivated by applications.
A specific feature of complex deterministic or stochastic systems is their ability to generate extreme events, i.e., tremendous short-time deviations from their mean behaviour. We are studying dynamical mechanisms which are able to create extreme events, we try to understand the rôle of precursors, and we consider statistical aspects for the detection and characterisation of extreme events. Two interesting results from recent work are worth mentioning: In a simple model of reactions of a system affected by extremes we found a parameter regime of relaxation oscillations, where the combination of random occurrence of events and reactions of a system generates an almost periodic sequence of above-threshold events. When predicting extreme events through the observation of precursors, we found processes where events are the better predictable the larger they are, which is counter-intuitive. In October 2006 we organised an international conference on extreme events in complex dynamics at the mpi**pks**.
In the future, we will focus even more on the issue of extreme events. For a better

understanding of underlying mechanisms we will put more emphasis on models. In view of management and prevention, we will in at least one example try to translate physical actions into human reactions and costs to society. This means that we intend to couple physical models of extreme events to models for human behaviour used in econophysics, being well aware of their hypothetical nature.

Cooperations

- W. Just, University of London; G. Radons, University of Chemnitz: Modelling of fast degrees of freedom through stochastic processes, Eigenvalues of Fokker Planck operators
- J. Peinke, University of Oldenburg: Surface wind, turbulence, and wind power turbines (consortium together with R. Friedrich, Münster; K. Schffarzyk, FH Kiel; C. Wagner, DLR Göttingen)
- S. Albeverio, University of Bonn, Modelling of highway traffic by time-dependent Fokker Planck equations
- C. Grebogi, University of Aberdeen: Influence of noise on deterministic dynamics
- N. Vitanov, IMB Sofia: data analysis of wind speeds, turbulence.

Division: Finite Systems
(Head: Prof. Dr. J. - M. Rost)

The group is interested in the non-linear dynamics of excited systems which consist of a finite number of particles, focusing on atoms and clusters. We have summarized our work over the last years regarding our two main areas of interest – ultracold coupled plasmas and the interaction of rare gas clusters with intense laser pulses – in two reviews (Physics Reports and Topical Review for J Phys B).

Research topics
Our interest in the area of ultracold gases has shifted towards phenomena of correlation in ultracold Rydberg dynamics. An ultracold gas is a very suitable environment to study the slow time scales and small energy differences of Rydberg atoms which can be viewed as embedded in a gas of cold (ground state) atoms (p. 99).
The scheme of embedding governs also our new perspective on clusters: Rare gas clusters doped with other atoms or molecules as well as clusters within superfluid helium droplets exhibit properties which are surprisingly different from the pure cluster when exposed to laser light. This has been documented in poorly understood experiments, where the doping was in the beginning more an accident due to an imperfectly prepared cluster target. Similarly, the embedding with a helium droplet is an elegant method to produce a cluster from an atomic beam and was thought to have little influence on the cluster itself.
We have started a new activity to investigate the response of (small) quantum systems to a combination of a laser pulse and external noise. If the noise is of comparable strength as the (non-perturbatively acting) laser pulse, the quantum system responds quite sensitively. Moreover, a time structure imprinted in the noise allows to selectively

address different types of binding, e.g., in a molecule nuclear or electronic motion. This kind of noise can be "designed" with the help of shaped laser light.
In a long time effort we investigate multiple ionization dynamics in atoms with classical mechanics. The goal of this work is twofold, first to provide a quantitative description for few-particle systems which have already too many degrees of freedom to be treated fully quantum mechanically, and second, to provide insight into the few-electron dynamics with the help of classical trajectories (p. 102). Our recent results lead to the unexpected hypothesis that not the two-body Coulomb problem is the fundamental building block of many-electron systems, but the helium-like three-body Coulomb problem.
Finally, we have continued our collaboration with experimental groups (Ron Phaneuf, Reno and Nora Berrah, Kalamazoo) to elucidate further the nature of collective dynamics in fullerenes and fullerene negative ions.

Methods
Our techniques range from full quantum approaches and density functional theory (TDLDA) over semiclassical approximations to a full classical treatment of microscopic phenomena including advanced techniques such as *tree codes* and *particle in a cell* formulations.

Perspectives for the future
Long range interaction phenomena in ultracold gases challenge theory due to their many-body nature. For the case of (dominant) Coulomb interaction in ultracold plasmas we have developed the theoretical tools for a good understanding of the phenomena. We also succeeded to find a suitable approach to correlation effects based on dipolar and van der Waals interaction of Rydberg atoms in neutral cold gases for specific laser excitation schemes. However, globally coherent many-body dynamics in cold gases is still a big challenge. To make progress, we will focus on the dynamical evolution of impurities in Bose-Einstein condensates and their experimental probing. There, explicit correlation effects can be built on top of a mean field description for the ultracold gas (condensate).

The work on interaction with clusters as well as atoms with laser light will be largely influenced by the new light sources which will gradually become available. These are the X-ray free electron lasers in Hamburg and Stanford and attosecond laser pulses in several labs around the world. While the latter open the way to monitor electron dynamics in atoms and extended systems (the period of the ground state electron in hydrogen is 24 attoseconds), the XFELs address time resolved probing on the femtosecond scale combined with atomic spatial resolution made possible by the X-ray wavelengths of the light.
We have started to explore alternative possibilities of imaging microscopic objects (clusters and large molecules) because standard imaging techniques will most likely not work: They destroy the object before enough photons are scattered, since the photo ionization cross section is larger than the scattering cross section of light in this parameter regime.
In the area of attosecond science we want to use the pump-probe scheme, well known from femtochemistry, to demonstrate the possibility of atomic "time of flight" mea-

surements. For instance it may be feasible that the first attosecond pulse (pump) creates a photo electron in one edge of, e.g., a metal cluster, while the second pulse (probe) stimulates the reabsorption of the electron at another edge. From the time delay τ between creation and reabsorption it may be possible to infer the distance the electron has traveled between the two pulses and in turn, one could "measure" microscopic distances. Similar pump-probe schemes we will also apply in the context of our quasiclassical study of few-electron dynamics in atoms.
We share the interest in attosecond dynamics with Andreas Becker's group in the department. With our complementary expertise we are well prepared to enter this emerging field of atomic attosecond phenomena.

Finally, we will further pursue the concept of embedded quantum systems, on the one hand side with two-component clusters as described before, and on the other hand by embedding small quantum systems in noise. The latter may either be directly generated by shaped laser pulses or be the consequence of collisions with a not further specified environment of massive particles.

Cooperations
With experimental groups
We have collaborated with the groups headed by Prof. Müller (Uni Giessen) and Prof. Phaneuf (Univ. of Nevada, Reno, USA) on collective excitation of electrons in complex systems by photons. A new collaboration on C_{60}^- has begun with Prof. Nora Berrah (Kalamazoo, USA). The collaboration with Prof. Kaindl (FU Berlin) and with Prof. Dörner (Uni Frankfurt) on photoexcitation of Helium has continued with joint publications. Furthermore, we have been in close contact with the groups of Prof. Weidemüller (Freiburg), Prof. Pillet (Orsay, France) and Prof. Raithel (Ann Harbor, USA) regarding the interaction of Rydberg atoms in ultracold gases and with Prof. Killian (Rice, USA) regarding ultracold plasmas.

With theoretical groups (some examples):
– on classical dynamics of quantum systems with A. Emmanouilidou (Eugene, USA)
– on semiclassical theory with A. Ozorio de Almeida (Rio, Brazil)
– on transport through single clusters and cluster arrays with M. Garcia (Kassel).

Local cooperations
The interaction with Prof. Rüdiger Schmidt's group from the TU Dresden has continued - the basis is the common seminar *Quantum Dynamics*. It takes place at the mpi**pks** with external speakers invited by both groups. Common research activities include *quantum adiabatic molecular dynamics* directly with R. Schmidt, as well as *semiclassical propagation techniques* and the effect of external noise with F. Großmann from the TU Dresden. A new link with the TU as well as with other institutes in the neighborhood has been established through our International Max Planck Research School and its monthly seminar which also takes places at mpi**pks**.

Research Group: Nonlinear Processes in Strong Fields
(Head: Dr. Andreas Becker)

The group hosts currently three Post-docs and two PhD students and is interested in the analysis of ultrafast nonlinear processes. Our activities include the dynamics of single atoms and molecules exposed to an external field, the generation and application of few-cycle and attosecond laser pulses as well as the propagation of ultrashort laser pulses in air. We approach these topics from different perspectives using analytical methods and models, S-matrix theories as well as ab-initio numerical quantum simulations.
A new focus of our work in recent years has been the development of ab-initio techniques for the direct integration of the time-dependent Schrödinger equation of few-body systems interacting with an intense laser pulse. In a joint work of the whole group a virtual laboratory has arised which allows for the efficient analysis and visualization of ultrashort atomic and molecular processes. In the applications we have addressed two vigorously discussed topics in strong field physics. First, we have proposed a model for nonsequential double ionization of an atom or molecule, in which there is taken full account of the correlation between the electrons, which has not been considered in the previous models (see report *A virtual laboratory for ultrashort processes in strong fields* p. 107). Second, we have been interested in the control of electron excitation and localization in atoms and molecules, which is one of the exciting goals of photochemistry and attosecond physics. We have explored this aspect on the basis of current laser technology using the techniques of pulse shaping and pump-probe schemes in the numerical simulations.
We have further considered the response of large molecules to an external field. Since ab-initio numerical integration techniques are limited to few-body problems, we have used as an alternative the S-matrix theory. This approach, that we have applied before to ionization of diatomics, has been now extended to fullerenes and to include vibrational excitation. We were able to provide an explanation of two unexpected strong-field phenomena, namely the deviation of the distributions in the vibrational states of an ion from a Franck-Condon distribution after ionization in a laser pulse and the suppression of ionization of fullerenes as compared to their companion atoms (see report *Molecules in intense laser pulses: S-matrix analysis of ionization and high harmonic generation* p. 104).
Another line of research has been the investigation of new schemes to generate ultrashort laser pulses. On the one side we have continued our work on high harmonic and attosecond pulse generation in a dense medium. Furthermore, in a collaboration with the experimental group of S.L. Chin (Quebec, Canada) we were able to demonstrate that tunable few-cycle laser pulses in the visible spectrum can be generated with high efficiency by four-wave mixing during the filamentation of near-infrared and infrared laser pulses in gases.
Finally, the dynamic interplay of Kerr self-focusing and defocusing of a femtosecond laser pulse from a self-generated plasma is known to form robust filamentary light channels over long distances. Most of the earlier theoretical studies have considered the dynamics of the pulse in the core of the filament only. But, our results obtained from numerical simulations and a variational approach have demonstrated the crucial role of a large spatial background energy reservoir of low intensity around the core for the long range filamentation of a femtosecond pulse.

Besides the scientific research we have been active in the organization of two international workshops, namely the International Seminar and Workshop *Intense laser-matter interaction and pulse propagation* (mpi**pks** Dresden, 1-24 August 2005) and the *International Symposium on Ultrafast Intense Laser Science 4* (Hawaii, 12-14 December 2005), as well as the *International Wilhelm und Else Heraeus Summerschool: Few-body dynamics in atomic and molecular systems* (Wittenberg, 10-23 September 2006). Both the mpi**pks** seminar and the summerschool have been attended by a large number of young Post-docs and PhD students, who have taken the opportunities to discuss the current status and the perspectives of the field with world-leading experts.

Perspectives

Exciting new laser technologies are the generation of carrier-envelope phase-locked few-cycle pulses and attosecond pulses. With our virtual laboratory we have now a numerical tool to study the temporal evolution of processes induced by such pulses. This will enable us to analyze e.g. the electron dynamics during single and double ionization of a target.
We further plan to extend our virtual laboratory to study the interaction of atoms with a highly charged ion. Experiments using the hydrogen atom as a target are under development at the MPI-K in Heidelberg.
Finally, we will continue our S-matrix studies on polyatomic molecules to explore how the geometrical structure and orbital symmetry of a polyatomic molecule leaves its footprints on high harmonic and photoelectron spectra. This may provide a spectroscopic tool to observe structural changes in the molecule on an ultrafast time scale.

Collaborations

We are part of two international collaborations, which were established in 2004, namely a Center of Advanced Science and Technology (COAST) on *Ultrafast Intense Laser Science* (coordinated by K. Yamanouchi, Tokyo, Japan) and a Special Research Opportunity Program on *Controlled electron rescattering: sub-A, sub-fs imaging of single molecules* (coordinated by M.Yu. Ivanov, Ottawa, Canada). Our collaboration with the group of Luis Plaja at the Universidad Salamanca, Spain, has been supported via a DAAD exchange project.

Experimental groups:
• with S.L. Chin (Québec, Canada) on (a) the propagation of femtosecond pulses in air and (b) the generation of tunable ultrashort laser pulses,
• with P. Agostini (at present at Ohio State University, USA) and S.L. Chin (Québec, Canada) on the fragmentation of molecules by intense laser pulses,
• with R. Dörner (Frankfurt) and P.B. Corkum (Ottawa, Canada) on the rescattering dynamics in strong field double ionization.

Theoretical groups:
• with N. Aközbek (Huntsville, USA) on two-color filamentation and the generation of tunable ultrashort laser pulses,
• with F.H.M. Faisal (Bielefeld) and A. Jaroń-Becker (Dresden) on strong-field ionization of molecules,
• with O. Kosareva and V.P. Kandidov (Moscow, Russia) on fragmentation of molecules by intense laser pulses,

• with J. Moloney (Tucson, USA) on third harmonic generation in light filaments,
• with L. Plaja and L. Roso (Salamanca, Spain) on correlated electron dynamics in few-cycle pulses.

Research Group : Nonlinear Dynamics in Quantum Systems
(Head: Dr. A. Buchleitner)

"Nonlinear Dynamics in Quantum Systems" deals with the complex dynamics of apparently simple quantum systems. "Complexity" arises from the destruction of symmetries through the strong coupling of few degrees of freedom, from the many degrees of freedom of an interacting many-particle system, from disorder or stochastic activation, and finally – as a specific quantum feature – from interference, decoherence, and entanglement. During the past years, our work focused on

- the representation of quantum mechanical entanglement measures in terms of suitable experimental observables (F. Mintert, L. Aolita);
- the dynamics of quantum entanglement under the influence of noise (M. Busse, C. Viviescas, I. García-Mata, O. Brodier, T. Gorin, A. Aragão, B.V. Fine, A.R. Ribeiro de Carvalho, F. Mintert);
- Ericson fluctuations, dynamical localization, and resonance-assisted tunneling in decaying one and two-electron Rydberg systems (J. Madroñero, A. Krug, S. Wimberger, C. Eltschka, A. Dudarev, P. Schlagheck);
- coherent backscattering of light from cold atoms (V. Shatokhin, C.A. Müller);
- the dynamics and decoherence of ultracold (interacting and non-interacting) atoms in periodic light potentials (A. Ponomarev, J. Madroñero, A. Kolovsky, S. Wimberger)

in close contact to ongoing experiments in quantum optics or atomic physics. Besides profound mathematical methods from operator analysis and quantum probability theory, also most advanced techniques of computational physics are employed on one of the currently most powerful parallel supercomputers worldwide, the IBM p690 at the Rechenzentrum Garching of the Max Planck Society.
In May and August 2006 Marc Busse and Alexej Schelle (both Ludwig Maximilians University of Munich) completed their diploma theses. M. Busse returned back to Munich for his PhD, while A. Schelle stays with the group, within a binational PhD program between the University Paris 6 (there under the responsibility of Dominique Delande) and the Ludwig Maximilians University of Munich. Furthermore we succeeded to attract two more PhD students in fall 2006 – Markus Tiersch (Dresden) and Hannah Venzl (Ulm) – as well as the new PostDocs Ming-Chiang Chung (Aachen), Fernando de Melo (Rio de Janeiro), and Sangchul Oh (Seoul). Carlos Viviescas, Artëm Dudarev, Thomas Gorin, Olivier Brodier, and Andrey Kolovsky left the group after the expiry of their guest contracts – C. Viviescas was appointed as a professor back at his home university in Bogotá, O. Brodier got a permanent position as a Maître de Conférence at Université de Tours, A. Dudarev finished his scientific carreer, T. Gorin went to Mexico, and A. Kolovsky returned to his home university at Krasnoyarsk.

Close links with research groups in Brazil, Poland, France, Italy, and Israel, in the first three cases funded through bilateral grants by DAAD and VolkswagenStiftung, were scientifically extremely fruitful and were maintained by the frequent exchange of young scientists. In particular, visits for several weeks by M. Busse and C. Viviescas to Warsaw and Cracow, several months visits of L. Aolita and A. Aragão, two PhD students of our partner group in Rio de Janeiro, here in Dresden, and a one month visit of A. Schelle to Paris should be mentioned.
The visitors program of the institute once more allowed us to host established (K. Dietz, S. Fishman, I. Guarneri, M. Kuś, H. Narnhofer), as well as promising young colleagues (F. Mintert, T. Wellens, S. Wimberger, K. Hornberger, P. Schlagheck, V. Shatokhin, T. Paul, M. Hartung, J. Bae, T. Barthel, D. Burgharth, B. Hiesmayr). A one month summer school on "Quantum Information", organized together with Richard Gill (Utrecht) and Rainer Blatt (Innsbruck), in September 2005 at mpi**pks** , was didactically and scientifically extremely successfull, and initiated several new scientific contacts and cooperations, many of which are documented by now. Part of the lecture courses of the school are presently being recollected for publication as a book. Specialized lecture courses on "Quantum Chaos" and "Quantum Information" were delivered by A. Buchleitner, under guest professorships or in the framework of summer schools, at the Université Catholique de Louvain (Belgium), at ICTP Trieste, and at the National Center for Theoretical Sciences, Hsinchu (Taiwan).
The research activities of the next years are defined by the following principle subjects of our current work:

I the quantum treatment of helium or helium-like atoms under the influence of static or oscillating electric fields, with a minimum of approximations;

II the dynamical characterization of entanglement in composed quantum systems subject to noise;

III the transport of photons or of interacting matter waves in disordered scattering media or in optical potentials.

Whilst the target of (I) is the approximation-free description of the fragmentation dynamics of the periodically driven three body Coulomb problem – realized in current experiments on the laser ionization of helium –, we aim at a general theory of the time evolution of quantum entanglement under Lindblad or more general incoherent dynamics – with the particular objective to define experimentally directly implementable measurement strategies. Under (III), we will focus on decoherence phenomena in the theory of interacting ultracold atomic gases, and of weak (and, possibly, strong) localization of light in scattering media with quantum structure.

Division: Biological Physics
(Head: Prof. Dr. F. Jülicher)

Our research focuses on active and dynamic phenomena in living cells. Starting from the physical properties of molecular processes (e.g. motor proteins) we characterize general mechanisms and principles that underly complex cellular systems (e.g. cell locomotion, cell division, sensory systems). We aim at a theoretical and quantitative

description in particular of dynamic processes in biological systems. Methods and concepts from statistical physics, non-equilibrium and nonlinear physics play a key role for a theoretical study of the collective behaviors of many interacting components, self-organization phenomena and the role of fluctuations. Our research ranges from the active physical properties of cells and their components to the communication between cells and the spatiotemporal organization of cells in tissues. Examples of our research activities are:

Active molecular processes: Protein motors are the prototype systems for active molecular phenomena in cells of animals and plants. They play a key role for cell locomotion, intracellular transport phenomena and cell division. Related processes are important when the cells replicates, transcribes and corrects the information of the genetic material (DNA). Our group studies the physical nature of force and motion generation on the molecular scale as well as situations where many active molecules operate collectively leading to new types of behaviors via self-organization phenomena.

Dynamics of cells and cellular structures: Cells are highly dynamic systems which constantly undergo movements and fluctuations. Examples are cell division, cell locomotion on solid substrates and swimming of cells in fluids. We study the dynamics of cellular structures such as the mitotic spindle, cilia, flagella and mechano-sensory hair bundles, driven by active molecular processes. The mitotic spindle is a cytoskeletal structure which plays a key role in the separation of duplicated chromosomes during cell division. In certain cases, a complex dynamics emerges which includes symmetry breaking and spontaneous oscillations which can be described quantitatively. Cilia are hair-like appendages of cells which stir fluids and propel swimming cells. Nonlinear bending waves emerge from the self-organization of motor proteins and elastic filaments.

Active soft materials: The cellular cytoskeletion is a polymeric gel-like material which is inherently active. It is driven by molecular processes in a non-equilibrium state. As a consequence, it exhibits unusual material properties. The cytoskeletal gel can generate spontaneous movements and flows and a complex dynamics. Starting with a microscopic description at the level of filaments and motor proteins, we develop a generic hydrodynamic description of active soft materials. The constitutive equations of these materials together with boundary conditions corresponding to adhesion and polymerization can capture essential features of the physics of cell locomotion on a solid substrate.

Organization of cells in tissues: An important model system for tissues are epithelia which are two dimensional sheets of cells in which important patterning processes take place during embryo development. An epithelium grows by cell divisions. In this process, it changes its shape and certain cells change in a precise manner their properties and cell types to form new morphologies. We study the physical properties of epithelia and tissues as soft materials. These materials are inherently active since cellular force generation and cell division can induce mechanical stresses and movements of cells. Tissues are visco-elastic and can exhibit fluid and solid behaviors. Pattern formation in the tissue results from the interplay of active material properties and cellular communication. We develop theoretical approaches to study the principles which

underlie these processes.

Communication between cells by morphogens: Morphogens are signaling molecules which are secreted by certain cells in a tissue and which convey signals to cells which are at a distance of several or many cell diameters.They typically form graded concentration profiles in a tissue and provide positional information to cells. We study transport processes which play a key role for the spreading of morphogens. In collaboration with experimental groups we could show that active transport through the cell interior plays an important role for morphogen transport. Based on the physical properties of active transport of morphogens in cells, nonlinear transport equations valid on larger scales can be derived which can account for the kinetics of morphogen gradient formation. The precision of the information conveyed by the gradient can be studied quantitatively and compared to predictions of theory. These approaches permit us in collaboration with biologists to characterize the role of different transport mechanisms in morphogen spreading and to study the robustness and precision of morphogen signaling.

Physics of sensory cells and hearing: Sensory hair cells of vertebrate ears are highly specialized mechanosensors which transduce vibrations to electrical signals. They enable our ears to operate over a dynamic intensity range of 12 orders of magnitudes and to detect extraordinarily weak signals using active and nonlinear amplification mechanisms. Nonlinear oscillators and their universal properties in the vicinity of oscillating instability represent an important conceptual framework to uncover the underlying principles of amplification in hearing. Our group studies active molecular processes in the hair bundle which generate oscillations as well as the role and amplitude of fluctuations which are associated with molecular processes. Universal properties of critical oscillators in the viscinity of oscillating instabilities are studied using field theoretic and renormalization group methods. A further example of our activities is the physics of nonlinear waves which, driven by active cellular processes propagate along the basilar membrane in the cochlea.

These research activities are carried out in close collaboration with experimental groups. Most notably is the collaboration with the Institut Curie in Paris and the AMOLF in Amsterdam in the context of a European Associate Laboratory as well as the links to the MPI of Molecular Cell Biology and Genetics (MPI-CBG) in Dresden. Our group operates a laboratory room with microscope facility which is located in the building of the MPI-CBG. There, experimental studies of oscillations of Min-proteins in bacteria are performed (Karsten Kruse). Furthermore we study physical properties of cell locomotion on solid substrates using Zebrafish Keratocyte cells which occur on fish scales. The strong links to the MPI-CBG consist of a joint research program built around three joint research groups. Our group is also linked to the International Max-Planck Research School on Cell Biology, Bioengeneering, and Biophysics which was initiated by MPI-CBG.

Future Perspectives

Because of the rapid development of molecular and cell biology, biological physics develops very dynamically and constantly broadens and deepens its scope. The Max Planck Institute for the physics of complex systems provides a special environment

for theoretical work in biological physics. The wide range of research in the area of complex systems allows for stimulating interactions and exchanges with other groups working e.g. on nonlinear systems. The vicinity to the MPI-CBG, the biotechnology center and the technical university provide a strong local environment which permits links to related research activities.
Of particular importance for the future is the strong and fruitful collaboration with the MPI-CBG. The joint research program between both institutes opens new developments in cell biology very quickly for theoretical approaches. This stimulates the development of new theoretical methods and also provides new impulses for biological research. The main focus of the joint research program with the MPI-CBG is the study of the behaviors of integrated cellular systems. Their function results from the interplay of many interacting components. The theoretical study of such complex systems moves more and more to the focus of general biological reserach, for example, in the context of the new and rapidly evolving field of Systems Biology. Many important biological processes, such as cellular signaling pathways and the regulation of cellular processes by gen expression become subject of theoretical approaches and physical descriptions. In this context, the understanding of how material properties, motion generation and other active processes are regulated by signaling systems will be of fundamental importance. Quantitative methods and theory will play an increasingly important role in the future for the study of complex biological systems.

Cooperations

- Max Planck Institute for Molecular Cell Biology and Genetics, Dresden
  - Collaboration with the groups of Jonathon Howard und Anthony Hyman on the dynamics of the cytoskeleton, cell division and the physics of motor proteins
  - Collaboration with Marcos González-Gaitán on tissue growth and the kinetics of morphogen gradients in the fruit fly Drosophila
  - Collaboration with Suzanne Eaton on the morphology of cells in tissues.
  - Collaboration with Andy Oates on the segmentation of vertebrates through oscillating and spatio-temporal gene expression patterns
  - Collaborations with Carl-Phillip Heisenberg on the study of cell movements and flows during the development of the zebrafish
  - Collaboration with Marino Zerial on the dynamics of the endosomal network in cells
- Cavendish Laboratory, Cambridge, UK
  - Collaboration with Thomas Duke on the physics of hearing and active wave phenomena in the cochlea
- Institute Curie, Paris
  Collaboration within a European Associate Laboratory
  - Collaboration with Jean-Francois Joanny and Jacques Prost on the physics of active gels, the dynamics of the cytoskeleton as well as cell locomotion

  - Collaboration with Pascal Martin on the role of fluctuations in mechanosensory hair cells (hair bundles)
  - Collaboration with Michel Bornens on the orientation of the mitotic spindle as well as on cytokinesis (the separation of the daughter cells after cell division)

- AMOLF, Amsterdam
  - Collaboration with Marileen Dogterom und Bela Mulder on the origin of contractile rings and on the dynamics of the cytoskeleton in plant cells

- Ben Gurion University, Beer-Sheva
  - Collaboration with Anne Bernheim-Groswasser on Active Gels

Research Group: Biological Physics of Olfaction: From Genes to Networks *(Head: Dr. M. Zapotocky)*

The group currently includes two postdoctoral researchers and one visiting scientist. We use techniques from statistical physics, nonlinear dynamics and soft condensed matter physics to study biological sensory systems, with emphasis on olfaction (the sense of smell) and mechanosensation. Our interests also extend more broadly into developmental biology and biochemical network theory. Our research has recently concentrated on three specific areas:

1. Signal transduction in olfactory sensory neurons:

In the cilia of olfactory sensory neurons, the initial external chemical signal (odorant identity and concentration) is transduced into an electrical signal. The corresponding signal transduction pathway is well characterized biochemically, and is known to include several feedback loops mediated by intra-ciliar calcium. In our previous work, we have used deterministic one-compartment models to examine the role of calcium-mediated feedback in the dynamics of signal transduction. More recently, we have been extending this work to include fluctuations and the effects of diffusion. In project "Response and fluctuations of a two-state signaling module with feedback" (page 128) we examine the kinetics and information transfer in a prototype signaling module consisting of a two-state stochastic point process with negative feedback. Using a path integral technique, we obtain explicit analytical results for the averages, auto-correlations, and response functions to first order in feedback strength; in addition, we investigate the strong feedback regime using Monte Carlo simulations. A surprising conclusion is that depending on precise parameter values, the negative feedback can either decrease or increase the signal-to-noise ratio at the output. Using an extension of this treatment to a 1-dimensional array of diffusively coupled switches we are presently examining the precision of olfactory signaling at very low odorant concentration.

2. Collective effects in axon guidance and targeting:

During development, connections among brain areas are formed by growing neural tubes (axons). In the prevalent picture of this process, each growing axon is independently guided to the proper target by sensing a spatially distributed chemical cue. We develop models in which axon-axon interactions play a dominant role, and proper

targeting thus becomes a collective effect. We idealize each axon as a directed random walk which has attractive contact interactions with other simultaneously growing axons. We have systematically characterized the dynamics resulting from the *turnover* of axons, a process in which the oldest fully grown axons die and are replaced by new growing axons. This corresponds to the situation in the mammalian olfactory system, where the turnover of sensory neurons persists into adulthood, and the connectivity pattern between the nasal epithelium and the olfactory bulb reaches its steady state only after 3-5 turnover periods. In the steady state, progressively larger bundles of axons are found at increasing distance from the epithelium, and the distribution of bundle sizes satisfies a scaling relation. In a heterogenous population of axons with type-specific interaction strength, we analyze the purity of the resulting bundles. We relate our results to the experimental data on targeting defects in the mouse olfactory bulb.

3. Regulation of Drosophila flight by mechanosensory feedback:

The aim of this project is to understand how the fruit fly uses mechanosensory input from its wings to enhance flight stability and maneuvrability. Flies have approximately 100 mechanosensory receptors in each wing; the pattern of the deformation of the wing is thus encoded in the timing of action potentials generated by these sensory neurons. The flight apparatus of Drosophila can be viewed as consisting of the engine (a set of power flight muscles) and two transmissions (sclerite hinges with attached small control muscles) which couple the power muscles to the left and right wing. The control muscles are influenced by the activity of the mechanosensory neurons in the wings; each transmission is thus dynamically regulated by a mechanosensory feedback loop. In our theoretical treatment, we couple a central nonlinear oscillator (the power muscles) to two linear mechanical systems with parameters controlled by the activity of the mechanosensors. Our initial goal is to capture the dynamics of a saccade, a fast 90 deg turn in the yaw plane. Within our framework, the saccade is initiated by a strong transient perturbation on the left or right side, and continues until the left and right wings are fully phase- and amplitude- synchronized. We analyze how the synchronization dynamics is influenced by the mechanosensory feedback, and compare the predicted courses of a saccade to experimental recordings from the laboratory of S. Fry (ETH Zurich). Using the genetic and physiological techniques developed in the group of J. Howard (MPI-CBG Dresden), we will then systematically perturb the activity of the mechanosensory neurons and examine the effect on flight. The project is partially supported by a grant awarded by the VolkswagenStiftung (with J. Howard and S. Frey).

Cooperations

With biology groups:
J. Howard, MPI for Cell Biology and Genetics, Dresden, and S. Frey, ETH Zurich
(mechanosensory control of insect flight)
P. Feinstein and P. Mombaerts, Rockefeller University, New York
(collective effects in axon guidance)

With theorists:
F. Jülicher, mpi**pks**
P. Borowski, University of British Columbia, Canada
M. Gopalakrishnan, Harish-Chandra Research Institute, India

G. Sibona, Universidad Nacional de Cordoba, Argentina
P. K. Mohanty, Saha Institute of Nuclear Physics, India

Research Group: Physics of Biological and Soft Matter
(Head: Dr. Ralf Everaers (until 12/06))

The group was founded in November 2002 and reached its typical size of two PhD students and four post-doctoral guest scientist in January 2004. Following the appointment of the group leader as a professor at the École normale supérieur de Lyon in 2006, activities in Dresden will come to an end in 2007. Our research interest are at the interface between material science and biological physics, where we regard biological systems as "living soft matter." We use methods from statistical physics with a particular emphasis on the combination of computer simulations with analytical and scaling theories.
The theoretical description of the interplay of lipids, proteins and nucleic acids in living cells requires similar methods as the analysis of gels and solutions containing colloidal particles, polymers or surfactant molecules. "Soft" condensed matter is strongly affected by thermal fluctuations, owes its name to its large susceptibility to external stresses, electric or magnetic fields and often exhibits unusual flow properties. Typically the systems possess or self-assemble into structures which are much larger than atomic or molecular scales. We use methods from statistical physics to study the relation between microscopic interactions, structure and dynamics at mesoscopic scales, and macroscopic physical properties or biological function. Our research is focused on three topics:

Polymer entanglement: Polymers have unique visco-elastic properties and are the basic structural element of systems as different as tire rubber and the cytoskeleton. A characteristic feature is the presence of topological constraints on a molecular scale. Similar to entangled ropes, polymer chains can slide past but not through each other. The standard model of polymer dynamics, the tube model, assumes that entanglements confine chain fluctuations to a narrow tube-like region along the coarse-grained chain contour. After having established the microscopic foundation of this highly successful phenomenological model by introducing a "primitive path analysis" (PPA) of the microscopic topological state (see the previous report for 2003/04), we have concentrated on deformation effects in entangled polymer networks. In particular, we have investigated the length-scale dependence of microscopic deformations, their manifestation in small-angle neutron scattering experiments with partially deuterated systems, and effects of chemical aging under strain.

Polyelectrolytes: In aqueous solution polymers with ionizable side-groups dissociate into charged macroions and small counter ions. Macromolecules of this type are commonly referred to as polyelectrolytes. Most water-soluble polymers fall into this class which comprises proteins and nucleic acids as well as synthetic polymers such as sulfonated polystyrene and polyacrylic acid. The treatment of the long-range electrostatic interactions is particularly complicated in the presence of non-polar, hydrophobic elements which typically have a very low dielectric constant compared to water. With the sup-

port of the Volkswagenstiftung we develop new simulation algorithms which allow the evaluation of electrostatic self-energies and charge-charge interactions in dielectrically inhomogeneous media.

DNA and chromatin: Genetic information is stored in the base sequence along two complementary strands of double-helical DNA molecules. In eucaryotic cells DNA is hierarchically compactified into chromatin fibers and chromosomes by association with proteins. The genetic information is replicated and transcribed by synthesizing complementary DNA or RNA strands along locally dissociated strands of the double helix. The relevant length scales range from 1 nm (the size of individual bases) to the total contour length of 2m of DNA in each human cell. We have worked on theories and computer simulations describing DNA elasticity and melting at the base-paire level, the structure of the 30 nm chromatin fiber, electrostatic interactions in DNA and chromatin, and topological constraints on chromatin decondensation during metaphase.

Cooperations

- Dr. G. S. Grest (Sandia National Laboratories, Albuquerque, USA): simulation of polymer melts and networks
- Prof. K. Kremer (Max-Planck-Institute for Polymer Research, Mainz): simulation of entangled polymers
- Dr. A. C. Maggs (ESPCI, Paris, France): Electrostatic interactions in soft condensed matter
- Prof. H. Schiessel (Lorentz Institut, Leiden University, The Netherlands): chromatin structure
- Prof. E. Straube (University of Halle-Wittenberg, Germany): analysis of tube confinement
- Prof. N. Uchida (Tohoku University, Sendai, Japan): simulation of actin solutions

Junior Research Group: Waves in Complex Media and Mesoscopic Phenomena
(Head: Dr. H. Schomerus (until 3/05))

This Junior Research Group existed from November 2000 and hosted since its inception a good dozen of young guest scientists for periods of 1-3 years. In 2005, the former head of the group took a permanent position of Reader in Theoretical Condensed Matter Physics at Lancaster University, UK.
The last former members left the mpi**pks** in autumn 2006. Apart from one individual who now works for industry, all other former members are still academically active, some of them on senior research positions (M. Hentschel at the mpi**pks**, J. Wiersig at Uni Bremen, M. Titov at Uni Konstanz, M. Zareyan at IASBS Zanjan, Iran).
The group dedicated its research to the electronic and photonic transport and dynamics in low-dimensional and mesoscopic quantum systems. It studied the interplay of

disorder, geometry, interactions, phase coherence, chaos, and various types of correlations in normal- and super-conducting as well as ferromagnetic and photonic materials. The group produced 81 peer-review publications in international journals, including 14 in Physical Review Letters.

Junior Research Group: Electronic Structure of Finite Systems
(Head: Dr. S. Kümmel (until 9/05))

The research focus of the Emmy Noether junior research group "Electronic structure of finite systems" was the investigation of the structure and, to an increasing extent, also the dynamics of electronic systems. Our favorite and most used theory was density functional theory and its time-dependent extension. One of the major goals of our research was to develop density functionals that allow for a reliable description of non-linear, nonperturbative electronic dynamics. These studies were motivated by atomic physics problems like non-sequential ionization and high-harmonic generation which are very successfully investigated experimentally. However, on the theoretical side the investigation of such effects is very much complicated by the fact that the time-dependent, correlated many-particle Schrödinger equation is numerically so difficult to solve that the long-ranged non-perturbative dynamics of even a seemingly simple system like the Helium atom can hardly be calculated without making far reaching approximations.
Time-dependent density functional theory seems ideally suited to bridge this gap because of its fundamentally different approach to quantum mechanics: Instead of working with the correlated wavefunction, it uses the particle number density as the basic variable. Thus, it is computationally much easier to handle. In addition, due to the fact that density functional theory works with intuitively accessible variables like the particle density and local potentials, it often leads to a clear physical interpretation of the observed phenomena. Pitted against these positive aspects is the major drawback of density functional theory: The fundamental functionals which incorporate the quantum mechanical effects of exchange and correlation into the theory are not known exactly and must be approximated. Investigating and pointing out central properties which functionals must have in order to reliably describe ionization dynamics was an important part of our work. Other projects were concerned with the interpretation of photoelectron spectra used in the determination of the structure of metal clusters and with the determination of the response properties of extended molecular systems.
These projects are now continued at the University of Bayreuth, Germany, at which Stephan Kümmel (former head of the Emmy Noether group) is now working as a professor of theoretical physics. With accepting the offer from Bayreuth, the Emmy Noether junior research group "Electronic structure of finite systems" ended. The joint projects and collaborations with international partners and with partners within mpi**pks** lead and contributed to the Focus Days „Electronic correlation in atomic and molecular dynamics“ which were organized jointly with M. Lein and J.-M. Rost as part of the conference "Atomic Physics 2005".

Junior Research Group: Many-body effects in mesoscopic systems
(Head: Dr. M. Hentschel (since 4/06))

The Emmy Noether group "Many-body effects in mesoscopic systems" began its work at the institut in April 2006. Besides the group leader, two Postdocs and two PhD students investigate consequences of Anderson orthogonality catastrophe on photoabsorption spectra and transport properties of realistic mesoscopic systems. A second, disjunct topic of the group's research concerns aspects of quantum chaos in optical microresonators. It is carried out by Postdocs of the Visitors Program and the group leader. These studies are also related to the activities of the *DFG-Forschergruppe 760* (Group of Researchers funded by the German Research Foundation, positively evaluated with final approval expected in April 2006) with the title "Scattering Systems with Complex Dynamics". Since October 2006, the group has its own weekly seminar on "Mesoscopic Systems". Furthermore, the group leader is the main organizer of the „Scientific Jam Session", a discussion forum for the young scientists (Postdocs and advanced PhD students) of the institut that meets on Friday afternoon since June 2006.

Many-body effects have always been of interest to the physcis community and often provoked the quest for new theories. One example is the x-ray edge problem that refers to deviations of the photoabsorption cross section of metals from the naive expectation. The progress in the fabrication of much smaller, nanoscale samples during the last 15 years has opened the possibility to repeat the experiments with those mesoscopic-coherent devices like metallic nanoparticles or quantum dots. The number of electrons is now reduced by orders of magnitude. Moreover, the model of Bloch electrons valid for metals has to be amended using concepts from the field of quantum chaos. Will this cause measurabele deviations in the many-body signatures and in transport properties? Such and similar questions are investigated in the Emmy Noether group.

That small systems can indeed show characteristics that qualitatively differ from the macroscopic case was exemplarily shown by the group leader for the photoabsorption cross section of generic-chaotic mesoscopic systems. Extension of these studies to regular systems is one main focus of the group's research. Presently, we investigate Andersons orthogonality catastrophe in circular and rectangular quantum dots as well as in systems with parabolic confinement potential. In this latter, experimentally relevant case we find characteristic shell effects. In continuation of this project we will identify their consequences for photoabsorption spectra and transport properties. Another system presently studied in the group is graphene. The special electronic properties at the Dirac points are clearly reflected in the behaviour of the Anderson overlap.

The second research topic of the group, namely the field of optical microresonators, comprises studies concerning semiclassical corrections to the ray picture on the one hand, and the investigation of the effect of an active medium (in lasing cavities) on the other hand side. More precisely, we study consequences of the Goos-Hänchen effect on the far field characteristics of microresonators and the relation, as well as possible differences, between resonance modes in passive and active cavities. These studies are of great practical importance for applications such as microlaser devices.

Perspectives
A future topic in the work on mesoscopic many-body phenomena will be the Kondo effect in nanoscale devices, in particular the interplay of Kondo and x-ray edge physics. In both cases, the density of states of electrons at the Fermi edge is changed and gives rise to Fermi edge singularities. Mesoscopic systems allow one to couple both effects in a manner not feasible in metals, thereby opening completely new possibilities for the study of many-body phenomena.
In the field of optical cavities we will address the question to what extent the results obtained for closed billiard systems (such as hierarchical states or the flooding of regular islands by chaotic states) are of relevance in open, optical systems. Moreover, we will investigate the issue of spontaneous emission in microlasers. To date, this effect is neglected in the models used. Its implementation in the Schrödinger-Bloch model is not only conceptionally desirable but also of practical relevance.
Eventually we would like to mention that the group leader will organize, jointly with Mark Raizen (University of Texas at Austin, USA) and Jan Wiersig (University of Bremen), the conference "New Frontiers of Quantum Chaos in Mesoscopic Systems" to be held at the institute in May 2008.

Collaborations
The connections of this junior research group to the national and international community are numerous and comprise both theoretical and experimental collaborations. Separated according to the two main research directions, these are:

Many-body effects in mesoscopic systems

- Continuation of the collaboration with Harold Baranger (Duke University, USA) and Denis Ullmo (Orsay, France) that was initiated during the group leader's Postdoc time at Duke University.

- Collaboration with Francisco Guinea (Madrid, Spain) on problems of Anderson orthogonality catastrophe in graphene.

Quantum chaos in optical microcavities

- Cooperation within the above-mentioned DFG research group, in particular with Jan Wiersig (University of Bremen), Roland Ketzmerick and Arnd Bäcker (Technical University of Dresden), and Henning Schomerus (Lancaster University, Great Britain).

- Continuation of the successful cooperation with the *experimental* groups of Takahisa Harayama and Takehiro Fukushima (ATR Wave Engineering Laboratories , Kyoto, Japan and Okayama Prefectural University, Japan) on the far field characteristics of oval microlasers (comparison of experiment with ray simulations).

- Contacts to the *experimental* group of Achim Richter (Technical University of Darmstadt) were recently established with the goal to measure the Goos-Hänchen shift at curved dielectric interfaces. Furthermore there are regular contacts to the groups of Chil-Min Kim (Paichai University, Daejon, Korea) and Sang Wook Kim (Busan National University, Korea).

Joint research program mpipks and MPI-CBG

Physics of Biological Systems

The joint research program 'Physics of Biological Systems' between the Max Planck Institute for the Physics of Complex Systems and the Max Planck Institute of Molecular Cell Biology and Genetics strengthens the collaborations between these two institutes in Dresden. The objective of the program is to develop new physical methods and concepts - experimental as well as theoretical - for analyzing biological systems. Three Junior Research Groups at the two institutes commenced their activities after the program started in 2004. The group of Dr. Karsten Kruse (The Physics of Cell Division) started in October 2004, is located at the mpipks and works on the principles of spatial and temporal organization of cells undergoing division. The group of Dr. Iva Tolić-Nørrelykke (Interior Design of the Cell) started in December 2004, is located at the Max Planck Institute of Molecular Cell Biology and Genetics, and studies how the cell organizes its interior over its lifetime. The group of Dr. Stephan Grill (Motor Systems) started in April 2006, is located at both institutes, and addresses how molecular machines function and interact to perform the dynamics within the living cell. A number of collaborations, joint group-meeting and a seminar series on the Physics of Biological Systems allow for high levels of interaction between these three groups and other groups within both institutes. This provides a unique research environment bringing together experimental biology and theoretical physics to shed light on the physical principles that underlie living systems.

Junior Research Group: Physics of Cell Division

(Head: Dr. K. Kruse (until 8/06))

The work in the group which was hosted at the mpipks from October 2004 to August 2006 concerned the study of physical aspects of cell division. Cell division provides a striking illustration of the necessity for living cells to spatially and temporally control subcellular processes. For example, first, the DNA has to be duplicated, then it has to be distributed evenly on the future daughter cells, and finally the cell has to be cleaved at a formerly specified division site. What are the principles underlying this orgnization in space and time? There is good evidence that cells are internally organized in a modular way. Our research is aimed at understanding specific modules operating during cell division by analyzing them as dynamical systems. To this end we use methods from non-equilibrium statistical mechanics and non-linear dynamics. The guiding idea in this endeavour is to isolate essential components of a module, which then allows for an understanding of possible basic mechanisms underlying its function. This should lead to the identification of mechanisms that are common to seemingly unrelated modules. The work focused on two modules:

The cytoskeleton. The cytoskeleton is an important structure of cells, that is essential not only for cell division, but also for cell locomotion or intracellular transport. It is a network of filamentous proteins, in eukaryotes mostly actin filaments and microtubules, that interact through a number of different associated proteins. In particular, motor proteins like myosins or kinesins use the chemical energy stored in ATP to gen-

erate forces in this network. Cells dispose of a variety of mechanisms to control and regulate the cytoskeleton. However, in vitro experiments have revealed the ability of motor-filament systems to self- organize. This leads to the question of how much of the reorganizations of the cytoskeleton observed in living cells can be accounted for by self-organization of cytoskeletal components? To study this question we have developed various descriptions of cytoskeletal dynamics that we now apply to different situations. In this context we have employed mesoscopic as well as macroscopic phenomenological approaches. We have applied these descriptions to various situations in vitro and in vivo.

The Min oscillations. An essential part of cell division is the determination of the division site. In *Escherichia coli*, a rod-shaped bacterium, division occurs with high precision in the middle, resulting in two equally sized daughter cells. Determination of the bacteria's middle depends crucially on the Min-system. This system consists of the proteins MinC, MinD, and MinE, where in particular MinC is an unspecific inhibitor of division. The Min-proteins oscillate between the two cell poles with a period of about 60s. As a consequence of the oscillations MinC inhibits cell division close to cell poles, such that division occurs most likely at the center. Work in the group aims at identifying possible mechanisms for the Min-oscillations and confronting theoretical predicitions with quantitative experiments.

Cooperations
Anne Bernheim-Groswasser (Ben Gurion University, Beer-Sheva), M. Dogterom (AMOLF, Amsterdam), Jonathon Howard (MPICBG, Dresden), Jean-Franǫis Joanny (Institut Curie, Paris), B. Mulder (AMOLF, Amsterdam), Jacques Prost (ESPCI, Paris), Petra Schwille (TU Dresden), Ken Sekimoto (Université Paris VII)

During the group's existence one habilitation (K. Kruse), one dissertation (G. Meacci) and one diploma thesis were prepared. Three further PhD-projects started (K. Doubrovinski, E. Fischer-Friedrich, S. Günther) and are now continued, respectively, at mpi**pks** (E. Fischer-Friedrich) and Saarland University (K. Doubrovinski, S. Günther). Meanwhile, K. Kruse has become full professor at Saarland University (W3) and G. Meacci has started as a post-doc at the IBM Thomas J. Watson Center in Yorktown Heights, USA. Finally, to the group belonged a guest scientist (A. Iomin), a post-doc (E. Nicola), and a guest student (R. Nguyen van yen, Ecole Normale Superieure, Paris). Amongst others, members of the group participated in 4 publications in Physical Review Letters and one report in Science magazine.

Research Group: Motor Systems
(Head: Dr. Stephan W. Grill (since 3/06))

Our group is interested in how molecular machines, the workhorses of the cell, function and interact to form the dynamical processes that are observed in living organisms. We focus on the physical mechanisms underlying the generation, coordination and regulation of force and movement in biological systems. This is done through a combined theoretical and experimental approach, with a focus on two systems that reach from

the scale of a single molecule to the scale of a single cell.

Transcriptional Systems. We study the mechanisms underlying the movement of RNA Polymerase II (RNAP II) along its DNA template at the single molecule level. RNAP II reads the genetic code that is stored within DNA and copies it to mRNA, which is subsequently read out and translated into protein. As all protein production starts by this information transfer process, RNAP II represents a central control point for cellular function and behavior. Specifically, we focus on the force dependence of rate-limiting off-pathway events during transcription, looking at the dynamics of backtracking, a state which is thought to be used in reducing the amount of copy errors. We have proposed that this molecular machine performs a one-dimensional random walk while it is fixing the error. We systematically study the implications of such a diffusive state on the lifetimes of the backtracked state and the general fidelity of transcription. Finally, we are developing a micromechanical model of transcription that will be able to relate the measured behavior in removing copy errors to the theoretically expected optimal behavior to which this machine is thought to have evolved to. We hope to ultimately reveal the details that are at the heart of transcription in the cells of higher organisms.

Cytoskeletal Systems. We study the mechanisms underlying cytoskeletal dynamics during the early growth of the embryo of the nematode worm *Caenorhabditis elegans*. The cytoskeleton is the mechanical scaffold of the cell which encompasses all the active mechanical processes that occur in a living system. *C. elegans* offers the possibility of pursuing a preturbative approach at a Systems-Biology level: For a particular cytoskeletal activity, we devise an initial theoretical description. To refine, we then perturb in a controlled manner, both mechanically and genetically, and study the subsequent response, both in theory and experiment. We have successfully applied this strategy to improve our understanding of spindle positioning during mitosis, and now focus on the cortical cystoskeleton that is localized beneath the membrane of a living cell. This meshwork of actin-based filaments is responsible for a number of important events in the development of any living organism, such as cell division. In particular, we study the mechanism of cortical polarization in asymmetric cell division, which is thought to be of importance in the division of stem cells. After breaking of symmetry and during this polarization event, two distinct cortical domains develop and their mechanical properties (visco-elasticity and actively generated tension) determine the respective sizes to which these domains grow. As these domains appear before the first division of the *C. elegans* embryo, they are able to 'read out' a body axis to control the spatial arrangement of future cellular and developmental events. We intend to describe the mechanical properties of these two distinct cortical domains in theory and experiment to ultimately reveal the precise biophysical properties and functions of all key cytoskeletal components involved in these dynamical processes.

Theory and Experiment. Our group is jointly appointed to the mpi**pks** and the MPI-CBG. We apply methods from non-equilibrium statistical mechanics and non-linear dynamics to devise theoretical descriptions which we then test using a high-resolution dual-trap optical tweezer (for single molecule experiments performed in reconstituted minimal systems), a UV-lasercutter (for mechanical perturbations of the living cell) and dosage-response RNA-mediated interference (for genetic perturbations of the living cell).

Cooperations
C. Bustamante, Howard Hughes Medical Institute and at the University of California, Berkeley: Transcription by RNA Polymerase II
C. Müller, European Molecular Biology Laboratory, Grenoble Oustation, Grenoble: Transcription by RNA Polymerase III
A. A. Hyman, Max Planck Institute of Molecular Biology and Genetics, Dresden: The mechanics of cortical polarization in *C. elegans*
J. Howard, Max Planck Institute of Molecular Biology and Genetics, Dresden: Optical tweezer technology and single cell perturbation experiments
E. Schäffer, Biotec Center, TU Dresden: Precise calibration of optical tweezers

Research Group: Interior Design of the Cell
(Head: Dr. Iva Tolić-Nørrelykke)

How does a cell organize its interior? Spatio-temporal organization is crucial for life at all levels of complexity, from macromolecules to cells, organs, and organisms. At the level of single cells, segregation of genetic material and a correct cell division relies on proper cell shape and position of organelles inside the cell. Mistakes in organelle positioning sometimes lead to cell death or diseases such as cancer.
We are a team of biologists and physicists investigating the dynamics of spatial order inside the cell. We use the fission yeast *Schizosaccharomyces pombe* as a model system because it has a simple symmetrical cell shape, a small number of cytoskeletal filaments, and highly developed genetics. We combine experimental methods (laser scanning microscopy, laser cutting, optical tweezers, mutants), advanced image analysis, and theoretical research at the interface of physics and biology.
Microtubules and the cell nucleus play a central role in organizing the cellular interior. We would like to understand the mechanisms that center the interphase nucleus, the processes that drive nuclear movements during mitosis and meiosis, as well as how the cell switches between different types of nuclear movements. We are focusing on the following topics:
Centering. How does an interphase nucleus find the cell center? The cylindrically shaped cells of fission yeast have a centrally placed nucleus and divide by fission at the cell center. A direct way to study how the cell positions its nucleus in the center involves mechanical perturbation of the nuclear position. We have developed a technique to move the nucleus within the cell using optical tweezers. These optical manipulations offer several advantages over the methods previously used to displace cell organelles, such as centrifugation: organelles can be displaced selectively; the manipulation can be performed exactly at a chosen time in the cell cycle; and, displacements as small as a few hundred nanometers can be detected because the image of the cell after the manipulation can be compared directly to the image before the manipulation. Our experiments show that when we displace the nucleus away from the cell center using optical tweezers, and then switch off the tweezers, the nucleus returns to the cell center. The force for the return of the nucleus is provided by microtubules, which push against the cell ends and thereby move the nucleus towards the middle of the cell.
How does a cell determine its division site? We are interested in the spatio-temporal coordination of nuclear events (chromosome segregation) and cortical activities (cytokinesis). Is the spatial cue for the division site provided by the position of the nucleus?

If the division site is established by a signal from the nucleus at a defined period of the cell cycle, then displacing the nucleus at an earlier time would result in a corresponding displacement of the division plane, whereas a later displacement would not affect the normal position of the division plane at the cell center. Our experiments, in which we displace the nucleus by optical tweezers, suggest that the division plane is indeed specified by the position of the nucleus. Moreover, the cell makes the decision where to divide at the very beginning of mitosis. Why so early, when a number of other cell types make that decision by the end of mitosis? The answer probably lies in the fact that the fission yeast nucleus is centered by microtubules during interphase but not in mitosis. Thus the establishment of the division plane at the beginning of mitosis may be an optimal mechanism for accurate division in these cells.

Alignment. How does the mitotic spindle become properly aligned within the cell? In all eukaryotic cells, spindle position with respect to the cleavage plane is important for a successful segregation of whole chromosome sets into daughter cells. In some cells, spindle axis determines the cleavage plane, thus also the size and fate of daughter cells. When and how does the spindle get aligned with the cell axis? There are several complementary mechanisms by which the spindle becomes properly aligned. Using confocal microscopy and high-precision tracking of spindle poles, we have identified three mechanisms of spindle alignment in fission yeast. First, interphase microtubules, which are aligned with the cell's longitudinal axis, serve as a template for the nascent spindle. Thus the spindle is aligned with the cell axis as it forms. Second, the cylindrical shape of the cell forces an elongating spindle to align with the cell axis. Finally, the third mechanism is based on astral microtubules, which push on the spindle poles against the cell edge and thus help to align the spindle.

Oscillations. What drives the nuclear oscillations in meiotic prophase (beginning of cell division in sexual reproduction)? During this phase in fission yeast the nucleus continuously oscillates between the two ends of the cell, with a period of about 5 minutes and a total duration of a few hours. Why are nuclear oscillations important? They may facilitate the spatial alignment of homologous chromosomes, which is required for their proper pairing during meiotic prophase. We would like to understand the mechanism that generates the oscillations. The oscillatory motion of the nucleus depends on astral microtubules that radiate from the spindle pole body and on cytoplasmic dynein, a minus-end directed microtubule motor. We are currently investigating the behavior of microtubules and dynein, as well as their role in the oscillations, using confocal microscopy, fluorescence recovery after photo-bleaching (FRAP), laser cutting of microtubules, and laser ablation of dynein foci. Future plans include theoretical modeling and computer simulations.

Cooperations

F.S. Pavone, LENS - European Laboratory for Non-linear Spectroscopy, University of Florence, Italy: Laser cutting and optical tweezers technology

K. Berg-Sørenesen and Lene Oddershede, Niels Bohr Institute, Copenhagen, Denmark: Subdiffusion in living cells and calibration of optical tweezers

K. Kruse, Max Planck Institute for the Physics of Complex Systems, Dresden: Modeling of nuclear oscillations

N. Pavin, University of Zagreb, Croatia: Modeling of nuclear oscillations

Chapter 3

Selection of Research Results

3.1 Charge Degrees of Freedom on Frustrated Lattices

Frank Pollmann, Peter Fulde and Erich Runge

Quantization of charge is a very basic feature in the description of the physical world. Therefore, the discovery of fractionally charged excitations came as a surprise to physicists. An early investigation by Su, Schrieffer, and Heeger [1] dates back to 1979 and deals with the chain molecule trans–polyacetylene $(CH)_n$. Fractionalization is also found in 2D in the much celebrated fractional quantum Hall effect (FQHE). It was Laughlin [2] who introduced this concept here. The question was left open whether or not fractionally charged excitations exist in 2D or 3D systems without a magnetic field. In [3] it was suggested by one of the authors that in a pyrochlore lattice, a prototype of a 3D structure with geometrical frustration, excitations with charge $\pm e/2$ do exist. In order to study frustrated systems with charge degrees of freedom, several 2D and 3D lattice models are considered. We mainly focus on a checkerboard lattice, which can be thought of as a projection of the pyrochlore lattice onto a plane. To be specific, here we consider a model Hamiltonian of spinless fermions

$$H = -t \sum_{\langle i,j \rangle} \left(c_i^\dagger c_j + \text{H.c.} \right) + V \sum_{\langle i,j \rangle} n_i n_j \tag{1}$$

on a crisscrossed checkerboard lattice. The operators $c_i (c_i^\dagger)$ annihilate (create) fermions on sites i. The density operators are $n_i = c_i^\dagger c_i$. We assume that half of the sites are occupied by fermions, i.e., $\sum_i n_i = \frac{N}{2}$ for a system with N sites. Our main interest is the regime $|t|/V \ll 1$.

For a moment, let us set the hopping integral t equal to zero. The ground–state manifold is then macroscopically degenerate: Every configuration that satisfies the so–called tetrahedron rule of having exactly two particles on each tetrahedron (crisscrossed square) is a ground state [4]. In other words, the system has a finite $T = 0$ entropy. Figure 1 (a) shows an example of such classical ground–state configurations. We will refer to configurations satisfying the tetrahedron rule as "allowed configurations". The classical ($t = 0$) ground states have the important property of being incompressible in the sense that no fermion can hop to an empty site without creating defects. In other

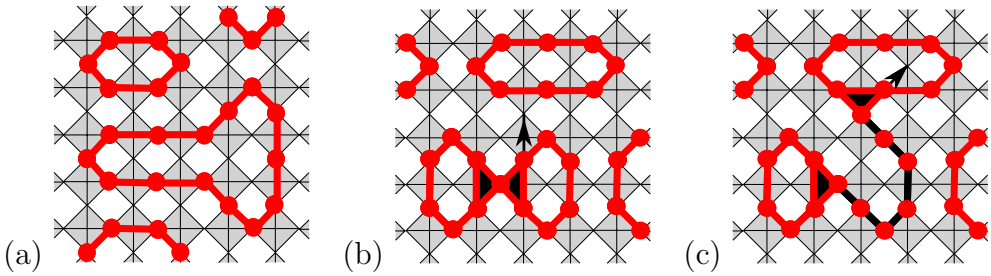


Figure 1: *Panel (a) shows an example of an allowed configurations on a checkerboard lattice at half filling. The occupied sites are connected by red lines. (b,c) Adding one fermion to the half–filled checkerboard lattice leads to two defects on adjacent crisscrossed squares. Two defects with charge $e/2$ can separate without creating additional defects and are connected by a string consisting of an odd number of fermions, shown by a black line.*

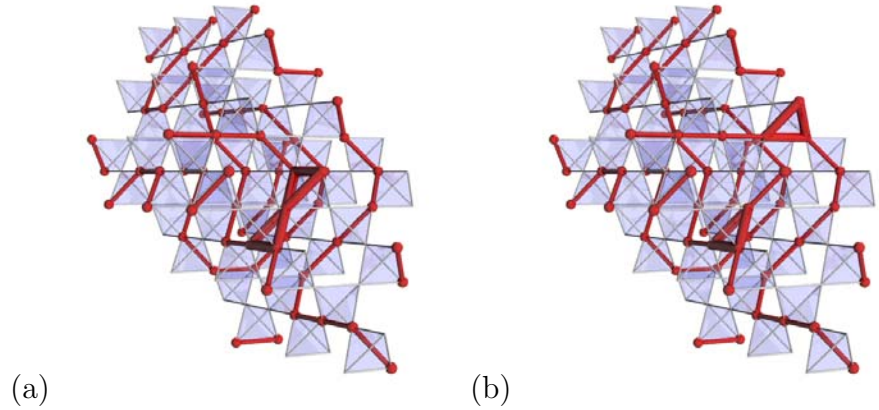


Figure 2: *Adding one fermion to the half–filled pyrochlore lattice leads to two defects on adjacent tetrahedra. Occupied sites are connected by red lines. The two defects with charge $e/2$ can separate without creating additional defects and are connected by a string consisting of an odd number of fermions.*

words, we have to violate the tetrahedron rule if we want to transform one allowed configuration into another.

Placing one additional particle with charge e onto an empty site leads to a violation of the tetrahedron rule on two adjacent crisscrossed squares (see Figure 1 (b)). The energy is increased by $4V$ since the added particle has four nearest neighbors. There is no way to remove the violations of the tetrahedron rule geometrically by simply moving the electrons. However, fermions on a crisscrossed square with three particles can hop to another neighboring crisscrossed square without creating additional violations of the tetrahedron rule, i.e., without increase of repulsive energy (see panel (c) in Figure 1). By these hopping processes, two local defects (violating the tetrahedron rule) can separate and the added fermion with charge e breaks into two pieces. They carry a fractional charge of $e/2$ each. The separation gains additional kinetic energy of order t. All above mentioned arguments for the existence of fractional charges on a 2D checkerboard lattice can be directly transferred to a 3D pyrochlore lattice at half filling (see Figure 2). For example, the fractional charges correspond to tetrahedra with three fermions. To our knowledge, this model gives the first realization of fractional charges in 3D systems.

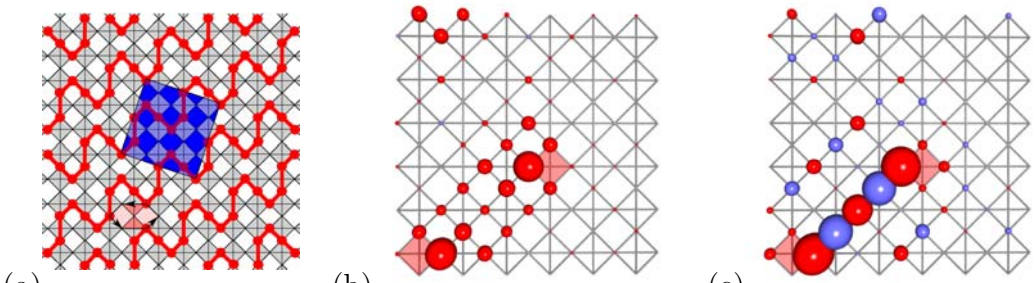


Figure 3: *Panel (a) shows one of several configurations of the half–filled checkerboard lattice maximizing the number of flippable hexagons. The unit cell contains* $\sqrt{20} \times \sqrt{20}$ *sites. Neighboring occupied sites (dots) are connected by a solid line. In panel (b), the local loss of kinetic energy due to the separation of two fractionally charged defects is shown. The radius of the dots is proportional to the local energy loss. The positions of the defect are indicated by red crisscrossed square. Red (blue) dots show an increase (decrease) of the local density (vacuum polarization due to two fractional charges) in panel (c).*

If we relax the constraint of having two fermions on each crisscrossed square and consider a very small but finite ratio t/V, quantum fluctuations come into play. The quantum fluctuations lead also to fractional charges, but do not change the net charge of the systems. Starting from an allowed configuration, the hopping of a fermion to a neighboring site increases the energy by V. One crisscrossed square contains three fermions while the other has only one fermion. Two mobile fractional charges with opposite charges $+e/2$ and $-e/2$ arise. The potential energy is lowered by the kinetic energy of the two defects leading to a reduction of the macroscopic degeneracy. Processes in lowest non–vanishing order in $\mathcal{O}(t/V)$ connect different allowed configurations and reduce the macroscopic degeneracy. An effective Hamiltonian H_{eff} acting on the subspace spanned by the allowed configurations is given to lowest non–vanishing order by ring–exchange processes $\sim t^3/V^2$ [5]. It includes ring exchanges around hexagons and reads

$$H_{\text{eff}} \;=\; -g \sum_{\{\hexagon,\hexagon\}} \big(\,|\, \hexagon \,\rangle\langle\, \hexagon \,|\, - \,|\, \hexagon \,\rangle\langle\, \hexagon \,|\, + \text{H.c.} \,\big), \qquad (2)$$

with the effective hopping–matrix element $g = 12\ t^3/V^2 > 0$. The sum is taken over all vertical and horizontal oriented hexagons. The pictographic operators represent the hopping around hexagons which have either an empty or an occupied central site. The signs of the matrix elements depend on the representation and the sequence in which the fermions are ordered. In passing, we mention that the fermionic sign problem of H_{eff} can be removed by a non–local gauge transformation and the low–energy excitations can therefore equivalently be described by hard–core bosons [6]. We can identify several quantum numbers in order to characterize different subensembles. A topological quantity, which is conserved by all local processes, i.e., ring–exchange processes, is the average tilt of a scalar height field [5]. Another useful set of quantum numbers are the numbers $(N_{\mathcal{B}}, N_{\mathcal{Y}}, N_{\mathcal{G}}, N_{\mathcal{R}})$ of particles on four sublattices. The conserved quantities of the effective Hamiltonian allow for a reduction of the numerical effort by exploiting the resulting block–diagonal form of the matrix representation. Furthermore, eigenstates can conveniently be classifed.

By means of exact numerical diagonalization, we find a long–range ordered ground

state as shown in Figure 3 (a) [7]. The 10–fold degenerate ground–states form squiggle configurations which maximize the number of flippable hexagons. Next we determine the changes of the local kinetic energy density due to the presence of two charges $e/2$. This is done by keeping two crisscrossed squares with fractional charges fixed at $\mathbf{0}$ and $\mathbf{r}$ and determining the ground state $|\psi_0^{\mathbf{0r}}\rangle$ as well as its energy. The result is shown in Figure 3 (b). One notices an increase of energy with respect to the vacuum in the region between the two charges. The increase is due to the topological changes caused by the string connecting the defects, i.e., it reduces the number of flippable hexagons. The energy increase is proportional to the length of the generated string and implies a constant confining force. A similar behavior is also found in the case of confined quarks. The confinement in our case results from a reduction of vacuum fluctuations and a polarization of the vacuum in the vicinity of a connecting string (Fig. 3 (c)). Consequently, we do not find free fractional charges on the checkerboard lattice, but instead we find bound pairs. In the considered limit, the bound pairs are expected to have a large spatial extent up to several hundred lattice spacings and might thus lead to unexpected physical properties at higher doping concentrations.

Our current interest focuses on a thorough investigation of the real 3D pyrochlore lattice. Even though the checkerboard lattice and pyrochlore lattice show many similarities, there exist certain differences between them, e.g., due to the higher spatial dimensionality [8]. Here, differences of the two lattices arise in the U(1) gauge theory which describes the low energy excitations of the considered systems [9]. The related compact electrodynamics is always confining in 2+1 dimensions while it allows for the existence of a deconfined phase in 3+1 dimensions [10]. Systematic exact diagonalization studies as well as the application of Monte Carlo techniques will provide a deeper insight and we hope to find a proof for the existence of a deconfined phase in a 3D pyrochlore lattice with free fractionally charged particles. In addition, a natural extension of the model is the inclusion of spin. This leads to a more realistic model and could provide a better link to experiments.

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3.2 Effect of Unconventional Superconductivity on the Magnetic Excitations in Layered Cuprates and Heavy-Fermion Compound UPd_2Al_3

Ilya Eremin, Jun Chang, Peter Thalmeier and Peter Fulde

Since the original pioneering work of Bardeen, Cooper, and Schrieffer on the microscopic origin of superconductivity and the discovery of an isotope effect on the superconducting transition temperature, the electron-phonon interaction has been considered for a long time as a main source of the Cooper-pair formation and, correspondingly, superconductivity. This general belief has been called in question after the discovery of the heavy-fermion and high-temperature superconductivity. In particular, the electron-phonon interaction is retarded in time, which is what puts ultimately a limit on the superconducting transition temperature because energy, and thus temperature, is conjugate to time. Moreover, the electron-phonon interaction is also local in space which usually leads to a total orbital moment of the Cooper-pair, $L = 0$, *i.e.*, s-wave symmetry of the superconducting wave function. At the same time in high-T_c cuprates and many heavy-fermion compounds the symmetry of the Cooper-pair wave function is higher than s-wave which is also higher than the symmetry of the Fermi surface. Due to this reason these superconductors are often called unconventional ones. There have been many scenarios as regard the non-phononic mechanisms of superconductivity like, for example, spin fluctuation-mediated Cooper-pairing or superconductivity through intra-atomic excitations and so on. At the same time, most of these proposals are at present qualitative and not quantitative and therefore, many questions have to be resolved.

One of the most interesting question concerning the non-phononic mechanisms of the Cooper-pairing is: what is the feedback effect of unconventional superconductivity on the bosonic excitations that in turn are supposed to drive the superconducting instability? For the usual 'conventional' electron-phonon mediated superconductors such a feedback effect of superconductivity on the phononic spectrum is known. In particular, below T_c, superconductivity induces shifts in the frequency and the linewidth of the acoustic phonons depending on their wavevector [1]. In this project, we have analyzed the feedback effect of unconventional superconductivity on the magnetic excitations in layered cuprates and on the magnetic excitons in heavy-fermion superconductor UPd_2Al_3. In both cases, Inelastic Neutron Scattering(INS) experiments reveal the formation of a magnetic resonance mode at temperatures $T < T_c$ and energies below $2\Delta_0$ [2, 3].

In high-T_c cuprates one of the most often considered scenarios of superconductivity is a Cooper-pairing mediated by an exchange of antiferromagnetic spin fluctuations which are peaked at the wavevector $\mathbf{Q}_{AF} = (\pi, \pi)$ (we set the lattice constant equal to unity) and characteristic frequency ω_{sf}. This interaction is generally repulsive due to its Coulomb nature and the solution of the BCS or Eliashberg gap equation is only possible for a symmetry higher than s-wave. In particular, for the typical Fermi surface topology in layered cuprates the solution of the gap equation yields $d_{x^2-y^2}$-wave symmetry of the superconducting gap, $\Delta_{\mathbf{k}} = \frac{\Delta_0}{2}(\cos k_x - \cos k_y)$. In the most simple case the dynamic spin response in layered cuprates could be analyzed within Random

Phase Approximation (RPA), its imaginary part measured by INS reads

$$\text{Im } \chi(\mathbf{q},\omega) = \frac{\text{Im}\chi_0(\mathbf{q},\omega)}{(1 - g_{\mathbf{q}}\text{Re}\chi_0(\mathbf{q},\omega))^2 + (g_{\mathbf{q}}\text{Im}\chi_0(\mathbf{q},\omega))^2} \quad , \tag{1}$$

where χ_0 is a bare particle-hole response function and $g_{\mathbf{q}}$ is a fermionic four point-vertex. In the superconducting state, the order parameter changes sign under transla-

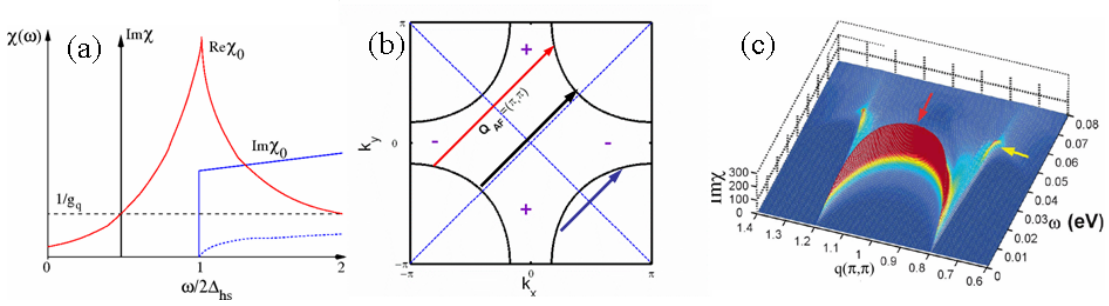

Figure 1: *Formation of the magnetic resonance peak in the superconducting state of layered cuprates. (a) Characteristic behavior of the real and imaginary part of the bare particle-hole response. Intersection of the real part with $1/g_{\mathbf{q}}$, marks the location of the pole in the RPA response function, χ (arrow). The dotted curve refers to the Im χ_0 in the s-wave superconductor. (b) Topology of the Fermi surface in layered cuprates. Dotted lines and signs denote the position of the nodes and positive or negative values of the $d_{x^2-y^2}$-wave superconducting gap. The arrows mark the scattering wave vectors. (c) Dispersion of the resonance peak as obtained within RPA [4].*

tion by $\mathbf{Q}_{AF}$, the BCS coherence factor for the pair-creation process, $1 - \frac{\varepsilon_{\mathbf{k}}\varepsilon_{\mathbf{k+q}} + \Delta_{\mathbf{k}}\Delta_{\mathbf{k+q}}}{E_{\mathbf{k}}E_{\mathbf{k+q}}}$, takes its maximum value on the Fermi surface, as opposed to the s-wave case where it is zero. The net result is (Fig.1(a)) that $\text{Im}\chi_0(\mathbf{Q}_{AF},\omega)$ has a step function jump from zero to a finite value at a threshold $2\Delta_{hs}$, where Δ_{hs} is the value of the superconducting energy gap at the 'hot spots' (points of the Fermi surface connected by $\mathbf{Q}_{AF}$ as shown in Fig. 1(b)). By a Kramers-Kronig relation, $\text{Re}\chi_0$ will then have a logarithmic divergence at $2\Delta_{hs}$. Thus, the full response function (1) will have an undamped pole at some energy less than threshold energy. Therefore, in a d-wave superconductor there is a spin triplet collective mode below the $2\Delta_0$ continuum edge. Away from $\mathbf{Q}_{AF}$, the resonance peak disperses downwards which results from the momentum dependence of the d-wave gap at the Fermi surface and the corresponding dispersion of the lowest threshold frequency where the jump in $\text{Im}\chi_0$ takes place (Fig.1(c)). In particular, for $\mathbf{Q}_i < \mathbf{Q}_{AF}$ the gap in the continuum decreases since the states closer to the diagonal of the first BZ are connected. As soon as $\mathbf{Q}_i$ connects states at the Fermi surface that lie on the diagonal, the resonance will be damped by the nodal gapless quasiparticles. For further decreasing values of $\mathbf{Q}_i$ a bound state is again possible which overall gives the dispersion of the resonance shown in Fig.1(c). Most important, the obtained results agree with the experimentally observed dispersion of the resonance peak [5].
In the heavy-fermion superconductor UPd_2Al_3 a magnetic-exciton mediated Cooper-pairing built on the dual nature of the $5f$ electrons has been proposed. It consists of localized $5f^2$ crystalline electric field (CEF) states which disperse into a magnetic exciton band due to intersite interactions and a conduction electron band formed by

remaining itinerant 5f electrons. The model successfully explains the formation of unconventional superconductivity in this compound based on the virtual exchange of the magnetic excitons between itinerant quasiparticles [6]. Due to the Ising-type anisotropy of the interaction between conduction electrons and magnetic excitons it has been previously found [6] that both, 'spin-singlet' $|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle$ with $\cos k_z$ momentum dependence and 'spin-triplet' $(S_z = 0)$ $|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle$ with $\sin k_z$ have the highest and degenerate superconducting transition temperatures. The $\cos k_z$ solution is observed experimentally in this compound. Due to the interaction of the magnetic excitons with

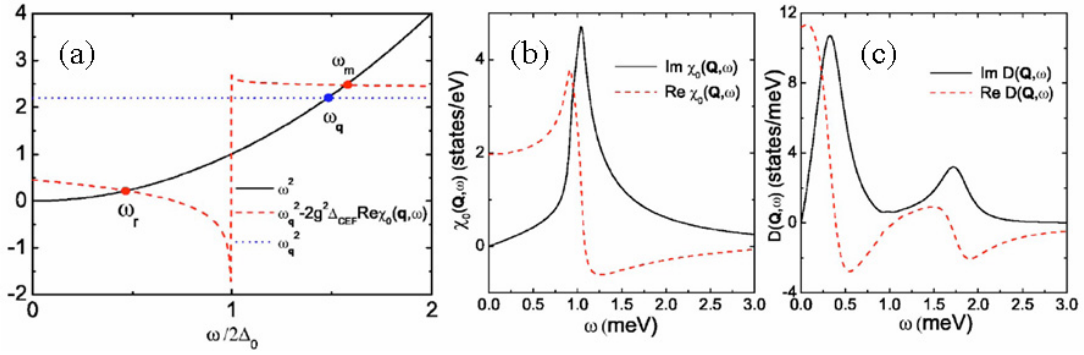

Figure 2: *Feedback of superconductivity on the magnetic exciton in UPd_2Al_3. (a) Illustration of the pole formation of Eq.3 at wave vector* $\mathbf{q} = \mathbf{Q}$*=*$(0, 0, \pi/c)$*. (b) Calculated real and imaginary parts of the longitudinal component of the conduction electron spin susceptibility. (c) The real and imaginary part of the total pseudospin susceptibility.*

conducting electrons, the feedback effect on the former results in

$$D = \frac{D_0}{1 - D_0\Pi_0} = -\frac{2\omega_{\mathbf{q}}}{\omega^2 - \omega_{\mathbf{q}}^2 + 2\omega_{\mathbf{q}}\Pi_0} \quad , \tag{2}$$

where $D(\mathbf{q}, v) = -\left\langle T_\tau a_{\mathbf{q}}(\tau) a^\dagger_{-\mathbf{q}}(0)\right\rangle_{FT}$ is the bosonic Green's function, and the magnetic exciton self–energy is $\Pi_0(\mathbf{q}, \omega) \approx g^2\chi_0(\mathbf{q}, \omega)$. Here g is the coupling constant and χ_0 is a conduction electron particle-hole bubble. The dispersion of the magnetic exciton in the presence of the coupling to the conduction electrons is given by

$$\omega^2 = \omega_{\mathbf{q}}^2 - 2g^2\Delta_{CEF}\mathrm{Re}\chi_0(\mathbf{q}, \omega) \quad . \tag{3}$$

where ω_q is the bare magnetic exciton dispersion. The solution of Eq.3 is illustrated in Fig.2(a). In the normal state, Reχ_0 is a constant at low frequencies determined in our case by the curvature of the Fermi surface along k_z-direction. Thus, the bare magnetic exciton acquires a linewidth and renormalizes slightly which changes the original position of $\omega_{\mathbf{q}}$ downwards. In the superconducting state due to the strong frequency dependence of Re$\chi_0(\mathbf{q}, \omega)$ (and/or Re Π_0) arising from the change of sign of the superconducting order parameters across $\mathbf{Q}$ (compare to the one discussed above for layered cuprates) one finds additional pole in Eq.(3) below $2\Delta_0$ as illustrated in Fig.2(a). Namely, the lowest pole ($\omega_r < 2\Delta_0$) occurs at very small damping (Imχ_0 is nearly zero) resulting in a resonance-like peak in Im$D(\mathbf{q}, \omega)$. The second crossing point is not visible in ImD due to a large peak in Imχ_0 implying strong damping around $2\Delta_0$

(see Fig.2(b)-(c)). The third crossing point, ω_m occurs at energies larger than $2\Delta_0$ and represents the effect of superconductivity on the magnetic exciton [7].
One should note, that in UPd_2Al_3 one finds two types of excitations below T_c since the energies of the magnetic exciton and the resonance peak are well separated. In cuprates, due to itinerant character of the magnetic excitations one finds always a single pole only. However, the main effect remains the same in both cases. Finally we point out that UPd_2Al_3 and layered cuprates are known examples where the unconventional nature of the superconducting order parameter yields a structure in the magnetic susceptibility. Therefore they can be regarded as model systems of unconventional superconductivity which can be studied by inelastic neutron scattering. Furthermore, such an interesting feedback effect can be also predicted for other unconventional phases like, for example, charge density wave with *d*-wave order parameter (DDW phase) [8]. This also can be tested experimentally.

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3.3 Magnetic Field Dependence of the Superconducting Gap Node Topology in Noncentrosymmetric Superconductors

Ilya Eremin, and James F. Annett

The existence of nodal points or lines in the energy gap of a superconductor or a Fermi superfluid, such as ^{3}He, is one of the main characteristics of unconventional symmetry pairing states. An important question is whether or not these nodes are accidental or are fully required by the fundamental symmetry of the pairing state. Second, one can ask whether or not the nodal points or lines are topologically stable, or whether they can in principle be destroyed by small perturbations. This question was discussed in a seminal paper by Volovik [1] in which he showed that point nodes, such as in ^{3}He-A, are diabolical points characterized by a Berry phase and topological

charge. Because of this property the nodal structure cannot be removed by small perturbations, such as a magnetic field. Very recently, Sato [2] has shown that for line nodes of the gap function, topological stability is only guaranteed if time-reversal symmetry is preserved. The topological structure of the nodal line can be classified as Z_2 (*i.e.*, the group {0,1} of integers modulo 2). Perturbations breaking time-reversal symmetry remove conservation of the relevant quantum numbers, and hence line nodes are not topologically stable against such perturbations.

In this project we have considered the effect of time-reversal symmetry breaking on the nodal topology in the noncentrosymmetric superconductors, using as an example the compound $CePt_3Si$ [3]. The absence of inversion symmetry along with parity-violating antisymmetric spin-orbit coupling (ASOC) makes possible in this compound a simultaneous admixture of singlet and triplet pairing components on the sheets of its non-Kramers degenerate, Fermi surface. Unconventional behavior, including zeros in the superconducting gap function is then possible, even if the pair wave function exhibits the full spatial symmetry of the crystal. Theoretical models of the superconducting state are based upon the existence of a Rashba type spin-orbit coupling

$$\hat{H}_{so} = \alpha \sum_{\mathbf{k},s,s'} \mathbf{g_k}.\sigma_{ss'} c^{\dagger}_{\mathbf{k}s} c_{\mathbf{k}s'} \tag{1}$$

as studied by Gor'kov and Rashba [4]. Here $\mathbf{g_k} = -\mathbf{g_{-k}}$ is a real pseudovector, by convention normalized so that $\langle g^2_{\mathbf{k}} \rangle_F = 1$ where $\langle \dots \rangle_F$ denotes an average over the Fermi surface, $\sigma = (\sigma_x, \sigma_y, \sigma_z)$ is the vector of Pauli matrices and $c^{\dagger}_{\mathbf{k}s}$ is the usual Fermi field operator. This spin-orbit coupling removes the usual Kramers degeneracy between the two spin states at a given $\mathbf{k}$, and leads to a quasi-particle dispersion $\varepsilon_{\mathbf{k}} = \epsilon_{\mathbf{k}} \pm \alpha |\mathbf{g_k}|$, splitting the Fermi surface into two sheets with a $\mathbf{k}$ dependent local spin orientation. A full symmetry analysis shows that conventional s-wave pairing ($\Delta_{\mathbf{k}}$ having full tetragonal symmetry) and a p-wave triplet pairing state with order parameter $\mathbf{d_k}$ parallel to the $\mathbf{g_k}$-vector, $\mathbf{d_k} \sim (-k_y, k_x, 0)$, are able to coexist [5]. In zero external field the diagonalization of the BCS Hamiltonian yields the quasiparticle energy dispersion,

$$E_{1,2}(\mathbf{k}) = \sqrt{(\epsilon_{\mathbf{k}} \mp \alpha g_{\mathbf{k}})^2 + |d_{\mathbf{k}} \mp \Delta_{\mathbf{k}}|^2}. \tag{2}$$

In the case where both singlet and triplet order parameters, $\Delta_{\mathbf{k}}$ and $d_{\mathbf{k}}$, can be chosen as real. Assuming that the p-wave gap component is dominant so that $\Delta_{\mathbf{k}}$ is smaller than the maximum value of $d_{\mathbf{k}}$ on the Fermi surface, then one of the Rashba split sheets of the Fermi surface will have a line node, where $\Delta_{\mathbf{k}} = d_{\mathbf{k}}$ and the other sheet will be nodeless. For a spherical Fermi surface and the simplest gap functions allowed by symmetry, $\Delta_{\mathbf{k}} = \Delta$ and $\mathbf{d_k} = d_0(-k_y, k_x, 0)/k_F$, the nodes are two horizontal circles around the Fermi sphere at $\pm k_z = $ const. as illustrated in Fig. 1(a). Let us now consider what will happen to the lines of nodes when time-reversal symmetry is broken by applying a weak Zeeman exchange field $\mathbf{H}$. If a weak c-axis field is applied, we find the spectrum becomes fully gapped, and the line node is removed. In effect the original line node is "accidental", arising from a particular cancelation between the s-wave and p-wave gap components $\Delta_{\mathbf{k}}$ and $d_{\mathbf{k}}$ at some particular value of k_z. When the symmetry breaking perturbation H_z is applied the crossing electron and hole-like levels interact and so an avoided level crossing occurs, hence removing the line node.

On the other hand consider the case of a $a - b$ plane magnetic field. The two Fermi surface sheets will be perturbed differently depending upon whether $\mathbf{H} \parallel \mathbf{g_k}$ or $\mathbf{H} \perp \mathbf{g_k}$.

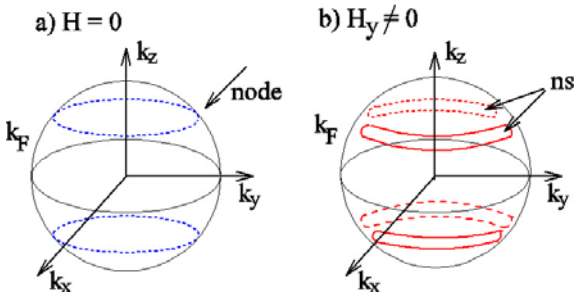

Figure 1: *Illustration of the influence of the ab-plane external magnetic field on the gap line nodes in $CePt_3Si$. (a) zero-field line nodes for $\pm k_z = const$ on one Rashba Fermi surface sheet; (b) $H_y \neq 0$ removes the node along the $\pm k_y$ direction and bifurcates the node elsewhere, yielding "boomerang"-like nodal topology.*

The latter case is essentially identical to c-axis magnetic field, and so for these parts of the Fermi surface the gap node is removed. On the other hand, for the regions where $\mathbf{H} \parallel \mathbf{g_k}$ the gap node is found to *bifurcate*. The reason for this is the following. The field perturbs the two Rashba sheets oppositely, because they have spin components parallel to the applied field $\mathbf{H}$. The corresponding superconducting state spectrum no longer obey the symmetry $E_{3,4}(\mathbf{k}, H_y) = -E_{1,2}(\mathbf{k}, H_y)$. A result is that one branch of the quasiparticle spectrum near the original line node now crosses zero twice, while the other remains non-zero. This implies that the gap node bifurcates. Note that the final spectrum can always be defined as positive, consistent with stability of the Fermi sea, after applying a suitable particle-hole transformation to the quasiparticle states. This sign change results in the bifurcated node.
The final nodal topology for $a-b$ oriented magnetic fields is shown in Fig. 1(b). For $\mathbf{k}$ vectors with $x-y$ components parallel to $\mathbf{H}$ the gap node is removed, while for $\mathbf{k}$ vectors with $x-y$ components perpendicular to $\mathbf{H}$ the gap node bifurcates. Overall this leads to the unusual "boomerang" shaped gap line nodes as shown in Fig. 1(b). This topological structure is consistent with the general Z_2 topological arguments of Sato [2]. The Z_2 gap node has two topological invariants, which in the presence of time reversal symmetry are independently conserved, leading to stability of the line node. But the symmetry breaking perturbation $\mathbf{H}$ removes the stability, leading to either node removal or node bifurcation depending on the field orientation. Finally, the effects we have discussed lead to a dramatic increase in the linear T coefficient in C_V/T, which should be visible experimentally in the single crystal samples that are now available. The appearance of these extra line nodes in a magnetic field and their large effect on the physical properties is surprising given the often stated argument that the non Kramers degenerate Fermi surface should suppress the effect of Zeeman interactions on the superconducting state.

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3.4 Frozen Local Hole Approximation

Elke Pahl and Uwe Birkenheuer

Introduction

The frozen local hole approximation (FLHA) is an adiabatic approximation which is aimed to simplify the correlation calculations of valence and conduction bands of solids and polymers or, more generally, of the ionization potentials and electron affinities of any large system. It is a quantum chemical *wavefunction*-based method which is conceptually very clear and allows for systematic improvement: based on self-consistent field calculations, electron correlation can be included successively by considering determinants of increasing excitation order in configuration interaction (CI) or related procedures. They yield approximate correlated wavefunctions from which all quantities of interest can be derived.

Of course, wavefunction-based methods are computationally very demanding. In order to arrive at manageable schemes for the description of solids or other extended systems, local orbitals have to be introduced and the local character of electron correlation must rigorously be exploited. Among these local schemes one can distiguish approaches which work in infinite systems and aim to truncate the excitation space by an appropriate configuration selection scheme (like the crystal orbital ADC formalism developed in our group [1]) and divide-and-conquer approaches which assemble the correlation effects from finite subsystems (embedded fragments). In particular, the local Hamiltonian approach has been used in the past quite successfully to describe the correlation effects on the band structure of covalent solids [2–4] and polymers [5]. Yet, this approach is quite involved and a more simpler, approximative way of computing the local Hamiltonian has been proposed by our group [6, 7].

In this work we address the question to which extent it is possible to simplify a correlation calculation on electron hole states by focusing on so-called "frozen" local hole configurations although, in reality, the electron hole is usually delocalized over the entire system. Intuitively, this frozen local hole approximation, is guided by the idea that the shape of the correlation hole which is carried along by a traveling electron is essentially invariant and is thus following the electron hole adiabatically.

Theory

Starting point for our correlation calculations is the Hartree-Fock (HF) ground state Slater determinant $|\Phi_0\rangle$ and energy E_0 of an N-particle system. The canonical HF orbitals $|\nu\rangle$ with orbital energies ϵ_ν are divided into the $N/2$ energetically lowest-lying orbitals which are occupied in $|\Phi_0\rangle$ and the unoccupied, virtual orbitals. Within these orbital subsets we can switch between delocalized canonical orbitals and localized orbitals, $\{|\nu\rangle\}$ and $\{|a\rangle\}$, using unitary transformations, such as

$$|a\rangle = \sum_\nu |\nu\rangle U_{\nu a} \tag{1}$$

for the occupied orbitals. In order to construct the correlated (N-1)-particle states of the system in mind, one first constructs so-called cationic reference states $|\Phi_i\rangle$ by removing one electron out of one of the occupied valence orbitals $|i\rangle$ in $|\Phi_0\rangle$. The

resulting states, either *canonical* ones $|\Phi_\nu\rangle$ or *local* ones $|\Phi_a\rangle$, are connected via

$$|\Phi_\nu\rangle = \sum_a |\Phi_a\rangle (U^{-1})^*_{a\nu} = \sum_a |\Phi_a\rangle U_{\nu a} \quad . \tag{2}$$

Including correlation effects one arrives at correlated wave functions $|\Psi_\nu\rangle$ with energies E_ν, and in analogy to Eq. (2) we then define so-called *correlated* local hole states $|\Psi_a\rangle$

$$|\Psi_a\rangle := \sum_\nu |\Psi_\nu\rangle U^*_{\nu a} \tag{3}$$

and an effective Hamilton $\hat{H}^{\text{eff}}$ with

$$H^{\text{eff}}_{ab} := \langle \Psi_a | \hat{H} | \Psi_b \rangle = \sum_\nu U_{\nu a} E_\nu U^*_{\nu b} \quad . \tag{4}$$

Evidently, the effective Hamiltonian is constructed such that diagonalizing its local matrix representation H^{eff}_{ab} precisely yields the desired correlated energies E_ν of the cationic states. Thus, provided one knows the correlated local hole states $|\Psi_a\rangle$ defined in Eq. (3), one can find the cationic energies by simply solving a small eigenvalue problem.

$$\begin{array}{lcll} \{|\Phi_\nu\rangle\} & \overset{U}{\longleftrightarrow} & \{|\Phi_a\rangle\} & \text{HF states} \\ \quad \text{MRCI} & & \text{FLHA} & \\ \{|\Psi_\nu\rangle\} & \overset{U}{\longleftrightarrow} & \{|\Psi_a\rangle\} & \text{correlated states} \end{array}$$

Figure 1: *Relation between the delocalized hole states on the HF level $|\Phi_\nu\rangle$ and the correlated ones $|\Psi_\nu\rangle$, and their localized counter parts $|\Phi_a\rangle$ and $|\Psi_a\rangle$.*

Within our frozen local hole approach we do not follow the above three-step process to construct the correlated local hole states $|\Psi_a\rangle$ but directly generate (as depicted in Fig. 1) a set of *approximate* correlated local hole states (CLHSs) $|\tilde{\Psi}_a\rangle$ by performing separate correlation calculations for each reference state $|\Phi_a\rangle$ during which the hole in the localized orbital $|a\rangle$ is kept frozen. This implies a rather stringent configuration selection where only those configurations are used in which the hole in $|a\rangle$ is maintained. In the case of an CI(SD) calculation (CI with single and double excitations), for example, the approximate localized hole states $|\tilde{\Psi}_a\rangle$ take on the following special form:

$$|\tilde{\Psi}_a\rangle = \alpha_a |\Phi_a\rangle + \sum_{x,v} \alpha^v_{a,x} |\Phi^v_{a,x}\rangle + \sum_{\substack{x,x' \\ v,v'}} \alpha^{v,v'}_{a,x,x'} |\Phi^{v,v'}_{a,x,x'}\rangle \quad . \tag{5}$$

The indices $x, x' \in \{\bar{a}, b, \bar{b}, ...\}$ run over all the remaining valence electrons, with $\bar{a}$ being the electron with opposite spin to the removed electron a, and v, v' denote the electrons in the virtual orbitals. Once suitable cut-off criteria are introduced this directly leads to an $\mathcal{O}(N)$ scaling of the FLHA with the system size. The fact that the configuration spaces for the different hole states $|\tilde{\Psi}_a\rangle$ overlap does not harm the procedure. On the

contrary, it is important to build up the correlation effects in the ultimate, delocalized hole states properly through a suitable mixing of the configurations in the final diagonalization step of the effective Hamiltonian (4),

$$|\tilde{\Psi}_\nu\rangle = \sum_a \lambda_a(\nu)|\tilde{\Psi}_a\rangle \qquad \text{where} \qquad \sum_b H^{\text{eff}}_{ab}\lambda_b(\nu) = \tilde{E}_\nu \sum_b S_{ab}\lambda_b(\nu) \quad . \tag{6}$$

Since the individual approximated CLHSs $|\tilde{\Psi}_a\rangle$ are not orthonormal with respect to each other, a generalized eigenvalue problem (with $S_{ab} = \langle\tilde{\Psi}_a|\tilde{\Psi}_b\rangle$) has to be solved here in order to arrive at the approximate canonical hole states $|\tilde{\Psi}_\nu\rangle$ and the associated approximate hole state energies $\tilde{E}_\nu$.

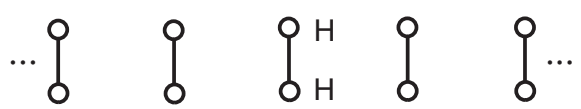

Figure 2: *Geometry of the $(H_2)_n$ ladders. The H_2 bond length is fixed at its molecular value of $R = 0.7417$ Å; the distance between the H_2 units is varied.*

Results

To analyze the frozen local hole approximation (FLHA) we choose two simple model systems, $(H_2)_n$ ladders (see Fig. 2) and linear H–$(Be)_n$–H chains with the Be–H distance being set to 1.37 Å which is the equilibrium distance found in all neutral chains of length n=4–10. *sp* cc-pVDZ basis sets are used for H and Be except for the terminating H atoms in the Be chains which are described by a reduced *s* cc-pVDZ basis [8]. We compare the results of the approximation with the results of the corresponding complete multi-reference CI(SD) (MRCI(SD)) calculation. All calculations were performed with the MOLPRO program package [9]. The computation of the Hartree-Fock ground state of the neutral system $|\Phi_0\rangle$ yields the canonical HF orbitals and energies. The energies of the cationic reference states are extracted from these orbital energies according to Koopman's theorem. Subsequently, the set of valence orbitals are localized by means of the Foster-Boys procedure [10] and used for the construction of the localized hole states $\{|\Phi_a\rangle\}$. Each $|\Phi_a\rangle$ is then separately correlated in a CI(SD) calculation with the above-described configuration selection.

The results for a $(H_2)_3^+$ ladder are shown in Fig. 3, where the total energies of the hole states on the frozen-orbital HF level, the MRCI(SD) level and the FLHA level are depicted in dependence of the distance between the H_2 units. The FLHA curves follow the reference data from the complete MRCI(SD) calculations very closely with the only noticeable slight deviations at the outer left edge of the potential curves. Essentially the same results were obained for the $(H_2)_5^+$ ladder.

In order to make sure that this excellent agreement is not only an artefact of the relatively weak van der Waals binding between the H_2 units, we choose predominantly covalently bound H–$(Be)_n$–H chains as second application. Again we found that for all systems considered, H–$(Be)_3$–H through H–$(Be)_5$–H, the FLHA and the "exact" MRCI(SD) data agree very well. Closer expection of the hole state wavefunctions of the Be_3H_2 system revealed [7] that there are indeed some up to 10% deviations in the CI coefficients of the approximate wavefunctions $|\tilde{\Psi}_a\rangle$ and the complete MRCI(SD)

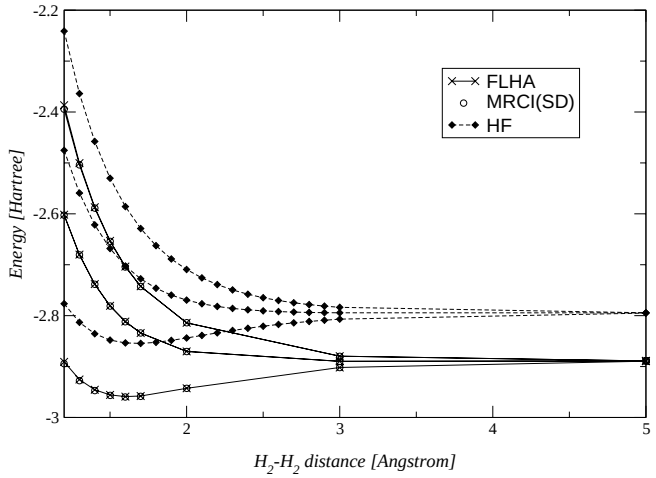

Figure 3: *Total frozen-orbital HF, MRCI(SD) and FLHA energies of $(H_2)_3^+$ as a function of the H_2–H_2 distance.*

wavefunctions $|\Psi_a^{\mathrm{MRCI}}\rangle$, but apparently, these deviations do not have any substantial impact on the total energy of the various correlated hole states.

Perturbative analysis

To understand, why the frozen local hole approximation (FLHA) works so well, we switch from the MRCI level of theory to quasi-degenerate variational perturbation theory (QDVPT) [11] and try to find the leading contributions in both, the "exact" hole state and the approximate hole states according to the FLHA. Within QDVPT the correlated wave functions $|\Psi_\nu\rangle$ of a system are written as

$$|\Psi_\nu\rangle = \hat{\Omega}|\Psi_\nu^{\mathcal{M}}\rangle \tag{7}$$

where $|\Psi_\nu^{\mathcal{M}}\rangle = \hat{P}|\Psi_\nu\rangle$ are the projections of the correlated wave functions $|\Psi_\nu\rangle$ onto the space $\mathcal{M}$ spanned by the local Hartree-Fock hole configurations $\{|\Phi_a\rangle\}$. In first order perturbation theory the wave operator $\hat{\Omega}$ which acts on the "model space" $\mathcal{M}$ and provides the full, correlated wave functions $|\Psi_\nu\rangle$ is given by [11]

$$\begin{aligned}\hat{\Omega} &= \sum_c |\Phi_c\rangle\langle\Phi_c| \\ &+ \sum_c \sum_{a<b,v} |\Phi_{ab}^v\rangle \frac{\langle vc||ab\rangle}{\varepsilon_v - \varepsilon_a - \varepsilon_b + \varepsilon_c} \langle\Phi_c| \\ &+ \sum_c \sum_{a<b,v<w} |\Phi_{abc}^{vw}\rangle \frac{\langle vw||ab\rangle}{\varepsilon_v + \varepsilon_w - \varepsilon_a - \varepsilon_b} \langle\Phi_c| \quad .\end{aligned} \tag{8}$$

Here, we take the zeroth-order Hamiltonian H^0 to consist of the diagonal terms of the Fock operator only, i. e., $H_{ij}^0 = \delta_{ij}\varepsilon_i$ with $\varepsilon_i = F_{ii}$. The perturbation then contains both, the off-diagonal terms $F_{ij} = \langle\varphi_i|\hat{F}|\varphi_j\rangle$, $i \neq j$ of the Fock operator $\hat{F}$ and the usual two- and one-electron contributions $\langle ij||kl\rangle$ and $\sum_a^{\mathrm{occ}}\langle ia||ja\rangle$ from the Møller-Plesset partitioning of the many-body Hamiltonian. Here and in the following, indices a, b, ... are understood to run over occupied localized orbitals while indices v, w, ... run over virtual orbitals. For arbitrary orbitals indices i, j, ... are used. The orbitals $|\varphi_i\rangle$ entering these expressions are the (localized) Hartree-Fock orbitals of the neutral N-electron system.

In the first step of the FLHA, the model space configurations and the excited configurations are restricted to those determinants which already contain a hole in a particular local occupied orbital $|\varphi_h\rangle$, such that the wave operator reduces to

$$\begin{aligned}\hat{\Omega}^{\mathrm{FLH}}(h) &= |\Phi_h\rangle\langle\Phi_h| + \sum_{a\neq h,v} |\Phi^v_{ah}\rangle \frac{\langle vh||ah\rangle}{\varepsilon_v - \varepsilon_a} \langle\Phi_h| \\ &+ \sum_{a<b,v<w} |\Phi^{vw}_{abh}\rangle \frac{\langle vw||ab\rangle}{\varepsilon_v + \varepsilon_w - \varepsilon_a - \varepsilon_b} \langle\Phi_h| \quad .\end{aligned} \tag{9}$$

Only single excitations $|\Phi^v_{ah}\rangle$ and double excitations $|\Phi^{vw}_{abh}\rangle$ with respect to the given local hole configuration $|\Phi_h\rangle$ show up here. Inspection of that equation reveals that these restricted wave operators are precisely the leading terms in the full wave operator $\hat{\Omega}$, in the sense that

$$\hat{\Omega} = \sum_h \hat{\Omega}^{\mathrm{FLH}}(h) + \hat{\Pi} \tag{10}$$

where the remainder

$$\hat{\Pi} = \sum_{a<b,v} \sum_{c\notin\{a,b\}} |\Phi^v_{ab}\rangle \frac{\langle vc||ab\rangle}{\varepsilon_v - \varepsilon_a - \varepsilon_b + \varepsilon_c} \langle\Phi_c| \tag{11}$$

contains all single excitations in which the three occupied spin orbitals $|a\rangle$, $|b\rangle$, and $|c\rangle$ are all *different*, while the leading terms are made up by all those contributions in which two of the hole indices coincide. Thus, up to first order perturbation theory the FLHA can be understood as a simple neglection of all three-distinct-spin-orbital single-excitation contributions to the wave operator $\hat{\Omega}$ and the resulting effective Hamiltonian (for details see Ref. [7]).

A further simplification of the FLHA can be achieved by treating the (N-1)-particle system with a frozen local hole on the Hartree-Fock level only. This has already been done with some success in our "simplified method" to correlation effects in band structures [6]. Orbital relaxation around the *localized* hole is the only effect which can be accounted for in this approach and we want to analyze here, to which extent the correlation effects in the (N-1)-particle system can be mimicked this way.

Removal of an electron from a fixed localized occupied spin orbital $|\varphi_h\rangle$ leads to the following modified Fock operator $\hat{F}^{\mathrm{FLH}}(h)$,

$$\begin{aligned}\langle i|\hat{F}^{\mathrm{FLH}}(h)|j\rangle &= F_{ij} - \langle ih||jh\rangle = \delta_{ij}\,\varepsilon_i + \langle i|V|j\rangle \\ \text{with}\quad \langle i|V|j\rangle &= (1-\delta_{ij})\,F_{ij} - \langle ih||jh\rangle\end{aligned} \tag{12}$$

Up to first order in the perturbation potential V the relaxed Hartree-Fock orbitals $|\tilde{\varphi}_i(h)\rangle$ which result from diagonalizing $\hat{F}^{\mathrm{FLH}}(h)$ under the constraint that $|\tilde{\varphi}_h\rangle$ remains unchanged read

$$|\tilde{\varphi}_i(h)\rangle = \begin{cases} |\varphi_i\rangle - \displaystyle\sum_{j\notin\{i,h\}} |\varphi_j\rangle \frac{\langle j|V|i\rangle}{\varepsilon_j - \varepsilon_i} & \text{for } i \neq h \\ |\varphi_h\rangle & \text{else} \end{cases} \tag{13}$$

and the corresponding Slater determinant becomes

$$|\Phi_h^{\mathrm{SCF}}\rangle = |\Phi_h\rangle + \sum_{a\neq h,v} |\Phi_{ah}^v\rangle \frac{\langle vh||ah\rangle}{\varepsilon_v - \varepsilon_a} + \mathcal{O}(V^2) \quad (14)$$

$$= \hat{\Omega}_{\mathrm{single}}^{\mathrm{FLH}}(h)|\Phi_h\rangle + \mathcal{O}(V^2) \quad (15)$$

where $\hat{\Omega}_{\mathrm{single}}^{\mathrm{FLH}}(h)$ is the restricted wave operator $\hat{\Omega}^{\mathrm{FLH}}(h)$ from Eq. (9) after neglection of all double excitations. Obviously, up to first order, the local frozen hole wave function obtained on the Hartree-Fock level is identical to the single-excitation correlated local hole state $|\tilde{\Psi}_h^{\mathrm{sgl}}\rangle = \hat{\Omega}_{\mathrm{single}}^{\mathrm{FLH}}(h)|\Phi_h\rangle$ of the system.
This result is somewhat surprising, at first glance, because it tells, that what formally looks like pure orbital relaxation around a frozen local *defect*, is actually bare electron correlation. That is not evident, because relaxation around a local hole is clearly distinct from relaxation due to the missing of an electron in a *delocalized* canonical orbital. Particularly in infinite systems the latter does not exist at all. But this result also tells, that performing a Hartree-Fock calculation around a frozen local hole rather than a much more demanding wavefunction-based correlation calculations is a rather promising approximation.

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3.5 *Ab Initio* Method for Excited States in Solids: Correlation Corrections to the Band Structure of Oxides

L. Hozoi, U. Birkenheuer and P. Fulde

Introduction

Advanced quantum chemical methods [1,2] allow to construct approximate wave functions for any system in mind at different levels of sophistication and accuracy and thus

offer a systematic route to converged results. Such wave-function based calculations can be routinely performed nowadays for small and medium size molecules. Algorithms to treat electron correlation effects in *infinite* periodic systems, however, have only been developed recently. The use of well-localized real space orbitals and local correlation schemes is crucial for these algorithms, because it not only allows a reduction in the computational effort, it also guarantees a more transparent physical picture of the effects and properties under investigation. Local correlation methods such as the incremental scheme [3,4] and the local Hamiltonian formalism [5–9] were applied in our group to the rigorous determination of both ground state and excited-state properties of infinite systems.
A new *ab initio* wave-function based method to study the electron correlation effects on band structures of oxide systems will be presented here. It is based on the "simplified method" first introduced by Fulde and Stoll [10] and analyzed in more detail by Pahl and Birkenheuer [11]. We choose bulk MgO as a prototype closed-shell ionic oxide, a realistic but at the same time still relatively simple insulating system, to prove the abilities of that new approach. We will identify the major correlation induced corrections to the valence *and* conduction bands of MgO and the closing of the Hartree-Fock band gap due to electron correlation.

Computational approach
The preceding periodic HF calculations for crystalline MgO were carried out with the CRYSTAL package [12]. Gaussian-type basis sets of triple-zeta quality were chosen from the CRYSTAL library, 8-511G for the Mg and 8-411G* for the more polarizable O ions [13]. For these basis sets the fundamental Hartree-Fock (HF) band gap was computed to 16.20 eV, 8.4 eV larger than the experimental value [14], and a low-laying conduction band complex of mainly Mg $3s$ and $3p$ character could be identified in the HF band structure which is well-separated from all the other conduction bands.
The Wannier functions associated with the HF valence and low-laying conduction bands were determined with the Wannier-Boys localization module [15] in CRYSTAL yielding s- and p-type Wannier functions for the two oxygen valence band complexes, respectively, and sp^3 hybrids for the conduction bands. The Pipek-Mezey localization procedure [16], as implemented in the MOLPRO package [17], was employed to separate these hybrids after projection onto the basis functions of the finite embedded cluster $\mathcal{C}$ into s- and p-type functions. The resulting virtual Wannier functions in the central, so-called active region $\mathcal{C}_\mathcal{A}$ of the embedded clusters are shown in Fig. 1. The norm of these projections is typically 99% and never below 98.5% of the original Wannier functions.
For the construction of the variational space to be used in the subsequent correlation and/or self-consistent-field (SCF) calculations we follow the strategy of a local modelling of the correlation hole proposed by Stollhoff and Fulde [18], and promoted further by Pulay and Saebø [19]. To this end, so-called projected atomic orbitals (PAOs) are constructed from the Gaussian basis functions associated with the active region $\mathcal{C}_\mathcal{A}$ of the embedded clusters by our CRYSTAL-MOLPRO interface [20] which also delivers the appropriate embedding potential.

Correlation corrections
Renormalization effects due to many-body interactions beyond the independent-particle approximation are handled as described in Refs. [10, 11] (see also report 3.4).

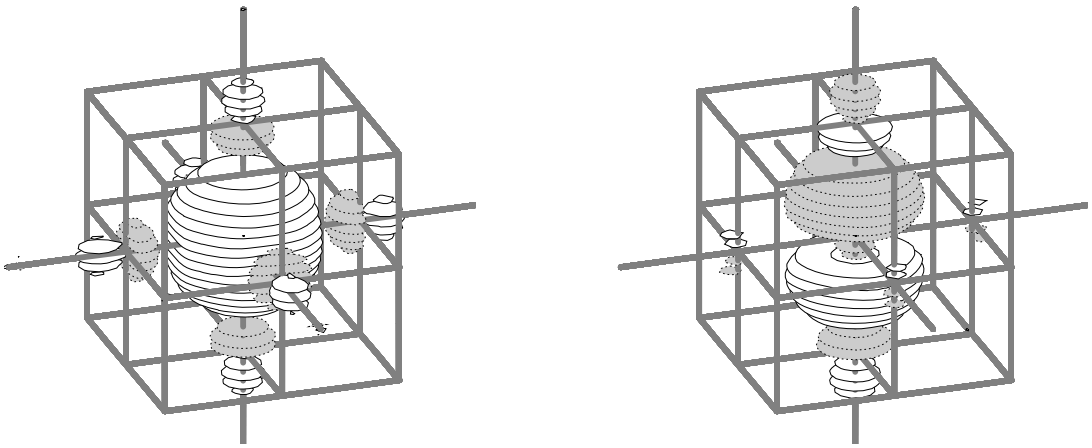

Figure 1: *Plot of the virtual Mg 3s- and 3p-like Wannier orbitals after projection onto a $Mg_{19}O_{14}$ cluster. They exhibit substantial weight at the neighbor oxygen sites.*

Relaxation and polarization effects in the immediate neighborhood of a localized oxygen *hole* were computed by separate restricted open-shell HF (ROHF) calculations on $O_{39}Mg_{30}$ clusters. The active region $\mathcal{C}_\mathcal{A}$ of this cluster contains the central $2p^5$ (or $2s^1$) O^- ion, the six adjacent Mg ions, and four of the twelve O^{2-} ligands in the next coordination shell in a planar configuration. All other ions of the cluster belong to the so-called buffer region $\mathcal{C}_\mathcal{B}$ which solely serves to improve the representation of the tails of the orbitals in the active region. The on-site relaxation effect is quite large, more than 2 eV, but there are also substantial relaxation/polarization effects due to the first oxygen neighbors. The values obtained for four planar O^{2-} ligands were multiplied by three in Table 1 to obtain an estimate of the effect of all twelve first oxygen neighbors. The correctness of this approach has been checked with smaller basis sets.
The low-energy *conduction* band states imply Mg $3s^1$ and $3p^1$ electron configurations. The ROHF calculations were performed on a $Mg_{19}O_{38}$ cluster with a MgO_6 kernel as active region. The on-site relaxation effects associated with the localized Mg $3s^1$ or $3p^1$ electron addition states turned out to be vanishingly small, while the relaxation effects at the adjacent O sites induce energy shifts of 0.80–0.85 eV.
It is known that differential correlation effects related to the existence of a different number of electrons in the N electron ground state and in the $(N\pm1)$ electron addition or electron removal excited states may be important. We investigated such correlation

ΔH_{ii}	O $2s$	O $2p$	Mg $3s$	Mg $3p$
On-site orbital relaxation	-2.64	-2.04	—	—
Nearset-neighbor orbital relaxation	-1.23	-1.20	-0.81	-0.84
Long range polarization	-1.80	-1.80	-2.25	-2.25
Total	-5.67	-5.04	-3.06	-3.09

Table 1: *Correlation induced corrections ΔH_{ii} to the diagonal elements H_{ii} of the effective Hamiltonian for the valence O $2s$, $2p$ and conduction Mg $3s$, $3p$ states. All numbers are in eV. Negative corrections induce upward shifts in the valence and downward shifts in the conduction bands.*

effects for the N and $(N-1)$ electron states by multi-reference CI (configuration interaction) calculations on $O_{19}Mg_6$ clusters with a O_1 kernel. We found that for a $2p$ hole the correction to the on-site matrix element of the Hamiltonian is $\Delta H_{ii} = +0.85$ eV, resulting in a downward shift of the $2p$ valence bands. A similar mechanism will determine an energy lowering of the $(N+1)$ electron addition states with respect to the N electron ground state, leading to a lowering of the conduction bands as well, and partial cancellation of these two corrections will occur, but the corresponding CI calculations for the N and $(N+1)$ electron states are not yet finished.

The data listed in Table 1 indicate that the on-site orbital relaxation and relaxation and polarization effects at the nearest oxygen sites in the presence of an extra electron or an extra electron hole add up to a reduction of the HF band gap of about 4.05 eV, that is, more than 45% of the difference between the HF and experimental values. Substantial corrections are therefore also expected from long range polarization effects. We employ the model of a dielectric medium to estimate these long-range relaxation effects,

$$\Delta H_{ii} = -\frac{\epsilon_0 - 1}{2\epsilon_0}\frac{e^2}{R_i} \quad , \tag{1}$$

where ϵ_0 is the static dielectric constant of the medium (9.7 for MgO) and R_i is the radius up to which the polarization effects have already been accounted for. We identify R_i with the mean radii of the first and second oxygen coordination shells, i.e., $(a\sqrt{2}/2+a)/2$ for the hole states and $(a/2+a\sqrt{3}/2)/2$ for the conduction band states where a is the lattice constant of MgO, and arrive at -1.80 eV for the O bands and -2.25 eV for the Mg bands. All together the polarization and relaxation effects in MgO lead to a reduction of the HF band gap of 8.1 eV, which is about 95% of the difference between the HF and experimental values.

We now turn to the correlation corrections to the off-diagonal elements H_{ij} of the effective Hamiltonian, the so-called hopping terms. To obtain the hopping term on the Hartree-Fock level 2×2 CI calculations in terms of frozen HF Wannier orbitals are performed,

$$H_{ij}^{\mathrm{HF}} = \langle \Phi_i^{N\mp1} | \hat{H} - E_0^{\mathrm{HF}} | \Phi_j^{N\mp1} \rangle \tag{2}$$

where $\Phi_i^{N-1} = \hat{c}_i \Phi^N$ and $\Phi_i^{N+1} = \hat{c}_i^\dagger \Phi^N$ are the frozen Hartree-Fock orbitals hole and electron addition states, respectively, and E_0^{HF} is the Hartree-Fock ground state energy of the neutral N electron system. To account for the polarization and relaxation effects

	t_{ij}^{HF}	Δt_{ij}
1NN:		
$3s - 3s$	0.41	0.01
$3p_{x(y)} - 3p_{x(y)}$	0.66	0.03
$3p_{x(y)} - 3p_{y(x)}$	0.72	0.05
$3p_z - 3p_z$	0.13	0.00
2NN:		
$3s - 3s$	0.36	0.01
$3p_x - 3p_x$	0.77	-0.03
$3p_{y(z)} - 3p_{y(z)}$	0.13	-0.01

Table 2: *The effective first (1NN) and second (2NN) nearest neighbor hopping terms* $t_{ij} = (H_{ij} - H_{ii}S_{ij})/(1-S_{ij}^2)$ *of energetically degenerate states with* $H_{ii} = H_{jj}$ *on the Hartree-Fock level (second column) and the correlation induced corrections* Δt_{ij} *(third column) for the low-lying Mg 3s and Mg 3p conduction band states (in eV).*

in the neighbor ligands the orbitals entering the $(N\mp1)$ particle wave functions are fully relaxed before they are used as non-orthogonal wave functions $|\Psi_i^{N\mp1}\rangle$ and $|\Psi_j^{N\mp1}\rangle$ in the 2×2 CI calculation.

For energetically degenerate states the resulting effective hopping term t_{ij}, which is defined as half of the energy separation between the two CI roots, is given by $t_{ij} = (H_{ij} - H_{ii}S_{ij})/(1 - S_{ij}^2)$ where S_{ij} is the overlap between the non-orthogonal wave functions. In the Hartree-Fock case where $S_{ij} = 0$ this reduces to $t_{ij} = H_{ij}$. The effective first and second nearest neighbor hopping terms of the more diffuse conduction band states are summarized in Table 2. Quite large $Mg_{28}O_{36}$ and $Mg_{36}O_{47}$ clusters were designed for that purpose for the first and second nearest neighbor hopping terms, respectively, with a Mg_2O_6 kernel for the former and a Mg_2O_9 kernel for the latter case.

The results listed in Table 2 show that optimizing the $(N+1)$ wave functions has only a minor effect (a few percent at most) on the electron hopping terms. No simple trend is discernable and some of the effective hoppings are slightly enlarged by taking into account short range relaxation and polarization effects and some are reduced. The main finding, however, is that all of the off-diagonal corrections are quite small and thus correlation induced changes in the width and the shape of the lower conduction bands are all very little in the case of MgO. A very different situation occurs in strongly correlated oxides such as the layered cuprates, where the existence of an antiferromagnetic spin background determines a reduction of the effective quasiparticle hoppings by a factor of four [21]. Regarding the longer-range polarization effects, we expect that their influence on the hopping terms is negligible.

The same kind of analyses was applied to the valence bands of MgO (not shown). Correlation induced changes in the range of 0.00–0.07 eV were found which is only slightly larger than the corrections for the conduction bands. Hence, for simple oxides such as MgO one has to conclude, that electron correlation essentially only shifts the energy bands, without any substantial change in the width or the shape of the bands. The reduction of the band gap due to electron correlation is reproduced quite nicely, leading to a band gap of 8.10 eV for MgO compared to the experimental value of 7.8 eV [14].

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3.6 Precursors of Extreme Events

Sarah Hallerberg, Holger Kantz

Not only after the December 2004 tsunami and the August 2005 hurricane humans have been realizing the vulnerability of our civilization by extreme events. Extreme events, as they are treated by the mathematical theory of extreme value statistics [1], are defined by some quantity (such as river level, wind speed, seismic activity) overcoming some pre-defined threshold. Extreme value statistics enables one (assuming stationarity and independence) to extrapolate from the frequency distribution of observed event sizes to event magnitudes one has never seen so far. Hence, the average probability of an event of given size can be obtained. However, a specific warning of a forthcoming event cannot be based on these results.

Unlike in weather forecasts, many phenomena lack a deterministic modelling or the proper knowledge of input data which might be needed for specific forecasts. In such cases, time series analysis is a promising alternative. Past records of a suitable quantity are used to learn about a given phenomenon in terms of time dependent structures and correlations.

Precursors of extreme events – Suppose that our knowledge about some phenomenon is limited to a time series S which is the time ordered sequence of measurements equidistant in time, $\{s_k\}$, $k = 1, \ldots, N$. On the basis of this time series, we define *events*. We convert the observed data into the event time series e_k, where $e_k = 1$ if an event takes place at time k and $e_k = 0$ otherwise. We study two types of events, namely threshold crossing of the observable itself, i.e., $x_k > \eta$, or threshold crossing of its increment, $x_{k+1} - x_k > \eta$. The first case is the framework of extreme value

statistics. The second is relevant in many applications, such as stock markets, where a crash is a large negative increment, wind power conversion, where a wind gust acting on a wind turbine is a large positive increment, and highway traffic flow, where the sudden reduction of velocity might cause car accidents.
In order to predict whether at time $k+1$ an event will take place, given past observations until time k, one could employ any time series prediction scheme for a forecast $\hat{s}_{k+1}$ of the measurement s_{k+1} and then compare $\hat{s}_{k+1}$ (or the increment with respect to s_k) to the threshold value η in order to predict the value $\hat{e}_k$, whether an event will follow or not. Corresponding prediction schemes might be linear [2] or nonlinear [3]. Their mutual drawback is that such a single valued prediction does not allow to determine probabilities for the event to follow, and that such predictions $\hat{s}_{k+1}$ are designed to minimize the root mean squared prediction error with respect to s_{k+1}, whereas for the optimal prediction of the events to follow we should minimize the classification error. The classification task is solved by the definition of precursors, which are quantitatifiable patterns on the time series. Observing that the time series elements $s_k, s_{k-1}, \ldots$ comply with a precursor with a given accuracy, one predicts the event to follow. Such approaches have been used in the prediction of epileptic seizures [4], of earthquakes [5], and of stock market crashes [6]. In this paper, we restrict precursors to being specific values of the observable itself, i.e., a precursor is an m-dimensional vector $\mathbf{x}_{pre} = (x_1, \ldots, x_m)$ with m being a parameter. Assuming that the time series S is a realization of a time discrete Markov process of order m, the maximal amount of (probabilistic) information which is available for predictions of events is the joint probability $p(s_k, s_{k-1}, \ldots, s_{k-m+1}, e_{k+1}) =: p(\mathbf{s}, e)$, where due to stationarity the time index k can be dropped and the index of e is always assumed to be one time step ahead of the time index of $\mathbf{s}$. Any precursory structure hence has to be extracted from this joint probability. In data analysis, the additional task is to estimate of this probability density from the observed time series data.
Construction of precursors – There are two competing ways to construct precursors, which both have been applied frequently, using either the *a posteriori PDF* or the *likelihood* [7]. If one constructs precursors in a retrospective way, one defines the precursor as the average structure preceeding events $e_k = 1$. Since the signals $\mathbf{s}_k$ before individual events $e_{k+1} = 1$ will follow the m-dimensional conditional probability distribution $p(\mathbf{s}|e = 1)$ (*a posteriori PDF*), optimal prediction of events will be achieved when defining the precursor by the maximum of this distribution, or, in the case of a multimodal distribution, defining several precursors by taking all maxima exceeding a given threshold. The rate of alarms is controlled by a threshold probability p_t such that an event $\hat{e}_{k+1} = 1$ is predicted for every k with $p(\mathbf{s} = \mathbf{s}_k|e = 1) > p_t$.
The alternative strategy takes those structures $\mathbf{s}$ for precursors for which the *likelihood* of an event to follow $p(e = 1|\mathbf{s})$, is maximal with respect to $\mathbf{s}$. Again, this probability density can have several maxima in $\mathbf{s}$, and again the introduction of the alarm volume leads to a simple threshold scheme: For a defined threshold probability p_t, one predicts $\hat{e}_k = 1$ iff $p(e = 1|\mathbf{s} = \mathbf{s}_k) > p_t$. If $\hat{p}(e = 1|\mathbf{s} = \mathbf{s}_k) > p_t$, an alarm is given. Both approaches were implemented as numerical algorithms on time series data which also estimate the relevant probabilities.
Quantification of the classification error – In order to compare different prediction schemes, their performance must be assessed in a quantitative way. While the total number of alarms is controlled by p_t, there are two different types of misprediction:

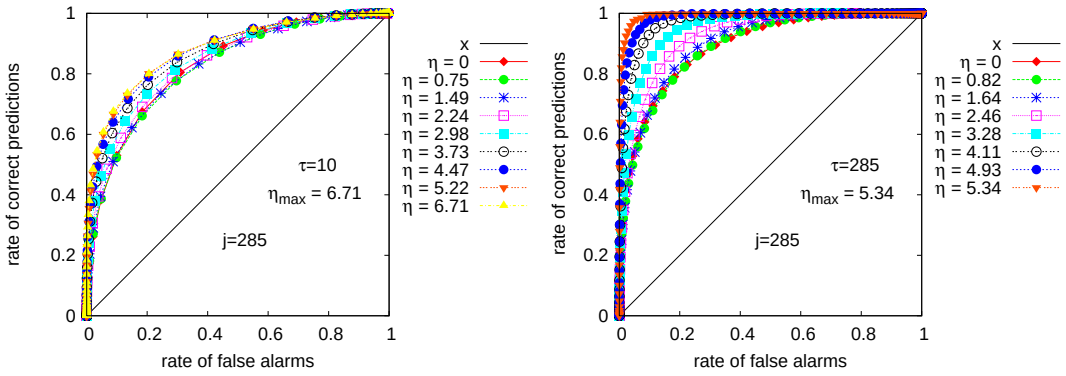

Figure 1: *The ROC curves for predictions of extreme positive increments, $v_{k+\tau} - v_k > \eta$, in free jet turbulence data, based on precursors defined by the likelihood. The left panel shows the exponential regime: The quality of the predictions is almost independent of the event size. The right panel shows the Gaussian regime, where larger events are clearly better predictable.*

false alarms and unpredicted events. The ROC (receiver operating characteristics) [8] statistics is a well established tool in signal processing in oder to quantify these classification errors. It compares the hit rate to the false alarm rate. A given prediction scheme is the better, the more the hit rate exceeds the false alarm rate. A random predictor without any predictive skill generates an equal rate of hits and false alarms, regardless of how many alarms are given, thus corresponding to the diagonal in a ROC plot.

Precursors and their performance – In [10,11] we study in detail the performance of the two different precursors on an auto-regressive model of order 1, AR(1), $s_{n+1} = as_n + \xi_n$. The advantage of choosing such an unrealisticly simple time series model lies in the fact that all relevant expressions can be evaluated analytically, so that the numerical observations can be traced back to properties of the process. There are two essential results. Firstly, choosing precursors through the *a posteriori* conditional PDFs is inferior to their definition through the likelihood. This is essential, since almost all machine learning algorithms rely on posterior PDFs. Secondly, the prediction skills of the precursors (both strategies) are in the examples of the AR(1) process the better the higher the threshold η used to define the events. In other words, in this examples one finds that the more extreme an event is, the better it is predictable on average. In the following we will refer to this effect as the *positive size dependence* of the quality of a prediction. We found the same properties numerically for wind speed data.

When are the more extreme events better predictable? – The slope of the ROC-curve at the origin can be used as summary index of the ROC curve, i.e., it quantifies the behaviour of the ROC plot in the region of small false alarm rates, which is of particular interest. For sufficiently simple processes we computed this slope analytically to some approximation. The results indicate that the size dependence of the quality of a prediction is influenced mainly by the probability distribution function (PDF) of the underlying stochastic process [11]. We investigated this phenomenon in detail for threshold crossing in sequences of gaussian, exponential and power-law distributed random numbers. The slope of the ROC-curve allows us to determine a criterion for the PDFs of the given process which tells us whether or not larger events

are better predictable. In the gaussian case the criterion reproduces the positive size dependence, found before for the AR(1)- process. In contrast to that the quality of the prediction decreases for larger events (*negative size dependence*) in sequences of power-law distributed random numbers. For sequences of exponential distributed random numbers the size dependence is sensitive to the choice of the precursor. It is negative for precursors constructed through the posterior PDF and almost neutral for precursors constructed through the likelihood.
Furthermore, we tested the criterion on experimental data measured in isotropic turbulence in a free jet experiment [9]: Velocity increments $v_{t+\tau} - v_t$ taken over short time intervals τ have an almost exponential distribution, whereas when taken with large τ their distribution is close to Gaussian [9]. Correspondingly, extreme events in the latter case are the better predictable the larger they are, whereas this is not the case for small τ (see Fig.1) [11].
Conclusions – Our work aims at a better understanding of the role of precursors of extreme events. As first steps, we have studied simple time series models. Currently, three main results exist: Percursors defined by the *likelihood* are superior to precursors defined by *a posteriori* distributions. In some processes, extreme events are the better predictable the larger they are. For this latter property we found and tested a condition to the stochastic process to be fulfilled. With a three months DAAD-fellowship, Sarah Hallerberg joined the group of Lenny Smith in London to study extreme events and precursors in meteorological data. From this we expect to learn about the validity of these results for processes with complicated temporal correlations and non-stationarities.

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3.7 Bouncing-Ball Orbits in Circular-Like Billiards

Eduardo G. Altmann and Holger Kantz

By linking dynamics to geometry billiards provide easily understandable examples of dynamical systems. The composition of a few simple curves already provides a complete picture of nonlinear Hamiltonian dynamics, where important fundamental questions such as the ergodic hypothesis were investigated [1]. Billiards are also keystone elements in different experiments and applications on mesoscopic (quantum dots, optical wave guides, lasers) and macroscopic (acoustic) scales [2, 7, 9, 12].

The use of simple curves to define a billiard introduces special symmetries in the system. Indeed, the most prominent billiards are composed of straight lines and arcs of circle. One consequence is the existence of *bouncing-ball orbits* colliding perpendicularly to parallel walls, e.g., in the Sinai [Fig. 1(a1)] and stadium [Fig. 1(a2)] billiards. The existence of such orbits prevents these systems from being fully chaotic (hyperbolic) despite being ergodic. It is widely recognized that the bouncing-ball orbits have a major influence on the decay of correlations [15], transport [15], and spectral properties [2]. It is usually argued that such orbits are exceptional (non-generic) since they arise from the special symmetry of the parallel walls and are destroyed by small perturbations of the billiard.

Contrary to this expectation, we show that orbits equivalent to the bouncing-balls appear in many different billiards possessing less obvious symmetries. The reason is that important classes of chaotic billiards can be obtained as spatially *localized* modifications of integrable ones, what is different from the usual KAM-like perturbations considered to be typical in Hamiltonian systems. For concreteness, we report results in mushroom and annular billiards, which are representative examples of modified circular billiard and where typically an infinite number of different families of bouncing-ball orbits exist. Such orbits have a strong effect on the decay of correlations and survival probability (in open systems) of chaotic trajectories for which a universal scaling exponent is deduced and verified numerically. Effect of such orbits in the quantum/wave mechanical version of such billiards is briefly discussed.

The distinguished feature of the bouncing-ball orbits is their marginal or neutral linear-stability. We consider 2-D billiards as systems defined by closed hard-walls inside which a pointwise particle experiences elastic collisions. In the discrete time system obtained applying the usual Poincaré section, marginal stability means that the eigenvalues λ_i of the Jacobian matrix of the dynamics are degenerate $\lambda_1 = \lambda_2 = 1$. Therefore perturbations grow/shrink linearly (as opposed to exponentially) in time[1]. In integrable systems (e.g., rectangular and circular billiards) these orbits are simply the trajectories with rational rotation number. They are surrounded by trajectories with irrational rotation number being thus stable. More interesting is the case of orbits with marginal stability embedded in a chaotic component, in which case they are marginally *unstable* periodic orbits (MUPOs). The existence of MUPOs is well known for the case of billiards with

[1] In the example of the billiards illustrated in Fig. 1(a,b) small perturbations of the collisional angle (with respect to the normal vector) $\theta = \theta_0 + \varepsilon$ lead to constant increment in time n of the displacement $\Delta\phi$ between the position of collision of the periodic orbit ϕ_0 and of the perturbed one $\Delta\phi_n = v_\varepsilon n$, with $v_\varepsilon \sim \varepsilon$. A perturbation in ϕ, maintaining $\theta = \theta_0$ constant, generically leads to an equivalent periodic orbit, what shows that marginally stable orbits usually appear as one-parameter families.

parallel walls (the bouncing-ball orbits mentioned above). We have reported in a previous publication the existence of such orbits for some parameters of the mushroom billiard [3] and more recently shown that an infinite number of such orbits typically exists in annular billiards [5, 6]. Our simple but relevant observation here is that such orbits exist whenever the dynamics of an integrable billiard is modified locally.

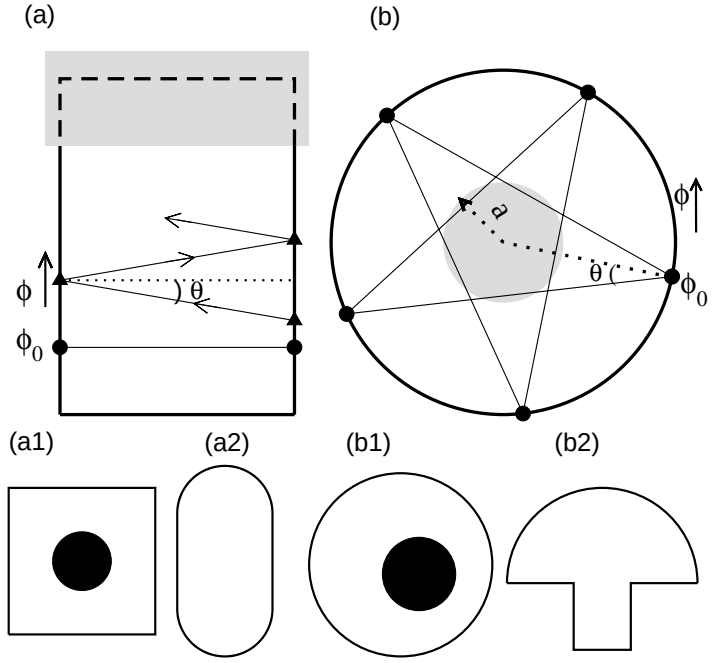

Figure 1: *Billiards with (a) parallel walls and (b) circular components. Periodic orbits indicated by •'s have marginal stability. We assume that in the gray regions the dynamics is defined in such a way that chaotic motion is possible. Examples of billiards with MUPOs: (a1) Sinai, (a2) stadium, (b1) annular [7], and (b2) mushroom [13].*

As concrete examples of the class of systems we are referring to, consider the four well-known billiards depicted in the lower part of Fig. 1. All of them can be obtained by redefining the dynamics in the gray region of the integrable billiards in Fig. 1(a,b). From a rectangular billiard [Fig. 1(a)] one obtains the Sinai billiard [Fig. 1(a1)] by inserting an inner circular scatterer and the stadium billiard [Fig. 1(a2)] by introducing a circular concave border. Similarly, from a circular billiard [Fig. 1(b)] one obtains the annular billiard [Fig. 1(b1)] by placing an eccentric circular scatterer and the mushroom billiard [Fig.1(b2)] by inserting a straight "hole" (see Refs. [3, 14]). The families of MUPOs are composed by: the orbits that bounce only in the rectangular walls in the first case and, in the second case, by the orbits that do not collide with the introduced obstacles (scatterers or holes) but that cross the circle of radius a being thus outside the regular region (the so-called whispering gallery) and inside the chaotic component [$a < R$ depicted in Fig. 1(b) is the radius of the smallest circle that incorporates all inserted obstacles]. It is evident that the procedure described above can be repeated for other integrable billiards and different obstacles or localized modifications.

It is interesting to compare the approach mentioned above of *localized* modifications of integrable billiards to the case of small *global* perturbations, as obtained, e.g., by applying a small magnetic field [4]. In this case the KAM theory [2] shows that most of the

[2]KAM theory is not strictly valid for billiards since the hard walls correspond to singular potentials. Nevertheless, in many billard systems the numerically observed scenario is in agreement with KAM predictions.

quasi-periodic orbits survive with only slight deformations, while all marginally stable periodic orbits disappear. Exactly the opposite happens for the localized modifications considered here: a wide range of quasi-periodic orbits disappear but there are families of periodic orbits with marginal stability that survive by avoiding collision with the introduced obstacles. In the case of circular-like billiards the obstacles lead to a sharp border between a regular and a chaotic component[3]. Inside the chaotic component no previous quasi-periodic orbit survive, while we have shown that an infinite number of different families of MUPOs typically concentrate close to the regular component [5,6]. We briefly mention next two of the most important consequences of the existence of families of MUPOs in a given system.

Trapping of trajectories:

When chaotic trajectories approach the families of MUPOs they stick close to them for a very long time performing an almost periodic motion. This stickiness phenomenon has a strong effect on the main dynamical properties of the chaotic trajectories, such as the decay of correlations and transport properties [5]. Based on previous results for the Stadium billiard [15], we have shown in Ref. [4] that the survival probability of an ensemble of trajectories close to a family of MUPOs decays asymptotically as

$$\rho(t) \sim t^{-\gamma} \text{ with } \gamma = 2. \tag{1}$$

This scaling behavior was numerically obtained in mushroom billiards [3], annular billiards [5][4], and piecewise-linear area-preserving maps [4]. This statistics is asymptotically equivalent to the survival probability mentioned above (see Ref. [4,5] for details). More generally, families of MUPOs and thus the scaling exponent of Eq. (1) appear in different systems showing sharply divided phase space, i.e., when the regions of regular and chaotic motion are separated by a simple curve [4]. This scaling has to be compared with the usual mixed phase space where an hierarchy of islands-around-islands and cantori exist in the phase space and typically it is observed that $\gamma < 2$ in Eq. (1). In the case of quantum and classical scattering in billiards with MUPOs one should expect a similar scaling for long times and regularities in the short time escaping rates (echoes) [3, 14].

Quantum billiard

Periodic orbits provide the semiclassical link between the classical and quantum dynamics [16]. Two aspects of the MUPOs described above make such orbits distinguished among all periodic orbits inside the chaotic component: (i) their marginal stability; (ii) the appearance in one parameter families. Recent microwave experiments designed to investigate this point have confirmed this semiclassical expectation by showing that MUPOs are indeed observed in the quantum spectra. One length spectrum obtained in a microwave cavity with the shape of an annular billiard is shown in Fig. 2 [6].

[3]MUPOs appear naturally also in piecewise linear maps with this property [4].

[4]Annular billiards may show additional KAM islands apart from the whispering gallery, in which case this exponent is reduced $1 < \gamma \leq 2$.

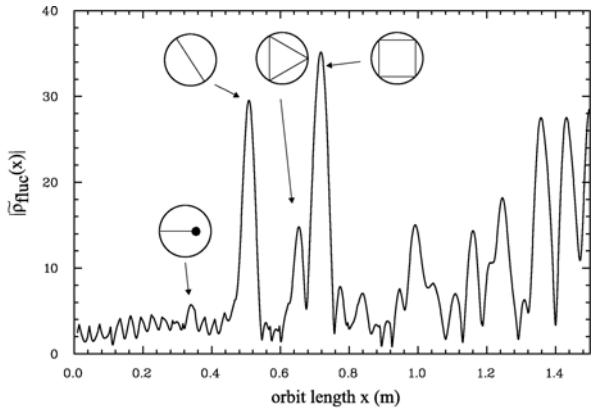

Figure 2: *Experimental length spectrum obtained in a microwave annular billiard with* $\delta/R = 0.48$ *and* $r/R = 0.12$*, where* $R = 0.125m$ *[6]. The peaks at* $x = 0.5$ *m,* 0.63 *m, and* 0.71 *m correspond to the diameter, triangular and rectangular orbit, respectively. While the two first orbits are inside the chaotic component, being thus MUPOs, the rectangular orbit is inside the whispering gallery being thus stable. The peak at* $x = 0.34$ *m corresponds to an unstable periodic orbit.*

Peaks at lengths corresponding to MUPOs are clearly identified and more pronounced than those corresponding to unstable periodic orbits. Moreover, changing the eccentricity δ/R of the inner scatterer of radius r/R it was verified that their strength (height of the peak in the length spectra) is proportional to the classical number of orbits present in the family [6]. It is well known that bouncing ball orbits in the stadium billiard affect the quantum spectrum [2]. Contrary to this, such results show the influence of the MUPOs orbits in a system with circular geometry and mixed chaotic-regular dynamics.

In general the MUPOs are important for those phenomena occurring in the chaotic component, specially those close to the border to the whispering gallery. In recent theoretical studies and microwave experiments, annular billiards were used to investigate chaos assisted tunneling [11, 12]. It was proved the distinguished role played by the so called "beach region" between the whispering gallery and the chaotic region, where an enhanced tunneling strength was observed. Our results provide a novel characterization of the beach region that is crucial for the formalization of such results.

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3.8 Correlation in Ultracold Rydberg Dynamics

Cenap Ates, Thomas Pohl, Thomas Pattard and Jan M. Rost

Apart from the well known creation of atomic and molecular Bose-Einstein-condensates the experimental realization of ultracold gases has also paved the way for novel dynamics of Rydberg systems whose slow time scales and small energy scales harmonize very well with an ultracold environment. This environment leads almost naturally in many situations to the formation of an ultracold plasma which has interesting properties in itself since it can be strongly coupled [1] and is easily accessible in the laboratory [2]. Another fundamental phenomenon, more related to Rydberg dynamics is the so called dipole blockade [3]. It implies that in an ensemble of cold atoms, ultimately one and only one atom can be Rydberg excited by a narrow banded laser, since the dipole-dipole interaction between the easily polarizable Rydberg atoms shifts the energy for the second Rydberg excitation out of the (laser-)resonance. In other words, correlation between Rydberg atoms prevents their excitation.
In the experiment, the situation is much more complicated through many side effects, e.g., the motion of the atoms or the laser excitation scheme. The latter can have a significant influence on the resulting Rydberg dynamics in the ensemble of cold atoms. And it is exactly the two step excitation scheme (see Fig. 1) used in the Freiburg and Michigan experiments [4, 5] which allowed us to formulate the correlated Rydberg dynamics for a large number of atoms in the ensemble.

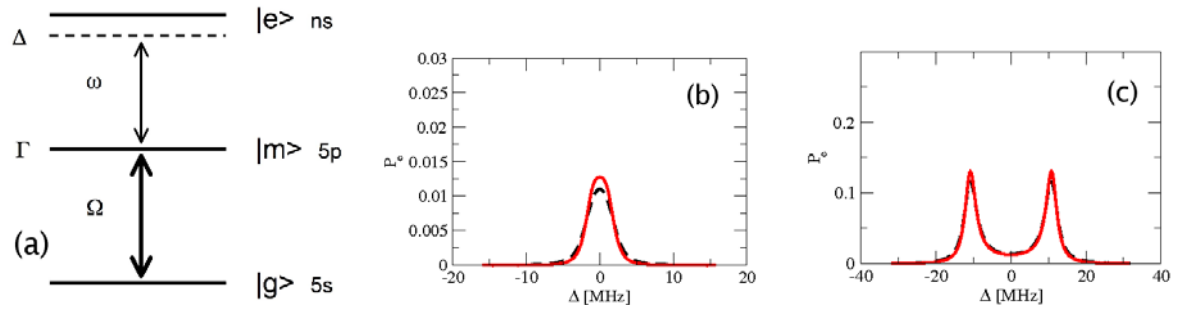

Figure 1: *(a) Sketch of the typical two-step excitation scheme, exemplified with the Rb atom: the lower state $|g\rangle$ and the Rydberg state $|e\rangle$ are optically coupled to an intermediate state $|m\rangle$. The Rabi frequency Ω of the lower transition is much larger than the Rabi frequency ω of the Rydberg excitation. Moreover, the intermediate level $|m\rangle$ decays with a rate $\Gamma \gg \omega$. (b) & (c): The population P_e of $|e\rangle$ according to (1) (solid) and the optical Bloch equation (dashed) for a laser pulse of length $\tau = 0.5\mu s$ and $\Gamma = 6\,MHz$. The other parameters are (in MHz) $(\Omega, \omega) = (4.0, 0.2)$ for (b) and $(\Omega, \omega) = (22.1, 0.8)$ for (c).*

Clearly, this must go hand in gloves with approximations since a fully coherent wavefunction of N atoms with the minimum of two states per atom (ground and excited) would require 2^N states. With a volume of only 5 atoms in each dimension one arrives with $N = 125$ already at 10^{38} states while about 10^9 states can be handled on a good PC.

The approximation we have formulated reduces the optical Bloch equation for the Rydberg excitation in the single atom three-level systems (see Fig. 1) to a rate equation of an effective two level system, whose solution for the Rydberg population P_e reads

$$P_e(\tau, \Delta) = P_\infty(\Delta) \left(1 - \exp\left[-\frac{\gamma(\Delta)\tau}{P_\infty(\Delta)}\right]\right), \tag{1}$$

where $P_\infty = P_e(\tau \to \infty, \Delta)$ is the steady-state occupation of $|e\rangle$. For typical Rabi frequencies [4, 5] and pulse lengths of $\tau \geq 0.5\,\mu$s, the excitation is well described by (1) and has the intuitively expected resonance shape with a single peak. However, also a double peak structure with maxima at finite detuning Δ can occur (Figs. 1b&c). The latter is due to the Autler-Townes splitting of the intermediate state $|m\rangle$ under strong driving of the $|m\rangle \leftrightarrow |g\rangle$ transition.

The description by a rate equation eliminates all coherences in the single atom three-level system but subsequently also in the interaction with other atoms in the ensemble. Hence, adding a second Rydberg atom leads merely to an additional (interaction induced) shift δ of the Rydberg level, already shifted by Δ through coupling to the laser (Fig. 1). Proceeding further to the gas, the effective shifts for all atoms at their positions can now be easily determined by creating randomly Rydberg excitations in accordance with the rates in a Monte Carlo procedure. Thereby, one obtains the global fraction of Rydberg atoms in the gas, e.g., as a function of the degree of excitation n (Fig. 2a), in qualitative agreement with the experiment. A similar qualitative agreement [7] has been achieved for the measured [5] counting statistics of Rydberg atoms which shows deviations from a Poisson distribution indicating interaction between Rydberg atoms [8].

However, the peculiar double-peak structure of the Rydberg population (Fig. 1) lead us

to the prediction that apart from an interaction induced blockade of Rydberg excitation, the opposite, namely an interaction induced *anti*blockade may also occur, i.e., an enhancement of Rydberg excitation. This should happen when the interaction shifts the Rydberg energy level out of the (laser)resonance but into resonance with one of the split peaks of P_e in Fig. 1b. This is indeed the case, as Fig. 2b reveals, but only if the atoms are regularly spaced in a lattice. Since the effect is rather robust against lattice defects (Fig. 2b), it should be possible to see it in an experiment, e.g., by creating an optical lattice with CO_2 lasers whose wavelength lead to the appropriate spacing of atoms of about $5\mu m$ [9].
We finally remark that the simple structure of (1) allows one to determine analytically the approximate boundary between blockade and antiblockade regime in the parameter plane of the Rabi frequencies (Ω, ω). In the limit $\omega \ll \Gamma \ll \Omega$, one has

$$\gamma = \frac{\Gamma\omega^2/\Omega^2}{2(1-4\Delta^2/\Omega^2)^2} \qquad P_\infty = \frac{1}{1+8\Delta^2/\Omega^2}\,. \tag{2}$$

From $\partial^2 P_e(\tau,\Delta)/\partial\Delta^2|_{\Delta=0} = 0$ and (2) we obtain a universal condition for the transition from the double to the single peak structure of $P_e(\tau,\Delta)$, which can be written as

$$g_0 = 2\ln(1+g_0) = 2.513\ , g_0 = \Gamma\tau\omega^2/\Omega^2. \tag{3}$$

Hence, for $\Omega \gg \omega$ single and double peak structures, and therefore the blockade and antiblockade regimes, are separated by a linear boundary of $\omega = \alpha\Omega$, where $\alpha^2 = g_0/(\tau\Gamma)$. From (2) one also notes the transient character of the double peak structure which vanishes for long laser pulses. Yet, experimentally accessible parameters, as, e.g., in [4], realize exactly the transient regime and therefore provide the conditions to see the antiblockade.

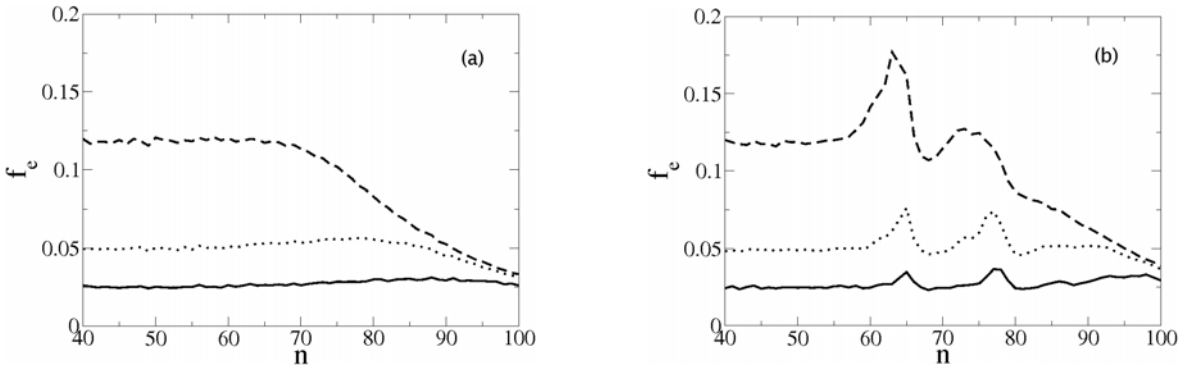

Figure 2: *(a) The fraction of Rydberg atoms f_e as a function of increasing excitation n and for laser pulse lengths of 1μs (solid), 2μs (dotted), and 5μs (dashed) at a gas density of $\rho = 8\cdot10^9 cm^{-3}$, and laser parameters as in Fig. 1c; (b) same as in (a) but for atoms on a cubic lattice of spacing $a = 5\mu m$ and with 20% defects (empty lattice sites). The peaks correspond to enhanced excitation for next neighbors, neighbors on the diagonal and the space diagonal of the lattice (hardly visible).*

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3.9 Classical Ionization Dynamics in Three-Electron Atoms

Agapi Emmanouilidou, Peije Wang and Jan M. Rost

The understanding of atomic structure requires a rigorous quantum mechanical approach which is, however, limited to small systems. Powerful quantum approximations have been developed such has Hartree Fock or densitiy functional theories.
Correspondingly accurate approximations for dynamical processes, e.g., multiple photoionization, involving long range Coulomb forces do not exist. A quasi classical approximation, on the other hand, does not only give quantitative results but offers also insight as was demonstrated for two-electron problems [1], in comparison to experiment and fully numerical quantum calculations.
Several reasons motivated us to tackle the three-electron problem in form of triple photo ionization of lithium quasiclassically: (i) There is good recent experimental data availbale to compare to [2]. (ii) Classical mechanics may offer through the existence of crucial trajectories a way to understand the rather complicated four-body dynamics.
We formulate the ionization quasiclassical single-photon ionization in two steps. First, the initial phase space distribution is constructed based on Wigner functions of the atomic ground state. Since for low and moderate photon energies we consider here, final state (i.e. dynamical) correlation is much more important than initial state (i.e. structural) correlation, we have taken a mean field initial state which greatly facilitates the determination of the Wigner function. Second, the photon is absorbed by one 1s-electron close to the nucleus and the (classical but fully correlated) dynamics of the three electrons is followed in time for a large number of randomly chosen initial conditions, registering all triply ionizing trajectories. This allows one in principle to determine all cross sections [3].
The classical results are rather accurate when held against the experiment or a meanwhile performed quantum calculation for the double differential cross section (see

Fig. 1). This allows us to look in more detail into the classical trajectories to extract a possible general mechanism of multiple ionization in atoms.

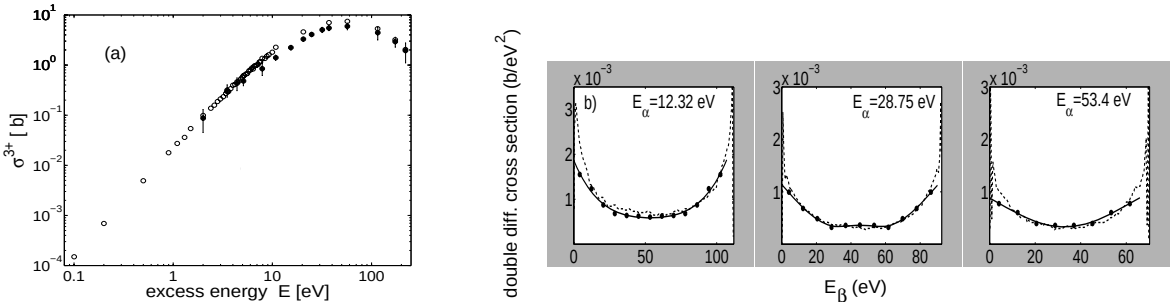

Figure 1: *Triple photo ionization from the ground state of lithium: (a) total ionization cross section from [3] (open circles) and experiment [2] (filled circles) as a function of excess energy E from the triple ionization threshold; (b) double differential cross section for fixed electron energies E_α as a function of electron energy E_β at $E = 115$ eV from [4], dashed line are ab initio results from [5].*

The trajectories are so many (total number of the order of 10^{10}, triple ionizing ones, dependent on the photon energy, between 10^3–10^5) that one needs an automated classification procedure to sort them. We have classified trajectories according to their energy-exchanging collisions among the electrons: clearly, for triple ionization enoung of the energy absorbed by the photo electron must be received by the other two electrons through collisions to enable them to leave the nucleus.

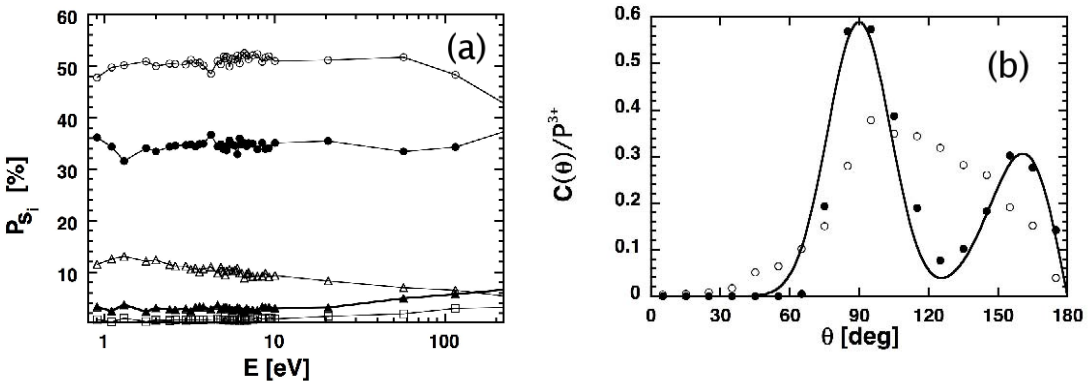

Figure 2: *(a) Percentage of trajectories belonging to collision sequences $s_1 = (12, 13)$ (open cirlces), $s_2 = (12, 23)$ (filled cirlces), $s_3 = (12, 13, 23)$ (open triangles), $s_4 = (23, 12, 13)$ (filled triangles) and others; (b) normalized probability density for the interlectronic angle $C(\theta)$ at $E = 0.9eV$ (open circles show $E = 420eV$ for comparison), the line is a fit, see [3].*

Hence, we have tried to classify all trajectories according to characteristic sequences of inelastic collisions ij of electron i with electron j in the presence of the nucleus, where the third electron is only a spectator during the collision, i.e., the energy in the helium-like sub-Hamiltonian H_{ij} containing the nucleus and the two colliding electrons ij is almost conserverd. More than 90% of all triple ionizing trajectories could be classified according to this scheme and two dominant sequences (accounting for 85%

of the ionizing events, see Fig. 2) emerged [3]. In the $(12, 13)$ sequence s_1 the 1s photo electron (1) collides with the other 1s electron (2) and afterwards with the 2s electron labeled as (3). In the other dominant sequence $s_2 = (12, 23)$, the first collision proceeds in the same way but in the second collision electron (2) shares some of its energy with the 2s electron (3). Secondly, the collision sequences imply in connection with the size of the electronic shells a charateristic time delay of the collisions of about 3 (1s-1s) and 60 attoseconds (1s-2s collision) after photo absorption. Probing these "times of flight" may be possible in the future with attosecond pulse technology [7]. Finally, a very general conjecture follows from these findings: it is not the two-body integrable (hydrogen-like) problem which is the fundamental building block of complex Coulomb problems. Rather it is the three-body (helium-like) system, since the four-body (lithium-like) systems can be decomposed in time into helium-like subsystems (the electron-electron collision hamiltonians). Due to the fact that atomic hamiltonians contain only two-body operators (electron-electron interaction) but not three-body terms or interactions involving even more particles, the decomposition into helium-like subsystems may be universal. We are presently extending our efforts to four-electron dynamics to investigate this question.

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3.10 Molecules in Intense Laser Pulses: S-Matrix Analysis of Ionization and High Harmonic Generation

Arvid Requate, Marcelo Ciappina, Andreas Becker

Of particular interest in the response of molecules to an intense laser pulse are the effects of the extra degrees of freedom, such as alignment, vibration and rotation of the nuclear frame, as well as of the multicenter nature of a molecule, which are absent in the case of atoms. The Intense-field many-body S-matrix theory (IMST) provides a systematic approach to investigate the dynamics of both simple diatomic and complex polyatomic molecules in intense laser fields (for a review, see [1]). In the leading order the S-matrix amplitude represents a direct transition of a single-active electron from the initial bound state to the final field-dressed plane-wave state (or Volkov state). The amplitude therefore takes account of the orbital symmetry and the angular momentum of the initial state, as well as the molecular geometry and the relative alignment of the

nuclear frame to the external field [2]. Recently, we have applied the IMST approach to ionization cum vibrational excitation of diatomics and the saturated ionization of large molecules, such as fullerenes.

Inelastic vibronic ionization of molecules

Ionization of molecules with vibrational excitation of the residual molecular ion (also named inelastic vibronic ionization (IVI)) is often the precursor of fragmentation of a molecule in a laser field. We have developed the IMST of IVI of molecules by incorporating the vibrational wave functions as factors to the electronic wave functions in the initial and final state [1, 3]. The theory is then applied to investigate the distributions of the vibrational states in the residual H_2^+ ion from ionization of the H_2 molecule. The comparison in Fig. 1 shows that the characteristic features of the calculated distributions [3] agree with those observed in a recent experiment [4]. In particular, a shift

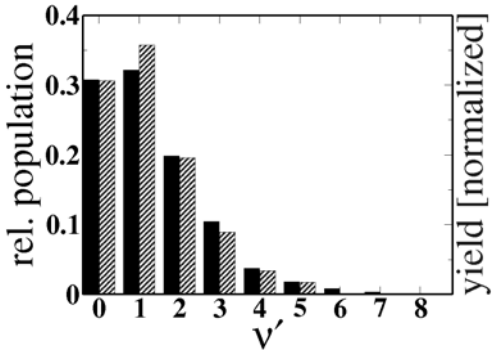

Figure 1: *Comparison of the normalized populations of the vibrational levels in H_2^+ (solid bars) with the normalized experimental yields (taken from [4], hatched bars) obtained in an intense laser pulse at a wavelength of 800 nm, a pulse duration of 45 fs and a peak intensity of $I_0 = 4.8 \times 10^{13}$ W/cm^2 [3].*

of the IVI distributions toward lower vibrational states as compared to the Franck-Condon distributions occurs both in experiment and theory. According to our analysis this unexpected result is due to the strong nonlinear dependence of the transition rates on the transition energy of the process. A Franck-Condon like distribution of IVI would have resulted only if the ionization rates for different inelastic vibrational channels would have been approximately constant. In a strong field however the increase of the transition energy, here towards the higher vibrational levels, results in a strong decrease of the electronic transition rate itself.

Saturated ionization of fullerenes

The fundamental interaction of photons with many-electron systems, such as complex atoms, molecules and clusters, is given by the independent sum of one-body interactions. This simple fact lies essentially behind the dynamical one-electron response of atomic and small molecular systems in laser induced single ionization processes. However, recent experiments on ionization of C_{60} at infrared laser wavelengths have revealed unexpectedly high saturation intensities for the fullerene and its multiply charged ions [5]. This has been interpreted [5, 6] to have shown that the hypothesis of an one-electron response fails for large molecules and to arise from a multielectron polarization effect. But, using the S-matrix theory we have demonstrated [7, 8], that the experimentally obtained saturation intensities can be also well reproduced within a single-active electron approach. This is exemplified in Fig. 2(a) for the results at $\lambda = 1500$ nm.

As can be seen from Fig. 2(b), we have found systematically higher saturation intensities (and therefore lower ionization probabilities at a given intensity) for the four

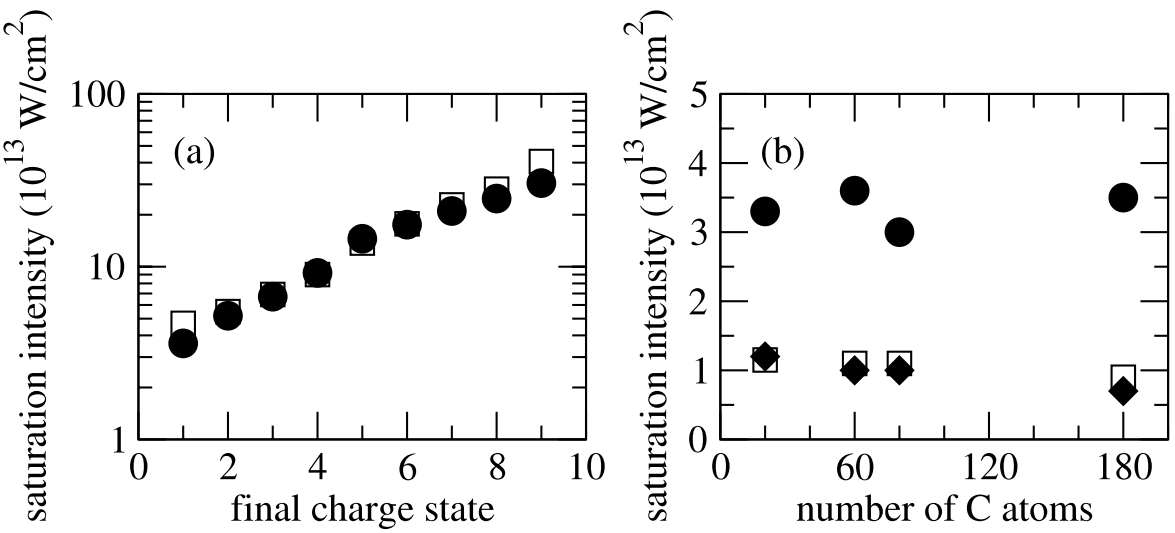

Figure 2: *(a) Comparison of the theoretical predictions for the saturation intensities of the first nine charge states of C_{60} (solid circles, [7]) with the experimental data (open squares, [5]). (b) Comparison of the saturation intensities for the four smallest fullerenes with icosahedral symmetry: full calculations (solid circles), model calculations (solid diamonds) and atomic tunneling predictions (open squares) [7]. All data at a laser wavelength of 1500 nm and a pulse duration of 70 fs.*

smallest fullerenes with icosahedral symmetry (solid circles) than those of the respective hypothetical companion atoms (open squares) with the same ionization potential, calculated using the atomic tunnel model. What is origin of this intriguing observation that fullerenes are harder to ionize than their companion atoms? According to our analysis it is due to the finite cage size and the 'multislit' interference effect between partial waves emitted from the different nuclei of the fullerene [7]. We have tested this explicitely by comparing the results of full calculations with those of fictitious model 'fullerenes', in which the cage size is put to zero and interference effects are omitted. The saturation intensities obtained for these test cases (solid diamonds in Fig. 2(b)) lie invariably below those for the real fullerene counterparts and are very close to those of the companion atoms.

We expect that the multislit interference effect leaves its footprints in photoelectron energy and high harmonic spectra. Preliminary results for the high harmonic yields based on the so-called Lewenstein model [9] show that indeed characteristic interference minima show up at the long infrared wavelengths. This may provide a spectroscopic tool to observe and characterize changes in the nuclear frame of large molecules on an ultrafast time scale.

This work has been done in collaboration with A. Jaroń-Becker (Technical University Dresden) and F.H.M. Faisal (University Bielefeld).

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3.11 A Virtual Laboratory for Ultrashort Processes in Strong Fields

Silvio Baier, Feng He, Arvid Requate, Camilo Ruiz, Andreas Becker

In intense light pulses the laser field strength equals or even exceeds the strength of the Coulomb fields that bind the electrons in the ground state of an atom or molecule. In this non-perturbative intensity regime exact solutions can be made by direct numerical integration of the time-dependent Schrödinger equation of a few-body system. Such simulations distinguish themselves just in the Hamiltonian of the respective Schrödinger equation. This has led us to develop a simulation program, which provides an unified basis for a number of intense field problems. It consists of routines for the propagation of the wavefunction on a grid and the post-processing of the data among others. The result is a virtual laboratory which allows us to analyze and visualize the evolution of ultrashort processes in strong fields. At present any three dimensional Hamiltonian can be efficiently implemented in short time. We have realized applications for the single-active electron dynamics in atoms [1], the control of electron excitation and localization in the dissociating hydrogen molecular ion, and a model for the two-electron dynamics in atoms and molecules [2, 3]. We are planning to implement a parallel version of the program in future. Below we exemplify our numerical studies via the results obtained for the nonsequential double ionization of the hydrogen molecule.

Calculations of double ionization beyond the 1D approximation

Computation of the quantum two-electron problem in a strong laser field constitutes a major challenge, since it involves six dimensions in space and one in time (for a review, see e.g. [4]). For the infrared frequencies of the widely used Ti:sapphire lasers at intensities of up to 10^{15} W/cm^2 it requires an extraordinary amount of computer resources. Under these circumstances, the dimensional reduction of the many-body problem is desirable. The conventional strategy is an one-dimensional approach, in which the motion of each electron is restricted to the axis of a linearly polarized laser field. Recent observations [5] of an emission of electrons out of the polarization plane suggest however that for the ejection of two electrons the 1D approach may be less accurate than in the single-electron case. We have therefore proposed an alternative strategy based on the atomic (or molecular) two-electron Hamiltonian in the field (Hartree atomic units, $e = m = \hbar = 1$ are used) [2]:

$$H(\mathbf{R}, \mathbf{r}, t) = \frac{\mathbf{P}^2}{4} + \mathbf{p}^2 - \frac{Z_{nucl}}{|\mathbf{R} + \mathbf{r}/2|} - \frac{Z_{nucl}}{|\mathbf{R} - \mathbf{r}/2|} + \frac{1}{r} - \frac{\mathbf{P} \cdot \mathbf{A}(t)}{c}, \qquad (1)$$

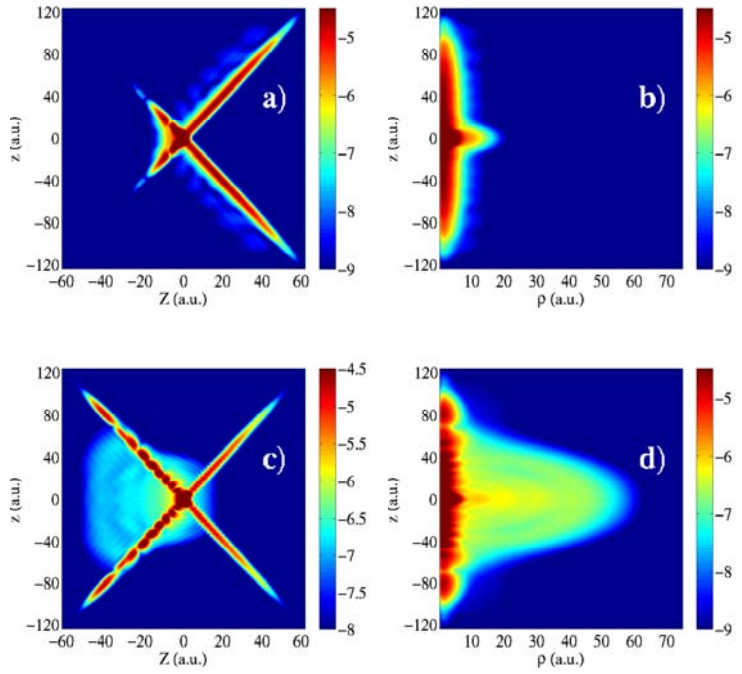

Figure 1: *Snapshots of the probability distributions (on a logarithmic scale) of a hydrogen molecule interacting with a three-cycle laser pulse at a wavelength of 800 nm and a peak intensity of* 2.9×10^{14} *W/cm*^{2} *[3]. A comparison of distributions integrated over* ρ *(left column) and* Z *(right column) at a maximum (upper row) and a zero (lower row) of the field is shown.*

where $\mathbf{R} = (\mathbf{r}_1 + \mathbf{r}_2)/2$ and $\mathbf{P} = \mathbf{p}_1 + \mathbf{p}_2$; $\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$ and $\mathbf{p} = (\mathbf{p}_1 - \mathbf{p}_2)/2$ are the center-of-mass and relative coordinates and associated momenta, respectively. Note that the field couples to the center-of-mass of the two electrons, but not to its relative coordinate. Therefore, for the case of linear polarization it is reasonable to restrict the center-of-mass motion to the field direction (here chosen as the Z-direction), while preserving the three-dimensional character of the electron-electron interaction mediated by the relative coordinate.

We have applied this model to the helium atom [2] and the hydrogen molecule with fixed nuclei along the direction of the field [3]. In these cases the system has azimuthal symmetry about the direction of polarization and the final model Hamiltonian has three degrees of freedom, which we have chosen as $\{Z, \rho, z\}$, where ρ and z are the transversal and longitudinal relative coordinate, respectively. Computations at the Ti:sapphire wavelength and intensities in the range between 10^{14} W/cm^2 and 10^{15} W/cm^2 are performed on a grid using the Crank-Nicholson method.

The numerical results show both in the atom as well as in the molecule two different pathways to nonsequential double ionization. This can be seen by the snapshots of the probability distribution for the molecular case in Fig. 1, taken shortly after a maximum (panels (a) and (b)) and at a zero of the field (panels (c) and (d)) [3]. While the panels on the left hand side show the $(Z - z)$ distributions, integrated over ρ, the panels on the right offer the complementary view of the $(\rho - z)$ distributions, integrated over Z. The diagonals in the $(Z - z)$ distribution represent the z_1 and z_2 axes and correspond to single ionization, while the double ionized population is found in between the z_1 and z_2 axes.

Shortly after the field maximum one sees an elongated structure in the $(Z - z)$ distribution (Fig. 1(a)), which is detached parallel to the z_1 and z_2 axes in the upper and lower triangle of the double ionization region. This contribution is due to field ionization of the previously singly ionized H_2^+ molecular ion. Since both electrons are released to opposite sides of the molecule, the correlation between the electrons is small, as can

be seen from the confinement of the distribution to low ρ in the respective $(\rho - z)$ distribution, integrated over Z (Fig. 1(b)). A thorough analysis has shown that this contribution arises from the excited states of the ion.
In the snapshots taken at the zero of the field one sees in Fig. 1(c) the correlated emission of two electrons at the same side of the core (in $-Z$-direction). In comparison with Fig. 1(b) the two electrons exhibit a strong transversal dynamics in the ρ-direction (Fig. 1(d)). Indeed, we observe that the smaller the interelectron separation along the polarization direction (reflected by the z-direction) the larger is the transversal distance (ρ coordinate) between the electrons. Previous 1D approaches did not take account of this transversal dynamics. Using additional absorbers we were able to confirm that both mechanisms are linked to the return of an initially singly ionized electron to the residual ion, as predicted in the rescattering model [6].
We acknowledge helpful advices of Torsten Goerke (mpi**pks**) during the development of the virtual laser laboratory. The work on the three dimensional model for correlated electron dynamics has been done in collaboration with L. Plaja and L. Roso (Universidad Salamanca, Spain).

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3.12 Experimental Determination of Entanglement with a Single Measurement

Steven P. Walborn, Paulo H. Souto Ribeiro, Luiz Davidovich, Florian Mintert and Andreas Buchleitner

Nearly all protocols requiring shared quantum information [1] for tasks as quantum-teleportation [2], or key-distribution [3], rely on entanglement between distant parties. However, entanglement is difficult to characterize experimentally. All existing techniques, such as entanglement witnesses [4] or Bell inequalities [5], disclose the entanglement of some quantum states but fail for other states: therefore, they cannot provide satisfactory results in general. Such methods are fundamentally different from entanglement measures that, by definition, quantify the amount of entanglement in any state. However, these quantities suffer from the severe disadvantage that they typically are *not* directly accessible in laboratory experiments.
Here, we report on the first direct experimental observation of an entanglement measure, namely concurrence [6] $C = |\langle\Psi^*|\sigma_y \otimes \sigma_y|\Psi\rangle|$ originally defined in terms of the

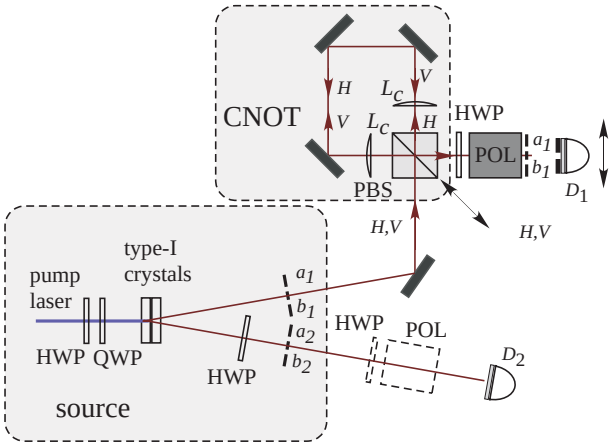

Figure 1: *Experimental setup for the measurement of entanglement using two copies of the quantum state. Photon pairs that bear entangement in two different degrees of freedom were created by pumping two type-I $LiLO_3$ crystals with a* 200 mW *HeCd cw laser (*442 nm*). Double-square apertures (*1 mm × 1 mm *squares,* 2 mm *center to center separation) placed* 1*m from the crystal face are used to select distinct spatial modes a and b. Detectors D_1 and D_2 use* 1.4 *mm circular and* 1×5 mm *rectangular detection apertures, respectively. Both were equipped with* 10 nm *FWHM interference filters (full-width at half-maximum,* 10 nm*). HWP, half-wave plate; QWP, quarter-wave plate; PBS, polarization beam splitter; LC, cylindrical lens; POL, polarization filter, CNOT, controlled-not. H and V indicate horizontal and vertical polarization.*

second Pauli matrix σ_y, and the transpose $\langle\Psi^*|$ of the original state $|\Psi\rangle$. The non-linear dependence on the system state – that constitues a fundamental property of *any* entanglement measure – is taken into account by considering a twofold copy of the state in question. Indeed, it has been shown that any m^{th} degree polynomial function of a density matrix ρ can be measured on an m-fold copy of ρ [7]. More precisely, the concurrence C of an arbitrary state $|\Psi\rangle$ can be defined as $C = 2\sqrt{P_A}$, where $P_A = \langle\Psi| \otimes \langle\Psi|A|\Psi\rangle \otimes |\Psi\rangle$ is the probability to observe the two copies of the first subsystem in an antisymmetric state, *i.e.*, a state that aquires a phase shift of π upon exchange of the constituents, and A is the correponding measurement operator [8].
In our specific setup, shown in Fig. 1, we created two copies of a bipartite quantum state using a photon pair obtained by spontaneous parametric down-conversion, where the polarization and momentum degrees of freedom each store one copy of the state $|\Psi\rangle$, respectively [9]. That is, both copies required for our measurement are carried by the same photon, which significantly facilitates the setup, since a measurement on only a single photon will be necessary. In fact, any required measurement can be realized efficiently with linear optics only [10].
With these two degrees of freedom, the entire system of two photons has polarization states spanned by $|H\rangle_i$, $|V\rangle_i$ ($i = 1, 2$ labels the two photons) and momentum states spanned by $|a\rangle_i$ and $|b\rangle_i$. Upon identification of the momentum state $|a\rangle_i$ as the equivalent of the polarization state $|H\rangle_i$ and analogously for $|b\rangle_i$ and $|V\rangle_i$, one can prepare two copies of an arbitrary input state $|\Psi\rangle$, one stored in each degree of freedom. As outlined above, the concurrence of $|\Psi\rangle$ is determined by the probability to observe the first photon in the antisymmetric state $|\psi^-\rangle = (|H\rangle|b\rangle - |V\rangle|a\rangle)/\sqrt{2}$, where we dropped the index '1', since from now on all considerations will concern only the first photon.

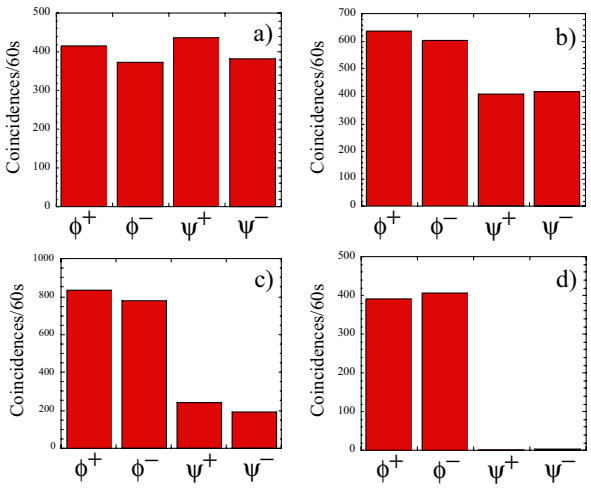

Figure 2: *Experimentally obtained count rates of the Bell-state measurement on the two-fold copy of input states* $\alpha|01\rangle + \beta|10\rangle$ *with a)* $|\alpha| = 0.71 \pm 0.02$, *b)* $|\alpha| = 0.53 \pm 0.01$, *c)* $|\alpha| = 0.35 \pm 0.01$, *and d)* $|\alpha| = 0.99 \pm 0.03$.

Since count rates rather than probabilities are accessible in laboratory experiments, one also needs to count events corresponding to the detection of the remaining Bell-states $|\psi^+\rangle = (|H\rangle|b\rangle + |V\rangle|a\rangle)/\sqrt{2}$, and $|\phi^\pm\rangle = (|H\rangle|a\rangle \pm |V\rangle|b\rangle/\sqrt{2})$. The probability P_A that determines concurrence, is then given by the count rate for the observation of $|\psi^-\rangle$ normalized by the sum of the count rates for all four Bell states.

The central building block for this Bell-state measurement in our specific experimental setup was a polarization-sensitive Sagnac interferometer containing two cylindrical lenses, as depicted in Fig. 1. The interferometer is used to perform a polarization-dependent rotation of the momentum modes, which is equivalent to a controlled-not (CNOT) operation. If the photon is vertically polarized, $|a\rangle$ evolves to $|b\rangle$ and vice versa; otherwise the momentum states remain unchanged [11, 12]. The crucial benefit of the CNOT operation is that it transforms the Bell-states such that the momentum and polarization states factorize:

$$\mathrm{CNOT}(|\psi^\pm\rangle) = 1/\sqrt{2}(|H\rangle \pm |V\rangle)|b\rangle = |\pm\rangle|b\rangle \tag{1a}$$

$$\mathrm{CNOT}(|\phi^\pm\rangle) = 1/\sqrt{2}(|H\rangle \pm |V\rangle)|a\rangle = |\pm\rangle|a\rangle. \tag{1b}$$

Thus, observing a photon with $|-\rangle$ polarization and momentum $|b\rangle$ *after* the CNOT, is equivalent to observing the state $|\psi^-\rangle$ *before* the CNOT operation, and analogously for the other Bell-states. Thus, the final measurement simply consists in detecting $|\pm\rangle$ polarized photons in the modes a and b. This can easily be carried out with two detectors positioned in the paths of modes a and b, and additional HWPs and polarization analyzers to discriminate the different polarizations. In particular, it should be emphasized that the four possible measurement results are the outcomes of a *single* measurement only.

In our experiment we measured the concurrence of states $\alpha|01\rangle + \beta|10\rangle$ with varying coefficients. The coefficients α and β of the polarization and momentum degrees of freedom were varied by rotating the HWP in the pump beam and shifting the apertures defining the momentum modes of photon 2, respectively. Fig. 2 shows the experimental count rates for observations of the Bell-states for four different states with increasing entanglement from a) to d). Experimentally-obtained concurrence C is depicted in Fig. 3 as a function of the varying coefficient α. The black dots show the experimentally obtained values, with error bars due to Poissonian count statistics. The theoretical

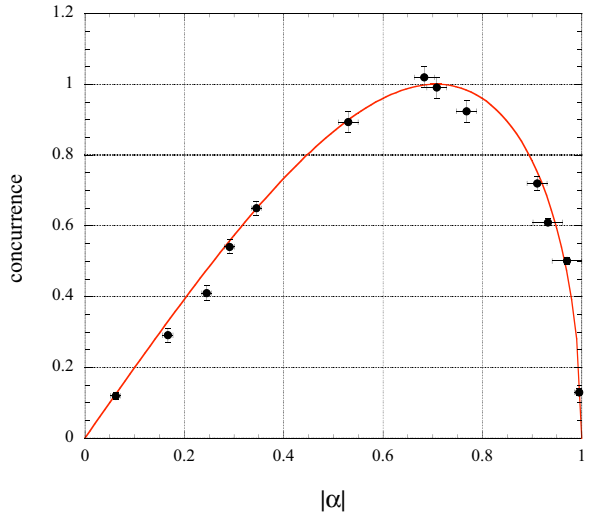

Figure 3: *Directly measured concurrence for states $\alpha|01\rangle + \beta|10\rangle$, as function of $|\alpha|$ with error bars due to poissonian statistics. The excellent agreement with theoretical value $C = 2|\alpha|\sqrt{1-|\alpha|^2}$ (shown as solid line) confirms the precision of the described measurement setup.*

value of $C = 2|\alpha\beta| = 2|\alpha|\sqrt{1-|\alpha|^2}$ is plotted as solid line and agrees virtually perfectly with the experimental observations. In particular, the maximum value $C = 1$ is obtained for $|\alpha| = 1/\sqrt{2}$, which provides an additional experimental evidence for the purity of the input states.

Our work [12] shows that it is possible to directly assess entanglement properties with few – in this case a single – local measurements. Whereas state reconstruction and subsequent mathematical determination of entanglement is a viable and succesfully demonstrated option for systems with few constituents, more efficient approaches are required for large objects. Our present experiment gives a proof of principle that indeed it is possible to circumvent the highly inefficient state reconstruction, and reliably characterize the entanglement properties of an unknown quantum state.

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3.13 Ericson Fluctuations in an Open, Deterministic Quantum System: Theory Meets Experiment

Javier Madroñero and Andreas Buchleitner

While erratic fluctuations of some experimental observable under changes of a control parameter come not too surprising in many-particle dynamics or in disordered systems [1–3], they still remain rather counterintuitive and for many a cause of discomfort in simple quantum systems with only few degrees of freedom – think of single electron or photon transport across two dimensional billiards [4], or of the ionization probability of a one electron Rydberg state under external forcing [5]. Here, classically chaotic dynamics substitute for disorder and many-particle interactions, though are expected to generate very similar – if not the same – statistical behaviour, in tantalizing contrast, e.g., to the clock-like regularity of Kepler like Rydberg motion. Hitherto, however, experimental evidence for chaos-induced fluctuations in the coherent quantum transport in low dimensional, strictly deterministic systems is scarce [4], since bona fide transport measurements require very high spectral resolution in the continuum part of the spectrum, together with the continuous tunability of a suitable control parameter. Here [6], we focus on a paradigmatic example in the realm of atomic physics – the photoexcitation of one electron Rydberg states in the presence of crossed, static electric and magnetic fields. Our contribution is motivated by recent experimental results [7] which probe the atomic spectrum above the field induced ionization saddle, and refines the interpretation of the experiments as the first observation of Ericson fluctuations in a strictly deterministic, open quantum system. Furthermore, this represents the first full-fledged, parameter-free quantum treatment of the truly three dimensional crossed fields problem at experimentally realistic spectral densities.

Ericson fluctuations are a universal statistical feature of strongly coupled, fragmenting quantum systems, first predicted [8] and observed [9] in compound nuclear reactions. They manifest as fluctuations in the excitation cross sections into the regime of highly excited, metastable resonance states, with typical decay widths larger than the average level spacing, such that single maxima in the cross section cannot be identified with single resonances any more, but are rather due to the interference of several of them. In particular, this implies that the typical scale of fluctuations induced by interfering decay channels is *smaller* than the typical width of individual resonances. In quantum systems with a well-defined classical analog, Ericson fluctuations can be understood as a hallmark of chaotic scattering [10].

Let us start with the Hamiltonian describing the single electron Rydberg dynamics subject to crossed electric and magnetic fields, in atomic units, and assuming an infinite mass of the nucleus:

$$H = \frac{\mathbf{p}^2}{2} + V_{\text{atom}}(r) + \frac{1}{2}B\ell_z + \frac{1}{8}B^2(x^2+y^2) + Fx\,. \tag{1}$$

Here, B and F are the strength of magnetic and electric field, respectively, and ℓ_z the angular momentum projection on the magnetic field axis. Note that, due to the mixing of all good quantum numbers of the unperturbed dynamics (the principal quantum

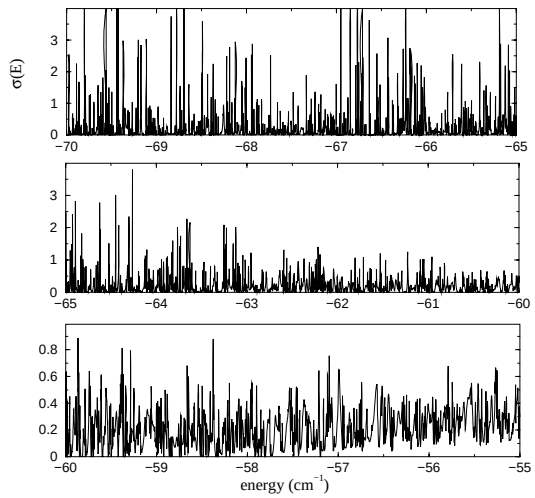

Figure 1: *Numerical photoexcitation cross sections, at magnetic and electric field strengths* $B = 2.0045$ T *and* $F = 22.4$ kV/m, *respectively, in the energy range* $E = -70.0 \ldots -65.0$ cm^{-1} *(top),* $E = -65.0 \ldots -60.0$ cm^{-1} *(middle), and* $E = -60.0 \ldots -55.0$ cm^{-1} *(bottom).*

number n, the angular momentum quantum number L, and the angular momentum projection M) by the crossed external fields, we are dealing with a truly three dimensional problem [11], and the only remaining constants of the motion are the energy E, and parity with respect to the plane defined by the magnetic field axis.

The experiments in [7] probe the energy range from -57.08 cm^{-1} to -55.92 cm^{-1} (corresponding to principal quantum numbers $n \simeq 43 \ldots 45$ of the bare atom), at fixed electric field strength $F = 22.4$ kV/m, and for three different values of the magnetic field, $B = 0.9974$ T, $B = 1.49$ T, and $B = 2.0045$ T. The electric field shifts the effective ionization threshold to -91.4 cm^{-1}, hence the experimentally probed energy range lies clearly in the continuum part of the spectrum. Invoking the scale invariance of the classical dynamics in a Coulomb potential, the specific choice of F and $B = 2.0045$ T corresponds to classically chaotic scattering [11] (where electric and magnetic field are of comparable strength, though incompatible symmetry).

We performed numerical diagonalizations of the complex dilated Hamiltonian (1) *precisely* for the experimental parameter values, though in a broader energy range, such as to illustrate the emergence of Ericson fluctuations from a smooth continuum background, with increasing Rydberg energies. Figure 1 shows the thus obtained photoexcitation spectra $\sigma(E)$, at magnetic and electric field strengths $B = 2.0045$ T and $F = 22.4$ kV/m, respectively, and in three different energy ranges, $-70.0 \ldots -65.0$ cm^{-1}, $-65.0 \ldots -60.0$ cm^{-1}, and $-60.0 \ldots -55.0$ cm^{-1}. The latter of these completely covers the experimentally probed energy interval. Clearly, individual resonances can be resolved in the two lower lying spectra, on top of an essentially flat continuum background. In contrast, the experimentally probed energy range is characterized by a strongly fluctuating continuum, with only few narrow structures on top, what immediately suggests the overlapping of an appreciable part of them. Inspection of the underlying distribution of resonance widths Γ_j along the energy axis, measured in units of the average local level spacing $\Delta = \langle E_j - E_{j-1} \rangle$, indeed comforts this picture, see Fig. 2: The weight of large resonance widths with $\Gamma_j > \Delta$ clearly increases as we probe higher lying energies, and amounts to approx. 65% of all contributing resonances, in the experimentally probed energy range. Many of the structures in $\sigma(E)$ are consequently due to the interference of decay channels through overlapping resonances.

A close comparison of our numerical cross section in the lower panel of Fig. 1 (and of Fig. 3 below) shows close similarity with the experimental signal [7], though no

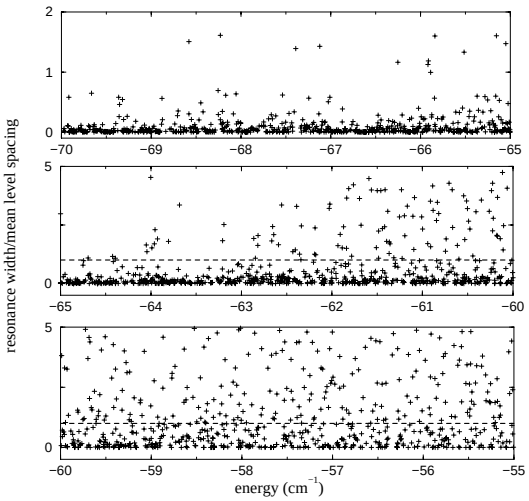

Figure 2: *Distribution of the resonance widths* Γ_j *contributing to the photoexcitation cross section, in units of the local mean level spacing* $\Delta = \langle E_j - E_{j-1} \rangle$*, over an energy range which spans the domain probed in the three plots of fig. 1, for the same values of* F *and* B*. The dashed line at* $\Gamma_j/\Delta = 1$ *separates isolated* ($\Gamma_j/\Delta < 1$) *from overlapping resonances* ($\Gamma_j/\Delta > 1$).

perfect coincidence is achieved. This, however, is anything but surprising, precisely

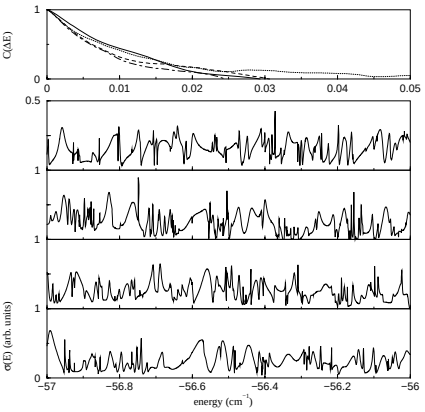

Figure 3: *Top: (Normalized) Autocorrelation functions* $C(\Delta E)$ *of the photoionization cross sections for magnetic field strengths* $B = 2.0045$ T *(full line),* $B = 1.49$ T *(dashed line),* $B = 0.9974$ T *(dotted line), and* $B = 0.563$ T *(dash-dotted line), at electric field strength* $F = 22.4$ kV/m*. The corresponding cross sections are shown in the subsequent panels, with increasing magnetic field strength from top to bottom. The characteristic correlation lengths* γ *of* $C(E)$ *deduced from our – parameter-free – numerical treatment, for the three largest values of* B*, are, from top to bottom:* $\gamma^{\rm th}[{\rm cm}^{-1}] = (0.0082,\ 0.0062,\ 0.0080) \pm 0.0005$ *– in very good agreement with the corresponding experimental values [7]:* $\gamma^{\rm exp}[{\rm cm}^{-1}] = 0.0083,\ 0.0065,\ 0.0081$.

due to the characteristic, extreme sensitivity of quantum spectra and cross sections with respect to tiny changes in the boundary conditions, in the regime of classically chaotic dynamics [4, 5]. Therefore, rather than scanning parameter space on a fine mesh, to reproduce the experimentally observed (but fragile!) cross section exactly, we calculate the autocorrelation function $C(\Delta E) = \langle (\sigma(E + \Delta E) - \langle \sigma \rangle)(\sigma(E) - \langle \sigma \rangle) \rangle$ of $\sigma(E)$, which is predicted [10] to have a Lorentzian shape with the characteristic width γ, $C(\Delta E) \sim 1/(\Delta E^2 + \gamma^2)$, in the regime of stronlgy overlapping resonances. The latter condition is indeed met by all the three values of the magnetic field employed in the experiments in [7], and Fig. 3 shows the autocorrelation functions, together with the excitation spectra from which they are deduced. γ is expected to be a statistically robust quantity, and we verified that its value remains unaffected by the sensitive parameter dependence of $\sigma(E)$ itself, within the error bars indicated. The respective values of the characteristic widths γ are in perfect agreement with the experimental values. In particular, also the nonmonotonous dependence of γ on the magnetic field strength B is recovered.

To complete the picture, we also display in Fig. 3 the excitation spectrum and the

associated cross section at a weak magnetic field $B = 0.563$ T (not recorded in [7]), where the classical dynamics of the associated Coulombic problem is near regular, since the electric field dominates the dynamics [11]. In contrast, the present result for rubidium exhibits a very similar structure as for stronger magnetic fields, certainly due to the destruction of the Coulomb symmetry by the multielectron core [12].

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3.14 Theory of Mitotic Spindle Oscillations

Stephan Grill, Karsten Kruse and Frank Jülicher

Complex dynamic processes in cells result from the interplay of a large number of molecular players. A prototype system for cellular dynamics is the cell cytoskeleton. The interaction of elastic filaments with force generating molecules such as motor proteins play essential roles in complex dynamic processes such as cell division. An important example for such dynamics is the movement and positioning the mitotic spindle. This biological structure consists of two asters of filaments called microtubules which radiate towards the cell periphery. The spindle microtubules interact with the chromosomes and physically separate the duplicated chromosomes during cell division. This structure must be correctly positioned within the cell for an asymmemtric cell division. Stem cells often divide asymmetrically, and these types of divisions are of fundamental importance in cell and developmental biology. They typically generate two daughter cells which are unequal and have different sizes. Such unequal divisions play an important role for the pattern formation of tissues in developing organisms.
The different sizes of daughter cells result from the fact that the plane of cell cleavage is shifted off center towards one side of the dividing cell. This is achieved by first physically displacing the mitotic spindle. Spindle displacements occur as a result of the action of motor proteins. In particular, motors in the cell periphery are attached close to the cell membrane in the so-called cell cortex. They interact with microtubules

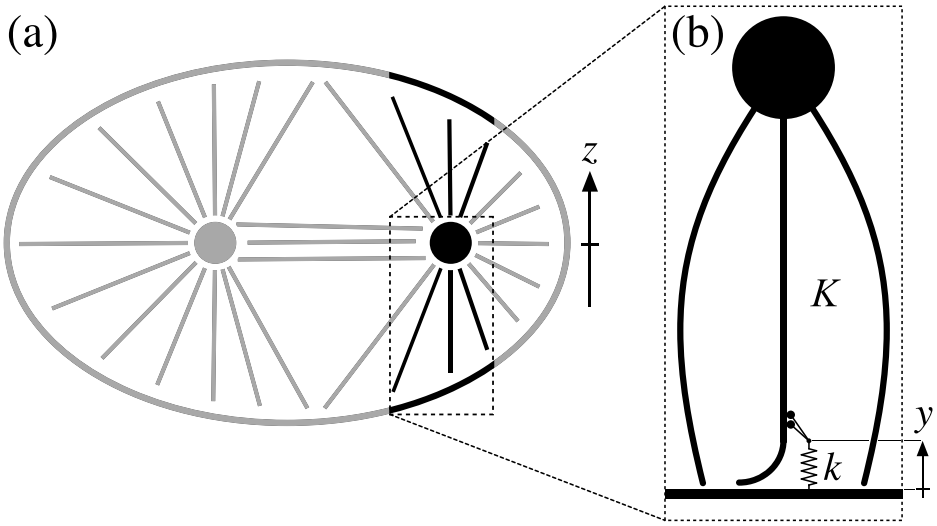

Figure 1: *(a) Schematic representation of the mitotic spindle in a single-cell stage C. elegans embryo. Microtubules (lines) radiate out from both spindle poles (solid circles). Cortical forces induce spindle pole displacements along the z-axis. (b) Interactions of the spindle pole with the lower cortex. Force generators are attached to the cortex via elastic linkers of stiffness k. The linker extension is denoted y. The bending rigidity of unattached microtubules provides a restoring force K.*

of the spindle and exert pulling forces, see Fig. 1. If the number of force generators on the two opposite sides of the cell is different, the spindle is effectively displaced by the action of motor molecules away from the cell center, resulting in an asymmetric division [1]. During this process, oscillations occur.

The physical principles underlying the movements of the mitotic spindle during cell division can be studied in living cells. An important model system is the first division of the fertilized egg of the nematode worm *Caenorhabditis elegans*. This first cell division is asymmetric and involves an interesting dynamics of the spindle. The spindle is displaced towards one pole of the egg while it undergoes spontaneous oscillations in a direction perpendicular to the displacement at the same time. This dynamics results from the interplay of force generators in the cell cortex and spindle microtubules [2]. Its quantitative analysis therefore provides valuable information about the molecular origins of spindle displacements.

The observed spindle oscillations can be understood as a collective phenomenon of many motor proteins which all pull on the spindle pole [3]. Since motors pull from opposite sides, they act antagonistically and generate no net force at steady state. However, the steady state can become unstable with respect to a collective oscillating mode. This instability and the properties of the resulting oscillations can be understood from the molecular properties of individual motors which have in the past been measured by single molecule experiments. The mechanical properties of a motor molecule is captured by a force-velocity relationship, which for a single motor is linear to a good approximation [4]:

$$v = v_0 - \alpha f_{\text{ext}} \quad , \tag{1}$$

where v_0 is the spontaneous velocity and the coefficient α characterizes the influence of an externally applied force f_{ext}. When a motors is in the vicinity of a filament, it

binds to the filament with a rate $\omega_{\rm on}$. The detachment rate $\omega_{\rm off}$ from the filament is a function of the applied force $f_{\rm ext}$ as has been shown in single motor experiments. This force dependence is key to understanding instabilities in the collective behaviors of motors. The strong increase of the detachment rate with increasing force $f_{\rm ext}$ can be described by [5, 6]

$$\omega_{\rm off} = \omega_0 \exp\{\frac{a|f_{\rm ext}|}{k_B T}\} \quad , \tag{2}$$

where ω_0 is the detachment rate in the absence of force and a denotes a molecular length scale. The action of many such motors which are attached to a solid object via elastic linkers of stiffness k can be described in a mean-field description. The net force of N motors is $F = -Nk \int y P_b(y) dy$, where $P_b(y)$ is the probability that a motor is bound to a microtubule with extension y of the elastic linker; see Fig. 1. The velocity of a motor on the microtubule is $v = \dot{y} - \dot{z}$, where $\dot{z}$ is the velocity of the microtubule itself. The bound probability $P_b(y)$ then satisfies an equation of the form [7]

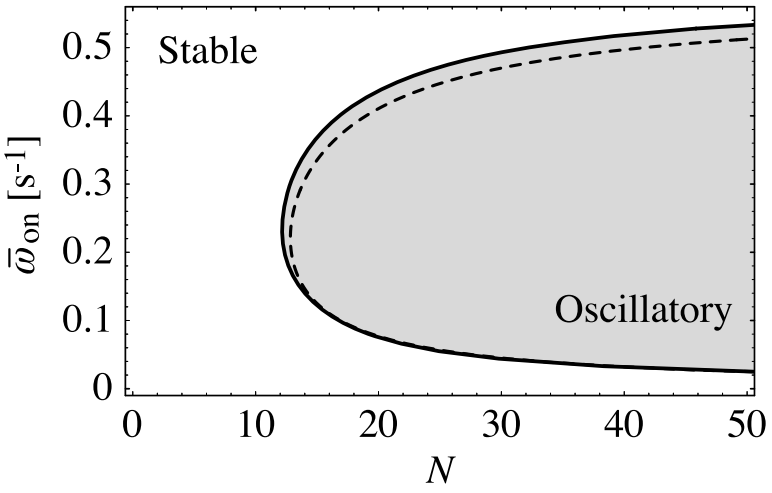

Figure 2: *(a) State diagram of mitotic spindle dynamics. The full (solid line) and the simplified equations (broken line) result in oscillating solutions inside the shaded region, while the non-oscillating solution is stable outside.*

$$\partial_t P_b(y) \quad + \quad \partial_y J_b = \omega_{\rm on} P_u - \omega_{\rm off} P_b \tag{3}$$

$$\partial_t P_u(y) \quad + \quad \partial_y J_u = -\omega_{\rm on} P_u + \omega_{\rm off} P_b \quad . \tag{4}$$

Here, the current in the bound state is given by $J_b = \dot{y} P_b$, where the velocity of linker extension is given by $\dot{y} = v_0 - k\alpha y + \dot{z}$. The motors in the unbound state relax on a fast relaxation time to an equilibrium distribution $P_u \sim \exp\{-ky^2/k_B T\}$.
At steady state, the force F generated by the motors is a nonlinear function of the velocity $\dot{z}$ and can exhibit dynamic instabilities. In order to discuss the dynamics of the spindle with its pole at position z, we write

$$\xi \dot{z} = -Kz + F_+ + F_- \quad . \tag{5}$$

Here ξ is the spindle pole viscosity and K characterizes a restoring force wich acts to center the spindle pole at $z = 0$. The forces of motors acting at the upper and lower sides are denoted F_+ and F_-, respectively.

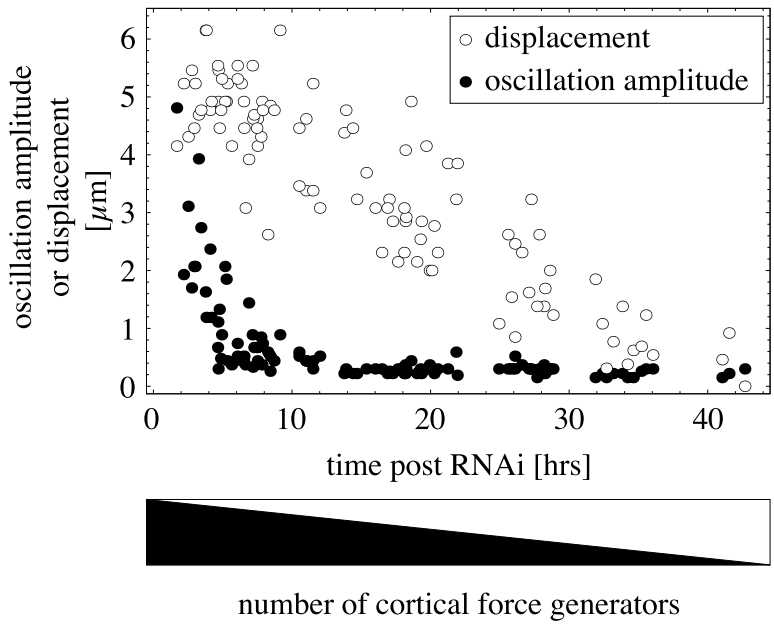

Figure 3: *The effect of a gradual reduction of the number N of cortical motors on spindle oscillations. As the time between RNA interference is increased, the displacement of the mitotic spindle (open symbols) changes gradually, while the oscillation amplitude (closed symbols) decreases sharply after a few hours. This is consistent with there being a threshold force beyond which oscillations arise spontaneously, as predicted by the model.*

The dynamic system of collective antagonistic motors can become unstable with respect to an oscillators instability. The state diagram of this system is shown in Fig. 2. The control parameters are the number of motors N as well as the binding rate $\omega_{\rm on}$. A linear stability analysis of the dynamic equations provides explicit expressions for the oscillation frequencies of the system. For slow oscillations, one can show that the system behaves like a simple nonlinear oscillator of the form

$$g\ddot{z} + (\xi - \Gamma)\dot{z} + Kz + B\dot{z}^3 = 0 \quad . \tag{6}$$

The coefficient

$$g \simeq \frac{2N}{\alpha\omega_{\rm on}}[\frac{f}{f_c}p^2(1-p)] \tag{7}$$

results from the force-dependence of the detachment rates and corresponds to an effective mass in the problem. Here, $f = v_0/\alpha$ is the stall force, $f_c = k_BT/a$ and $p = \omega_{\rm on}/(\omega_{\rm on} - \omega_{\rm off})$ is the fraction of bound motors. The coefficient

$$\Gamma \simeq \frac{2N}{\alpha}[\frac{f}{f_c}p(1-p) - p] \tag{8}$$

corresponds to negative friction which leads to an instability as soon as $\Gamma > \xi$. The oscillation frequency at the instability is $\omega = (g/K)^{1/2}$. The nonlinearity described by the coefficient B is a consequence of collective rupture of motors from the filament.
The mechanisms for moving and positioning an object via the action of antagonistic and processive motors is general and also applies to other situations within the living cell where motors act in large numbers and work in opposition. For example, motors

of different directionality have been shown to transport cargo in tissue or organelles within cells. Regarding the oscillations of the mitotic spindle that are observed in different living cells, our physical mechanism can account for the observed shape of oscillations, their frequency and amplitude. We have used parameter values for the single-motor properties measured in single motor experiments. Comparing experiment and theory, we were able to determine the spindle friction $\xi \simeq 10^{-6}\,\mathrm{N\,s/m}$ and the spindle centering force described by the coefficient $K \simeq 4 \times 10^{-6}\,\mathrm{N/m}$.
The predictions that follow from the scenario proposed above can be tested experimentally by studying the first cell division of the *C. elegans* embryo. Our theory suggests that oscillations occur because cortical motors are activated and the critical value in motor number is exceeded, at which the antagonistic system becomes unstable with respect to oscillations. The number of active force generators can be manipulated experimentally via a protein called GPR-1/2, which is part of a signaling system in the cell which regulates cortical motors and the forces that drive spindle displacements. By using an RNA interference technique, the amount of GPR-1/2 protein can be selectively reduced. The longer the time post interference, the fewer GPR-1/2 protein remains in the living embryo. This is in turn thought to reduce the number of cortical motors that are present. The consequence of this experiment is displayed in Fig. 3, where both the observed spindle displacement as well as the observed amplitude of oscillations is shown as a function of the time an embryo was fertilized after treatment of the worm with the interference technique. While the displacement of the spindle decreases gradually, the oscillations amplitude vanishes abruptly. This is indicative that the system crosses an oscillating instability, a clear prediction of the theory. Because spindle displacement decreases gradually with time post interference, the number of active force generators is continuously decreased in a smooth fashion. These results indicate a scenario where the cell increases the number of active force generators during division on one side of the cell to achieve spindle repositioning. To be able to displace the spindle robustly in the natural environment of the embryo, it does so by placing a large number of antagonistically acting motors on the cortex. The result is that an instability is exceeded and oscillations appear. Finally, a careful determination of the oscillation period as a function of time during oscillations shows that the frequency decreases with time, which suggests that the rate ω_{off} is decreased and thus the processivity is increased in order to activate force generators [8].
In summary, we have shown that a simple physical mechanisms for an oscillating instability based on collectively operating motors occurs during cell division in the *C. elegans* nematode worm. This instability is a consequence of cellular regulation of force generators in the cell which ultimately control the movements of the mitotic spindle.

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3.15 Hydrodynamic Flow and Synchronization of Beating Cilia

Andrej Vilfan and Frank Jülicher

Many eucaryotic cells possess cilia or flagella, which are motile, whip-like structures on the cell surface [1]. While certain cells such as sperm swim using a single flagellum other cells use several or a large number of cilia for propulsion in a fluid. Epithelial cells such as those on the surface of the airways of the respiratory tract use densely ciliated surfaces to transport fluids. Hydrodynamic flows generated by cilia play a key role during the embryonal development of higher organisms. In all mammals, the left-right symmetry of the embryo which leads to positioning the heart at the left side of the body, is broken with the help of nodal cilia. These cilia rotate rapidly and generate a hydrodynamic flow with chiral asymmetry which presumably transports signalling molecules in a left-right asymmetric manner and thus controls the breaking of this symmetry [2].
All these cilia are based on the same microscopic structure. They are formed by a regular arrangement of microtubule doublets which are filaments of the cytoskeleton. Microtubules are arranged in a cylindrical geometry. Motility is achieved by the action of a large number of motor proteins which generate forces in the cilium while consuming a chemical fuel. As a consequence, the cilium produces periodic deformations of its shape in three dimensional space [3].

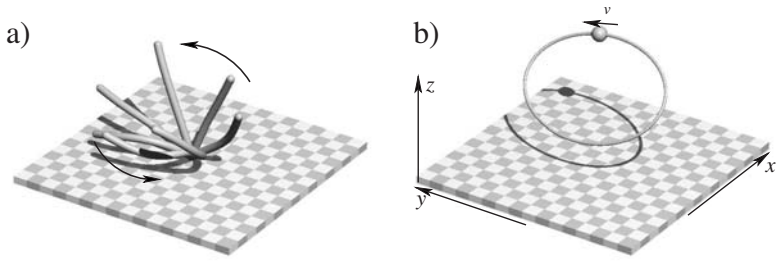

Figure 1: *(a) Schematic representation of the beating motion of a cilium on a surface. It consists of an effective stroke pushing fluid, followed by a recovery stroke closer to the surface. (b) Simplified representation of the ciliar beat by a small sphere, moving on a tilted elliptical trajectory. This configuration has the essential symmetries of a beating cilium. It generates a net hydrodynamic flow along the surface.*

We describe the hydrodynamic flows generated by a cilium which emerges from a surface and periodically stirs a fluid by its beating motion (Fig. 1). Our minimal

model of the ciliary beat captures the essential features and symmetries - the difference between effective stroke and recovery stroke of whip-like beating as well as the tilted rotatory motion of nodal cilia. We replace the cilium by a small sphere of radius a (essentially describing the center of mass position of the cilium), which moves on a fixed trajectory in the vicinity of a planar surface (defined as the plane $z = 0$). The trajectory of the bead is elliptic, the phase of the oscillation (the position along the trajectory) is described by an angle ϕ. The asymmetry of the ciliary beat is reflected in the fact that the two principal axes (denoted A and B) are different, and that the ellipse is tilted with respect to the surface as described by the parameter C.
The hydrodynamic flow field generated by the sphere moving on a tilted ellipsoidal trajectory can be calculated as a solution to the Stokes equation together with no-slip boundary conditions on the surface. The instantaneous flow field can be written as $\mathbf{v}(\mathbf{x}) = \overleftrightarrow{G}(\mathbf{x}_i, \mathbf{x})\mathbf{F}_i$, where $\mathbf{F}_i$ is the force the particle located at $\mathbf{x}_i$ exerts on the fluid. The propagator $\overleftrightarrow{G}$ can be expressed as a sum of a stokeslet, an anti-stokeslet, a source-doublet and a stokes doublet [4]. The far field is given by

$$\overleftrightarrow{G}(\mathbf{x}_i, \mathbf{x}) \approx \frac{3}{2\pi\eta}\frac{z_i z}{r^3}\begin{pmatrix} \cos^2\beta & \sin\beta\cos\beta & 0 \\ \sin\beta\cos\beta & \sin^2\beta & 0 \\ 0 & 0 & 0 \end{pmatrix} \tag{1}$$

where $\tan\beta = (y_i - y)/(x_i - x)$ and $r^2 = (x_i - x)^2 + (y_i - y)^2$.

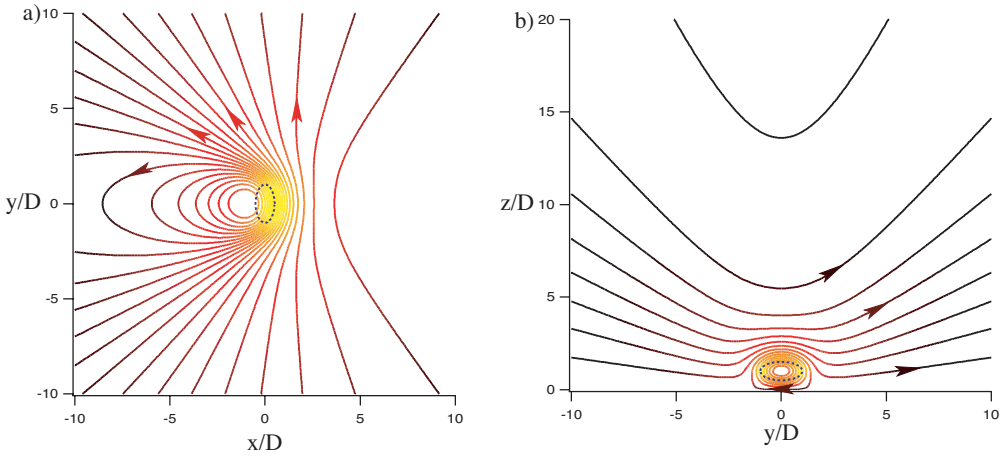

Figure 2: *(a) Flux lines describing the time averaged fluid flow generated by a sphere moving on a tilted elliptical path shown in the x-y plane. (b) Same flow field displayed in the y-z plane, for $x = 0$. Black lines correspond to low fluid velocity, yellow lines to high velocity. The dashed lines indicate the projections of the ellipsoidal trajectory of the sphere.*

As the particle moves periodically along a tilted ellipsoidal trajectory, a time-periodic hydrodynamic flow field is generated. Because of the symmetry of the trajectory and in particular the tilt, the flow generated in the forward direction at the largest distance from the surface differs from the flow during the time when the particle is close to the surface. As a consequence, a net average flow $\bar{\mathbf{v}}(\mathbf{x}) = \frac{1}{T}\int_0^T \mathbf{v}(\mathbf{x}, t)dt$ exists with a

far-field given by

$$\bar{\mathbf{v}} = \frac{9\pi aBC}{T}\frac{yz}{|\mathbf{x}|^5}\begin{pmatrix} x \\ y \\ z \end{pmatrix} \quad . \tag{2}$$

Here T denotes the period of motion. A dynamic equation for the moving sphere can be writted by assuming that internal forces generate a constant force in a direction tangential to the ellipsoidal path. The particle velocity is then determined from the relation $\mathbf{F}_i = \overleftrightarrow{\gamma}\mathbf{v}_i$, where the friction tensor depends on the height z over the surface:

$$\overleftrightarrow{\gamma}_i = \gamma_0 \left(\overleftrightarrow{I} + \frac{9}{16}\frac{a}{z_i}\begin{pmatrix} 1 & & \\ & 1 & \\ & & 2 \end{pmatrix} \right) \quad . \tag{3}$$

The net flow field which results from this description is displayed in Fig. 2.
This simplified generic model for the motion and hydrodynamics of a beating cilium can be used to study hydrodynamic interactions between different cilia. Here, we focus on the simple case of two cilia which are arranged relative to each other at a distance vector $\mathbf{x} = \mathbf{x}_1 - \mathbf{x}_2$, see Fig. 3(a). Each cilium is described by a sphere which is driven by

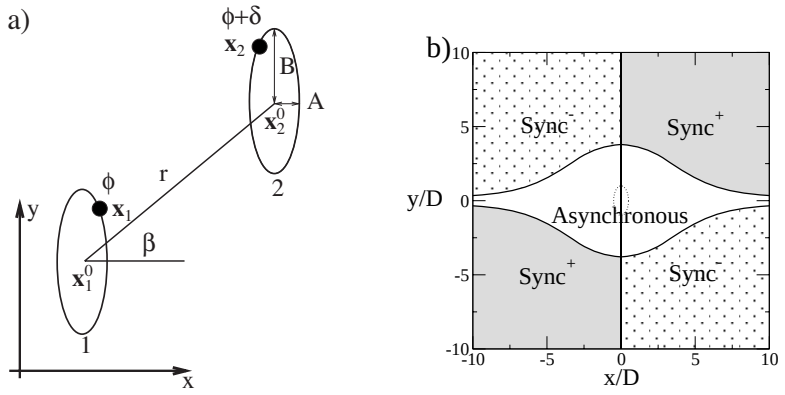

Figure 3: *(a) Top view of an arrangement of two beating cilia represented by ellipsoidal trajectories. The distance r and the angle β are indicated. (b) The state diagram as a function of the distance vector $x = x_2^0 - x_1^0$, $y = y_2^0 - y_1^0$. Three different regions are indicated. In the region of asynchronous beat, two frequencies occur. Two synchronous states can be distinguished with equal (Sync$^+$) and opposite (Sync$^-$) phase of both cilia in the limit of large separation r.*

a constant internal force on a tilted periodic trajectory. The velocity of motion results from a balance of this internal force with hydrodynamic friction which results from the relative speed between particle and fluid. Since the second moving sphere generates a fluid flow at the position of the first, the instantaneous velocity of a sphere depends on the position and velocity of the second. As a consequence, the equations of motion of the two spheres are hydrodynamically coupled. The system can be described as two nonlinear phase oscillators which are coupled via the propagator $\overleftrightarrow{G}$. The nonlinear dynamics of this system exhibits several different types of behaviors, depending on the geometry of the particle trajectories as well as on the distance and relative orientation of the particles, see Fig. 3. In the case of synchronized cilia, the phase difference between

both particles along their trajectories is constant. Interestingly, synchronization occurs for larger distances $r = |\mathbf{x}_1 - \mathbf{x}_2|$. Note that even though both particle trajectories have the same geometry, the arrangement shown in Fig. 3 (a) breaks their symmetry. As a consequance, there exists an asynchronous state in which they oscillate with different frequencies. This situations occurs typically for small r.
We have shown that the hydrodynamic far field around a periodically beating cilium has generic properties which do not depend on the detailed beating pattern. Its main features can thus be generated by a sphere moving on a tilted elliptical trajectory. This simplified description can be used to study hydrodynamic interactions between cilia. A natural extension of our work is the generalization to a periodic lattice of cilia attached to a surface. Such situations correspond to some epithelial cells which generate fluid flows on their surface and to microorganisms such as paramecium. In all these cases, the ciliary beat is organized in metachronal waves which result from hydrodynamic and steric interactions between cilia. In different cells, these waves of ciliary strokes propagate along the surface in different directions relative to the one defined by the working stroke [5]. Other examples for hydrodynamically stirred surfaces are realized in experiments where bacteria are attached to surfaces and their flagella rotate, driven by bacterial rotary motors. In this situation, where the arrangement of the flagella is more disordered, complex and disordered flow patterns have been observed [6]. The extension of our study to many hydrodynamically coupled cilia and metachronal waves is left for future work.

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3.16 Statistics of Neural Shot Noise

Benjamin Lindner

Stochastic Processes in Neurophysics
All our sensations are mediated by small electric discharges across the cell membrane of nerve cells (neurons) [1]. These discharges are called action potentials or spikes; their occurrence in time is thought to encode information solely by means of the instances in time (not by the shape of the stereotypic action potential, cf. Fig. 1).
The statistics of *spike trains* and their relation to sensory stimuli has long been studied within the framework of stochastic point processes. There are several internal and external sources of fluctuations that require a statistical description of neural activity [2]. The main source of noise in neural networks is synaptic background activity: neurons *in vivo* that are not directly stimulated (e.g. neurons in the visual cortex

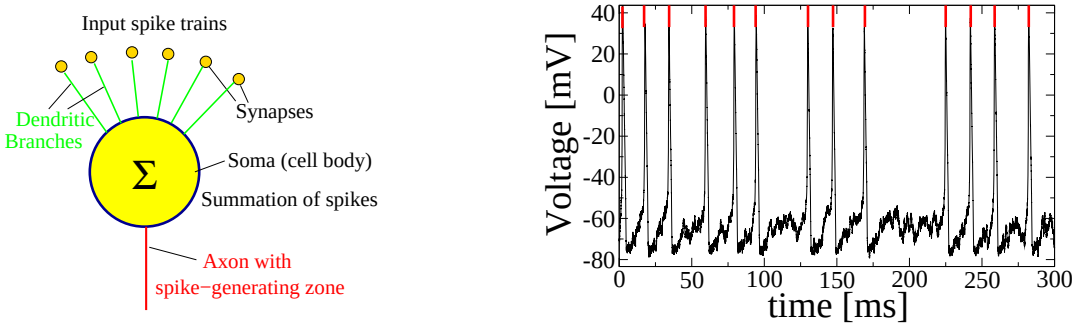

Figure 1: *Left: Scheme of a neuron that receives many* $(10^2 - 10^4)$ *spike train inputs from other neurons via synapses on the dendritic branches. If the input is sufficiently strong, an action potential or spike is generated in the axon. Right: Voltage trace of a stochastic model neuron (Hodgkin-Huxley model) showing randomly occurring action potentials due to the noisy synaptic input. Information is entirely encoded in the spike train (red bars).*

when the animal or human is in the dark) still fire spontaneously in a highly irregular fashion and at low rate ($1 - 10$ Hz). Every neuron in the net is connected to hundreds or thousands of other neurons and receives their spikes through excitatory (driving the neuron towards firing) or inhibitory (driving the neuron away from firing) synapses. These shot noise inputs are summed up in the cell soma. Because of the large number of connections, the low activity of all presynaptic cells adds up to a considerable stochastic input. Various proposals have been made to explain possible roles of this neural noise for the signal transmission and processing in neurons (see e.g. [3,4]).

Statistics of the shot noise

The single synaptic input spike train has certainly some temporal structure. It is, for instance, known that neurons cannot fire action potentials in short succession — there is an absolute (1ms) and a relative refractory period (several ms) after the last spike during which a new spike is impossible or unlikely, respectively. Other features like neural bursting and adaptation lead to more complex temporal correlations.

However, in the soma many of these spike trains are summed and if we assume (in first approximation) that the different spike trains are independent, one might be tempted to think that the resulting spike train (the superposition of all synaptic inputs seen in the spike generating zone in the axon) is completely random without any temporal correlations. Indeed, in the overwhelming majority of theoretical studies it has been assumed that the input noise is a Poisson shot noise (known in physics as electron shot-noise e.g. in a vacuum tube or in semi-conductors) which has a flat power spectrum, i.e. no temporal correlations. In addition, in many experiments such a Poisson shot noise was used *in vitro* in order to mimic realistic synaptic noise. In a recent study [5], it has been shown, however, that temporal correlations in the input to a neuron or neural network can lead to qualitative changes in network dynamics and signal transmission properties of single neurons.

The justification of the Poissonian approximation boils down to the following question: Is the superposition of many independent (non-Poissonian) spike trains a Poisson process? Let us consider independent spike trains $x_i(t) = \sum \delta(t - t_i)$ that share the same

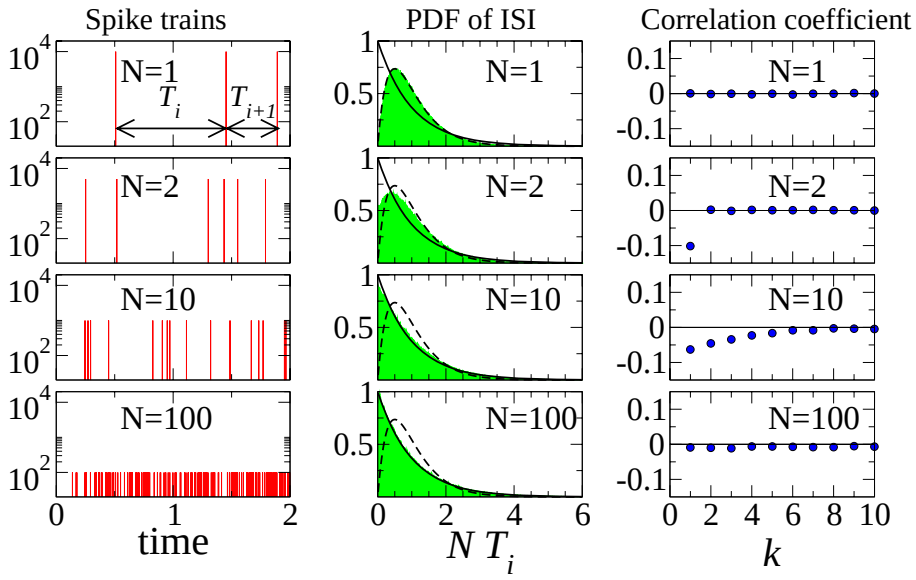

Figure 2: *The statistics of the superposition of spike trains for different numbers of synapses: resulting spike trains (left panels), ISI densities (middle panels), and serial correlation coefficient of two intervals lagged by an integer k. The single spike train ($N = 1$, upper row) has a non-Poissonian statistics, all intervals are mutually independent (the SCC is zero for all lags). The formula for the interval density (dashed line in the mid panel) is given in the text. Adding a few spike trains (middle row) results still in a nonexponential interval density and also leads to correlations among ISIs. For a large number of spike trains, the statistics seem to converge to Poissonian with exponential ISI density (solid line in the mid panels) and vanishing correlation coefficients at all lags. The resulting spike train, however, is* not *Poissonian as shown below.*

stationary non-Poissonian statistics with spike rate r and let us considered

$$X(t) = \frac{1}{N} \sum x_i(t) \tag{1}$$

where the prefactor is a normalization.
Commonly, researchers have referred to a proof by Khinchine [8] to answer the above question with a yes. Apparent numerical evidence for the Poissonian nature of the superposition is demonstrated in Fig. 2 for a specific choice for $x_i(t)$. We choose the single spike train to be a renewal process with a probability density for the intervals between successive spikes (interspike intervals — ISIs) that obeys an α function $p_\alpha(T) = 4r^2 T \exp[-2rT]$. The power spectrum of the spike train is not flat $S_\alpha = r[2r^2 - (\pi f)^2]/(4r^2 + (\pi f)^2)$; it exhibits a dip at low frequencies as many neurons do due to the neural refractory period. In Fig. 2 we show the ISI density and ISI serial correlation coefficient for the superposition of N spike trains. As we add more and more spike trains the probability density of ISIs tends to an exponential function (cf. Fig. 2, mid column). Furthermore, all the ISI correlation coefficients vanish (cf. Fig. 2, right column) and the resulting spike train seems to converge to a renewal process (i.e. all ISIs are statistically independent). A renewal process, however, is uniquely determined by its ISI density — if the density is exponential we deal with a Poisson process. Hence, the statistics in Fig. 2 seems to imply that $X(t)$ converges to a Poisson process as

$N \to \infty$. A similar line of reasoning has been used in the literature by different authors.

Is the superposition of random spike trains Poissonian?
I recently showed [9] that under reasonable assumptions the statistics of neural shot noise is *not* Poissonian if the input spike trains do not obey a Poissonian statistics in the first place. This is obvious when looking at the power spectrum of the spike train:

$$S_{XX} = \langle \tilde{X}\tilde{X}^* \rangle = \frac{1}{N^2} \sum_{n,k} \langle \tilde{x}_n \tilde{x}_k^* \rangle = \frac{1}{N} S_{xx} \tag{2}$$

where the tilde and the asterix denote the Fourier transform and complex conjugated, respectively, and where we have used that the single spike trains $x_n(t)$ are statistically independent. The above relation states that if the spectrum of the single process is not flat (e.g. peaked at certain frequencies), this feature will be maintained in the spectrum of the superposition irrespective of the value of N, thus we never obtain a Poisson process with flat power spectrum. This is demonstrated numerically and analytically for the simple example used before in Fig. 3 (l.h.s.). The dip seen in the spectrum of the single spike train is conserved as we add more and more spike trains, hence it is also present in the effective input in the spike generating zone of the stimulated cell.
There is a paradox here: from the point of view of the ISI statistics the process $X(t)$ seems to converge to a renewal process (all correlation coefficients vanish) with exponential ISI density. However, looking at the spectrum, we find a non-Poissonian statistics because the power spectrum is proportional to that of the single process, i.e. in general the spectrum is not flat.

Resolution of the paradox
Although each correlation coefficient tends to zero, the sum of all correlation coefficients remains finite even for $N \to \infty$. This is seen in Fig. 3 (r.h.s.). Thus, the process $X(t)$ is *not* a renewal point process but a nonrenewal process with strong cumulative memory. Consequently, the conclusion from vanishing SCC and exponential ISI density to Poissonian statistics is wrong. Although the ISI density indeed converges to an exponential function, the resulting process has still the same spectral statistics as the single process. A closer inspection shows that the assumptions made in the classical proof by Khinchine do not apply to the neurobiological problem [9].

Implications for models of neural communication
The simple arguments that I have used here show that caution must be used when applying seemingly intuitive approximations in neural modeling. The spectral statistics of the single presynaptic input is still seen when the soma sums over many synaptic inputs. In particular, models that employ the so-called diffusion approximation of neural spike train input (replacing the shot noise by a Gaussian noise) should use a "colored" (i.e. a non-flat spectrum implying temporally correlations) instead of white Gaussian noise. Continuous noise models exist that reproduce a spectrum with reduced power at low frequency (so-called green noise) or with peaks at finite frequency (harmonic noise). The inclusion of such processes in stochastic neuron models remains an exciting subject of future studies.

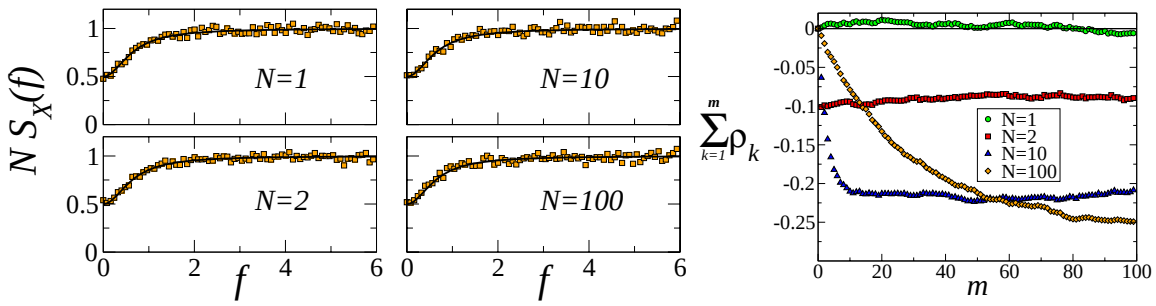

Figure 3: *Left: Power spectra of the superposition of spike trains for different numbers N of superposed processes $x_n(t)$. As seen the shape of the spectra is maintained and* does not *converge to a flat (Poissonian) spectrum. Right: Partial sum of the first k correlation coefficients. Although each single coefficient vanishes as $N \to \infty$, the sum converges to a finite value indicating a nonrenewal property of the superposition of spike trains.*

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3.17 Response and Fluctuations of a Two-State Signaling Module with Feedback

Manoj Gopalakrishnan, Peter Borowski, Frank Jülicher, and Martin Zapotocky

In the work presented, we develop a systematic analytical framework to study the dynamics of the simple auto-regulatory module shown in Fig. 1. The module consists of a single protein that switches between active (A*) and inactive (A) states. In

the active state, a certain molecular species C is produced with a fixed rate. The accumulation of C increases the A*→A transition rate (Fig. 1a), leading to negative feedback on the production of C. In addition, C is removed at a fixed rate independent of the activation state.

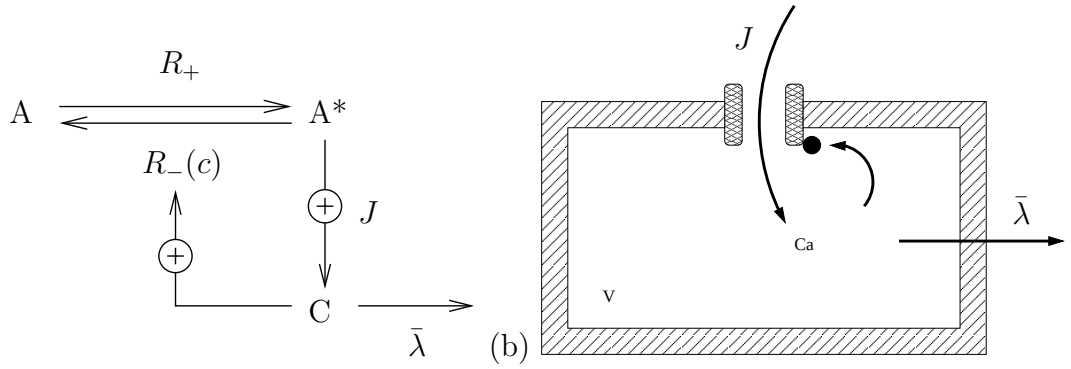

Figure 1: *(a) The simple two-component auto-regulatory signaling module with negative feedback studied in this paper. The product C (with concentration c), generated with rate J in the active state A*, enhances the deactivation rate R_-. C is removed with a rate $\bar{\lambda}$ independent of the activation state of A. An input signal encoded in a temporal change $R_+(t)$ is transduced into an output signal $c(t)$. (b) A channel in the open state permits the entry of ions (rate J) into a small compartment of volume V. The ions, once inside, increase the closing rate of the channel, and are also removed from the compartment at a constant rate $\bar{\lambda}$.*

Without the feedback, the activation and deactivation kinetics would be described by a two-state Poisson process. In the presence of feedback, the deactivation rate, at any given time, becomes dependent on the history of transitions, and makes the effective two-state kinetics non-Markovian. We use a path-integral technique to analytically evaluate the effects of weak feedback, and investigate the strong feedback regime with Monte Carlo simulations.

A specific example of the physical realization of our module is a single ion channel connected to a small cellular compartment (Fig. 1b). This can be viewed as an idealization of calcium signaling in a short segment of the olfactory cilium, or in a synaptic spine. The state of the channel at time t is represented by $S(t)$, with $S = 1$ being the open state and $S = 0$, the closed state. Let us denote by $\bar{c}(t)$, the ion concentration inside the compartment at time t. The kinetics of $\bar{c}$ is described by the equation

$$\frac{d\bar{c}}{d\bar{t}} = \frac{J}{V} S(t) - \bar{\lambda}\bar{c}(t). \tag{1}$$

In the above equation, J represents the molar current of ions entering the cell through the channel in the open state, $\bar{\lambda}$ represents the total rate of removal of ions by membrane pumps, and V is the volume of the compartment. The channel kinetics is specified by the opening rate R_+ and closing rate R_-. We assume the existence of a negative feedback corresponding to a rate R_- that increases with increasing ion concentration. If the effect of the feedback is weak, one may expand to linear order and write

$$R_-(\bar{c}) \approx R_-^0 + \bar{\alpha}\bar{c}(t), \tag{2}$$

where R_-^0 is the closing rate of the channel when no ions are present in the compartment and the coupling parameter $\bar{\alpha}$ specifies the feedback strength. We further assume that, in general, an external signal is received by the module as a change in the opening rate (due, e.g., to the binding of extracellular ligands to the channel). Unless otherwise noted, however, we assume that the opening rate is not time dependent. A path integral treatment of a Markovian two-state system with time-dependent transition rates has been given by Goychuk an Hänggi in [1].
In the following we adopt a dimensionless formulation of the problem. The inverse of the intrinsic closing rate R_-^0 is chosen as the unit of time, and the ratio $J/(\bar{\lambda}V)$ (i.e. the maximum achievable ion concentration) is the unit of c. The rescaled closing rate then takes the form $r_- = \frac{R_-}{R_-^0} = 1 + \alpha c$, where $\alpha = \frac{\bar{\alpha}J/V}{\lambda R_-^0}$ is the dimensionless feedback coupling constant. Fig. 2 shows the typical dynamics of the system (obtained in Monte Carlo simulations) for several values of the dimensionless opening rate r_+ and dimensionless extrusion rate λ.

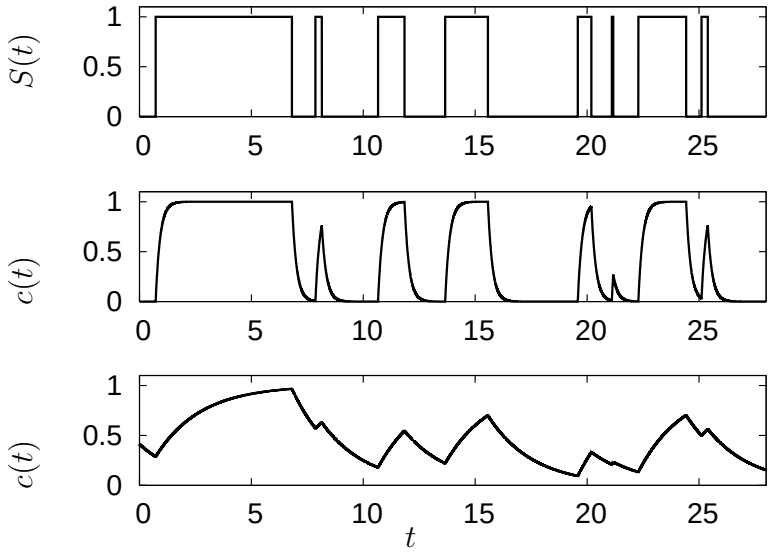

Figure 2: *The figure illustrates the kinetics of channel openings and Ca^{2+} concentration for two typical runs, with $r_+ = 0.5$ and $\lambda = 5$ (top and middle) and $\lambda = 0.5$ (top and bottom) in the absence of feedback ($\alpha = 0$). Note that for larger λ, $c(t)$ almost follows the step-like kinetics of $S(t)$.*

In order to formulate a path-integral description, we define the functional $\mathcal{P}_{ij}[t_0, t; \{\tau_k\}_{k=1}^N; c_0; N]$ of $S(t)$ with $t > t_0$. It represents the probability that a certain time evolution of the system from $S(t_0) = i$ and $c(t_0) = c_0$ to $S(t) = j$ is realized. This time evolution is characterized by the set of times $\{\tau_k\}_{k=1}^N$ at which the state switches from $S = 0$ to 1 or from $S = 1$ to 0. In order to write down the functionals $\mathcal{P}_{ij}$ in the explicit form, we make the transformation from flip-times $\{\tau_i\}_{i=1}^N$ to time-interval variables $\{t_j, t'_j\}_{j=1}^m$ with $m = N/2$, where the $\{t_j\}$ denote the time intervals when the channel is closed and the $\{t'_j\}$ when it is open. In the absence of feedback, the probability to remain in the initial channel state for the length of each time interval is $\exp(-r_+ t_j)$, resp. $\exp(-t'_j)$. The full probability functional then has the form

$$\mathcal{P}_{00}^{(0)}[0, t; \{t_i\}, \{t'_i\}; 2m] = r_+^m e^{-F_{00}(0,t;\{t'_i\};m)}, \tag{3}$$

with the weight factor F_{00} given by

$$F_{00}(0,t;\{t_i'\};m) = r_+ t + (1-r_+)\sum_{i=1}^{m} t_i'. \tag{4}$$

In the presence of the feedback-coupling to $c(t)$, the expression for $\mathcal{P}_{00}$ is modified to

$$\mathcal{P}_{00}[0,t;\{t_i\},\{t_i'\};c_0;2m] = r_+^m \prod_{i=2}^{2m}{}' \left(1+\alpha c(\tau_i)\right) e^{-F_{00}-\alpha \sum_{j=1}^{2m-1}{}'' \int_{\tau_j}^{\tau_{j+1}} d\tau c(\tau)}, \tag{5}$$

where the prime (double prime) on the product- or sum-symbol indicates that the running index is always even (odd). A key simplification is that after expanding Eq. 5 to first order in the dimensionless feedback strength α, calcium concentration terms enter only as linear prefactors of the exponential term $\exp(-F_{00})$. The evaluation of the Green's function

$$G_{00}(t_0,c_0;t) = \sum_N \int_0^t dt_1 \int_0^{t-t_1} dt_1' \int_0^{t-t_1-t_1'} dt_2 ... \int_0^{t-\cdots-t_m} dt_m' \mathcal{P}_{00}[t_0,t;\{t_i\},\{t_i'\};c_0;2m] \tag{6}$$

is then done most conveniently in terms of Laplace-transformed variables and is carried out in Ref. [2].

We skip the resulting lengthy expressions for the functions $G_{ij}(t_0,c_0;t)$, and present below some of the explicit results for the averages and correlations in the steady state, to first order in feedback strength α. We also show results from Monte Carlo simulations for strong feedback. The analytical first order perturbation theory is found to be adequate up to $\alpha \approx 0.2$, as demonstrated in the insets of the figures.

The mean fraction of open channels in the steady state (which is equivalent to the steady state calcium concentration in our dimensionless units) is found to be

$$\langle S\rangle = \langle c\rangle = \frac{r_+}{1+r_+}\left(1-\alpha\frac{r_+ + \lambda}{(1+r_+)(1+r_+ +\lambda)}\right) + O(\alpha^2). \tag{7}$$

As expected, the negative feedback always decreases the mean open fraction. In Ref. [2], we show that the corresponding expression obtained from mean-field analysis underestimates the effect of feedback, and becomes equivalent to Eq. 7 only when the calcium dynamics is slow compared to the channel dynamics, i.e. when $\lambda \ll r_+$ and $\lambda \ll 1$.

In Fig. 3a, the steady state average $\langle S\rangle = \langle c\rangle$ is plotted as a function of the opening rate r_+, for various values of α. This is analogous to a dose-response curve, if the mean calcium concentration is interpreted as the response of the system to an external stimulus that modifies the opening rate of the channels. We observe that feedback shifts the response towards higher r_+ values by closing the channels more often. However, the 'dynamic range' of sensitivity (e.g. the range of r_+ covered between 5% and 95% of the response) is found to be increased with feedback: the curves become less steep for large α.

In Fig. 3b we show the variance $(\delta c)^2$ of c in steady state as a function of r_+ for various feedback strengths. The fluctuations are generally suppressed by feedback (except at very high r_+). As we showed above, however, the mean response $\langle c\rangle$ is decreased by feedback as well. A convenient measure of the precision of signal transduction is the

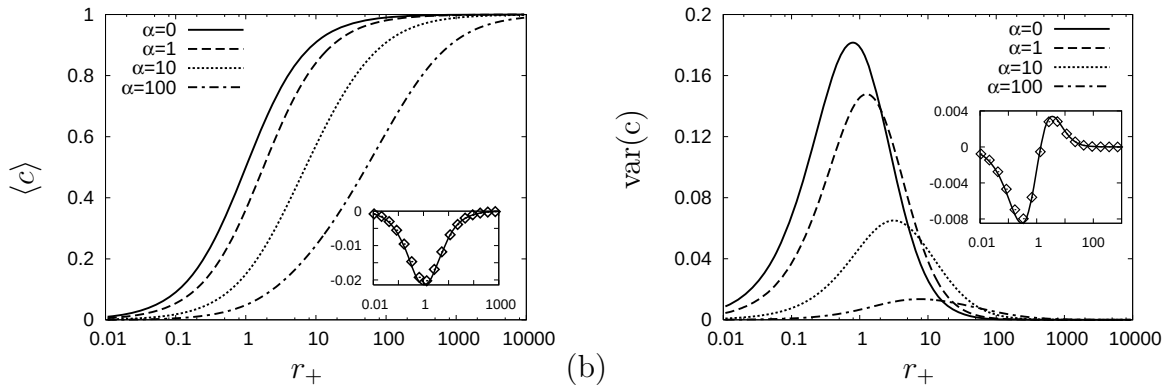

Figure 3: *(a) The numerically obtained mean calcium concentration $\langle c \rangle$ in the steady state plotted as a function of the opening rate r_+. (b) Variance in c in the steady state plotted as function of r_+.* ***Insets:*** *Difference between the cases $\alpha = 0.1$ and $\alpha = 0$. The line represents the term linear in α from the analytical treatment, symbols indicate numerical results.*

coefficient of variation, defined as the ratio of the standard deviation of calcium to its mean in the steady state. The analytical result to first order in α is

$$\frac{\delta c}{\langle c \rangle} = \sqrt{\frac{\lambda}{r_+(1+r_++\lambda)}} \left(1 + \alpha \, \frac{(r_++\lambda)(-1+r_++2\lambda)}{2(1+r_++2\lambda)(1+r_++\lambda)}\right) + O(\alpha^2). \qquad (8)$$

Clearly for $\lambda > \frac{1}{2}$ the relative fluctuation is increased for any value of r_+, while for sufficiently small λ it is increased when r_+ is large and decreased when $r_+ < 1$. The precision of output can thus be improved by feedback when the input is weak (r_+ is small).

We now briefly discuss the autocorrelation and response functions. The autocorrelation of the channel variable $S(t)$ in the steady state is found to be

$$\mathcal{C}_S(t) = \frac{r_+}{(1+r_+)^2} e^{-(1+r_+)t} + \alpha \left(B_1 e^{-(1+r_+)t} + \right.$$
$$\left. C_1 e^{-\lambda t} + D_1 e^{-(1+r_++\lambda)t} + E_1 t e^{-(1+r_+)t}\right) + O(\alpha^2). \qquad (9)$$

The coefficients B_1, C_1, D_1, E_1 are algebraic functions of r_+ and λ and are given in Ref. [2]. We observe that the first order correction term introduces two new time scales. Furthermore, the feedback introduces a term non-monotonic in time, whose sign depends on the relative values of λ and r_+. Fig. 4 shows the auto-correlation function for the channel state in the case of strong signal ($r_+ = 6$). In general, one notes that the effect of increasing feedback is to reduce the characteristic time scale of decay of the correlations. When the feedback parameter is very large, the channel auto-correlation function briefly becomes negative before vanishing at longer times. This anti-correlation in the channel state may be interpreted physically as the rapid closing of an open channel by the Ca^{2+} which enters through it.

In Ref. [2], we compute the linear response functions for our system, and show that the main effect of the feedback is to widen the range of frequencies effectively sensed by the system. Using our results for the autocorrelation and response functions, we also quantify the deviation from the fluctuation-dissipation theorem in our non-equilibrium system.

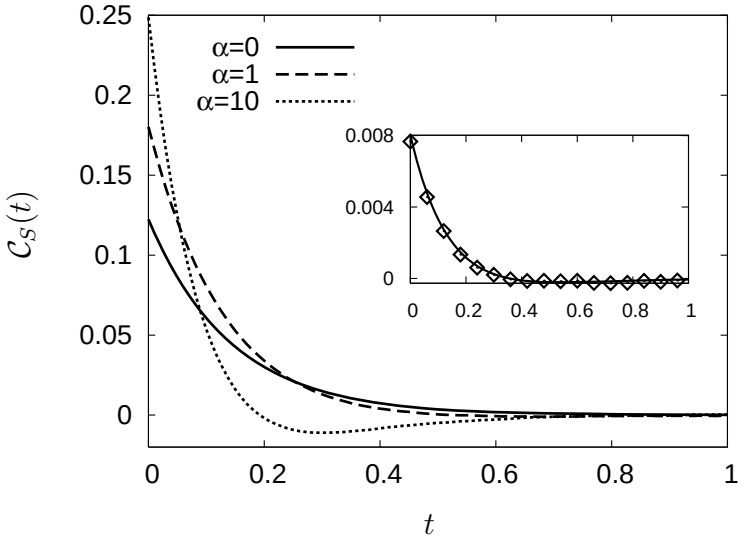

Figure 4: *Autocorrelation function for $S(t)$ in the steady state for $\lambda = 5$ and $r_+ = 6$.* ***Inset:*** *Difference between the cases $\alpha = 0.1$ and $\alpha = 0$. The line represents the term linear in α from Eq. 9.*

Our principal conclusions from this study may be outlined as follows. We find that the rate of extrusion of Ca^{2+} ions, λ, is the single most important control parameter of the model. When λ is large, the short-time scale dynamic response of the system is improved by negative feedback. In addition, the negative feedback increases the range of sensitivity of the system, while at the same time suppressing the response to weak signals. For small λ, the coefficient of variation in calcium was reduced with feedback, for weak stimuli. This might help the system to differentiate between stimuli of different magnitudes in this regime. In general, however, having a small λ was found to adversely affect the dynamic response characteristics.

Starting from the relevant experimental literature [3], we obtained estimates for the dimensionless parameters used in our model for the specific case of the vertebrate olfactory cilium. We find for the opening rate $r_+ \approx 10^{-5} - 20$ depending on the concetration and identity of the odorant. The parameter governing the calcium dynamics is $\lambda \approx 20$ and the feedback parameter α is of the order of 1. The large value of λ indicates that in this case, the biological system evolved so as to use the feedback to improve the temporal precision of signaling at intermediate and high odorant concentration, rather than to improve the detection of weak stimuli. This is in general agreement with recent experimental work [4] that showed enhanced detection of low odorant concentrations in olfactory cilia with artificially suppressed calcium feedback.

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3.18 Nanoscale Dielectric Response

Ralf Everaers, I. Pasichnyk, and A.C. Maggs

The project aims at developing improved implicit solvent models based on a new family of algorithms for calculating electrostatic interactions in (bio-)molecular simulations. These algorithms [1] generate long ranged electrostatic interactions *dynamically* via *local* interactions between charges, the medium and the electric field. They are based on the formulation of free energy functional for the electric field $\mathbf{D}$:

$$U_{elec} = \int \frac{\mathbf{D}_\mathbf{r}^2}{2\epsilon_\mathbf{r}} \mathrm{d}^3\mathbf{r}. \tag{1}$$

combined with local or cluster (worm) Monte Carlo updates which modify the field degrees of freedom as well as the position of charges while conserving Gauss' law, div $\mathbf{D} - \rho = 0$. These algorithms should be contrasted with classical methods of simulation of charged media in soft condensed matter where the long ranged electrostatic interaction is calculated explicitly.

An example of the importance of dielectric effects arise in the the Born solvation (self) energy of an ion, $q^2/8\pi a\epsilon$ where a is an atomic scale. The strong preference of ions for aequous solutions is explained by the low Born energy in water with $\epsilon \approx 80$ compared to $\epsilon \approx 2-5$ for non-polar fluids such as oil. To show that we are indeed able to evaluate electrostatic (solvation) self-energies and charge-charge interactions in dielectrically inhomogeneous media, we have worked out illustrative cases in simple geometries for which analytical results exist. The figure demonstrates that the algorithm generates conventional electrostatics in dielectric media [3] including the zero-frequency component of the Lifshitz interaction [2].

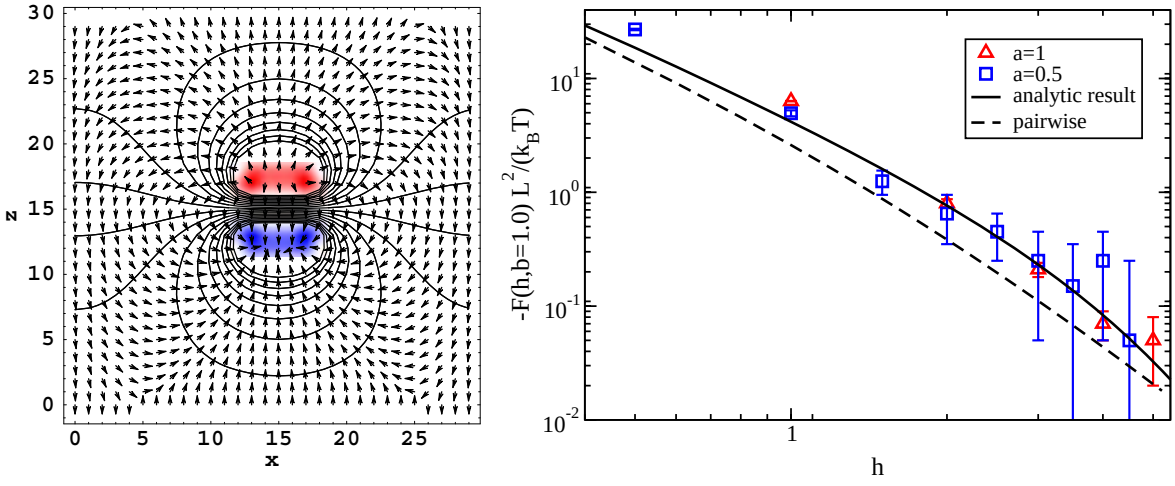

Figure 1: *L.h.s.: Dielectric sphere in a capacitor. Arrows indicate the minimized vector field* $\mathbf{E}$*, lines designate equipotential surfaces, and colors show the induced charge density,* q^{ind}*. R.h.s.: Distance dependent Lifshitz interactions in a slab geometry. Simulation (symbols) vs. analytical results (lines).*

Our main result [4] concerns the simulation of the non-local dielectric response on the nm-scale

$$\mathbf{D}_\mathbf{r} = \int \epsilon_{\mathbf{r},\mathbf{r}'} \mathbf{E}_{\mathbf{r}'} \mathrm{d}^3\mathbf{r}' \tag{2}$$

implying the existence of scale dependent dielectric effects

$$\mathbf{D}(\mathbf{q}) = \epsilon(\mathbf{q})\mathbf{E}(\mathbf{q}). \tag{3}$$

In the case of water, the dielectric constant drops to $\epsilon = 20$ at a wavelength which is comparable to the Bjerrum length of a monovalent ion (7Å); below a wavelength of ∼5Å, ϵ diverges and becomes *negative*. Moreover, many situations of practical interest require the inclusion of non-linear effects such as dielectric saturation or surface ordering and alignment.

To treat these effects, we have developed a generalization of the Marcus energy for polarizable media written in terms of the true, independent thermodynamic variables in the problem: the electric polarization of the medium, $\mathbf{P}$, and the displacement, $\mathbf{D}$. There are two contributions to the energy of a dielectric medium. Firstly, the energy density $\mathbf{E}^2/2 = (\mathbf{D}-\mathbf{P})^2/2$ of the electric field; secondly, an elastic polarization energy, $G(\mathbf{P})$, due to short ranged interactions between molecules. G can be expressed as a general quadratic function of $\mathbf{P}$ with a *short ranged kernel* $K_{\mathbf{r},\mathbf{r}'}$ which varies from place to place in a heterogeneous system and contains *all* the material properties

$$U = \int \frac{(\mathbf{D}_\mathbf{r} - \mathbf{P}_\mathbf{r})^2}{2} \mathrm{d}^3\mathbf{r} + \int \frac{\mathbf{P}_\mathbf{r} K_{\mathbf{r},\mathbf{r}'} \mathbf{P}_{\mathbf{r}'}}{2} \mathrm{d}^3\mathbf{r}\mathrm{d}^3\mathbf{r}' \tag{4}$$

Furthermore, $\mathbf{D}$ is constrained by Gauss' law, div $\mathbf{D} - \rho = 0$. Our simulation algorithm uses local or cluster (worm) Monte Carlo updates which modify $\mathbf{D}$ and $\mathbf{P}$ while conserving div $\mathbf{D}$. By analytically investigating the stationary points of the functional and their stability, we have shown that this formalism is capable of reproducing the full range of the linear dielectric response seen in nature including negative dielectric constants.

By choosing appropriate kernels K we can introduce semi-microscopic models of dielectric media with a great variety of dielectric properties. A systematic approach is to use a Landau-Ginsburg expansion of the free energy for the polarization field. However our simulation technique is *not* limited to linear models. We have shown that we can study freely rotating dipoles with long ranged electrostatic interactions at practically unchanged computational costs. Such models have long been used to describe polar solvents and exhibit a saturation of the polarization degrees of freedom when interacting with strongly charged objects. Thus we were able to show that our approach allows the efficient investigation of electrostatic interactions in heterogeneous, non-linear and non-local dielectric media.

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3.19 Statistical Physics of DNA at the Base-Pair Level

Nils B. Becker, Christian Simm, Sanjay Kumar and Ralf Everaers

We are interested in the elasticity, thermal denaturation and folding of DNA and RNA at the base respectively base-pair level.
In the first part of the project, we have concentrated on the biological function of elastic deformations of B-form DNA. Our approach is to combine experimental data obtained by crystallographic, biochemical and biophysical methods as well as simulation results, and to establish theoretical relationships between them on the basis of the rigid base–pair model of DNA elasticity [1].
In this description, the Watson–Crick base pairs building up the DNA helix are represented as a rigid bodies. There are six degrees of freedom of relative rotation and translation between neighboring base–pairs. To a first approximation, thermal fluctuats are governed by a quadratic deformation energy. Both equilibrium structure and stiffness are sequence dependent. There are competing sets of structural and elastic parameters for this model, which were extracted from molecular dynamics (MD) simulation of DNA and from a data base of high–resolution DNA crystal structures.
Our first step consisted in testing these parameters sets (and combinations of them) against an independent biochemical experiment which measures the binding affinity of the bacteriophage 434 repressor to mutated binding sites. As shown in Fig. 1a, the central four base pairs of the binding site are not directly contacted by the protein. Nevertheless biochemical experiments show that protein–DNA binding affinity varies up to 200-fold depending on their sequence. This effect is called ïndirect readoutänd due to the sequence-dependent structure and elasticity of dsDNA. We found [2] that predictions for the relative binding affinities varied strongly with the employed parameter set and that satisfactory agreement is obtained with a new, hybrid crystal–MD parametrization.
Based on this result, we worked on the identification of DNA subsequences in protein–DNA complexes which are optimized for indirect readout. Fig. 1b illustrates that such subsequences are not characterized by a particularly small *absolute* elastic energy, rather the deformation free energy is small *relative* to other sequences adopting the same structure. These statements can be given a clear meaning in a Statistical Mechanics framework [2]. Fig. 1c shows that our marker for indirect readout shows a clear signal exactly at the known indirect readout site of the 434 repressor.
Finally, we have developed a systematic coarse–graining procedure to established the connection between DNA elasticity on the base-pair level and recent single–molecule assays, which probe the elastic properties of DNA on a mesoscopic scale of hundreds of base–pairs [3]. Results are much less sensitive to the details of the employed parameterization on the microscale and compare well, without additional adjustable parameters, to direct mesoscopic measurements. For example, we reproduce the recently reported negative twist–stretch coupling of DNA [4].
In the second part of the project, we reconsidered the classical problem of DNA thermal denaturation. Depending on the GC-content of long chains, melting occurs in 1 M NaCl solutions in a temperature interval between 355 to 390 K. A detailed analysis of differential melting curves for intermediate length chains reveals the existence of discrete peaks

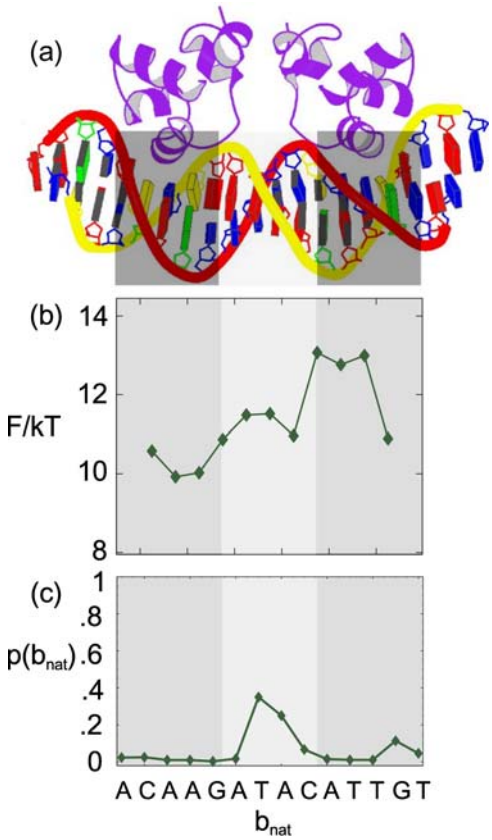

Figure 1: *(a) Crystal structure of bacteriophage 434 repressor protein bound to the OR2 operator sequence. (b) DNA deformation free energy profile computed from the structure. (c) Our local marker for indirect readout shows a peak at the non-contacted bases, shaded in light grey.*

corresponding to the successive opening of AT-rich regions of the chain. Both standard theoretical descriptions of DNA thermal denaturation, the nearest-neighbor (NN) model of oligonucleotide melting [5] and the Poland-Sheraga (PS) model of polynucleotide melting [6], are based on sequence-dependent parameters describing the free energy gain per nearest neighbor pair of stacked and paired bases in the double helix. The standard approach deals with the secondary structure of polynucleotides, but neglects the embedding of the molecule in three-dimensional space and the resulting long-range (in terms of chemical distance) interactions. Is it possible to preserve the polymer model underlying the PS-approach? Explicit models of associating polymers automatically account for the subtle (but universal) polymer contributions to the free energy. In addition, they include fluctuations in situations without pre-determined secondary structure, generate an ensemble of three dimensional structures and provide direct acess to the response to external mechanical forces. Our work has focused on lattice models. Besides investigating generic aspects of the coil-globule transition and force-induced unzipping [7–9], we have shown [10] how to parameterize a lattice model [11] in such a way as to provide a *quantitative* and *unified* description of the thermal denaturation of DNA oligomers and polymers. Deriving the DNA specific parameters of the lattice model from the nearest-neighbor and the Poland-Sheraga descriptions is, in principle, simple, since all models are defined on the same length-scale. Essentially, one has to count and group microstates of the lattice model and match the corresponding contributions to the partition function of the PS-model term by term. In particular,

- we translate the sequence dependent free-energy gain $\Delta h_{NN} - T\Delta s_{NN}$ per stacked

pair of neighboring base-pairs to a pairing free energy for overlapping chain sections in the lattice model;

- we express the initiation terms $\Delta h^0_{ini} - T\Delta s^0_{ini}$ as the sum of the entropy of mixing at standard conditions and a (capping) free energy penalty for the ends of double-helical chain sections;

- we interpret the PS cooperativity parameter σ for loop formation in terms of an interfacial (forking) free energy between coiled and helical sections of a double-stranded complex.

The lattice model has no adjustable parameter corresponding to the loop exponent c [6], because it implicitely accounts for generic polymer contributions to the entropy loss due to loop closure, as well as intra- and inter-loop excluded volume interactions.

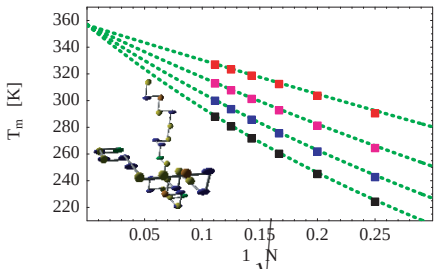

Figure 2: *Melting temperatures of Poly-A/Poly-T oligonucleotides as a function of chain length. SantaLucia [5] nearest neighbor model (lines) in comparison to data points calculated from exact enumeration results for the lattice model [10]. Inset: partially folded chain in the lattice model.*

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3.20 Pattern Formation in Bacteria

Giovanni Meacci, Elisabeth Fischer-Friedrich and Karsten Kruse

Living cells display a host of different spatial and temporal structures. Examples are circadian rhythms, which enable a cell to anticipate the repeating alternation between day and night, or sheet-like cellular protrusions called lamellipodia, which enable cells to crawl on a substrate. Revealing the mechanisms generating these structures is an important step on the way to understanding cells. In a physical system out of themrodynamic equilibrium, patterns can be formed by self-organization of its constituents. Is self-organzation a helpful concept to understand pattern formation on a subcellular level?

As an example where this seems to be the case, we discuss in the following our work on the dynamics of the Min system in the bacterium *Escherichia coli* [1]. It consists of three proteins and is essential for directing division to the center of this rod-shaped cell. The dynamics of these proteins provides a striking example of pattern formation in living cells: they are periodically shuffled from one end of the rod-shaped bacterium to the other and back with a period of about a minute, see Fig. 1. The functional role of these oscillations is to suppress cell cleavage in the vicinity of the ends which then leaves the cell center as only possible site for division. We aim at understanding the mechanism underlying these oscillations by employing theoretical as well as experimental techniques.

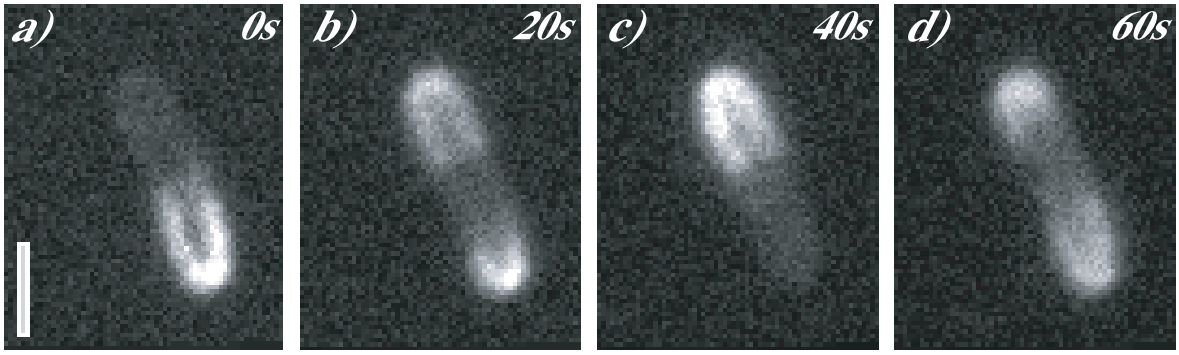

Figure 1: *Oscillations of MinD in E. coli. a-d) Fluorescence images of MinD which has been fused to green fluorescent protein (GFP) in a cell at subsequent time points separated by 20s. Scale bar: 1μm.*

The generation of this spatiotemporal pattern relies on the presence of two of the Min system's proteins, MinD and MinE. By binding Adenosine-Tri-Phosphate (ATP), MinD undergoes a conformational change. Subsequent to this conformational change, MinD has a high affinity for binding to the inner bacterial membrane. While MinD is bound to the membrane, its ATP is hydrolyzed resulting in Adenosine-Di-Phosphate and inorganic Phosphate. The ensuing conformational change leads to release of MinD from the membrane. The rate at which ATP bound to MinD is hydrolyzed is sped up about a hundredfold after MinD has formed a complex with MinE. The formation of MinDE-complexes occurs by recruiting MinE to the bacterial inner membrane through membrane-bound MinD. The dynamics of MinD- and MinE-exchange between

the membrane and the cytoplasm, which is the part of the bacterium surrounded by the membrane, is schematically shown in Fig. 2. Together with the diffusion of MinD and MinE, these processes, however, are not sufficient to generate the observed spatiotemporal oscillations.

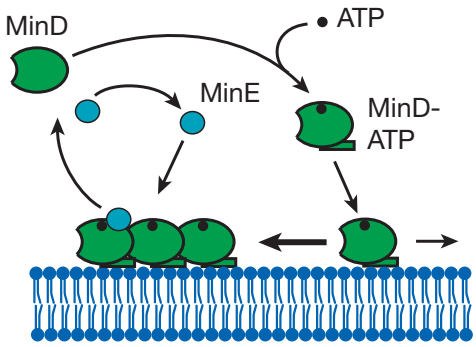

Figure 2: *Schematic representation of the Min protein dynamics. In its ATP-bound form, cytoplasmic MinD (green) attaches anywhere to the membrane. Attractive interactions between membrane-bound MinD moving on the membrane lead to the formation of MinD aggregates (thick arrow). MinE (blue) binds to membrane-bound MinD. It induces ATP hydrolysis which eventually leads to detachment of the MinDE complex from the membrane.*

Strong evidence exists that MinD bound to a membrane forms aggregates. In experiments involving the binding of MinD to vesicles, the formation of tight MinD helices deforming the vesicle have been observed [2]. Also in living bacteria experimental data suggest the existence of MinD helices [3]. The formation of these aggregates together with the elementary dynamics of MinD and MinE described in the previous paragraph has been shown to be sufficient for self-organization of the end-to-end oscillations as observed experimentally [4].

Two classes of processes leading to the formation of MinD aggregates have been studied. In cooperative aggregation (CA) models, free MinD molecules attach with the membrane with a higher probability in regions with membrane-bound MinD than in regions free of MinD. In aggregation current (AC) models, MinD binding to the membrane occurs with equal probability anywhere. Once bound to the membrane, MinD forms aggregates through. Currently, there is no experiment that would allow to distinguish between the two mechanisms. In our work, we focus on the AC mechanism [5–7].

Consider the limiting case of infinitely fast diffusion of MinD and MinE when detached from the membrane. In that case, the distribution of proteins in the cytoplasm, i.e., not bound to the membrane, becomes homogenous and does not change with time. Hence, attention can be focussed to the dynamics on the membrane. We describe the distribution of MinD molecules and MinDE complexes on the membrane by the fields c_d and c_{de}, respectively. The dynamic equations read

$$\partial_t c_d = \omega_D(c_{\max} - c_d - c_{de}) - \omega_E c_d - \nabla \cdot \mathbf{j}_d \quad (1)$$

$$\partial_t c_{de} = -\omega_{de} c_{de} + \omega_E c_d \quad . \quad (2)$$

The reaction terms are linear in the protein densities and the parameters characterize the attachment of MinD, ω_D, the attachment of MinE, ω_E, the detachment of MinDE complexes, ω_{de}, and the maximal protein density on the membrane, $c_{\max}$. The current j_d describes transport of MinD and has the form

$$\mathbf{j}_d = -D_d \nabla c_d + c_d(c_{\max} - c_d - c_{de})[k_1 \nabla c_d + k_2 \nabla \triangle c_d] \quad . \quad (3)$$

Here, k_1 and k_2 characterize the interaction between MinD molecules. For sufficiently large values of k_1 the homogenous distribution becomes unstable. The resulting state is oscillatory if the rates satisfy $\omega_{de}^2 < \omega_D \omega_E$, see [6].

Initially, the analysis was carried out assuming the distributions of Min proteins to be invariant under rotations around the bacterium's long axis. It revealed that the oscillatory solutions of Eqs. (1) and (2) display all qualitative features of the Min-protein dynamics observed in *E. coli*. Since the distribution of Min proteins in bacteria are not rotationally symmetric, we also performed an analysis of the dynamic equations in a bacterial geometry [7]. In this case, we found in addition to rotationally symmetric solutions also chiral solutions. In these states a traveling wave moving along the cells circumference is superimposed onto the pole-to-pole dynamics, see Fig. 3. The existence of these solutions can be traced back to the coupling of several unstable modes. Remarkably, without any modification, our dynamic equations thus generate solutions with the same symmetry as of the observed MinD helices.

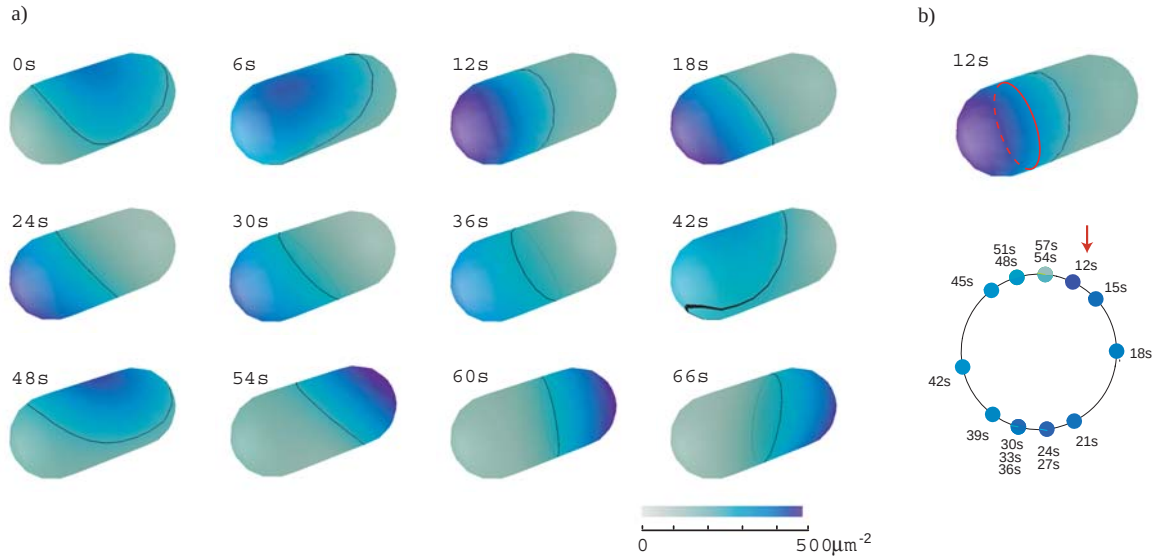

Figure 3: *Chiral solution of the dynamic equations (1) and (2). a) Concentration of membrane-bound MinD, $c_d + c_{de}$. The black line on the bacterium indicates an iso-concentration curve. In addition to the pole-to-pole oscillations, the distribution turns around the long axis. b) Location of the maximum MinD concentration on the red circle indicated on the left for the solution presented in (a). Color code as in (a).*

According to our calculations, waves of Min proteins should also be observable in situations where a flat membrane is immersed in a buffer containing MinD, MinE, and ATP. We analytically determined the asymptotic linear spreading velocities of these waves and found good agreement with the numerically obtained values. As we did not find wave solutions using CA models such an experiment might be able to distinguish between the two model classes.
A weakness of all models was for a long time that the values of their parameters were experimentally unknown. As a first step, we measured the diffusion constants of MinD and MinE as well as their residence times in the cytoplasm between release from the membrane and rebinding. In a collaboration with the group of P. Schwille at the TU Dresden, we employed to this end fluorescence correlation spectroscopy (FCS). This technique exploits the fluctuations of a fluorescence signal emanating from a small volume about a femto liter in size. The autocorrelation function of these fluctuations

depends on the dynamic processes through which fluorescently labeled molecules enter and leave the detection volume. By fitting the expected correlation curve to the data, key parameters of the underlying dynamic process can be determined.
In the case of the Min oscillations, the applicability of FCS hinges on the existence of quasi-steady states, i.e., intervals of about ten seconds during which the protein distributions do not change appreciably in the course of an oscillation period, see [8]. Through these measurements we were able to determine the diffusion constants of unbound MinD and MinE, which are both of the order of $15\mu\mathrm{m}^2/\mathrm{s}$. A second time scale visible in the correlation curve could be interpreted either as resulting from diffusion of membrane-bound proteins or from the exchange of molecules between the cytoplasm and the membrane. The corresponding fits of the correlation curve are equally good so that based on our data it is not possible to distinguish between the two processes. For the diffusion constants of membrane bound MinD and MinE we obtained about $0.2\mu\mathrm{m}^2/\mathrm{s}$ a value which is sufficient to allow for the formation of MinD helices through aggregation of membrane bound molecules.

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3.21 Long-Time Signatures of Short-Time Dynamics in Chaotic Quantum-Decay

Thomas Gorin

In recent years, there has been considerable interest in the interplay of universal behavior described by random matrix theory and system specific behavior described by semiclassics in mesoscopic systems. If we consider either diffusive or chaotic systems, there exists a time scale which separates system specific from universal behavior, the Ehrenfest time [1]. The combination of semiclassics and random matrix theory has been termed SRMT. In the present work, we analyze effects in the long-time behavior of a decaying quantum system, which stem from the interference with processes on a short time scale (before the Ehrenfest time).
An alternative point of view is provided by the classic example of a single resonance whose shape gets distorted by the existence of some coherent background [2]. We may associate the broad background with some prompt decay process, and the narrow

resonance with the decay on a long time scale. In that sense the distortion is an effect which falls precisely into the category discussed above. In order to arrive at the situation there, we just have to increase the number of decay channels, and go from the tunneling regime to ballistic couplings. This very quickly leads to strongly overlapping resonances, where individual resonance line shapes can no longer be observed. In that regime we study the *form factor* of the decay cross section, as a means to quantify these interference effects.
In this work, we consider the quantum analog of a classical chaotic scattering system, in a regime where the number of resonances M (below a given excitation energy) becomes very large, while the number of open channels N remains finite. Then we assume that by some mechanism, the system is excited into a state which has overlap with the scattering solutions of the system, thereby leading to decay. We focus on the total decay cross section $\sigma(E)$, which is given in terms of these overlaps. We consider the Fourier transform of the autocorrelation function of $\sigma(E)$, the *form factor*. Up to normalization, it is equal to the return probability of the excited state. For quantum-chaotic systems, the cross section autocorrelation function has been calculated analytically within random matrix theory [3]. In Ref. [4] (and references therein), this result has been generalized to take the effects of direct decay processes.

Quantum map approach
In order to model the dynamics of a decaying system, we use the efficient quantum map approach. It has the advantage that time is discrete, which makes it easier to quantify and to steer the prompt decay processes by properly choosing the initial state (the state of the system after the excitation).
As pointed out in Ref. [5], the open kicked rotor can be thought of as a generic model for open ballistic chaotic quantum dots. To see the analogy, we imagine a classical chaotic billiard, where one can quantize the classical Poincaré map in Birkhoff coordinates. The result would be a unitary operator T, defined on the boundary of the billiard. Since the dynamics is assumed to be chaotic anyway, we pretend that the dynamics is periodic, with the evolution over one period (the average one-bounce time) given by T. Now, we discretize the boundary and replace T with the Floquet operator F for the chaotic kicked rotor. For the study of generic properties, the actual dynamics of the system does not really matter (as long as it is sufficiently chaotic). Finally, the ballistic openings are implemented, by choosing some sites on the boundary to be perfect absorbers for the evolving wavefunction.
The open kicked rotor has been used previously to describe transport in systems with a finite Ehrenfest time [1] (and references therein). However, in our case, it was essential to modify the model in order to conserve time reversal invariance when the quantum map is connected to decay channels. In the case of time reversal invariance the Floquet operator can be written as the product of two unitary matrices: $F = F_{\rm out}\, F_{\rm in}$. To introduce decay, we specify an N-dimensional subspace (spanned by the column vectors of p) within the M-dimensional Hilbert space of F. That subspace provides the interface between the closed system and the decay channels. For ballistic decay (ideal coupling) we define $Q = \mathbb{1} - p\,p^T$ and obtain the time-reversal symmetric open quantum map

$$\psi(n+1) = F_{\rm in}\; Q\; F_{\rm out}\; \psi(n)\;, \tag{1}$$

which describes how the internal wave function ψ is degraded sequentially in successive

decay attempts, where the integer n is the stroboscopic time. For a short excitation pulse which leaves the system in the internal initial state $|\alpha\rangle$, the quantum map yields

$$\psi(n) = \begin{cases} (F_{\rm out}^\dagger\, Q\, F_{\rm in}^\dagger)^{-n}\, |\alpha\rangle & :\ n \leq 0 \\ (F_{\rm in}\, Q\, F_{\rm out})^{n}\, |\alpha\rangle & :\ n \geq 0 \end{cases} \tag{2}$$

for the forward and reversed time evolution of the system. With time $t = n/M$ measured in units of the Heisenberg time, the stroboscopic form factor is

$$\hat{C}(n/M) = M\, |\langle\alpha|\psi(n)\rangle|^2 = \langle\alpha|\psi(n)\rangle\, \langle\alpha|\psi(-n)\rangle\ . \tag{3}$$

Direct processes

We incorporate quasi-deterministic fast processes by assuming that part of the initial amplitude escapes during the first iteration of the map. Note that the form factor contains the forward, but also the backward (time-reversed) evolution. Hence, it will be sensitive to direct decay in either direction. To study this dependence quantitatively, we assume the following decomposition for the initial state:

$$|\alpha\rangle = |\alpha_0\rangle + F_{\rm out}^\dagger\, p\, |\alpha^+\rangle + F_{\rm in}\, p\, |\alpha^-\rangle\ . \tag{4}$$

While $|\alpha_0\rangle$ leads to purely indirect decay, $\|\alpha^\pm\|^2$ gives the probability for direct decay within the first step of the open map, forward (backward) in time. In [6] we computed the random matrix prediction for the form factor analytically, and showed that it depends on $|\alpha\rangle$ only via the parameters $\|\alpha_0\|^2$, $\|\alpha^+\|^2$, $\|\alpha^-\|^2$, and $\langle\alpha^+|\alpha^-\rangle$. Note that an excitation process which preserves time reversal invariance excites the system into a state $|\alpha\rangle$ with real coefficients. In that case, $|\alpha^+\rangle = |\alpha^-\rangle$ must hold such that the decay process becomes symmetric in time. If we imagine a sharp excitation pulse at $t = 0$ (instead of a stationary excitation), we discover that at most half of the initial wavepacket can leave the system directly.

Dynamical model simulations

For the numerical simulations, we used the Floquet matrix of the kicked rotor in position representation. We used parameters such that all unitary symmetries in the system were broken and only the time reversal symmetry was left. For $|\alpha\rangle$ we used Gaussian minimal-uncertainty wavepackets, chosen such that the state would take the desired routes to direct decay with certain probabilities. We simulated ensemble averages by changing the kick strength in quantum mechanically large, but classically small steps.

In Fig. 3 (taken from Ref. [6]) we show a series of numerical simulations for maximally asymmetric decay, $\|\alpha^+\|^2 = 0$, $\|\alpha^-\|^2 + \|\alpha_0\|^2 = 1$. The figure illustrates the interference-effects of quasi-deterministic decay in the form factor at long times, as well as the validity of our theory. To clarify the significance of these effects in a single experiment, we considered the integrated form factor

$$Y(t) = \frac{2}{t\,\hat{C}(20)} \sum_{m=20}^{Mt} \frac{\hat{C}(m/M)}{C_0(m/M) - C_{01}(m/M)}\ . \tag{5}$$

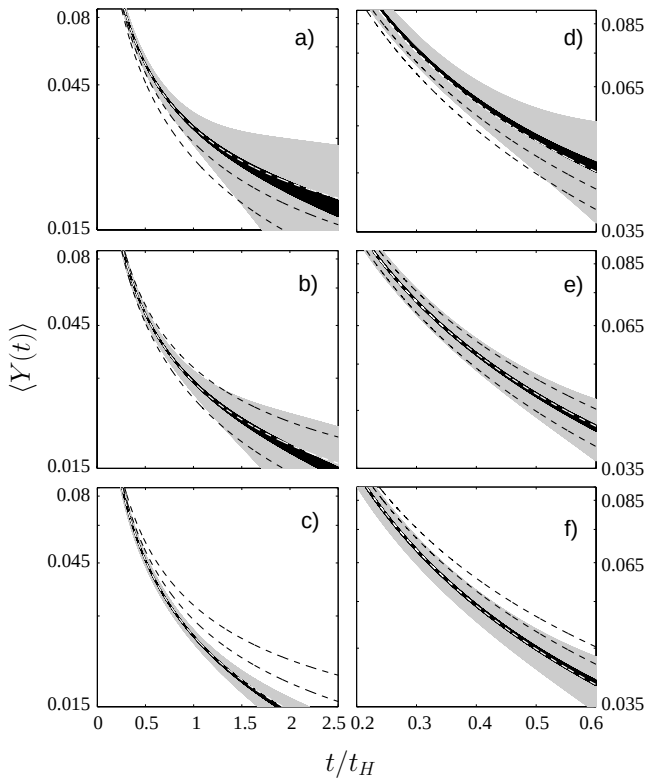

Figure 1: *Numerical data and theory for the integrated form factor $Y(t)$, for $N = 20$ channels (left panels) and $N = 50$ channels (right panels). The overlap of the initial state with the regions of fast decay is given by $\|\alpha^-\|^2 = 0$ (a), 0.595 (b), 0.907 (c), 0 (d), 0.571 (e), and 0.906 (f). Areas in gray represent the standard deviation of $Y(t)$, while areas in black represent the standard deviation of $\langle Y(t) \rangle$ when the average is taken over 100 samples. The dashed lines show the theoretical curves for the different values for $\|\alpha^-\|^2$; the respective theoretical curve corresponding to the numerical result is plotted in light gray.*

It efficiently suppresses fluctuations in time, such that only sample-to-sample fluctuations survive. $C_0(t)$ is the universal form factor in the absence of direct processes, and $C_{01}(t)$ is theoretical form factor in the limit $\|\alpha_0\|^2 \to 0$. The sample-to-sample fluctuations are shown in Fig. 3 by the gray areas, while the expected standard deviation for the average over 100 samples is shown in black. The dashed lines show the different theoretical curves, obtained from our theory, that fit best to each of the numerical results. The figure shows that the fluctuations decrease considerably as the probability for direct decay is increased. This means, that the presence of direct processes can be excluded with higher confidence than their absence. It also shows, that fewer channels allow more precise estimates for the probability for direct decay.

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3.22 Derivative Discontinuities in Time-Dependent Density-Functional Theory

Michael Mundt and Stephan Kümmel

Time-dependent density-functional theory (TDDFT) has become one of the most widely used theories for investigating time-dependent processes in atoms, molecules and solids. TDDFT describes the dynamics of an electronic system in terms of only its time-dependent electron density. Due to the resulting numerical simplicity, the theory allows one to approach on a first principles basis problems that are too complex for wave-function based methods. This is particularly important for the area of nonlinear, non-perturbative electronic excitations, since solving the fully time-dependent, three-dimensional Schrödinger equation is totally out of reach for larger systems. The advances in laser technology and the increasing interest in nonlinear phenomena, on the other hand, call for a reliable theoretical tool to explore these regimes. TDDFT offers the chance to be this tool.

One of the most fundamental quantities in TDDFT is the exchange-correlation potential. In this project a previously overlooked property of the exchange-correlation potential which has far reaching consequences for describing strong-field phenomena was investigated. When a finite system is exposed to a strong, ionizing field, e.g., the electrical field of a pulsed laser, some of the electronic density can move far away from the system's center. Simulating this process in TDDFT typically leads to a situation where the density that remains bound integrates to a fractional number of electrons. From *static* DFT it is known that fractional particle numbers lead to a "jump" in the exchange-correlation potential, and this jump has a profound influence on physical properties like band gaps of solids and response properties of molecules. Although this fact had been known for many years, so far it had not been investigated how the *time-dependent* exchange-correlation potential depends on the particle number. This question lies at the heart of why TDDFT fails for a paradigm problem, the strong-field double ionization of the Helium atom [1]. In the present project [2] we showed that the *time-dependent* exchange-correlation potential must jump discontinuously whenever the particle number crosses an integer value. We further demonstrated that such a discontinuity appears naturally in the theory of the time-dependent optimized effective potential. The latter is the proper way to include orbital functionals into Kohn-Sham density functional theory. Thus, orbital functionals can be a natural and successful way towards a reliable description of strong-field phenomena on a TDDFT basis.

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3.23 Many-Body Effects in the Mesoscopic X-Ray Edge Problem

Swarnali Bandopadhyay, Georg Röder, and Martina Hentschel

Many-body phenomena such as the Kondo effect or Fermi edge singularities have always been of great interest in condensed matter physics. The progress in the fabrication and investigation of micro- and nanoscale samples, such as quantum dots or metallic nanoparticles, during the last 15 years suggests to study many-body effects in the *mesoscopic* regime – thereby combining the richness of many-body physics with the unique opportunities of the mesoscopic world. Here, we theoretically address the x-ray edge problem [1] in mesoscopic systems [2, 3].

In the photoabsorption process underlying the x-ray edge problem for metals, an x-ray excites a core electron into the conduction band. Two counteracting many-body responses of the system lead to deviations from the naive expectation in the form of a peaked or rounded photoabsorption edge. Besides the Mahan-Nozières-DeDominicis response that is present under certain conditions, Anderson orthogonality catastrophe constitutes an universal many-body response mechanism of the system to the sudden appearance of the core hole left behind. As a result, the overlap between the unperturbed and perturbed many-body ground states tends to zero in the thermodynamic limit [4]. This does not hold, however, in the mesoscopic regime where the typical number of electrons in the system ranges from less than a dozen to a few thousands. Although these numbers might, on first sight, suggest that there are still *many* particles involved, the considerably smaller system size can be appreciated once compared to the 10^{23} electrons typical for metallic samples. As characteristic for many-body phenomena, the Anderson overlap vanishes (only) as a power law in the number of particles.

Other differences to the metallic case are the presence of fluctuations inherent to the mesoscopic regime as well as the coherent dynamic of the ballistic electrons that, moreover, depends on the geometry of the system. At this point ideas and concepts from the field of quantum chaos enter classic condensed matter physics and can cause qualitatively different behaviour of the metallic and mesoscopic system, respectively. For example, based on a Fermi golden approach to the photoabsorption cross section [1] it was shown that an edge that is typically rounded in the metallic case develops a (slight) peak as the size of the system is reduced to the mesoscopic-coherent scale [2], cf. Fig. 1. Here, chaotic dynamics of the electrons was assumed [2, 3].

In the following, we focus on Anderson orthogonality catastrophe in regular mesoscopic systems. We solve the Schrödinger equation exactly and model the sudden appearance of a core hole (or a comparable potential) as a rank-one perturbation [1, 3] of certain strength v_c acting at a position $\vec{r}_c$. The relation to the physical reality is established by relating the perturbation strength to the experimentally observable phase shift at the Fermi energy [3]. The perturbed single-particle energies can be found numerically. One appealing feature of a rank-one perturbation is that all quantities of interest, in particular the Anderson overlap, can be computed from the unperturbed and perturbed single-particle energies alone (unless they can be taken as independent random variables).

Results for the Anderson overlap as a function of filling (of a conduction band with N

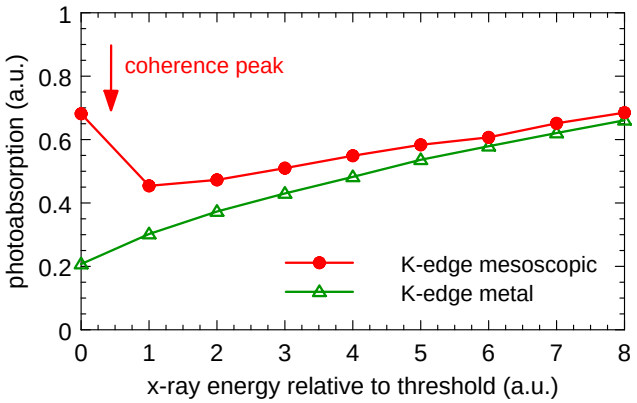

Figure 1: *Photoabsorption spectra for a chaotic-coherent mesoscopic system (filled circles mark the average values) and a metallic probe (open triangles). The different dynamics of electrons in mesoscopic systems results in a coherence peak at the K-edge threshold as opposed to a rounded edge observed in metals.*

levels) and perturbation strength are shown in Fig. 2. The upper left panel is the so-called bulklike situation, referring to a system with equidistantly spaced unperturbed energy levels and uniform wave function amplitudes throughout the system – the situation that, apart from the finite number of particles, mimics the metallic case. In the rank-one model used here, the Anderson overlap shows a characteristic dependence on the filling due to bound any effects and for otherwise equal conditions, will diminish with increasing system size [3]. Now turning to a circular quantum dot with hard walls as a simple example of a regular mesoscopic system, fluctuations superimposed on the bulklike structure are clearly visible, see the upper right panels of Fig. 2. They originate in the non-uniform distribution of the wave function in the system. For a single-particle wave function with large (modulus of the) amplitude at the position of the perturbation, the effectively felt perturbation strength is increased and the Anderson overlap decreases. Consequently, the result will depend on the position of the perturbation as is illustrated in Fig. 2.

A more involved situation arises in the experimentelly well established case of quantum dots with parabolic confinement potential [5], cf. lower row in Fig. 2. Here, the unperturbed energy levels form degenerate shells with 1,2,3, ... electrons. For clarity, let us assume that the degeneracies are lifted by a small magnetic control field that equidistantly separates the formerly degenerate levels within one shell but does not disturb the overall shell structure. Assuming uniform wave function amplitudes (bulklike case, lower left panel) and very small perturbation strengths, each shell individually resembles the bulklike behaviour [6]. Towards larger perturbation strengths, the shell structure remains clearly visible and is superposed on the bulklike behaviour shown in the panel above. Taking now the correct wave functions into account, mesoscopic fluctuations depending on the position of the perturbation again become evident as shown in the remaining two panels of Fig. 2. The shell structure is still prominent but modified due to the specific spatial dependence of the wave functions, and the electrons appear in bunches of a few electrons. The consequences of Anderson orthogonality catastrophe on the photoexcitation and photoabsorption spectra of regular mesoscopic systems are presently under investigation and will be published elsewhere [6]. They can be addressed, for example, in experiments where the core level is replaced by a suitable impurity level which are possible using nowadays state-of-the-art technology. Such measurements are also well suited to experimentally confirm the existence of the coherence peak discussed in Fig. 1 above for chaotic mesoscopic systems.

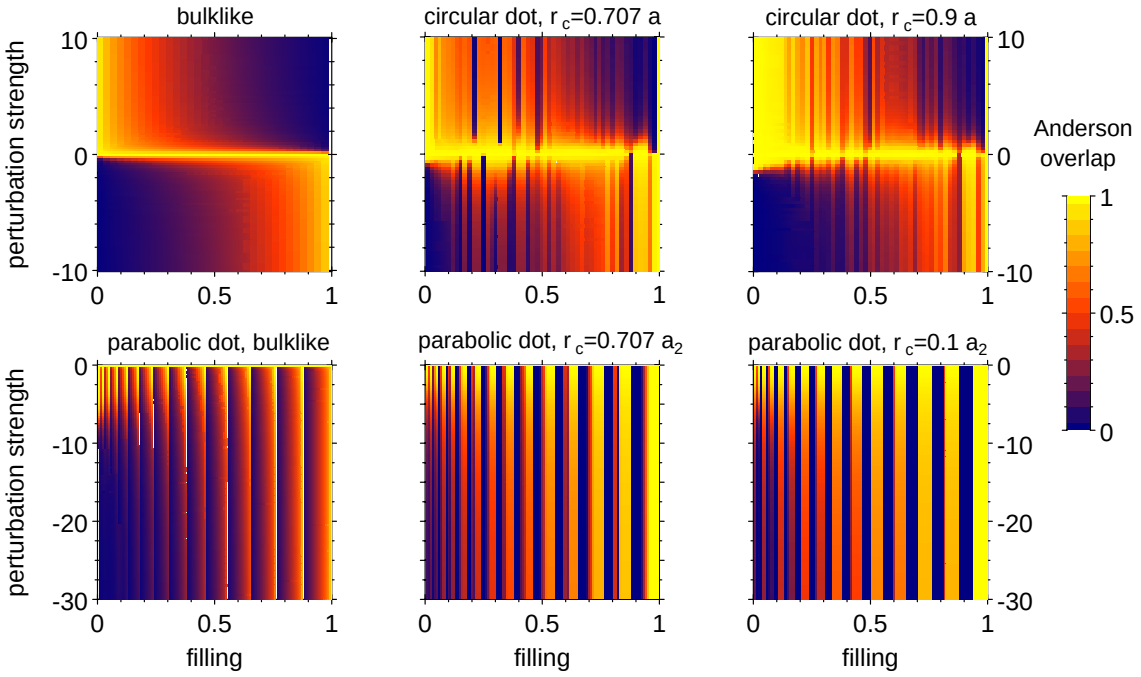

Figure 2: *Anderson orthogonality catastrophe in various mesoscopic systems. Shown in color scale is the Anderson overlap as a function of band filling and perturbation strength. Top row: Non-degenerate bulklike case (left panel) and the case of a circular quantum dot (radius a) with two different positions r_c of the perturbation considered (right panels, $N = 100$ levels). Mesoscopic fluctuations, induced by the spatial variations in the wave function amplitudes, are evident. Lower row: Same for the degenerate case of a parabolic quantum dot ($N = 120$, a_2 is the oscillator length). In the bulklike case (left panel), pronounced shell effects are superposed on the structure observed for the nondegenerate case (cf. panel above). The shell effects survive the induced mesoscopic fluctuations but are modified (right panels).*

The physics that we describe here, namely the sudden perturbation of a (mesoscopic) Fermi sea of electrons by a localized potential, is of importance not only in the context of the x-ray problem but also for mesoscopic transport. It is interesting to note that a bunching behaviour of electrons similar to the one described above has been reported in transport measurements on quantum dots with up to 200 electrons by Ashoori and coworkers [7]. Their measured electron addition spectra did not show an even spacing in gate voltage. Rather, pronounced correlations were observed such as electron additions grouped in bunches containing 2 to 6 electrons. It was argued that tunneling of electrons into different spatial areas of the dot could explain this behaviour. Here, we provide qualitative support for this idea based on a full many-body analysis of the Anderson overlap [6].

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3.24 Interphase Microtubules Align the Mitotic Spindle

Sven K.Vogel, Isabel Raabe, Aygül Dereli, Nicola Maghelli, and Iva Tolić-Nørrelykke

For a successful cell division, the mitotic spindle has to be properly positioned and aligned with respect to the cell cleavage plane in order to segregate the chromosomes to the future daughter cells. In some cell types spindle position determines the cell division site, which in turn affects cell shape and size, as well as tissue organization. Key questions are when and how the spindle gets aligned with the cell axis.
In the fission yeast *Schizosaccharomyces pombe*, interphase microtubules (MTs) position the nucleus [2, 5]. The nucleus then positions the cell division plane [2, 6]. It is unclear how the spindle orients, with respect to the predetermined division plane, to ensure that the chromosomes are segregated across this plane.

Initial spindle alignment is determined by the alignment of the interphase MTs. In the cylindrically shaped cells of fission yeast, interphase MTs lie approximately parallel to the cell axis. The spindle pole body (SPB) duplicates long before mitosis; the two parts are connected and attached to the outside of the nuclear envelope and to interphase MTs [8]. At the onset of mitosis the interphase MTs disassemble, while the two SPBs begin to move apart by growth and sliding of interpolar MTs. We noticed that the SPBs separated apparently along the axis of the interphase MT to which they were attached [1]. This observation led us to hypothesize that interphase MTs guide the alignment of the duplicated SPB prior to mitosis, which in turn defines the initial alignment of the mitotic spindle parallel to the cell's longitudinal axis, see Fig. 1A-C. This hypothesis predicts that impaired interphase MTs should lead to misalignment of newly formed spindles. If the interphase MTs are, on average, not much longer than the cell width, they may be less constrained by the cell shape and hence more misaligned than long MTs. As a consequence, the spindles formed in the following cell division may be misaligned. This hypothesis was tested using a $mal3\Delta$ mutant: Mal3 protein associates with MTs and suppresses MT catastrophe, thus $mal3\Delta$ cells have short interphase MTs [10]. In comparison with wild type, we found that the newly formed $mal3\Delta$ spindles were significantly more misaligned, often clearly following the axis of the interphase MT to which they were attached [1]. This result is consistent with the above hypothesis that the axis of a nascent spindle follows the axis of the interphase MT attached to the SPB.

To further test the role of MTs in spindle alignment, we depolymerized interphase MTs chemically. The cells without interphase MTs displayed highly misaligned spindles. Misaligned spindles were also found in a mutant [9] where interphase MTs are typically detached from the SPB. In summary, initial spindle alignment follows the alignment of the interphase microtubules attached to the SPB. Detachment of the SPB from interphase MTs, predominance of short misaligned interphase MTs, as well as absence of interphase MTs, lead to misalignment of nascent spindles, see Fig. 1D.

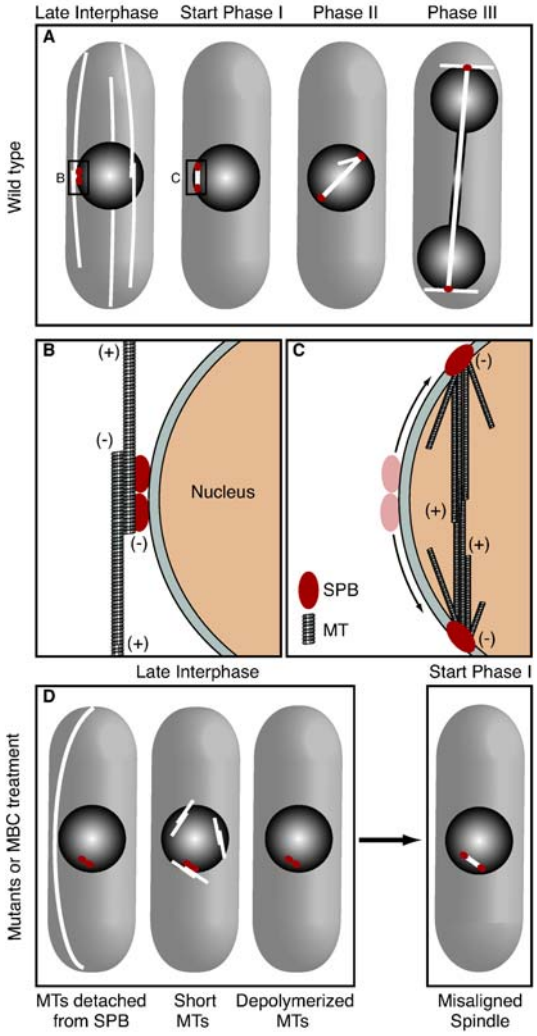

Figure 1: *A model for spindle alignment in fission yeast: Interphase microtubules (MTs) determine the initial alignment, while the cell shape and astral MTs make final corrections during Phase III (anaphase). (A-C) In wild-type cells, interphase MTs align the duplicated spindle pole body (SPB) with the cell's longitudinal axis, setting the axis for future SPB separation. Consequently, the nascent spindle is well aligned with the cell axis (B-C). This alignment is later lost through random movements of the spindle, but the loss of alignment does not delay entry into Phase III (anaphase), i.e., there is no alignment checkpoint. Spindle alignment is corrected in Phase III, when the elongating spindle is constrained by the cell shape and assisted by pushing forces of astral MTs. (D) Defects in interphase MT dynamics and attachment of MTs to the SPB lead to misaligned spindles at the beginning of the subsequent mitosis.*

Spindle Orientation Checkpoint does not operate in fission yeast. We asked whether spindle alignment affects progress through mitosis. A number of recent studies have suggested a Spindle Orientation Checkpoint (SOC) in fission yeast [7], analogous to the established SOC in budding yeast [11]. According to the SOC idea, well-aligned spindles start anaphase on schedule, whereas misaligned spindles exhibit a metaphase delay until they become aligned.

A direct way to test the idea of SOC is a single-cell analysis of the correlation between spindle angles and the progress through mitosis. If SOC operates, then the cells that have a misaligned spindle should exhibit a longer metaphase than the cells with aligned spindles. Surprisingly, we found no correlation between the duration of metaphase

and the spindle angle [1]. This result is not consistent with a checkpoint for spindle alignment per se (SOC) in fission yeast.
Why does fission yeast, in contrast to budding yeast, proceed with mitosis without checking the spindle alignment? The answer probably lies in the different geometries of the two yeasts. The cylindrical shape of fission yeast cells facilitates mitosis: the cell shape forces an elongating spindle to align with the cell's longitudinal axis, which results in a correct separation of the genetic material towards the tips of the future daughter cells. The budded shape of budding yeast, on the other hand, provides a difficulty for mitosis: one pole of the spindle, which is formed in the mother cell, has to pass through the narrow neck into the bud. Thus, a checkpoint mechanism for the spindle position and alignment is necessary in budding yeast to ensure that the bud actually receives a nucleus.

Initial misalignment of the spindle can lead to cells without a nucleus. If the degree of early spindle alignment does not affect progression through mitosis in normal growth conditions, then what is the biological significance of spindle alignment? We hypothesized that proper spindle alignment promotes correct segregation of the two sets of chromosomes across the division plane. Spindle alignment depends on three mechanisms: interphase MTs align the spindle at the beginning of mitosis, whereas cell shape and astral MTs align the spindle during anaphase. In order to test the significance of the first mechanism (interphase MTs), we perturbed the other two (cell shape and astral MTs) by treating the cells with a MT-depolymerizing chemical. We first treated the cells during metaphase to abolish the cell shape and astral MTs mechanism, but not the interphase MTs mechanism, and measured the frequency of equal nuclear segregation (1 nucleus per daughter cell) versus unequal nuclear segregation (0 or 2 nuclei per daughter cell). All the cells finished mitosis normally, with equal nuclear segregation ($n = 16$ out of 16 cells).
Next, we treated the cells with a MT-depolymerizing chemical before mitosis to abolish all three mechanisms of spindle alignment. Remarkably, 31% of the cells segregated the nuclei unequally ($n = 137$). Moreover, the cells with highly misaligned spindles at the beginning of mitosis showed unequal nuclear segregation more frequently than the cells with initially aligned spindles [1]. Our explanation of these results is that, even when elongating slowly, aligned spindles typically cross the cell cleavage plane before its closure because they elongate nearly perpendicular to this plane. Misaligned spindles, on the other hand, start elongating almost parallel to the cell cleavage plane, thus, the cell cleavage often confines the spindle to one daughter cell. Our results suggest that the mechanism of spindle alignment by interphase MTs is important for correct nuclear segregation in conditions where the other alignment mechanisms (cell shape and astral MTs) are impaired and may, therefore, be of evolutionary advantage.

Summary. Fission yeast spindles attain proper alignment by three mechanisms: driven by interphase MTs, as revealed in our recent study [1], and by cell shape and astral MTs, as shown in our previous work [3], see Fig. 1. At the very beginning of mitosis, the newly formed spindle is already well aligned with the cell's longitudinal axis. We propose that the interphase MTs attached to the duplicated SPB serve as a template for SPB separation during spindle formation. Our results suggest a novel role for interphase microtubules: in addition to determining the nuclear and, consequently,

the division plane position [2, 5, 6], they also determine the initial alignment of the mitotic spindle [1]. Proper spindle alignment, in turn, facilitates correct segregation of chromosomes across the division plane. This work in fission yeast may help to clarify similar mechanisms in other cell types where spatial cues in interphase determine the initial position of the mitotic spindle before the subsequent cell division [4].

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Chapter 4

Details and Data

4.1 PhD Program

The training of PhD students is one of the central educative tasks of the mpi**pks**. It is realized through a large institute PhD program, our leading role in the IMPRS "Dynamical Processes in Atoms, Molecules and Solids" (see next section) and our participation in the IMPRS "Molecular Cell Biology and Bioengineering" which is coordinated by the Max Planck Institute for Cell Biology and Genetics.
Prospective PhD students have several options of contacting scientific advisors at mpi**pks**. PhD position openings funded through external grants are advertised in scientific journals and on the internet pages of the institute. In addition there is a permanent advertising of PhD positions funded through the Visitors Program on the internet pages of the institute and in several information booklets. Finally, a significant part of PhD students is recruited through personal contacts with potential scientific advisors at mpi**pks**. Since the begin of operation of the International Max Planck Research School the number of PhD students substantially increased.
The success of this strategy is well documented in previous scientific reports of mpi**pks**. In 2005 we had a total of 29 PhD students at mpi**pks**, including 7 students from abroad (these numbers count all students, i.e. including those who finished their PhD studies or just started their studies during that year). The respective numbers for 2006 were a total of 35 PhD students at mpi**pks**, including 8 students from abroad. We counted 6 successful final PhD exams for the year 2005 and 6 exams for the year 2006.
Besides their scientific work at mpi**pks** our PhD students use several further types of activities to strengthen their academic and communicative skills. In addition to lecture courses offered at the TU Dresden the mpi**pks** provides lecture courses on modern topics of theoretical physics on a regular basis. PhD students can join workshop talks and seminar lectures of the Workshop and Seminar Program of mpi**pks**. Many of them participate actively in these events by presenting short talks or posters. Our institute organizes annual PhD Student Days (1-2 days). All students of mpi**pks** participate in this meeting and present short talks on their current research results. A PhD student exchange program with East European countries like Poland or Czech Republic, which is supported by the Max Planck Society, allows our students to visit cooperating research groups and to present talks, as well as to coach visiting PhD students from those groups at mpi**pks**. The mpi**pks** offers financial and logistic support for joining German language courses for our PhD students from abroad in order to help with

integration into the German speaking community.
A growing number of PhD students pass the final PhD exams at the TU Dresden. Still, some students are obtaining the PhD degree from various universities throughout Germany. After obtaining the PhD degree most of our students continue their research work by accepting PostDoc positions at research institutions in various countries. A significant part is also successfully applying for positions in companies in such areas as applied research, informatics, finance and consulting. The mpi**pks** organizes regular alumni meetings of former PhD students with discussion rounds to provide a transfer of experience for our present PhD students.

4.2 International Max Planck Research School

The International Max Planck Research School for "Dynamical Processes in Atoms, Molecules and Solids" (hereafter referred to as IMPRS) started its operation in January 2005. It belongs to the 4th round of approved research schools of the Max Planck Society.
The IMPRS is a collaboration of the following institutions

- Technische Universität Dresden — TUD
- Forschungszentrum Dresden-Rossendorf — FZD
- Leibniz Institute for Solid State and Materials Research — IFW
- Max Planck Institute for Chemical Physics of Solids — MPI-CPfS
- Max Planck Institute for the Physics of Complex Systems
- Institute of Low Temperature and Structure Research — ILTSR (Polish Academy of Science Wrocław/Poland)

It was founded to attract talented students, who want to obtain a PhD in atomic, molecular or solid state physics, to Dresden. The research focus is on dynamical processes and comprises theoretical and experimental work. PhD students do their research in one of the participating groups and take part in the seminar and lecture program offered by the IMPRS.

PhD students of the school
The IMPRS has admitted so far 37 PhD students. Whereas about one third of the students are Germans, the other two thirds come from all over the world. The dominating countries are Poland (4 students), Romania (3), Ukraine (3) and China (3). The affiliation to the participating partners is as follows, TUD: 7, FZD: 1, IFW: 10, MPI-CPfS: 2, mpi**pks**: 10, ILTSR: 4. The four Polish students are inscribed in Wrocław universities and are financed by grants of the Klaus-Tschira Foundation. Three of them spent about a year of their PhD studies at the IFW and the MPI-CPfS, respectively, in Dresden and were for this stay financially supported by the IMPRS.
In the starting phase of the IMPRS (spring 2005) we admitted PhD students who had started their PhD projects in one of the partner institutions before the foundation of the IMPRS. Two of them, Andreas Neudert and Christian Thiele, both IFW, have

already obtained their doctoral degree.

Seminar and lecture program
One of the regular meeting points for all students is the monthly IMPRS seminar. Each seminar starts with a pre-talk given by an IMPRS student, followed by an invited talk given by an external speaker. These speakers are invited on proposals by supervisors and students from the participating research groups and thus cover the broad scientific spectrum of the IMPRS.
The lecture program follows the schedule of the Technische Universität Dresden with winter (October – February) and summer (April – July) terms. The lectures are given by professors from the university and young researchers from the various partner institutions including the mpi**pks**. We offer about four lectures per term. They are open to students from the Technische Universität Dresden. Participation of the IMPRS students in the lectures is monitored by a credit-point system.

Figure 1: IMPRS *meeting in Gohrisch (Sächsische Schweiz) in October 2006.*

Scientific events
In connection with the official opening ceremony in September 2005 we started a series of IMPRS meetings held in autumn somewhere in the Sächsiche Schweiz (see Fig. 1). In these meetings the PhD students present their work in extended talks to provoke discussions among all students including those working in different fields. Furthermore, contact to the newly arrived students of the IMPRS is initiated.
We plan to establish regular spring schools with a different scientific focus each year. At these schools the lectures are given by senior researchers. The first one of this series was organized by our Polish partners in May 2006 in Wrocław and dealt with modern aspects of superconductivity.
In February 2006 a presentation skill seminar lead by Kerstin Kathy Meyer-Ross (Max-Planck-Institut Informatik, Saarbrücken) took place at the mpi**pks**. In this one-and-a-

half-day course the students worked on their presentation technique.

Organization and administrative matters
The school is operated by the IMPRS board with the following members:

Prof. Dr. Jan-Michael Rost (chairman, mpi**pks**)
Prof. Dr. Roland Ketzmerick (TUD)
Prof. Dr. Michael Loewenhaupt (TUD)
Prof. Dr. Gotthard Seifert (TUD)
Prof. Dr. Helmut Eschrig (IFW)
Prof. Dr. Yuri Grin (MPI-CPfS)
Prof. Dr. Peter Fulde (mpi**pks**)
Prof. Dr. Jozef Sznajd (ILTSR Wrocław)
Dr. Ulf Saalmann (coordinator, mpi**pks**)

There are two board meetings a year, where the board discusses and decides all matters regarding the operation of the IMPRS. This comprises the admission of new students, the distribution of the IMPRS resources (in particular grants), the seminar and lecture program, organization of summer/winter schools or other IMPRS meetings.
The executive board, consisting of Prof. Rost, Prof. Loewenhaupt and Dr. Saalmann, meets if required. It does in particular a pre-screening of the numerous applications we get. The "daily coordination", i. e. contact to students, application and admission procedure, advertisements, organization of the lecture and seminar program and maintenance of the web-page (`http://www.imprs-dynamics.mpg.de`), is done at the mpi**pks**.

4.3 Workshop and Visitors Program

The Visitors Program of mpi**pks** hosts guest scientists for a period of usually up to two years. Excellent working conditions are offered to the qualified, mostly young, scientists. This also includes logistic help, e.g., for finding suitable accommodation, solving visa problems etc. The close collaboration with administrative units responsible for, e.g., the computational and technical equipments of the offices allows the guest scientists to fully concentrate their efforts on research. Informal Tea Seminars, a weekly *Young Scientists Jam Session* and financial support for joining German language courses help to integrate our guest scientists fast and easily into the local community. Many guest scientists participate actively in the events of the Workshop and Seminar Program of mpi**pks**.
During 2005 the mpi**pks** hosted 111 guest scientists with contracts for at least three months, and 114 during the year 2006. We enjoyed a large number of senior scientists who used their sabbatical time for long-term research stays at mpi**pks**. This led to an enhancement of transfer of experience to young scientists at the institute. In 2006 the institute decided to install an *Advanced Study Group* each year at mpi**pks**. These groups will consist of 3-5 experienced researchers, who join forces to do cutting-edge research on a topic from the field of the physics of complex systems. The first *Advanced Study Group 2007* will start its activities in March 2007.

The guest scientists are usually linked to the research groups at mpi**pks**. In some cases they conduct more independent research, which leads to synergetic effects, including recent temporary collaborations at the institute on *Bose-Einstein condensation*. Synergetic effects are also enhanced due to the possibility to listen to talks and lectures within the Seminar and Workshop Program of mpi**pks** (see p. 168).
In addition to the regular positions of the Visitors Program the institute annually offers a Distinguished PKS Postdoctoral Position for experienced postdoctoral scientists for up to three years. PKS Fellows do research in areas related to but not directly represented by the work done in the mpi**pks** research groups. Two PKS Fellows are currently working at mpi**pks**: *Dr. Kay Hamacher* on *Computational Methods for Investigating Structures and Functions of Molecular Systems*, *Dr. Benjamin Lindner* on *Modelling of Nonequilibrium Processes in Biological Physics*, see report on p. 159. Two PKS fellows have left the institute: *Dr. Abhik Basu* (*Statistical Dynamics of Nonequilibrium Systems*) took a researcher position at the Saha Institute of Nuclear Physics in Calcutta, and *Dr. Joachim Brand* (*Physics of Bose-Einstein Condensates*) accepted a lectureship at the Massey University Auckland.
Together with the TU Braunschweig the institute supports a junior professorship (*Prof. Ilya Eremin*, see report on p. 161). *Prof. Eremin* is teaching at Braunschweig, and is conducting research work at mpi**pks**.
To strengthen the transfer of knowledge and experience at mpi**pks**, the institute awards annually the Martin Gutzwiller Fellowship to a senior scientist with exceptional contributions in the area of the physics of complex systems. Gutzwiller Fellows spend up to one year at mpi**pks** and have the possibility to nominate a young guest scientist for the Visitors Program. The 2005 and 2006 fellows were *Prof. Lawrence S. Schulman* and *Prof. Steven L. Tomsovic* (see report on p. 163).
A considerable number of guest scientists leave the institute for permanent positions in the academic sector, besides many others who continue with postdoctoral positions at other institutions in Germany or abroad. Several guest scientists leave for positions in the non-academic sector, such as applied research, informatics, finance or consulting.
In addition to the long-term guest scientist positions the Visitors Program also hosts many short-term visits (for up to three months). These visits are usually due to collaborations of the research groups at mpi**pks** with other institutes. Their number reached new levels, 242 during the year 2005 and 230 during the year 2006.

4.3.1 PKS-Fellowship

Report by *Dr. Benjamin Lindner*: Stochastic Processes in Neurophysics

Sensory neurons transmit information via stereotypic electric discharges of the potential across their membrane known as *action potentials* or *spikes*. Since this neural activity displays a strong random component, the neural coding of sensory information should be studied within the frame work of stochastic nonlinear dynamical systems.
I am interested in how different aspects of the neural dynamics (for instance, temporal and spatial correlations, feedback with temporal delay, synaptic short-term plasticity, and, of course, noise) affect the transmission and processing of sensory information. Using methods from statistical physics, I aim at analytical solutions as well as fast simulation algorithms for simplified yet realistic models of neural activity and sensory

processing.

Projects at the mpipks

With *Rafael Vilela De Oliveira* (Postdoc at the mpi**pks**) I work on the role of temporal and spatial correlations in the input to simple model neurons. I study the role of synaptic shot noise for the dynamics of the subthreshold membrane potential together with *Lars Wolff* (Diploma student). At the mpi**pks** I have also turned to auditory systems and the signal transfer by sensory hair cells. In collaboration with *Prof. Frank Jülicher*, *Kai Dierkes* (PhD student), and *Diana Claußnitzer* (Diploma student), I work on the stochastic dynamics of single and coupled hair cells, developing analytical approaches for their spectral statistics. I also collaborate with *Ernesto Nicola* (Postdoc at the mpi**pks**) studying models of nonlinear Brownian motion and their application to molecular motors and self-propelled motion in biology.

External collaborations

With *Brent Doiron* and *Andre Longtin* from the University of Ottawa (Canada), I developed a theory of spectral measures in biological neural networks with time-delayed global feedback. Another project in collaboration with *John Lewis* (Dep. of Biology, University of Ottawa) deals with short-term plasticity of synaptic transmission and its role in signal transmission. With *Maurice Chacron* at the University McGill in Montreal (Canada) I pursue the study of correlations in sequences of interspike intervals and their implications for neural coding. I also studied the related problem of correlations in the sequence of escape times with *Tilo Schwalger* from the Humboldt University Berlin.

Further activities

During the last semester I gave lectures on *Stochastic Processes* at the Technical University Dresden. Currently, I am preparing a workshop on stochastic processes in the life sciences ("Noise in Life") that will take place in November 2007 at the mpi**pks**.

Acknowledgment

Let me acknowledge the efforts of the Visitor's program, of the administration, and of the IT service at the mpi**pks** for providing just the perfect conditions for our scientific work here at the institute. Special thanks go to Prof. Frank Jülicher for a number of inspiring discussions and his general support of my work.

Articles completed and written at the mpipks

- B. Lindner, B. Doiron, and A. Longtin: *Theory of oscillatory firing induced by spatially correlated noise and delayed feedback* Phys. Rev. E **72** (2005) 061919.
- B. Lindner: *Correlations in sequences of first-passage times* AIP Proc. **800** (2005) 323.
- B. Lindner: *Superposition of many independent spike trains is generally not a Poisson process* Phys. Rev. E **73** (2006) 022901.
- B. Lindner: *Diffusion aktiver Brownscher Teilchen in einer Raumdimension* in *Physik Irreversibler Prozesse und Selbstorganisation* ed. T. Pöschel, H. Malchow, and L. Schimansky-Geier, Logos-Verlag (2006).

- M. Chacron, B. Lindner, and A. Longtin *Threshold fatigue and information transfer* submitted.
- B. Lindner: *The diffusion coefficient of nonlinear Brownian motion* submitted.
- B. Lindner and T. Schwalger *Correlations in the sequence of residence times* submitted.
- B. Lindner, A. Longtin, and J.E. Lewis *Broadband coding with dynamical synapses* submitted.

4.3.2 Junior Professorship

Report by *Dr. Ilya Eremin*: Unconventional superconductivity and magnetism in strongly correlated electronic systems

The study of unconventional superconducting materials such as the heavy-fermion superconductors and the high-Tc cuprates has been at the forefront of scientific research over the last two decades, and revealing their mystery is still one of the most challenging topics of condensed matter physics. Many unconventional superconductors are highly correlated and complex systems whose phase diagrams include magnetic, superconducting, and charge ordered phases in close proximity. Generally, I am interested in studying both analytically and numerically the possible mechanisms of the unconventional superconductivity and their fingerprints and consequences for the spin and the charge dynamics. Furthermore, I am also aiming to understand deeper the aspects of the co-existence and competition between unconventional superconductivity and magnetic and charge ordered phases.

Projects at the mpipks
Together with J.-P. Ismer (Ph. D. student at the mpi**pks**) I work on the understanding the behavior of the spin excitations in the normal and superconducting state of hole- and electron-doped cuprates and their evolution with doping. More recently, together with P. Fulde and Jun Chang, I have also turned to study the feedback of the unconventional superconductivity on the spin dynamics in the heavy-fermion superconductors such as UPd_2Al_3. (see also the contribution on p. 75). I also collaborate with M. Korshunov (INTAS postdoctoral research fellow at mpi**pks**) studying magnetism on the triangular lattices in application to the lamellar cobaltates.

External collaborations
With D. K. Morr and E. Rossi from the University of Illinois at Chicago (USA), and A. Chubukov from University of Wisconsin at Madison (USA) we have studied the resonant excitations in the superconducting hole-doped as well as in the electron-doped cuprates. Our cooperation with UIC is supported through the bilateral DAAD grant. Another project in collaboration with J.F. Annett (Physics Department, Univeristy of Bristol, UK) applies to the study of the non-centrosymmetric superconductors (see also the contribution p. 76). Together with F. Nogueira (Free University of Berlin) I have analyzed the spin and charge Josephson currents between two non-uniform superconductors. With ARPES group from IFW Dresden (S. Borisenko, M. Knupfer, and others) we have performed an analysis of the ARPES experimental data in layered

cuprates and their connection to the inelastic neutron scattering experiments. Most recently, with W. Brenig (TU Braunschweig) we have pursued a study of the many-body effects in the lamellar cobaltates (Na_xCoO_2) as a function of the doping concentration. This work was also partly done in collaboration with the group of V. Anisimov from the Institute of Metal Physics (Ekaterinburg, Russia). Very recently together with J. Sichelschmidt (MPI CPFS, Dresden) and B.I. Kochelaev (Kazan state University, Russian Federation) we have initiated a combined theoretical and experimental study of the electron spin-resonance in the heavy-fermion Kondo compound $YbRh_2Si_2$ supported through the Volkswagen foundation.

Further activities

My duties as a junior-professor include not only scientific research which is done at the mpi**pks** but also teaching at the Physics Department of the Technical University of Braunschweig. During the last two years I have given the following specialized courses there: Special Chapters from Advanced Quantum Mechanics (Winter semester 2005/2006), Group Theory I (Summer semester 2006), Group Theory II and Quantum Electrodynamics (Winter semester 2006/2007). Furthermore, I have also given lectures for the graduate students of the International Max Planck Research School at the Spring Seminar held in Wroclaw, May 22-25, 2006. Together with Prof. Peter Lemmens from TU Braunschweig I am organizing the Internal Symposium of Division Low Temperature Physics of the German Physical Society Spring Meeting in 2007 on Superconductivity and Magnetism of lamellar cobaltates. Currently, I (together with Profs. James F. Annett and Dirk K. Morr) am preparing a workshop on the physics of unconventional superconductors (Competing Orders, Pairing Fluctuations, and Spin Orbit Effects in Novel Unconventional Superconductors) that will take place in June-July 2008 at the mpi**pks**.

Acknowledgment

I would to thank Prof. Peter Fulde for his general support of my work and inspiring discussions on the physics of the strongly correlated electronic systems. Let me also acknowledge the continuous support and help of the faculty members at TU Braunschweig, in particular, Prof Wolfram Brenig, Prof. Peter Lemmens, and Prof. Gertrud Zwicknagl as concerns my work in Braunschweig. My special thanks are to the efforts of the Visitors program of the mpi**pks** and generally to the staff members of the mpi**pks** for providing the excellent working conditions for our research at the institute.

Articles completed and written at the mpipks

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- J. Chang, I. Eremin, P. Thalmeier, and P. Fulde: Theory of magnetic excitations in the heavy-fermion superconductor UPd_2Al_3, Phys. Rev. B **75** (2007) 024503.
- T. Mayer, M. Eremin, I. Eremin, and P.F. Meier, Spin dynamics in HTSC cuprates: The singlet-correlated band (or t-J-V) model and its applications. J. Phys.: Condensed Matter **19** (2007) 116209.

- M.M. Korshunov, I. Eremin, A. Shorikov, and V.I. Anisimov, Electronic theory for the itinerant in-plane magnetic fluctuations in Na_xCoO_2, Pisma Zh. Eksp. Teor. Fiz. **84** (2006) 769 [JETP Lett. **84** (2006) 650].

- T. Dahm and I. Eremin, Comment on: "Spin dynamics of the Electron-Doped High-T_c Superconducting Cuprates", Phys. Rev. Lett. **97** (2006) 239701.

- I. Eremin and J.F. Annett, Magnetic field dependence of the superconducting gap node topology in non-centrosymmetric $CePt_3Si$, Phys. Rev. B 74 (2006) 184524.

- J.-P. Ismer, I. Eremin, and D.K. Morr, Dynamical spin susceptibility and the resonance peak in the pseudogap region of underdoped cuprate uperconductors, Phys. Rev. B 73 (2006) 104519.

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- J.-P. Ismer, I. Eremin, E. Rossi, and D.K. Morr, - Resonance peak in electron-doped cuprates, submitted to PRL, cond-mat/0702375.

- D.S. Inosov, S.V. Borisenko, I. Eremin, A.A. Kordyuk, V.B. Zabolotnyy, J. Geck, A. Koitzsch, J. Fink, M. Knupfer, B. Buechner, H. Berger, and R. Follath, Relation between the one-particle spectral function and dynamic spin susceptibility in superconducting $Bi_2Sr_2CaCu_2O_8$, cond-mat/0612040, submitted to PRL.

- Ilya Eremin, Dirk K. Morr, Andrey V. Chubukov, Karl Bennemann: Spin susceptibility in bilayered cuprates: resonant magnetic excitations, cond-mat/0611267, submitted to Phys. Rev. B (regular article).

4.3.3 Gutzwiller-Fellowship

Ratcheting up energy by means of measurement

L. S. Schulman

During my stay at the MPI I was involved in many projects, but one in particular was stimulated by the informal scientific give and take characteristic of the institute. A publication on this topic has already appeared [1], and another is on the way [2].
The question that got me going arose from work that Sergej Flach and Ricardo Pinto were doing on interactions of quantum breathers with an external field. What degree of coherence could be expected between ground and excited states after interaction with the field? I assumed that the textbook answer to this question was that if the field was in a coherent state the final state would be coherent; if not, not. Shortly after this I ran into a textbook author [3], who confirmed my impressions, but who offered an argument I did not understand. So for reasons of good conscience, I set out to establish the result on my own.

As usual, with coherent states everything is elegant. I model both the system with "ground and excited states" (call it $\mathcal{A}$) and the field (call it $\mathcal{B}$) to which it is subjected as harmonic oscillators. Suppose that during their temporary contact the Hamiltonian is

$$H = \omega_a a^\dagger a + \omega_b b^\dagger b + \gamma \left(a^\dagger b + b^\dagger a\right) , \tag{1}$$

with the usual notation (this is the Jaynes-Cummings model). γ is a non-zero constant during the period of contact, $0 \le t \le T$. Let the initial state be a coherent state,

$$\psi(0) = |z_a, z_b\rangle = e^{-|z_a|^2/2 - |z_b|^2/2} e^{z_a a^\dagger + z_b b^\dagger} |0,0\rangle , \tag{2}$$

for $z_a, z_b \in \mathbb{C}$, and $|0,0\rangle$ the $\mathcal{A}$-$\mathcal{B}$ ground state. Then it is an exercise to show that

$$\psi(T) = |z'_a, z'_b\rangle , \qquad \text{with } \begin{pmatrix} z'_a \\ z'_b \end{pmatrix} = U \begin{pmatrix} z_a \\ z_b \end{pmatrix} , \tag{3}$$

and U is a unitary matrix directly related to the quantities ω_a, ω_b, γ and T (see [2]). Thus if you start with a coherent state, it stays that way (and in particular, stays unentangled). Since the ground state of $\mathcal{A}$ is the coherent state $z_a = 0$, the levels in the final state of $\mathcal{A}$ are indeed coherent.
On the other hand, if the field is initially in a Fock state, i.e., an eigenfunction of the number operators,

$$\psi(0) = \frac{(a^\dagger)^{n_a}}{\sqrt{n_a!}} \frac{(b^\dagger)^{n_b}}{\sqrt{n_b}} |0,0\rangle , \tag{4}$$

the result is completely different. Using the same U that appeared in Eq. (3), the final state is highly entangled (even if $n_a = 0$):

$$\psi(T) = \frac{1}{\sqrt{n_a!}\sqrt{n_b!}} \left(U_{11} a^\dagger + U_{12} b^\dagger\right)^{n_a} \left(U_{21} a^\dagger + U_{22} b^\dagger\right)^{n_b} |0,0\rangle . \tag{5}$$

So far, so good; but it turns out that this satisfying answer does not survive more general circumstances. First though I take up a variation on the theme. Because of previous work on repeated scattering in a gas [4, 5], I was curious about the following scenario. Let there be a container holding many exemplars of type $\mathcal{A}$ and type $\mathcal{B}$ oscillators (no longer necessarily thought of as fields or atoms), and let them scatter and re-scatter off one another. That is, when any two of them are close they have interaction $\gamma \left(a^\dagger b + b^\dagger a\right)$, as above. Thus after a particular $\mathcal{A}$ ("$\mathcal{A}_1$") meets a particular $\mathcal{B}$ ("$\mathcal{B}_1$") they separate and $\mathcal{A}_1$ goes off to meet some $\mathcal{B}_2$, and similarly for $\mathcal{B}_1$. How does one describe the state of this multi-particle system? It is a standard and justified procedure to drop $\mathcal{A}_1$-$\mathcal{B}_1$ correlations when they separate. Of course that now standard procedure (related to the *Stosszahlansatz*) got Boltzmann into trouble, but I'll assume that reversibility and recurrence issues do not enter. Now Boltzmann was only concerned with momentum and position correlations, but for us the same considerations apply to *quantum entanglement*. The upshot is that the density matrix after a scattering, $\rho_{\mathcal{AB}}$, is replaced by $\rho_{\mathcal{A}} \otimes \rho_{\mathcal{B}}$, where (e.g.) $\rho_{\mathcal{A}} \equiv \mathrm{Tr}_b(\rho_{\mathcal{AB}})$ [6].
Conservation of total boson excitation number ($a^\dagger a + b^\dagger b$) in Eq. (1) leads to a peculiar prediction. A numerical simulation of the $\mathcal{A}$-$\mathcal{B}$ gas showed that each component, $\mathcal{A}$ and $\mathcal{B}$, evolved to an exponential distribution; that is, the probability that (e.g.) an $\mathcal{A}$ particle was excited to its n^{th} level is const$\cdot \exp(-\lambda_a n)$. What is peculiar is that

$\lambda_a = \lambda_b$: they drop with the *same* exponential. Since in general $\omega_a \neq \omega_b$, equipartition is lost. If you could separate the $\mathcal{A}$'s and $\mathcal{B}$'s using a field unrelated to their mutual interaction, you could use the different temperatures to convert heat to work, violating the second law of thermodynamics. (Do not start looking for venture capital; I will disable this perpetuum mobile below.)

I discussed this with several people at the MPI. Luiz Davidovich, who was visiting for a conference, suggested that I try this on the spin-boson model (with coupling $g(a^\dagger + a)(b^\dagger + b)$), to see if my result was an artifact of the Jaynes-Cummings boson conservation law.

This led to an even greater surprise. Not only was the second law of thermodynamics compromised, but the first law was violated as well [7]. The *total* boson number was gradually increasing with time! My first instinct was to accept an obvious solution: I had messed up the numerics. I have trouble writing two lines of algebra without a silly error creeping in; 50 lines of Schulman-authored computer code certainly represents a weak link in the chain of reasoning!

I contacted my long-time collaborator, Bernard Gaveau (Univ. Paris VI) who became intrigued, and undertook an analytical calculation of the effects of replacing $\rho_{\mathcal{AB}}$ by the tensor product of its partial traces, $\rho_{\mathcal{A}} \otimes \rho_{\mathcal{B}}$. He found that for a large class of interactions and for short times, the energy actually increases. This meant that I'd have to take my simulations seriously.

Perhaps I am guilty of over-dramatization: even as I worked on this problem I knew where trouble could be hidden, but until forced to take this feature seriously I sought other explanations. The particles were separating (justifying the partial trace) and then encountering other particles, from which they would again separate. One could think of the coupling "constants," γ and g as time-dependent. For a time-dependent Hamiltonian there is no reason to expect energy conservation. However, particles scatter off one another all the time, and their separation does not conflict with energy conservation. Even in abstract scattering theory [8] one uses the idealization of "in" and "out" states, representing states of the particles without their interaction. In this case, the turning off of the interaction at early and late times causes no violation of energy conservation.

What is distinctive in this problem is the nature of the interaction. The spin boson interaction, $(a^\dagger + a)(b^\dagger + b)$, when written as a coordinate interaction, is of the form xy, with x and y the oscillator coordinates. If x and y are position variables, as the particles separate, the force does not weaken. So the interaction really must be turned off and on. I developed two physical pictures of this process.

One picture of what's happening imagines the variables associated with $\mathcal{A}$ and $\mathcal{B}$ to be internal particle variables. When the motion of the particles bearing those variables brings them together one gets coupling. In this picture the coupling "constant" is a function of the position coordinates: $g = g(\boldsymbol{r}_a, \boldsymbol{r}_b)$. The source of the energy that enters the internal modes is now clear: it's the kinetic energy of the moving particles. As that's transferred to the internal degrees of freedom, they stop moving, and finally the energy-increasing repeated separations cease occurring.

A second perspective is more of an open systems approach: I imagine there is some external system whose job it is to turn the coupling off and on. This would be like ratchet models of muscular motion [9,10], where the turning off and on of an asymmetric potential induces directional motion in diffusing particles. But this turning off and on

is not free! It costs energy, which is precisely the job of ATP to provide. (Similar remarks resolve our Jaynes-Cummings paradox as well.)
So finally the laws of thermodynamics are intact. What one learns from this is that the destruction of entanglement may come at a surprising price, and that its effects can be felt at the thermodynamic level.

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4.3.4 Collaboration with Experimental Groups

A number of joint collaborations with experimental groups in Germany, Europe and the US has been partially supported by mpi**pks**. The following list summarizes these collaborations for the period 2005-2006.

- *Cell movements and flows during the development of the zebra fish* with C. P. Heisenberg (Dresden)
- *Dynamics of the Endosomal network* with M. Zerial (Dresden)
- *Dynamics of the cytoskeleton, cell division and the physics of motor proteins* with J. Howard, A. Hymann (Dresden)
- *Tissue growth and the kinetics of morphogen gradients in the fruit fly Drosophila* with M. Gonzalez-Gaitan (Dresden)
- *Morphology of cells in tissues* with S. Eaton (Dresden)
- *Segmentation of vertebrates through ocillating and spatio-temporal gene expression patterns* with A. Oates (Dresden)

- *Physics of hearing and active wave phenomena in the cochlea* with T. Duke (Cambridge)
- *Physics of active gels, the dynamics of the cytoskeleton as well as cell locomotion* with J.-F. Joanny, J. Prost (Paris)
- *Role of fluctuations in mechanosensory hair cells* with P. Martin (Paris)
- *Orientation of the mitotic spindle as well as on dytokinesis* with M. Bornens (Paris)
- *Origin of contractile rings and on the dynamics of the cytoskeleton in plant cells* with M. Dogterom, B. Mulder (Amsterdam)
- *Active Gels* with A. Bernheim-Groswasser (Amsterdam)
- *Fragmentation of molecules by intense laser pulses* with P. Agostini (Ohio) and S. L. Chin (Quebec)
- *The propagation of femtosecond pulses in air and the generation of ultrashort tunable laser pulses* with S. L. Chin (Quebec)
- *The rescattering dynamics in strong field double ionization* with R. Dörner (Frankfurt a. M.) and P. Corkum (Canada)
- *Far-field characteristics of oval-shaped mircolasers: Comparison between experiment and theory* with T. Harayama (Kyoto)
- *Quanten information* with S. Walborn, P. Souto-Ribeiro, L. Davidovich (Rio de Janeiro)
- *Photoemission in high-Tc* with M. Knupfer, S. Borisenko (Dresden)
- *Neutron Scattering* with D. Reznik, L. Pintschovious (Karlsruhe)
- *Short-range antiferromagnetism in an optimally-doped high Tc superconductor* with T. Harayama (Karsruhe)
- *Ultracold glasses* with H. Strehlow (Berlin)
- *Spin-current control* with P. Mohanty (Boston)
- *Physics of Josephson junction networks* with A. Ustinov (Erlangen)
- *Cold atom ratchets in optical potentials* with M. Weitz (Bonn), F. Renzoni (London
- *Collective excitation of electrons in complex systems by photons* with A. Müller (Giessen), R. A. Phaneuf (Nevada)
- C_{60}^- with N. Berrah (Kalamazoo)
- *Photoexitation of Helium* with G. Kaidl (Berlin), R. Dörner (Frankfurt)
- *Interaction of Rydberg atoms in ultracold gases* with M. Weidemüller (Freiburg), P. Pillet (Orsay), G. Raithel (Ann Harbor)
- *Ultracold plasma* with T. Killian (Rice)

4.3.5 Conferences, Workshops and Symposia 2005-2006

1. *Semiconductor Physics and Technology*
   Japan-Germany Colloquim: February 14 - 16, 2005 — 25 participants
   Scientific coordinators: K. Iga, J. Weber

2. *Collective Quantum States in Low-Dimensional Transition Metal Oxides*
   Workshop: February 22 - 25, 2005 — 87 participants
   Scientific coordinators: W. Brenig, B. Büchner, C. Gros, P. Lemmens

3. *Korrelationstage 2005*
   Workshop: February 28 - March 5, 2005 — 153 participants
   Scientific coordinators: F. Gebhard, M. Lang, G. Zwicknagl

4. *Aspects of Quantum Chaotic Scattering*
   Workshop: March 7 - 12 , 2005 — 82 participants
   Scientific coordinators: Y.V. Fyodorov, T. Kottos, H.-J. Stöckmann

5. *Strong Correlations and ARPES: Recent Progress in Theory and Experiment*
   Seminar and Workshop: March 29 - May 6 , 2005 — 105 participants
   Scientific coordinators: J. Fink, K. Matho, E. Müller-Hartmann

6. *Nanoscale Fluctuations in Magnetic and Superconducting Systems*
   Workshop: May 10 - 14 , 2005 — 67 participants
   Scientific coordinators: H. Alloul, E. Dagotto, P. Hirschfeld, A. H. MacDonald

7. *MPG-MOEL Symposien*
   Workshop: May 23 - 25 , 2005 — 73 participants
   Scientific coordinators: F. Krausz, H.-W. Spiess, G. Wegner

8. *Towards the Future of Complex Dynamics: From Laser to Brain*
   Workshop: May 30 - June 1 , 2005 — 59 participants
   Scientific coordinators: M. Bär, H. Kantz, A. Torcini

9. *Classical and Quantum Dynamical Simulations in Chemical and Biological Physics*
   Workshop: June 06 - 11, 2005 — 77 participants
   Scientific coordinators: U. Kleinekathöfer, J. Knoester, M. Schreiber

10. *Nonlinear Dynamics in Biophysics*
    Seminar and Workshop: June 20 - July 15, 2005 — 83 participants
    Scientific coordinators: C. Grebogi, R. Koberle, J. Kurths

11. *Quantum Simulations via Analogues*
    Workshop: July 25 - 28, 2005 — 31 participants
    Scientific coordinators: R. Schützhold, W. G. Unruh

12. *Intense Laser-Matter Interaction and Pulse Propagation*
    Seminar and Workshop: August 1 - 24, 2005 — 107 participants
    Scientific coordinators: A. Becker, S. L. Chin, N. Moiseyev

13. *International Summer School on Quantum Information*
    Seminar and Workshop: August 29 - September 30, 2005 — 118 participants
    Scientific coordinators: R. Blatt, A. Buchleitner, R. Gill

14. *Critical Stability of Few-Body Quantum Systems*
    Workshop: October 17 - 22, 2005 — 50 participants
    Scientific coordinators: A. Jensen, L. Wiesenfeld

15. *Atomic Physics 2005*
    Workshop: November 28 - December 2, 2005 — 79 participants
    Scientific coordinators: M. Lein, S. Kümmel, J.-M. Rost

16. *370. Wilhelm und Else Heraeus-Seminar*
    Workshop: January 4 - 6, 2006 — 30 participants
    Scientific coordinators: F. Krauss

17. *Dissipative Solitons*
    Workshop: January 23 - 29, 2006 — 65 participants
    Scientific coordinators: N. Akhmediev, L. Pismen, Y. Pomeau

18. *Dynamics on Complex Networks and Applications*
    Workshop: February 6 - March 3, 2006 — 91 participants
    Scientific coordinators: J. Kurths, M. A. Matias, A. E. Motter

19. *Quantum Disordered Systems, Glassy Low-Temperature Physics and Physics at the Glass Transition*
    Workshop: March 13 - 14, 2006 — 63 participants
    Scientific coordinators: C. Enss, H. Horner, S. Hunklinger, R. Kühn

20. *Cold Atoms Meet Condensed Matter*
    Workshop: March 27 - 31, 2006 — 66 participants
    Scientific coordinators: I. Bloch, Ch. Bruder, W. Zwerger

21. *Trends in Condensed Matter Physics*
    International Symposium: April 5 - 7, 2006 — 203 participants
    Scientific coordinators: P. Fulde

22. *Non-Equilibrium Dynamics in Interacting Systems*
    Seminar and Workshop: April 18 - May 5, 2006 — 83 participants
    Scientific coordinators: J. Kroha, A. Muramatsu, I. Perakis

23. *Quantum Coherence, Noise and Decoherence in Nanostructures*
    Workshop: May 15 - 26, 2006 — 101 participants
    Scientific coordinators: Ch. Bauerle, G. Schön, A. Zaikin

24. *Correlated and Many-Body Phenomena in Dipolar Systems*
    Workshop: May 29 - June 2, 2006 — 53 participants
    Scientific coordinators: N. Bigelow, H. Sadeghpour

25. *XXX. International Workshop on Condensed Matter Theories*
    Workshop: June 5 - 10, 2006 — 61 participants
    Scientific coordinators: F. Fulde, H. Reinholz, G. Röpke

26. *Physics of Biological Systems*
    Workshop: June 19 - 23, 2006 — 90 participants
    Scientific coordinators: F. Jülicher, J. Howard, A. Hyman

27. *Constructive Role of Noise in Complex Systems*
    Workshop: June 26 - July 21, 2006 — 84 participants
    Scientific coordinators: A. Neimann, A. Pikovsky

28. *Dynamics and Relaxation in Complex Quantum and Classical Systems and Nanostructures*
    Seminar and Workshop: July 24 - October 6, 2006 — 89 participants
    Scientific coordinators: B. Altshuler, V. Falko, A. Ludwig, K. Wiese, I. Aleiner

29. *Interactions, Excitations and Broken Symmetries in Quantum Hall Systems*
    Seminar and Workshop: October 2 - 7, 2006 — 57 participants
    Scientific coordinators: A. Mirlin, F. von Oppen

30. *Extreme Events in Complex Dynamics*
    Seminar and Workshop: October 23 - November 3, 2006 — 70 participants
    Scientific coordinators: S. Albeverio, V. Jentsch, H. Kantz, S. Ruffo

31. *Polymorphism in Condensed Matter*
    Workshop: November 13 - 17, 2006 — 64 participants
    Scientific coordinators: K. Binder, H. Emmerich, B. Nestler

32. *Atomic Physics 2006*
    Seminar and Workshop: October 23 - November 3, 2006 — 70 participants
    Scientific coordinators: J.-M. Rost

33. *Nonlinear Dynamics of Acoustic Modes in Finite Lattices: Localization, Equipartition, Transport*
    Workshop: December 6 - 8, 2006 — 53 participants
    Scientific coordinators: A. Giorgilli, S. Flach

4.3.6 Workshop Participation and Dissemination of Results

Statistics of Workshop participation

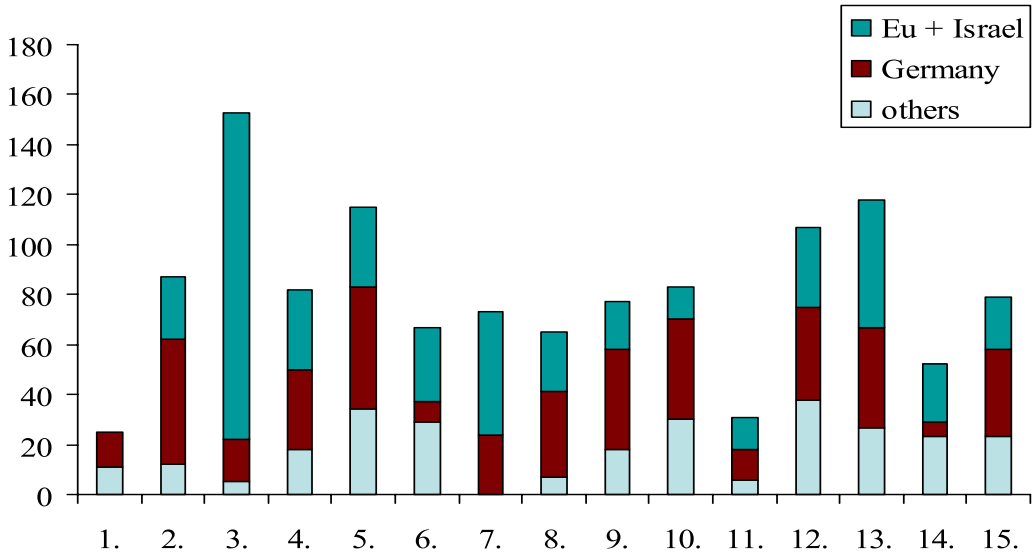


Figure 1: *Number of Workshop/Seminar participants in the year 2005.*

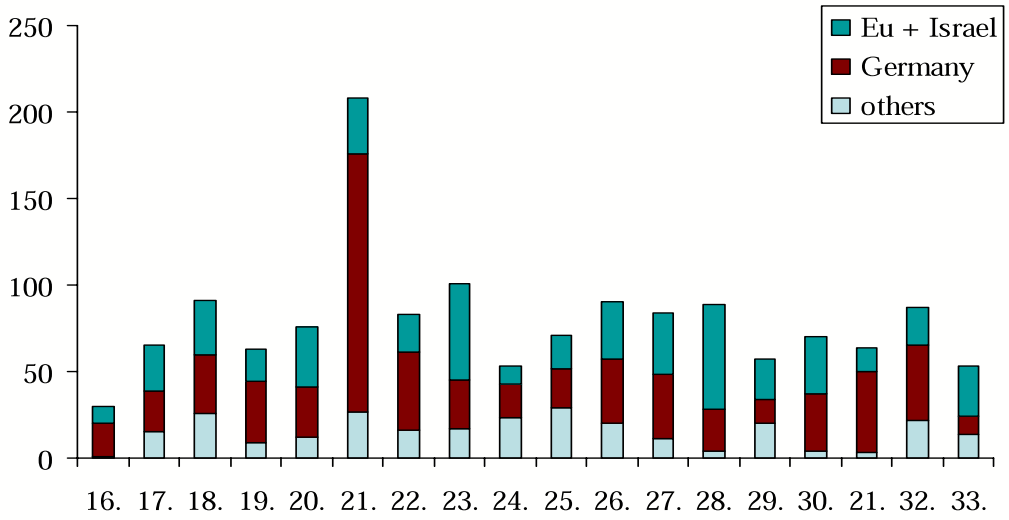


Figure 2: *Number of Workshop/Seminar participants in the year 2006.*

Dissemination of Workshop Results

As the topics of Workshops and Seminars at mpipks are focusing on new and emerging fields of the physics of complex systems, scientific coordinators often consider the option of publication of proceedings, lecture notes or monographs related to the results of their event. The mpipks supports such efforts in various ways. The following list summarizes the relevant publications:

- Workshop:
  Quantum Simulations via Analogues
  Lecture Notes in Physics, Springer Verlag, (to be published)
- Workshop:
  Aspects of Quantum Chaotic Scattering
  Journal of Physics A 38 **15**, L241-262, 3247-3474 (2005)
- Workshop:
  Dynamics on Complex Networks and Applications
  Physica D **224**, 1 - 214 (2006)
- Workshop:
  Intense Laser-Matter Interaction and Pulse Propagation
  Lecture Notes in Physics, Springer Verlag, Vol. **718** (2007)(to be published)
- Workshop:
  Dissipative Solitons
  Lecture Notes in Physics, Springer Verlag, (to be published)

4.3.7 Workshop Reports

Semiconductor Physics and Technology

Japan-Germany Colloquium, Scientific coordinators: K. Iga, J. Weber
On february 14th-16th, the 2nd Japanese German Colloquium entitled Semiconductor Physics and Technology was held at the Max Planck Institute for the Physics of Complex Systems in Dresden. The meeting was organized by the Bonn office of the Japan Society for the Promotion of Science (JSPS) under its director Prof. Yasuo Tanaka, in collaboration with Prof. Jrg Weber from the Institute of Applied Physics (IAP) of the University of Technology Dresden. The opening address was presented by the JSPS executive director Prof. Kenichi Iga, who introduced the major activities of JSPS and presented an overview of the present Japanese semiconductor technology in the area of photonics and optoelectronics. During the meeting, scientists from Japan and Germany presented various topics covering semiconductor nanostructures, organic semiconductors, photonic crystals, spintronics and semiconductor crystal growth. The main focus of the Colloquium was the transition from fundamental research to applications such as high-performance infrared semiconductor lasers, organic transistor integrated circuits for large-area sensors, organic LEDs and solar cells, optical switches and terahertz emitters. The stimulating atmosphere of the Colloquium helped to initiate and foster collaborations between the participating scientists.

Collective Quantum States in Low-Dimensional Transition Metal Oxides

Workshop
Scientific coordinators: W. Brenig, B. Büchner, C. Gros, P. Lemmens
Insgesamt 80 Teilnehmer aus Deutschland, Japan, Frankreich, der Schweiz, den USA haben in Rahmen von diesem Workshop die neusten experimentellen und theoretischen Ergebnisse zu 'kollektiven Quanten-Zustände in niedrigdimensionalen Übergangs-Metallen' diskutiert. Diese internationale Zusammenkunft hat gleichzeitig als Abschlusskonferenz des gleichnamigen Schwerpunktprogrammes 1073 der DFG fungiert. Das Thema ist dabei eingebettet in verwandte Gebiete wie das der korrelierte Elektronen und der quantenkritische Phänomene. Nach Ansicht der Organisatoren ist es gelungen im Rahmen des Workshops Fachleute aus Experiment und Theorie zusammenzubringen und der internationalen Zusammenarbeit weitere Impulse zu geben.
So hat Elbio Dagotto (Florida State University) eine allgemeine Einführung ber 'Complexity in transition metal oxides' gegeben und John Tranquada (Brookhaven National Laboratory) zu 'Universal magnetic excitation spectrum for cuprate superconductors'. Dieses sind zwei Beispielen von Übersichtsvorträgen, welche der allgemeine Diskussion einen Rahmen gegeben haben. In sehr interessanten Vorträgen wurden dann über Neuentwicklungen berichtet, wie z.B. von Götz Uhrig (Universitt Köln) ber 'Magnetic excitations in low-dimensional spin systems by continuous unitary transformations' und von Mats Johnsson (Stockholm University) 'Novel routes to quantum spin systems and low dimensional compounds'.
Die Stimmung war whrend der Konferenz sehr gut und intensive Diskussionen wurden im Anschluss an die Vorträge geführt, sowie während der Pausen. Eine ganze Reihe von jüngeren Teilnehmern konnten sich einen guten Einblick in dieses lebendige Forschungsfeld verschaffen und ihre Ideen vorstellen.

Aspects of Quantum Chaotic Scattering

Workshop and Seminar
Scientific coordinators: Y. V. Fyodorov, T. Kottos, H.- J. Stöckmann
Quantum scattering is a topic of interdisciplinary interest ranging from nuclear, atomic, molecular, and mesoscopic physics to quantum optics, quantum chaos and pure mathematics. However, the interchange of knowledge, and of the techniques developed independently in the different fields is still quite limited. It was the goal of the current workshop to bring researchers from different disciplines together, aiming in promoting new cooperations, and guiding new theoretical directions and technological applications. From comments provided by a large number of participants (ranging from positive to overly enthusiastic) we can conclude with high confidence that the goal was successfully achieved.
The total number of participants was more than 80, exceeding by far our originally envisaged figure of 50 participants. One of the main goals was to ensure the appropriate mixture between less experienced young researchers and more senior scientists, giving the opportunity to the former group of participants to interact and present themselves. To this end, there was a poster session on the first day of the conference. In addition, more than one quarter of the talks was given by scientists of younger generation.
On the theoretical side the contributions covered a large variety of subjects ranging from semiclassical approach to chaotic scattering (Smilansky, Prange, Gaspard, Ketzmerick,

Seligman, Schanz, Jacquod, Schomerus, Silvestrov), scattering from random media (Ossipov, Weiss, Shapiro, Smolyarenko, Garcia- Garcia, Mirlin) and systems with surface disorder (Mello, Freilikher), to the effect of dephasing (Beenakker, Sokolov, Casati) and absorption (Savin) in chaotic scattering. The conference was focused also in scattering from quantum dots and mesoscopic devices (Brouwer, Lewenkopf, Weidemüller), and applications scattering to random lasers (Hackenbroich), microlasers (Nöckel, Viviescas), atomic physics and quantum optics (Kolovsky, Guarneri, Buchleitner, Stania, Mehlig).
More than one third of the talks was given by experimentalists. The presented topics ranged from transport and wave function measurements in chaotic microwave systems (Kuhl, Richter, Sirko, Legrand, Anlage), light transport through random media and random lasers (Gennack, Cao, Lagendijk) and sound propagation in disordered systems (Van Tiggelen, Weaver, Ellegaard). It should be stressed that it seems to be the first time that all three communities joined at one workshop, although a considerable overlap in concepts used in different research directions involved was evident. This meeting almost surely will facilitate a further fruitful exchange of ideas between those fields.
The success of the conference is also reflected in the fact that the IOP asked the organizers to serve as Editors on a special issue on *Trends in Quantum Chaotic Scattering* published by Journal of Physics A: Mathematical and General. The corresponding call for papers was announced and distributed to the participants.
Finally we would like to acknowledge the excellent organization of the event by the mpi**pks** staff and the very friendly atmosphere there which was an important ingredient for the success of the conference.

Strong Correlations and ARPES: Recent Progress in Theory and Experiment

Workshop and Seminar
Scientific coordinators: J. Fink, K. Matho, E. Müller-Hartmann
The CORPES05 seminar was organised by the Max Planck Institute for the Physics of Complex Systems mpi**pks**) in Dresden, from March 29th to May 6th 2005; the more intense workshop took place in the week of April 4 - 8. Scientific coordinators were Jrg Fink from the Leibniz Institute of Solid and Materials Research, Dresden, Konrad Matho from the Center for Low Temperature Research, Grenoble, and Erwin Mller-Hartmann from the University of Kln. There were several reasons to stage these events in 2005. One hundred years ago, in the first of five famous papers of his annus mirabilis, Albert Einstein postulated the dual nature of light at once particle and wave and thereby explained the photoelectric effect, among other phenomena. This work was also singled out by the Nobel committee in 1921. The photoelectric effect has since become the basis of one of the most important techniques in solid state research. A rapidly advancing field is angle-resolved photoelectron spectroscopy (ARPES). One decade ago, the focus was on the determination of the band structure of solids. Since the advent of new photon sources from undulators in synchrotron radiation facilities, new analysers with two-dimensional detectors, and new cryo-manipulators it is now possible to measure the spectral function near the Fermi level with high angular (momentum) and energy resolution. One can extract the electronic self-energy function which describes the many-body interactions of the charge carriers. This is of particular

importance for strongly correlated systems, in which interactions influence the transport and other material properties beyond the mean-field level. Presently, the main focal points for theorists are unconventional superconductors, heavy fermion compounds and low dimensional systems. The purpose of the workshop and the seminar was to strengthen the interface between ARPES and the many-body theory and to explore new ways of analysing a rapidly increasing wealth of experimental data. In the opening talk of the workshop Philippe Aebi of Fribourg asked the provocative question: Do we even understand ARPES results from simple systems such as Cu-metal? In fact, the still poorly understood process of exchange between photon and electron, manifest in the matrix element effects, remained a unifying theme throughout the meeting. Photon sources such as laser light and soft X-rays present new challenges to theory. The central topic was the measurement and interpretation of ARPES results on high-temperature superconductors. Several speakers discussed the evidence for a simultaneous presence of electron-electron, electron-phonon and magnetic interactions in the spectral function. Understanding the dominant mechanism in the dressing of the charge carriers at the lowest energies is of particular interest since it is related to the origin of the attraction that causes superconductivity. Mike Norman of Argonne gave an excellent overview to the Dresden physics community in the mpi**pks** colloquium. Other highly correlated systems such as heavy fermions, transition metals with poorly understood polaronic effects, new oxide superconductors and low dimensional systems were treated in both the seminar and the workshop. Finally, in a well attended lecture to the Dresden public, Stefan Hfner of Saarbrcken described a century of the photoelectric effect, from the few facts Einstein knew when he made his bold interpretation to the electronic technology of the 21st century. CORPES05 took place in the pleasant atmosphere of the mpi**pks**, favoring discussions in the lecture hall and around the posters. Nearly all important groups working in the field of ARPES and in the theory of strongly correlated systems were represented. Young scientists, many of them benefiting from financial support of the International Institute for Complex Adaptive Matter (IICAM), were impressed by the possibilities of the ARPES technique and by the recent developments in the theory of correlated systems. Participants frequently expressed the conviction that CORPES05 should be a starter in a series of similaNanoscale Fluctuations in Magnetic and Superconducting
Systemsr events to highlight further developments of a fast moving field.

Nanoscale Fluctuations in Magnetic and Superconducting Systems

Workshop, Scientific coordinators:
H. Alloul, E. Dagotto, P. Hirschfeld, A. H. MacDonald

- **Purpose.** The NANO05 workshop was based on the premise that three different classes of materials of current interest–cuprates, manganites, and dilute magnetic semiconductors–displayed nanoscopic inhomogeneities and that participants from the three communities could learn from one another's approaches to these problems.

- **Participants.** Response to the initial announcement was very strong, as these problems are perceived as very important and timely. Ultimately 67 people attended from the original 80 applicants, with two invited speakers cancelling at

the last minute. Of the 67 attendees, geographical distribution was good with 23 participants from N. America, 41 from Europe and 4 from Japan. There were eight women among the participants (3 speakers), a reasonable total for conferences in this area. Eleven participants were junior researchers (postdoc or student).

The quality of the participants was very high. The workshop managed to attract one or two key players from every subdiscipline, experimental and theoretical, in the three areas, and some from related outside areas. These included T. Dietl (Polish Acad. Sci.), D. Argyriou (Otto Hahn), D.-H. Lee (Berkeley), L. Brey (Madrid), J.C. Davis (Cornell), H. Eisaki (Tokyo), A. Yazdani (Princeton), B. Keimer (Stuttgart), H. Ohno (Japan), N. Samarth (Penn St.), T. Devereaux (Waterloo), J. Mannhart (Augsburg), M. Fogler (La Jolla), M. Sigrist (ETH), L. Gor'kov (Tallahassee), G. Zarand (Budapest), J. Cibert (Grenoble), J. Moore (Berkeley), G. Blumberg (Lucent), Y. Ando (CRIEPI) and J. Zaanen (Stanford/Leiden).

- **Talks.** With one or two exceptions, the quality of the talks was remarkably high. In particular, the 40-min. review talks were mostly quite successful with explaining basic concepts of the subfield to the "outside" audiences. Many participants commented that they learned a good deal about problems in parallel subfields from these talks.

- **Discussions.** In the discussion periods after the talks, discussion was spirited and generally lasted well beyond the allotted time, which posed no problem since this had been anticipated in the schedule. Despite encouragement of participants to pose "naive" questions outside their subfield, most discussion during this period was joined by experts in the given field. During the scheduled periods in the late afternoon, however, when it was hoped comparisons and contrasts between the different materials classes could be drawn, participants were tired and these planned discussions did not take place. Many participants commented that they had excellent private and small group discussions during the many breaks built into the schedule, however.

- **Excursions/social activities.** Very successful and well-organized.

- **Scientific highlights.**

  - J.C. Davis presented evidence that dopant atoms, now imaged with STM, are the source of nanoscale inhomogeneity in the BSCCO-2212 system.
  - H. Eisaki showed data correlating T_c suppression by different rare earth impurities with the areal change in volume occupied by the impurity, and demonstrated a linear T_c vs. ρ_{2D} supression.
  - J. Bobroff showed that the asymmetry of the NMR lineshape in the superconducting state of the cuprates could be used to extract information on the local density of states shifts around impurities.
  - F. Rullier-Albenque presented data suggesting the Nernst effect in underdoped cuprate pseudogap phase might be due to defects.

- T. Valla showed that improved sample quality and nodal resolution allowed the observation of an ARPES nodal relaxation rate which dropped below T_c, in agreement with optics.
- J. Mannhart showed that the boundary resistance of a high-T_c grain boundary falls linearly with increasing T in the normal state.
- T. Nunner suggested that the dopant-gap correlations in Cornell STM experiment can be explained by assuming that the superconducting pair interaction is modulated by impurities.
- D. Broun showed that YBCO materials can be made extremely homogeneous, and reported a linear-T relaxation rate in BSCCO-2212.
- Y. Ando presented evidence that the insulating state in the cuprates revealed when T_c is supressed in field is an unknown type of field-induced localization associated with field-stabilized stripe or impurity-induced magnetization.
- D. Argyriou showed that the charge and orbital ordering fluctuations in half-doped manganites freeze out near room temperature, leading to a polaronic glassy phase.
- D.-H. Lee proposed that incommensurate magnetic fluctuations are responsible for the lack of an obvious pseudogap near the antinodal point in underdoped LSCO.
- T. Dietl showed that the critical temperature and hysteresis modulation-doped II-VI quantum wells can be explained by including antiferromagnetic interactions in Monte Carlo simulations.
- H. Ohno discussed studies of domain wall motion in (Ga,Mn)As devices with high spin transfer efficiency.
- Ilya Vekhter emphasized scenarios in which electronic systems with competing orders could form glassy phases even in the absence of disorder.
- M. Fogler explained why disorder effects in 2DEGs could be nonperturbatively strong due to regions where the local density is driven to zero by dopant impurities.

MPG-MOEL Symposien

Workshop, Scientific coordinators: F. Krausz, H.-W. Spiess, G. Wegner
Inhalt des Symposiums: Ein Anliegen unserer Veranstaltung war es, auf die enorme Breite des Einsatzes der Magnetischen Resonanz hinzuweisen. Obwohl alle Teilnehmer aus dem Gebiet Magnetische Resonanz kamen, kannten sich selbst die Arbeitsgruppenleiter untereinander nur teilweise. Durch das strukturierte Programm und die gemeinschaftlichen Rahmenveranstaltungen hatten alle Teilnehmer vielfältige Gelegenheit, sich und ihre Forschung kennen und schätzen zu lernen. Dies wurde immer wieder mit Dank zum Ausdruck gebracht. Teilnehmerkreis: An unserem Symposium nahmen neben 17 Arbeitsgruppenleitern, die Übersichtsvorträge hielten, fast 30 Nachwuchswissenschaftler (Doktoranden, Postdocs und bereits habilitierte Wissenschaftler) teil. Diese hatten Gelegenheit, ihre Poster den Teilnehmern zusätzlich in fnfminütigen Kurzbeitrgen zu prsentieren. Hierdurch hatten wir alle einen sehr guten berblick ber

diesen Teilnehmerkreis. Ich bin sicher, dass sich hieraus konkrete Forschungskooperationen mit Austausch von Gastwissenschaftlern ergeben. Das hohe Interesse an der Teilnahme der jungen Leute wurde auch dadurch demonstriert, dass die Teilnehmer aus den MOEL die Kosten fr An- und Abreise selbst übernahmen. Die Nachwuchswissenschaftler aus den MOEL waren von der Veranstaltung geradezu begeistert und brachten dies mir gegenüber auch bei zwischenzeitlichen Begegnungen auf anderen Konferenzen immer wieder zum Ausdruck. Konkrete Kooperation: Trotz der Kürze der Zeit, die seit dem Symposium vergangen ist, kann ich bereits von einer konkreten Kooperation berichten: Seit einiger Zeit pflegen wir eine lockere Zusammenarbeit mit dem Direktor des National Insitute of Chemical Physics and Biophysics, Tallinn, Estland, Dr. Ago Samoson. Er hat mit seiner Gruppe hat MAS-NMR-Probenköpfe mit der weltweit höchsten Rotationsfrequenzen entwickelt. Diese Expertise ist fr uns von groem Interesse. Deshalb haben verabredet, unsere Kooperation zu intensivieren und durch einen Vertrag zu formalisieren. Angesichts der gegenwärtigen Umbruchsituation in Estland sind solche Kooperationen fr unsere aueruniversitären Partnerinstitute besonders wichtig und ich wäre Ihnen sehr dankbar, wenn Sie unsere Initiative unterstützen könnten. Weiterfhrung - Science and Art in Europe: Nach dem zuvor gesagten ist klar, dass ich eine Weiterführung der Veranstaltungen Science and Art in Europe auerordentlich begrüen würde. Ich freue mich deshalb sehr, dass Tschechien Interesse an der Organisation der nächsten Symposium-Reihe angemeldet hat. Ich selbst hatte Kollegen aus Slovenien angesprochen, die ebenfalls Interesse zeigten. Generell herrschte bei meinen Gesprchen die Meinung vor, dass gerade auch die zentrale Eröffnungsveranstaltung in Berlin das Symposium ber den wissenschaftlichen Austausch hinaus wesentlich bereichert hat. Gerade unsere Gäste aus dem Ausland haben die Gelegenheit begrüt, dabei kulturelle aber auch wissenschaftliche Anregungen aus den verschiedenen Ländern zu erhalten.

Classical and Quantum Dynamical Simulations in Chemical and Biological Physics

Workshop
Scientific coordinators: U. Kleinekathöfer, J. Knoester, M. Schreiber
The workshop which took place at mpi**pks** from June 5 to 11, 2005 covered so diverse topics as molecular dynamics in the gas phase, coherent control, dissipation and nanostructures, exciton transfer in organic and biological systems, as well as modelling of biomolecules. Although each of those topics is already interdisciplinary, the themes and the investigated objects are so distinct that separate research communities have developed treating these fields. On the other hand, the topics are sufficiently close and overlapping, especially concerning methods and techniques, that fruitful exchange between the participants evolved during the workshop week as anticipated in the proposal. Due to lively discussions, which developed after the talks, in the coffee breaks, during the poster sessions, and in the leisure time, the interdisciplinary interaction and the information exchange between the different fields was considerable. Many participants have explicitly expressed their gratitude for the broad scope of the workshop and the stimulating atmosphere that was created.
The scientific program of the workshop had been proposed, because recent technological breakthroughs such as ultrafast pulsed lasers and crystallography of macromolecules

improved the experimental tools of physicists working, in particular, in the area of chemical and biological physics. On the other hand, high-performance computing has significantly enhanced the possibilities for simulations of such systems as demonstrated in the workshop. For small systems with a few degrees of freedom it is possible to treat the dynamics fully quantum mechanically. The workshop showed a huge variety of phenomena that these small systems exhibit including the possibility of a coherent laser-pulse control of specific reactions. Of course, in large and more complex physical systems it is impossible to treat all degrees of freedom quantum mechanically. Several speakers described the appropriate modelling with a few relevant modes, treating the rest of the system as a thermal bath. In this way the dissipation and excitation transfer in tailor-made nanostructures like molecular wires and donor-acceptor complexes with varying bridge length in between can be simulated. However, many of the numerous system-bath models are not directly connected to an atomic-level description of the system of interest. But atomic-level details are known nowadays also in biological physics from, e.g., X-ray crystallography of a crystallized version of the macromolecules. It was shown, that the treatment of static and dynamical properties for big molecules even within a surrounding liquid of protein structures is possible by classical molecular-dynamic simulation on an atomic level. Force-field-based simulations were presented, several orders of magnitude faster and cheaper than quantum calculations. Hybrid approaches enable to cover several orders of magnitudes in size and in time. Not only static properties of biomolecules have been simulated, but also dynamical processes like the conversion of light into chemical energy in light harvesting bacteria have been described.
The total number of 75 participants included 45 speakers, most of them invited. The majority of the talks described the modelling and the simulations. Selected experimentalists provided a stimulating overview over spectroscopic observations and coherent control which are nowadays feasible. Some speakers and nearly all of the other participants presented their research on posters during two long evening sessions, in which the discussion lasted (supported by beer and wine) beyond midnight. The speakers came from 11 different countries, the other participants covered 17 countries. On behalf of all the participants the organizers thank the mpi**pks** for making this workshop possible and for the generous support. In particular, we are grateful for the organizational support by Katrin Lantsch who treated all management issues promptly, efficiently, and always with a smile.

Nonlinear Dynamics in Biophysics

Workshop, Scientific coordinators: C. Grebogi, R. Koberle, J. Kurths
We had an extremely successful event with about 80 participants including a large number of top scientists in the field and a substantial number of students and research fellows. The Workshop/Seminar emphasized the applications of nonlinear dynamics in biology. Since biology is the natural playground for dynamics and, why not, physics, this event was markedly relevant for future developments in the field. The event was particularly concerned with mathematical and data-based modelling of biological systems grounded on nonlinear dynamics.
The four-week long event was partitioned as the following:
The first week was made up of a series of short courses on nonlinear dynamics in

topics that were relevant to biological systems, and seminar talks. The lectures on the short courses were delivered by Holger Kantz mpi**pks**), Juergen Kurths, Marco Thiel and Niels Wessel (Potsdam University), Celso Grebogi (University of Sao Paulo) and Roland Koberle (University of Sao Paulo at Sao Carlos). The Monday Colloquium was delivered by Alexander Borst (MPI fuer Neurobiologie). The short courses, attended by most of the young people present at the event, set up the tone for the Workshop held in the second week. Initial collaborative work was already organized in the first week. The second week was highlighted by the Workshop with the presence of a large number of invitees of international stature in the field. We had over 30 talks during this week. The Monday Colloquium was this time delivered by Alain Arneodo (Ecole Normale Superieure du Lyon). Most of the 80 participants took part in the Workshop. We had also poster sessions during this week. Of course, the much appreciated excursion and the romantic sightseeing tour through Dresden at night took place during this week. The third and the fourth weeks were dedicated to seminars and collaborative research. We had 27 seminar talks in this period and a lot of time for scientific discussions and collaborative work. The Monday Colloquium was delivered by Alessandro Moura (University of Sao Paulo) in the third week and Leo van Hemmen (TU Muenchen) in the fourth week.
This was an important and unforgettable event that, of course, could not be realized without the generous support of mpi**pks** and the commitment of its Mitglieder and staff, especially the staff involved with the visitors program. Research collaborations were seeded at this event and led to relevant scientific work.

Quantum Simulations via Analogues

Workshop, Scientific coordinators: R. Schützhold, W. G. Unruh
Since it is at present impossible to construct universal quantum computers, quantum-mechanical systems can nowadays be simulated on classical computers with exponential effort only. However, the dynamics of specific quantum systems can also be obtained by constructing analogues that resemble the equations of motion for important observables. Many analogues are theoretically well understood but lack the experimental foundations. The workshop aimed at providing an overview on theoretical and experimental possibilities of the construction of such analogues and related systems.
The atmosphere of the workshop has been strongly enriched by experienced researchers such as William Unruh (University of British Columbia, Vancouver, Canada) who introduced the phenomenon of Hawking radiation in the MPI colloquium. Grigori Volovik (LTL, Hut, Finland) helped with his enormous experience both on the experimental and theoretical side.
Researchers such as Jakob Yngvason (Institut für Theoretische Physik der Universität Wien, Austria), Uwe R. Fischer (Eberhard-Karls-Universität Tübingen, Germany), Ralf Schützhold (TU Dresden, Germany) have shared their theoretical experience and discussed proposals for future analogues. The experimental expertise was represented by renowned scientists such as Peter Skyba (Institute of Experimental Physics, Kosice, Slovak Republic) and Bernard Barbara (Laboratoire Louis Neel, Grenoble, France).
The workshop was taken as an opportunity by several postdocs and PhD-students to present their research projects in talks of 35 minutes (plus 10 minutes for questions/discussions), some of them presented their first talk to an international audience.

The presentations raised lively discussions afterwards and provided the young scientists with the opportunity to gain knowledge about alternative methods. In breaks especially included for individual discussions in the workshop program, all researchers had the chance to talk about the specific ideas in greater detail. The controversial discussion with experienced scientists is a major ingredient of the education of young researchers.
Apart from the training aspect for young researchers, the workshop enabled the exchange of ideas among both experimentalists and theoreticians. The experimental talks have increased the awareness of experimental possibilities and difficulties. Theoretical presentations have demonstrated that the experimental implementation of quantum-mechanical analogues may be achievable with current experimental means.
In a more general context, the workshop enabled young and senior researchers to initiate and extend networks for future communication and collaborations. It is planned to publish selected lectures of this workshop in a book in the series Springer lecture notes in physics.

Intense Laser-Matter Interaction and Pulse Propagation

Workshop, Scientific coordinators: A. Becker, S. L. Chin, N. Moiseyev
The aim of the seminar and workshop was to bring together the currently best experts and promising young scientists on the fields of interaction of intense ultrashort laser pulses with atoms, molecules and clusters and the propagation of high peak power pulses in optical media. Among the more than 100 participants from 23 countries there was a balance between established and young scientists, researchers from experiment and theory, physicists and chemists. A main focus was to give the graduate students and post docs an overview of the theoretical approaches, computational methods and experiments, which have been carried out and are under investigation, as well as of the challenges for the future.
During the seminar leading scientists gave an introduction to the basic phenomena and the current trends in series of lectures (two 90 min lectures, each morning from Monday to Friday). The focus of the first week was on theoretical and computational methods of photo induced dynamics in strong laser fields (F.H.M. Faisal, N. Moiseyev, U. Peskin) and the formation of laser filaments in optical media (J. Moloney). In the second week different aspects of the response of molecules to a strong field were introduced and discussed (W. Hill III, H. Kono, D. Tannor). The seminar was completed with a focus on the generation and application of attosecond pulses (P. Agostini) and an introduction to relativistic optics (R. Sauerbrey). Interaction between the graduate students and post docs with the experts were inspired by joint work on computer projects, a discussion on open problems (named by the lecturers), short talks by the participants as well as social activities in the afternoons and evenings.
The international workshop focused on the most last achievements, among them were: *High harmonics and attosecond science and technology.* The generation of intense radiation from high harmonics and its application to generate pulses in the sub-femtosecond regime is currently one of the most vividly discussed topic in the field. The measurement of a two-photon two-electron ionisation with high harmonics in the soft X-ray regime was presented. Different aspects of the observation of attosecond electron dynamics with and without attosecond laser pulses were discussed.

Molecules and clusters in intense fields. A wide spectrum of theoretical approaches, ranging from numerical simulation techniques to the combination of wave packet approaches with S-matrix methods, to investigate phenomena in complex targets, such as molecules and clusters, were discussed. These talks were complemented by the presentation of experimental observations of the ionisation and Coulomb explosion of small diatomic molecules, the dynamics of atoms in the rearrangement of molecular ions and the dissociation of large molecules and clusters.
Coherent Control. It was shown how experimental techniques to shape a laser pulse in intensity, phase and polarisation allow to coherently control the response of a molecule to an optical field. While the control mechanisms in the non-perturbative intensity regime are still widely unknown, impressive theoretical progress in understanding the optimisation of processes at low intensities were presented.
Femtosecond interaction and propagation. Several reports showed the current joint efforts of experiment and theory towards an understanding and control of the formation of laser filaments. The importance of these studies became obvious from presentations on the perspectives how to use femtosecond plasma channels for atmospheric research.
Relativistic super-intense optics and applications. An overview of the generation of highest laser intensities and the possible applications for laser induced particle acceleration was given.
Young scientists presented their results in more than 70 posters during two poster sessions, which were times of vivid discussions among the participants of the workshop.
A special event of the workshop was a panel discussion on the filamentation of femtosecond laser pulses in optical media. During one afternoon the leading experts openly discussed the current understanding of the physics as well as the challenges and open problems towards an application of this interesting phenomenon. According to the reaction of the panel members it was one of the few opportunities where people did freely exchange their points of view on the same field of interest.
R. Sauerbrey gave a public evening lecture on *Die Kraft des Lichts. Physik mit Hochintensitätslaser*, which was well attended by approx. 150 guests. A vivid discussion between the guests and the speaker at the end of the lecture as well as over snacks and wine in the lobby concluded the evening.
We thank the Max-Planck-Institut für Physik komplexer Systeme for all the support in organising the seminar and workshop. We also acknowledge partial support by the Core-to-Core Program on Ultrafast Intense Laser Science (Japan Society for the Promotion of Science), the Priority Area Program on Control of Molecules in Intense Laser Fields (MEXT, Japan) and the Minerva Foundation.

International Summer School on Quantum Information

Workshop, Scientific coordinators: R. Blatt, A. Buchleitner, R. Gill
The purpose of our "International Summer School on Quantum Information" was to provide intense training for a selection of approx. 60 (approx. 10 of which from Dresden University or from mpi**pks**) promising and highly motivated students or young Post-Docs, in the field of Quantum Information. The lecture program extended over four weeks, with two 90 minutes lectures every morning, and one 90 minutes lecture, the monthly mpi**pks** Colloquium, seminars, extra lectures, open problems and dictionary sessions during the afternoon. Most lecturers contributed a series of five lectures (à 90

minutes), distributed over four weeks. The various lecture courses covered the entire realm of quantum information science, from mathematical foundations over algorithmic and theoretical aspects to experimental implementations. Along a steep learning curve, starting out at the basics, students were guided to cutting edge research. The seminar program was composed by talks delivered by the School's students, to introduce their respective fields of expertise/interest, and to stimulate scientific exchange and discussion. The rather diverse background of the students was nicely reflected by the diversity of the covered material. Dictionary sessions were used as a complementary tool, such as to clarify jargon specific of the different subcommunities which meet under the wide roof of quantum information: In that framework, lecturers or advanced participants of the School volunteered (ad hoc) to explain key words which had not been sufficiently clarified during lectures or seminars, on the blackboard.
The course and seminar program was dense, and, on average, the students certainly were well occupied to absorb and digest the offered material. The institute's infrastructure – the library with special material on the School's subject area on display, the seminar and discussion rooms, the guest house facilities, and, last but not least, the ping-pong table placed at the ground floor of guest house 1 –, its crew (visitors program, computer support, technical and administrative staff), and the fortunate selection of participants created an intense and creative atmosphere, building scientific and personal contacts which are likely to last. During the year after the School, several cooperations emerged, participants visited each other at their respective institutions, and some cooperation projects initiated at mpi**pks** already led to common publications by various participants. It should be stressed that the total duration of four+one weeks is a crucial ingredient for the success of such event, since mutual trust and familiarity need time to grow.
The School closed with a one week international conference on the topic, with approx. 120 participents, half of which were the School's students. The best seminar contributions of the School were upgraded to talks during the conference, and the concerned students did a splendid job. Students of the School were also actively participating as conference chair persons, and could present their own scientific work during prominently placed poster sessions.
The theory lectures of the School will be published under the title "Theoretical Foundations of Quantum Information", in the series Lecture Notes of Phyics, by Springer Verlag, in 2007.

Critical stability of few-body quantum systems

Workshop, Scientific coordinators: A. Jensen, L. Wiesenfeld

Aim and Purpose: Almost all subfields of physics are confronted with interesting problems related to few-body physics at the edge of stability as demonstrated at previous meetings at ECT* in 1997, 2003 and Les Houches in 2001. Few-body physics are often the result of selecting the crucial degrees of freedom within many-body systems. Being close to stability or close to thresholds often enhance effects of the related degrees of freedom. This is not subfield specific but rather a general observation at least within physics. The broader universal picture is fruitful but also essential in communications between people from different subfields.

The feed back from previous workshops were very positive both during the workshops and afterwards when participants expressed views on successful and less successful meetings. These participants had apparently lots of relevant information to exchange with each other. This encouragement is one reason why we followed up by organizing the present workshop on similar topics and appealing to similar, but not identical, groups of people. The other convincing reason for taking the trouble to organize a new workshop were the developments in the field of few-body physics at the edge of stability. Almost all subfields of physics contribute with interesting problems of this nature. The concepts, ideas, methods and techniques are often similar or identical in the different subfields, but not equally well-known and not developed to the same degree of refinement. The usual meetings do not often appeal to the interdisciplinary aspects or at least bringing people together from rather separated physics communities is not often successfully achieved.

The idea of the present meeting was to bring together people with overlapping interests and supplementary knowledge from fields ranging from quantum chemistry via condensed matter, molecular, atomic, nuclear to mathematical physics. With such a variety of subfields it is essential to have overlapping interests in concepts, ideas or techniques. Smaller groups from the same community begin too easily to speak only to each other. The selection of participants therefore had to be very careful to promote exchanges between people genuinely interested in the deeper understanding of the problems addressed. We started with persons we knew individually to have the required qualities. We added some by recommandation, and some after they registered for participation.

We wanted contributions within the main theme of critical stability from as many subfields as possible and with a significant number of both topics and participants in common with the previous workshops. This more or less adiabatic development ensures both continuity and renewal. We planned a smaller shift of relative weighting towards inclusion of more molecular and condensed matter physics. This resulted in more atomic and molecular physics, and more classical non-linear physics at the expense of nuclear and hadron physics. We wanted to allow the participants to present the work they find most interesting. This gives a workshop influenced by the actual participants, it gives enthusiasm and discussion of the most recent results. The theme still remains as spelled out in the title.

The continuity of people was rather easy to keep as many previous workshop participants already had expressed their interest in the meeting, and when invited they accepted immediately. The participants should present a relatively broad distribution in age reflecting a mixture of experience and youthful energy, but all eager to learn. The level of the meeting should accordingly not be too technical unless the basis is presented at the meeting. Knowledgeable phd-students and post docs must be able to follow the essential pieces.

Structure and content: The worshop was kept within one full week beginning monday morning and closing on friday afternoon. The scientific program is reflected in the titles of the talks presented. The themes were in the announcements divided into 9 main topics:

- Weakly Coulomb or gravitational-bound few-body states

- Weakly short-range-interaction bound few-body states
- Continuum structure and few-body decay properties
- Dynamical few-body problems near instability
- Correlation in boson-fermion and mixed condensates
- Few-body correlation within many-body systems
- Exotic structures: Efimov, tango, Borromean, halo states
- Lower-dimensional systems
- Semi-classical methods

We divided the presentations into 9 sessions, one morning and one afternoon every day except wednesday afternoon. In each session were 4 speakers with a coffee break in the middle. Every speaker had 30 minutes to give the talk. The 15 minutes reserved after each talk for discussions were fully exploited almost every time. The last talk on friday were replaced by a discussion. In addition to the oral contributions we had about 10 poster contributions. They were mostly presented by the younger participants.
There was about 50 participants from 19 countries. A number of very knowledgeable scientists participated as well as a few capable phd-students and some postdocs. The most prominent participants were:
J. Briggs (Germany), atomic physics
J.B. Delos (USA), fractal and chaos theory
P. Duclos (France), mathematics
N. Elander (Sweden), molecular and chemical physics
C.H. Greene (USA), atomic and molecular physics
M. Hussein (Brazil), nuclear physics
R. Littlejohn (USA), mathematical physics
V. Ostrovsky (Russia), atomic physics
J.M. Richard (France), hadron physics
The institution mpi**pks** was very efficient in providing the physical framework, the infrastructure and the help with the necessary individual arrangements. Everything was so smoothly running that both the participants and the external organizers could concentrate fully on the content of the workshop. This clearly means that all the necessary underlying work is carried out. When no problems are visible it is easy to forget the fine-tuned machinary. This smooth running was characteristic throughout the organization from the planning stages to completion of the actual workshop.

Difficulties and achievements: The difficulties are the superficial differences in different subfields like notation, specific units, unessential simplifying assumptions invalid for other applications. The common features are too easily hidden. Much is known in one field and not in another and exchange of information would speed up the research. However, to identify similarities of approaches in different fields may be very difficult but also very useful. Progress would clearly be faster if we could ßpeak the same languageänd immediately distribute the knowledge from one field to another. Collaboration across subfield barriers would be welcome and an efficient method to transmit new insight.

We started by inviting about 27 key speakers, then made one general announcement of the meeting and asked for applications to attend. The final selection resulted in about 50 participants. This is an ideal number covering many different subfields still with several individuals within each. This number allowed time for an oral presentation for most participant while the remaining about 10 presented posters. To focus and get acquainted with the topic we asked for abstracts for distribution in advance. This was not meant to tie down the speakers to exactly those topics, but such written information is a very useful tool for communication across boundaries of different subfields. Unfortunately we missed here the opportunity to ask for the practical information of key references in these abstracts.

To prevent evaporation of the information after the last day of the workshop we decided to produce proceedings. For an interdisciplinary meeting these written tracks have turned out to be very useful both for people who wants to recall specific contributions and for people who wants to get an orientation of topics in a different subfield discussed at the workshop. Often the proceedings are produced too late and with too little new content to be of any value. Traditionally proceedings have also been blamed for preventing free discussion, but this certainly has not been an observable effect at these workshops. The proceedings are scheduled to appear in one issue of Few-Body Systems in the beginning of 2006. Each paper is subject to normal refereeing. The agreement with the journal is that the responsible (organizers and J.-M. Richard) guarantee the quality.

The presentations and discussions included surveys and examples of a number of methods as well as precise theoretical investigations of various few-body systems very close to the threshold of stability. Some talks were of review character of a field or a technique, some talks were much more specialized, some talks started with a soft introduction then turning into specifics, some talks were to a large extent presenting qualitative features without technical details. The content was left to the speakers, which were attempted selected with interest and capability to communicate and learn from people across subfields boundaries.

Specific applications to problems distributed throughout physics were addressed, i.e., transition states in chemical reactions, semiclassical approximations, vibrations of hydrogen molecular clusters, threshold laws for multifragmentation, zero-range interactions, universal scaling laws, level distances in resonating quartz blocks to test universal laws of symmetry breaking, symmetries in few-body fragmentation, photo disintegration of atoms and nuclei, three and four-nucleon states, the pentaquark, atom-positron physics, cold atomic bosonic and fermionic gasses, thermalization in integrable quantum gasses, excitons in quantum wires, quantum dots.

The meeting was very lively with lots of enthusiastic discussion and many pieces of useful information were exchanged. We used our contacts, knowledge and experience to organize this workshop. We think it essentially worked out as planned. We did not want just another conference, it should be a workshop with lots of discussion. The unifying aspects were to a large extent techniques, but also concepts proved to be useful in different subfields. As for the previous workshops, future research projects will be affected by this one and probably new collaborations initiated.

Dissipative solitons

Workshop, Scientific coordinators: N. Akhmediev, L. Pismen, Y. Pomeau
The workshop "Dissipative solitons" has been hosted by the Max Planck Institute for Complex Systems mpi**pks**) in Dresden from 23 till 29 of January 2006. Leading experts from 15 countries gathered together to discuss the present state of the art in this hot area of research. The list of lecturers consisted of around 40 authorities, including scientists from Scotland, Israel, UK, France, USA, Germany and many other countries from around the world. Each lecturer presented highly innovative approach to the subject within his own field of research. The 65 participants of the workshop shared their ideas in this multidisciplinary subject that incorporated ideas from physics, biology, chemistry, medicine, mathematics and the modern technology of optical communications and laser systems. The poster session and the panel discussions held within the workshop were highly exciting events that generated a new vision of the concept. The concept of dissipative solitons comes from a combination of soliton science, theory of systems far from equilibrium and the notion of 'self-organization'. As the lecturers clearly demonstrated, examples of dissipative systems can be found everywhere. Grass patches in nature, small droplets oscillating on a surface of a liquid, patterned organic films on a substrate, avalanches on mountain slopes these are all examples of objects that can be classified as dissipative solitons. The complexity of these objects can be very high. Every living thing can be considered as a dissipative system. Each organism needs a continuous supply of energy and/or matter for its existence. All the energy obtained has to be dissipated. This is the reason for the general term Dissipative system. An internal flow of energy and matter occurs continuously. When the flow stops, the structure disintegrates. There are many common features and useful properties of dissipative systems that can be used beneficially in technology. The distinctive feature of these systems is self-organization. The latter becomes essential for very small object sizes (nano-scales) and ultra-short time frames (femto- and atto-seconds), where control over the objects becomes difficult. Control over their shape becomes practically impossible when the structure moves. Then, the only way to prevent the structure from disintegration is self-organization. These principles can be applied successfully to technological devices and man-made systems such as ultra-short-pulse lasers, wide aperture laser systems and all-optical information transmission lines. The subject of dissipative solitons is a new rapidly-developing area of research. A multi-author book "Dissipative solitons" has been published by Springer in 2005. The comprehensive approach developed at the present workshop increased dramatically our knowledge of dissipative solitons, and created absolutely new and useful ideas for fundamental science and technology. The workshop allowed to enrich and to crystallize the notion of dissipative soliton. This event established "Dissipative solitons" as a legitimate scientific key-word. It was agreed that dissipative localized structures constitute a general type of organization in nature. The follow up of the workshop will be continued in various forms in other countries. The workshop "Dissipative Optical Solitons" will be organized by N. Rosanov in the framework of the XII International conference "Laser Optics - 2006", St.-Petersburg, Russia, in June 25-30. (http://www.ilph.spb.ru). Prof. Velarde is planning to organize similar workshop in Madrid, Spain. Thus, the present workshop has served as a seeding event for a broader set of meetings around the world on this subject.

Dynamics on Complex Networks and Applications

Workshop, Scientific coordinators: J. Kurths, M. A. Matias, A. E. Motter
This program, DYONET06, was held at the mpi**pks** between February 6th and March 3rd, 2006. The four-week Conference was structured in the following way: School, Workshop, Seminar I, and Seminar II.
Main focus: The Conference focused on the emerging field of dynamics on complex networks. This field combines concepts from the areas of complex networks, statistical physics, and nonlinear dynamics, and has as an essential underpinning a strong interaction among different disciplines and between theory and applications. Altogether, 27 invited speakers, other 67 participants (out of over 200 applications), and the three coordinators participated in the meeting.
Senior participants: The participants included leading experts working in these fields, such as J. Bader, E. Bollt, S. Bornholdt, G. Caldarelli, P. Hänggi, M. Hasler, S. Havlin, J. Jost, J. Mendes, E. Ott, L. Pecora, A. Politi, S. Redner, S. Solla, A. Vespignani, and D. Zanette. Furthermore, two mpi**pks** Colloquia were delivered by Z. Toroczkai (protein conformation networks) and M. Ghil (complex-systems modeling of Earth), in the second and fourth weeks, respectively. The meeting also hosted an evening lecture (in German) by B. Blasius (networks, chaos, and synchronization of ecological systems).
Young scientists: 34 out of the 80 talks given in the Workshop, School and Seminars were presented by young scientists (typically at the postdoctoral and junior faculty level, but also included a few Ph D and even diploma students). For instance, the diploma student M. Schäfer presented an interesting work on the propagation of failures on networks, which has been subsequently published in PRL. The majority of the 25 posters presented in the meeting was by young participants. A two-minute oral presentation of each poster was arranged, so that the poster presenters could reach a wider audience. During each Seminar week, a day was arranged in which Ph D students could briefly present their work and get interesting feedback from the more senior participants.
Scientific results: This Conference helped crystallize the emerging field of dynamical phenomena on complex networks as a promising area of interdisciplinary research. The works presented in the conference included research efforts in established areas such as epidemic spreading, traffic congestion, cascading failures, and synchronization of coupled oscillators, and that are just at the forefront of the current research on network dynamics. These works reflect a new trend within the area of complex networks, where along with the study of the purely structural and evolutionary properties that gave birth to the area, there has been an increasing interest in the interplay between the structure and the dynamics of complex networks. The combination of contributions from experts primarily working in different areas, such as nonlinear dynamics, statistical physics, and life sciences, was a very unique and outstanding aspect of the Conference. This helped create a stimulating atmosphere of discussions that is expected to foster the creation of a common framework for the study of dynamical processes on complex networks and can result in potentially important collaborations across disciplines. Our overall evaluation of the Conference is very positive. The Conference generated exciting discussions, the average attendance in the activities was high, and the level of most contributions was excellent. In order to disseminate the scientific out-

puts of the Conference, we are organizing the publication of a Special Issue in Physica D with ca. 25 original selected papers and also a Springer's Book with review articles from distinguished participants.

Acknowledgments: We would like to thank MPI for the Physics of Complex Systems for generous support and the ideal environment to carry out the Conference. In particular, we would like to acknowledge the Guest Program of the *mpi***pks**, specially Marita Schneider for her extremely efficient, dedicated, and competent contribution in handling all the issues related to the organization of the Conference.

Cold Atoms Meet Condensed Matter

Seminar and Workshop
Scientific coordinators: I. Bloch, Ch. Bruder, W. Zwerger

CATCOM 2006 took place from March 27 to March 30, 2006. There was a total of 76 participants (29 professors, 31 postdocs, and 16 PhD students). 29 of the participants were affiliated with German research institutions, 35 with European ones outside of of Germany, and 12 participants came from the U.S. or Japan. We had to turn down a considerable number of potential participants: there were about twice as many applications as open slots.

The main focus of the conference was on the interface between the very active research field of ultracold atoms and - more generally - atomic and molecular physics with condensed-matter physics. In the last couple of years, a very fruitful exchange of ideas and concepts has taken place between both fields. For instance, cavity QED experiments have been realized with Cooper-pair boxes replacing single atoms, while quantum phase transitions have been studied in a perfectly tunable system with cold atoms in optical lattices. Further examples include active cooling techniques adopted from laser-cooling which are now applied to cool nanomechanical resonators into the quantum limit of zero or just a few phonons, or the realization and study of Bose-Einstein condensates on a microchip. A number of recent theoretical proposals have also considered combinations of cold atoms and molecules or ion-trap configurations with solid-state devices like single-electron boxes or with nanomechanical resonators.

We had invited 17 speakers, all of which accepted our invitation without hesitation. Two of them [P. Zoller (Innsbruck) and R. Schoelkopf (Yale)] were unable to attend the workshop but were replaced by speakers from the group [P. Rabl] or by an outstanding alternative [J. Doyle (Harvard)]. All of the invited speakers are internationally leading experts in their field and gave excellent talks. Nobel-laureate W. Ketterle (MIT) and R. Grimm (Innsbruck) gave fascinating accounts of their experiments on pairing phenomena in ultracold quantum gases. J. Reichel (ENS Paris) and C. Zimmermann (Tübingen) reported on progress in atom-chip experiments, and D. Bouwmeester (Santa Barbara), K. Schwab (Cornell), and K. Karrai (LMU München) talked on various aspects of cooling of mechanical degrees of freedom. S. Haroche (ENS, Paris) provided an authoritative introduction to cavity-QED experiments with Rydberg atoms while S. Girvin (Yale) reported on cavity-QED theory and experiment in superconducting structures. In the area of cold atoms the most recent advances with Fermions in optical lattices and with two-dimensional Bose-Einstein condensates were reported by T. Esslinger (ETH Zürich) and J. Dalibard (ENS, Paris).

The invited talks were complemented by a (small) number of contributed talks and

the poster session. Because of the high scientific standing of most of the participants, the poster session had a very high level as well. Out of the 16 PhD students that participated, 2 gave talks, and most of the others presented posters.

The talks, discussions, and posters at CATCOM 2006 demonstrated that the field is developing rapidly and has great prospects. In particular, it brings together scientists from areas which had been separated for a long time and thus opens many really new areas of research beyond the traditional directions.

To conclude: in our opinion, CATCOM 2006 was a great success: S. Girvin (Yale) called it "one of the best conferences I ever attended". This success was made possible by the superb infrastructure of the mpi**pks**and the excellent and always friendly support of Claudia Pönisch.

Quantum Coherence, Noise and Decoherence in Nanostructures

Seminar and Workshop
Scientific coordinators: Ch. Bauerle, G. Schön, A. Zaikin

The Seminar and Workshop took place at mpi**pks** in Dresden on May 15-26, 2006 and were mainly focused on recent progress in investigations of coherent phenomena, noise and interaction-induced decoherence in a variety of nanoscale structures of different dimensions such as quantum dots, quantum wires, nanorings, solid state qubits, hybrid normal-superconducting systems, disordered two-dimensional electron structures etc. Some of the key subjects covered during the Seminar and Workshop were transport of interacting electrons in disordered conductors, low temperature electron decoherence in metals and semiconductors, decoherence and quantum computation, shot noise and full counting statistics, metal-isulator phase transition in 2D structures, persistent currents in nanorings, mesoscopic superconductivity and spintronics.

Over 100 participants from Europe, USA, Canada, Japan, Israel and Taiwan took part in the meeting. The program included 76 oral presentations, both invited and contributed, as well as two poster sessions. Invited talks were presented by a number of leading experts in the field who covered major recent achievements in both theory and experiment. Younger participants presented their recent results in the form of short talks and posters.

Among the most important participants and results presented by the inivted speakers let us mention R.A. Webb "Shot noise and decoherence in nanostructures", Y. Gefen "Decoherence in Mach-Zehnder interferometer", A. Finkelstein "Metal-insulator transition in disordered two-dimensional electron gas", S. Kravchenko "Critical behavior of the spin susceptibility near the 2D metal-insulator transition", J. Mooij "Superconducting nanowires as quantum phase slip junctions", T. Klapwijk "Spin triplet supercurrent through the half-metallic ferromagnet CrO_2", G. Zarand "Theory of inelastic scattering from quantum ipurities", M. Büttiker "Dephasing and inelastic scattering from voltage probes", U. Weiss "Counting statistics of open point contact tunneling", K. Ensslin "Shot noise in quantum dots", H. Grabert "Josephson junctions as on-chip detectors", P. Lindelof "Superconducting contacts to carbon nanotubes", P. Mohanty "Realizing quantum nanomechanics", Y. Nakamura "Decoherence in flux qubit", S. Tarucha "Probing and manipulating spin effects in quantum dots" and J. Clarke "Entanglement of two flux qubits with controlled interaction". Many other participants also made important contributions and presented interesting new results. Let us also

mention the high quality of talks of many young scientists as well "scientific newcomers" from related fields.
¿From our viewpoint the meeting was definitely a success. It has clearly responded to the two main goals we have set : (i) to bring together leading scientists working in different sub-fields of condensed matter physics in order to discuss recent advances in the field, to visualize further research prospects and to promote new research collaborations and (ii) to bring together top level scientists and young researchers, to stimulate lively interaction and exchange of ideas between them. We have gotten an extremely positive feedback from many of the invited speakers who have also encouraged us to repeat a similar meeting in the future.
We would like to thank mpi**pks** for its hospitality and excellent infrastructure provided for our participants. We would also like to thank the team of secretaries for their kind assistance in organizing the Workshop.

Correlated and Many-Body Phenomena in Dipolar Systems

Workshop, Scientific coordinators: N. Bigelow, H. Sadeghpour
A workshop on recent developments in the emerging subfield of dipole-dipole interaction in atomic, molecular, and mesoscopic systems was held at mpi**pks**-Dresden from May 29 to June 2, 2006. The workshop was attended by about 55 practitioners in the field, from the US, EU, Russia and Japan, and 41 invited long- and short-talks were presented. An accompanying poster session, joined by a menu of fine German beers, was a popular hit with the workshop participants.
The organizers arranged the sessions along permanent and induced electric and magnetic dipole lines: a session was devoted to metastability, and crystalline phase transitions could be induced by tuning the induced dipole-dipole interactions in optical standing lattices using ultracold quantum degenerate Bosonic and Fermi gases. Gora Shlyapnikov described how a spinor BEC would exhibit supersolid behavior in an optical lattice. Another talk by Guido Pupillo theorized the existence of a quantum phase transition from a superfluid to a triangular crystal.
Two sessions (one full day) were allocated to attempts at creating ultracold dipolar (polar) molecules and techniques in manipulating them. Such molecules are progressively being touted as ideal laboratories for precision measurements of the fine structure constant and the electric dipole moment. Collisional and magnetic field quenching of transitions, which normally lead to depletion of molecules from the traps, were discussed. In one such talk, Jun Ye discussed how Stark decelerated OH molecules were used to measure the lowest lambda-doublet lines with an order of magnitude improvement in accuracy.
A full day was devoted to discussion of magnetic dipoles and spinors. Recent creation of the fully spin-aligned chromium BEC was reported by Tilman Pfau. This is the first measurement of the observable mechanical effect of dipole-dipole interaction in an ultracold gas. The stability of such a BEC and the effect of long-range spin-orbit interaction in a spinor BEC were discussed.
Another full day was allocated for discussion of induced electric dipoles in Rydberg-Rydberg collision and spectroscopy. Major developments in manipulating many-body long-range interactions in Rydberg electron collision in ultracold atomic samples, frozen Rydberg gas, van der Waals blockade, spontaneous evolution into plasma and other

coherence and statistical properties of cold and ultracold Rydberg gases, were reported. Such phenomena as blockade of multiple excitations hold promise for construction of quantum logic gates.
A session on dipolar aggregates, clusters, nanoparticles and complex molecules, but not necessarily cold, reported on interesting developments, such as ferroelectric domain formation, and spectral broadening of absorption lines due to dipolar interaction.
One of the decidedly advantageous aspects of holding the workshop at the MPI-Dresden was its friendly and accommodating atmosphere. This is particularly helpful for young and aspiring researchers who find easy access to senior faculty and speakers. The office facilities are first-rate. Particular to this workshop, was the availability of top-notch researchers from different areas of AMO and condensed matter physics with expertise on dipolar interactions. Having experts from different subfield on the same floor was welcomed by the participants and especially so, by the junior members of the workshop. Finally, and definitely not last, the workshop organizers benefited enormously from the expertise and assistance of a fine and devoted staff at mpi**pks** for all sorts of things, from the mundane to even arranging for a fine social tour of the city. We are indebted to all at mpi**pks**, Prof. Dr. Jan-Micheal Rost for the hospitality and above all to Ms. Claudia Poenisch, who so expertly guided everyone and us.

XXX. International Workshop on Condensed Matter Theories

Workshop, Scientific coordinators: P. Fulde, H. Reinholz, G. Röpke
The 30th International Workshop on Condensed Matter theories was held at the mpi**pks** June 5-10, 2006, under the sponsorship of the Max-Planck-Institute Physics for Complex Systems, Dresden. It was organized by the institute (Prof. P. Fulde, M. Schneider as local organizer) and the University of Rostock (Prof. G. Röpke, Dr. H. Reinholz), Prof. M. Das (Canberra, Australia) and Prof. R. Bishop (Manchester, UK) from the Workshop's International Advisory Committee. The International Workshop on Condensed Matter Theories is an annual scientific meeting since its inception in Sao Paulo, Brazil in 1977, and the longest continuously running yearly event. Originally initiated as an initiative to get together US and Latin American physicists, the workshop is now held at varying places all over the world, e.g. India, Australia, Argentina, Japan, US. Within these places, the institute was a special highlight as the venue for the 30th anniversary.
This series of Workshops is devoted to the development and promulgation of advanced methods for the description of condensed many-body systems. Adhering to the tradition, the Workshop has been interdisciplinary, where the emphasis was placed on the common concerns of theorists applying advanced many-particle methods in such diverse areas as solid-state, low-temperature, nuclear, particle, statistical, and biological physics as well as in quantum field theory, quantum information and the theory of complex systems. This corresponds closely to the expertise of the hosting institute.
The list of participants consisted of regularly attending well established scientists, e.g. J. Clark, R. Bishop, B. Malik, A. Proto, as well as a considerable number of newly interested and mainly locally based (German) speakers. The interchange of points of view between participants with distinct scientific interests in modern techniques for the description of condensed many-body systems gave rise to a highly stimulating atmosphere.

Prominent speakers highlighted advances in the very broad fields of applications which incorporated high-temperature superconductivity (M. Das/Canberra, H. Gross/Berlin), Density functional theory (P. Gori-Giorgi) and Bose-Einstein condensation (R. Zimmermann), low dimensional systems along with quantum dots (D.E. Logan/Oxford), mesoscopic systems (E. Suraud/Toulouse) and magnetic properties (C. E. Campbell). It shall be emphasized that the contributions by U. Schollwöck/Aachen (quantum information), H. Stolz/Rostock (Bose-Einstein condensation) and J. Tiggesbäumker/Rostock (cluster physics) with experimental background were particularly stimulating. A poster presentation was organized for young participants to present their results. A number of scientists working in Dresden or who habe been peviously working at the mpi**pks** participated as well, e.g. Eschrig/Dresden, G. Zwicknagel/Braunschweig and E. Runge/Ilmenau.
In a special session the birthdays of Susanna Hernandez (Buenos Aires) and Mikko Saarela (Oulu) who made considerable contributions to the physics of 4He were celebrated with talks by the jubilees as well as E. Krotscheck (Linz) , M. Miller (Washington) and J. Boronat (Catalunya). In Honour of the 100th birthday of the late Sir Nevill Mott a presentation to the general public was given as an evening lecture by G. Röpke.
The Workshop encouraged cross-fertilization between different approaches to various many-body systems and promoted continuing collaborative efforts involving groups of regularly attending Workshop participants and newcomers in order to increase the stem of the Workshop participants by younger scientists. As a result, common publications of participants are expected. The Proceedings of the Conference will be published as a volume by World Scientific.
The workshop finished with a business meeting of the International Advisory Committee. The members expressed their gratitude to P. Fulde and the hosting institute for the excellent workshop facilities and the financial funding. It was decided to hold the next meeting of the Workshop in Bangkok/Thailand in December 2007.

Constructive Role of Noise in Complex Systems

Workshop, Scientific coordinators: A. Neiman, A. Pikovsky
The main focus of the meeting was on the role of fluctuations and noise in complex systems. The meeting was organized as a 3 week seminar with lectures and intensive discussions followed by one week workshop.
We were happy to have lectures presented by leading researches in the filed of statistical physics, biophysics, medical physics and nonlinear dynamics: Christian van den Broeck (University Hasselt); Werner Ebeling (Humboldt University, Berlin); Jordi Gracia-Ojalvo (Technical University, Barcelona); Frank Juelicher mpi**pks**); Pavel Krapivsky (Boston University); Peter Haenggi (Augsburg University); Juan Parrondo (University of Madrid); Peter McClintock (Lancaster University); Peter Tass (Research Ceneter Juelich); Lev Tsimring (University California San Diego); Lutz Schimansky-Geier (Humboldt University, Berlin). Lectures were also given by young prominent scientists such as Brent Doiron (New York University), Benjamin Lindner mpi**pks**) and Eric Lutz (Augsburg University) who will definitely shape the field in the near future. P. Haenggi gave a mpi**pks** colloquium talk, and W. Ebeling presented a public lecture.

We had a large group of graduate students participated both in the seminar and in the workshop. During the seminar all students gave 20 min oral presentations. For some of them this was their first talk in an international scientific meeting. During the workshop all students presented their results at two poster sessions. Our scientific newcomers did extremely well and had opportunity to have informal and intensive discussions with senior participants.
As results of this meeting we would like to underline two aspects. First, from a broad theoretical point of view the meeting showed increased interest in the field of fractional Brownian motion and kinetics and in the field of quantum fluctuations. Another hot topic is related to applications of modern theories of statistical physics and nonlinear dynamics to small systems on nanoscale and biological systems. Remarkably, in both latter examples one studies point processes with correlated events, what makes the importance of unified theoretical approaches evident.
We consider the seminar/workshop as extremely successful, and are thankful in the name of all participants to the Max Planck Institute for the perfect organization and to the Office of Naval Research Global for support.

Dynamics and Relaxation in Complex Quantum and Classical Systems and Nanostructures

Workshop, Scientific coordinators:
B. Altshuler, V. Falko, A. Ludwig, K. Wiese, I. Aleiner
The international Seminar and Workshop Dynamics and Relaxation in Complex Quantum and Classical Systems and Nanostructures was devoted to quantum transport and field theories of quantum disorder, a fast-growing field of charge and spin dynamics in nanostructures (including manipulation of multi-qubit systems and spins in quantum dots), and to theories of disordered and strongly interacting classical systems. The programme started with a three-week Workshop focused on the theory of phase coherence and de-coherence in qubits, interaction and localization in one and two dimensions and fundamental issues in classical disordered systems. The recent progress in the field theory of pinning and its relation to chaos, random fields and fermions, as well as to the new results on non-integrable quantum field theories and disordered classical systems have been brought up by Miguel Ortuo (Murcia), Pierre Le Doussal (ENS Paris), Kay Wiese (ENS Paris) and Giuseppe Mussardo (SISSA Trieste). They have shown spectacular theoretical results in this field, which were confirmed by the extensive numerical simulations by Alan Middleton (Syracuse). Igor Lerner (Birmingham) has shown how to apply statistical field theory methods to study critical phenomena in computer networks (in application to email traffic and distribute computing). Finally, Igor Aleiner (Columbia Univ NY) and Denis Basko (Princeton) have presented the new theory of the interactions-driven localisation transition in disordered systems. The issue of decoherence has been discussed in relation to a very broad range of complex quantum systems and devices, ranging from Luttinger liquid formed on the edge of a two-dimensional quantum Hall effect system [Yuval Gefen (Weizmann Inst), Dima Feldman Brown University), Ady Stern (Weizmann Inst)], superconducting and quantum dot spin qubits [Yuri Galperine (Oslo), Rosario Fazio (Pisa), Valery Pokrovsky (Univ Texas), Baruch Horovitz (Haifa), Elisabetta Paladino(Catania)], quantum wires and dots [Leonid Glazman (Minneapolis), Alessandro Silva (ICTP Trieste), Bjrn Kubala

(Bochum), John Jefferson (Qinetiq)]. During the middle part of the Seminar, the main attention has been given to the spin-related effects in quantum nanostructures. Naoto Nagaosa (Tokyo Univ), Arturo Tagliacozzo (Naples), Yaroslav Tserkovnyak (UCLA), Leon Balents (UCSB) discussed theories related to the spin-orbit coupling in 2D electron gases and quantum dots, with one week fully dedicated to the discussion of the spin Hall effect. Alexander Tartakovskii (Sheffield) has reported an amazing observation of the bistable behaviour of nuclear polarisation in optically pumped quantum dots, with the theory of this new effect developed by Alan Russell and Vladimir Falko (Lancaster). The culmination of the Seminar was in the one-week Graphene Conference. In 2004, the group of A. Geim at Manchester has separated individual graphene flakes (atomically thin graphitic monolayers and bilayers) from pyrolitic graphite crystals and produced the first graphene-based field-effect transistor. Since then, Geims group and P. Kim and H. Stormer at Columbia University NY have processed individual graphene flakes into microstructures and measured their transport characteristics while varying the carrier density in graphene sheets from the electron (n) to the hole (p) channels. The most recent technological development in graphene has been that of E. Rotenberg (Lawrence Berkeley National Lab) who have grown monolayer and bilayer graphene on a silicon carbide substrate and performed angle-resolved photoemission measurements confirming the features of the electronic band structure of these materials. All these and other more recent developments have been reported by the world leaders in the field: Andre Geim (Manchester), Philip Kim (Columbia University NY), Walter de Heer (Georgia Tech), Eli Rotenberg (Berkeley). The recently performed measurements of Raman spectra have been reported by Klaus Ensslin (ETH Zurich) and Andrea Ferrari (Cambridge). Alberto Morpurgo (TU Delft) has shown the results on the first operational graphene-based Josephson proximity effect transistor. The advancement of theory has been described by the repsentatives of most of the groups involved in graphene research. Edward McCann (Lancaster), Alexander Altland (Koln) Igor Aleiner (Columbia University), Matthew Foster (UCSB), Igor Gorny (Karlsruhe), and Vadim Cheianov (Lancaster) formed the complete picture of the quantum interference effects in graphene. Vladimir Falko (Lancaster), Fracisco Guinea (Madrid) and Antonio Castro Neto (Boston) reviewed the most unusual properties of this new material derived from its band structure. Vladimir Falko, Louis Brey (ICMM Madrid) and Herbert Fertig (Univ. of Indiana Bloomington) delivered the peculiar theories of quantum Hall effect in graphene, which Janis Pachos (Leeds) and Yasuhiro Hatsugai (University of Tokyo) related to the index theorem in application to this two-dimensional crystal. The Graphene Conference was great success. It attracted a lot of interest from community (55 participants came to Dresden on a very short notice). This was the first Conference entirely dedicated to this new material, and, now, it will be followed by the focused workshop in KITP in Santa Barbara (January 2007) and possibly by the ESF Conference in 2008. All components of the Seminar have been productive and met their goals. Half of the Seminar participants were junior researchers who collaborated with the senior participants and engaged themselves in numerous discussions. The atmosphere of the meeting was informal, with a lot of open fruitful discussion.

Interactions, Excitations and Broken Symmetries in Quantum Hall Systems

Workshop, Scientific coordinators: A. Mirlin, F. von Oppen
QHSYST06 took place in Dresden from October 2 to October 7, 2006. There were a total of 60 participants, out of whom 16 represented Germany, 26 other European countries and Israel, and 18 the Overseas (USA and Japan). The program consisted of 31 invited and 5 contributed talks, as well as 16 poster presentation. If proof was needed, this workshop unambiguously demonstrated that a quarter century after the discovery of the integer quantum Hall effect (IQHE) in 1980 and the fractional quantum Hall effect (FQHE) in 1982 the field of quantum Hall (QH) physics continues to develop rapidly, remaining one of the most active research areas of modern physics. The Workshop program was structured in thematic sessions, with 3-5 interrelated talks in each of them. The talks by leading experimentalists who reported a large number of remarkable new results, were complemented by theoretical talks where many fascinating novel concepts were proposed. In view of space limitations, we can only mention some of the highlights of the Workshop: Magnetotransport and quantum Hall effect in graphene Recent breakthrough in manufacturing of single-and double-layer graphene structures have triggered a flurry of research activity in this area. The transport measurements demonstrated a number of remarkable properties of these systems, including novel types of the quantum Hall effect, related to the Dirac nature of carriers in graphene. The interest in these systems is given additional impetus by expectations that graphene-based structures may play a key role in future nanoelectronics. Experimental aspects of this exciting field were presented at the conference by A. Geim (Manchester) and A. Yacoby (Harvard). Theoretical developments on the QHE in graphene were summarized by V. Falko (Lancaster). Quantum Hall interferometry Quantum coherence in the quantum Hall regime as probed by edges state interferometers attracts a lot of interest. Pioneering experiments by the Weizmann Institute group were presented by M. Heiblum (Rehovot). The theory of these experiments was discussed by J. Chalker (Oxford). The presentations by Y. Gefen and A. Stern (both Weizmann Institute) discussed prospects of using QH interferometers for confirming the fractional and nonabelian quasiparticle statistics in the FQHE. Non-abelian statistics and quantum computation Applications of the QH physics to the fi@eld of quantum computations was also addressed. The most actively pursued proposal at present is to use FQH states with non-abelian statistics of excitations, as discussed in talks by S. Simon (Lucent), E. Rezayi (Los Angeles), and J. Jain (Pennsylvania). In his talk at the mpi**pks** Colloquium, organized during the Workshop week, K. von Klitzing (Stuttgart) reviewed the unique role played by the QHE in metrology. To summarize: The talks, discussions, and posters at QHSYST06 demonstrated that the field is very active, with many fascinating new develoments. Approximately 40

Extreme Events in Complex Dynamics

Workshop
Scientific coordinators: S. Albeverio, V. Jentsch, H. Kantz, S. Ruffo
Extreme events challenge our highly complex civilized life in many ways, such as in the form of extreme precipitation events and floods, by earthquakes, by network failures (power supply, Internet, traffic networks), by extreme socio-political events and by extreme economical events. Despite of their high potential damage, extreme events do

not receive sufficient attention in all of the corresponding specific disciplines. In parallel and only partly connected to real world phenomena exist mathematical theories such as the theory of large deviations and extreme values statistics, and fundamental work in statistical physics on systems exhibiting large fluctuations.
On the workshop the current state of research related to extreme events was presented, by invited and contributed talks and by an extensive poster session. It was fully interdisciplinary including applications. Experts in, e.g., meteorology (L.A. Smith), climatology (M. Ghil), mathematical finance (D. Sornette) geology (S. Hergarten), avalanche research (M. Lehning), traffic flow (K. Nagel, D. Helbing) presented and discussed their phenomenology of extreme events. Statistical physicists (Z. Racz, P. Holdsworth) and mathematicians (P. Imkeller, S. Steinebach) discussed recent theoretical results, numerical simulations and laboratory experiments relevant for the issue. The seminar was devoted to physical and mathematical theories and consisted in tutorials in extreme value statistics (Z. Racz), theory of large deviations (R.S. Ellis), atmospheric turbulence (J. Peinke), and stochastic processes (R. Mahnke). It served particularly young scientists to obtain an overview of relevant theoretical concepts for the research in extreme events. Younger participants presented their work by talks during the seminar and in a poster session during the conference.
Recent results, among them the claim of Bramwell, Holdsworth and Pinton of a universal distribution of fluctuations found in turbulence as well as in critical phenomena, suggest that a global point of view would reveal surprising commonalities between extremes in very different systems. The conference initiated the very relevant discussion about how far extreme events can be studied under unifying aspects and how far common theoretical descriptions will be possible and useful. Many interactions between participants from different disciplines during the conference showed clearly that it is highly beneficial for all participating disciplines to establish the research on extreme events on a more abstract level as a field in complex systems research. It served to collect the current knowledge, to explore potentially relevant theoretical concepts and model classes, and to explore the forefront of the different fields which can contribute to a theory of extreme events. The conference helped to make a step towards identifying sufficient and necessary conditions for a system to create extreme events, identifying mechanisms and precursors of extreme events, and advancing theories such as extreme value statistics and the theory of large deviations into a state applicable to nonlinear, long range correlated processes.

Nonlinear Dynamics of Acoustic Modes in Finite Lattices: Localization, Equipartition, Transport

Workshop, Scientific coordinators: A. Giorgilli, S. Flach
The aim of the workshop was to bring together different groups of researchers working on models strictly related to the celebrated nonlinear chain of Fermi–Pasta–Ulam. Needless to say, this has been the first nonlinear model to be investigated by numerical methods.
The list of invited people included: (i) mathematicians and physicists who are specifically working on the FPU system, both from numerical and from analytical viewpoint; (ii) researchers working on special solutions of nonlinear lattices, namely periodic orbits and breathers; (iii) people interested in related phenomena, including conductiv-

ity, molecular dynamics, nanoparticles, Anderson localization and transport, biological models.
The program included more that 30 long (invited) talks, a few short talks and poster sessions. Among the invited talks I shold mention in particular those delivered by Serge Aubry, Boris Altshuler, Leonid Bunimovich and Luigi Galgani. Senior participants included Giancarlo Benettin, Tassos Bountis, Giulio Casati, George Chechin, Roberto Livi, Antonio Politi and Stefano Ruffo. I should also mention that it was a great pleasure to see many young researchers among the participants, most of them presenting interesting work. It may also be noticed that the group of italian people was quite numerous, in consideration of the long–standing tradition of studies related to the FPU problem in italian universities, in particular Milano, Padova and Firenze.
The workshop has been very successful in joining together expertise and knowledge on different problems. Comments that I have heard from many, especially young, participants were very positive. I should say that the main goal of the workshop, namely making people with different interests, experience and knowledge to interact taking the FPU problem as a common basis, has been fully reached. As a personal remark, I discovered with great pleasure a number of results strictly related to the dynamics of the FPU chain, in particular those related to the study of periodic orbits, traveling waves and transport, that I was not copmpletely aware of. It seems likely that new international collaboration will be born in the next future, thanks to the opportunity of encounter and of exchange of knowledge offered by this beautiful workshop.

4.4 Externally Funded Research and Relations to Industry

4.4.1 DFG Projects

Individual Projects

- *Experimentelle und theoretische Untersuchung von räumlich lokalisierten Anregungen in nichtlinearen Gittern*, Dr. S. Flach
- *Probabilistische Verfahren zur Vorhersage raumzeitlicher Strukturen des Autobahnverkehres*, Prof. H. Kantz
- *Modellierung schneller chaoticher Freiheitsgrade durch stochastische Prozesse*, Prof. H. Kantz
- *Kohn-Sham Dichtefunktionaltheorie mit exaktem Austausch für Grund- und angeregte Zustände*, Dr. S. Kümmel
- *Moderne und universelle first-principles Methoden für Mehrelektronensysteme in Chemie und Physik*, Dr. U. Birkenheuer
- *Wechselwirkung in ultrakalten Atom- und Molekülgasen*, Prof. J.-M. Rost, Dr. T. Pattard
- *Directed Transport within Hamiltionian Dynamics: From Theory to Cold Atoms Experiments*, Dr. S. Flach

Schwerpunktprogramme

- *Elektronenstruktur und Magnetismus (SPP 1153)*, Dr. U. Saalmann
- *Zeitreihenanalyse von Bifurkationen elasto-plastischen Typs auf der Grundlage von extrem kurzen Beobachtungszeiten (SPP 1114)*, Prof. H. Kantz
- *Development of a wavefunction-based ab-initio-method of group II metals applying (SPP 1145)*, Dr. B. Paulus
- *Spectral proberties of interacting cold atoms in optical lattices (SPP 1116)*, Dr. A. Buchleitner

Sonderforschungsbereiche und Nachwuchsgruppen

- *Emmy-Noether-Gruppe: Elektronische Struktur endlicher Systeme*, Dr. S. Kümmel
- *Emmy-Noether-Gruppe: Vielteilcheneffekte in mesoskopischen Systemen*, Dr. M. Hentschel
- *SFB 463 Seltenerd-Übergangsmetallverbindungen: Struktur, Magnetismus und Transport*, Prof. P. Fulde
- *SFB 609 Modellierung von Erstarrungsvorgängen unter Magnetfeldeinfluss*, Prof. H. Kantz

4.4.2 BMBF Funding

- *Verbundprojekt Windturbulenzen und deren Bedeutung für die Nutzung von Windenergie: Statistische Analyse und stochastische Modellierung von Windböen*, Prof. H. Kantz

4.4.3 EU Funding

- Marie Curie RTN *Unifying Principles in Non-Equilibrium Pattern Formation*, Dr. U. Thiele
- ESF-Network *Arrays of quantum dots and Josephson junctions*, Dr. S. Flach

4.4.4 Additional External Funding

- HLRB Grand Challenge Projekt: *Spectral Properties of Atomic Rydberg States in Intense Electromagnetic Fields*, Dr. A. Buchleitner
- HFSPO Research Grant *The driving microtubule forces for cytokinesis checkpoint and early G1 cell spreading*, Prof. Dr. F. Jülicher
- Robert Bosch Stiftung, *Netzwerk Lehrerweiterbildung in Sachsen*, Prof. H. Kantz, U. Gneisse
- Japan Society for the Promotion of Science, *Ultrafast Intense Laser Science*, Dr. A. Becker
- NSERC Canada, *Controlled electron rescattering: sub-A, sub-fs imaging of single molecules*, Dr. A. Becker

- VW-Stiftung, *New algorithms in charged soft and biological matter*, Dr. R. Everaers
- VW-Stiftung, *Neuronal Control of Flight in Drosophila*, Dr. M. Zapotocky
- VW-Stiftung, *Electron spin resonance of Kondo ions in heavy fermion compunds: experiment and theory*, Prof. I. Eremin
- DAAD, *Entanglement and decoherence in open quantum systems* , Dr. J.-M. Rost
- DAAD, *Dynamik von Mehr- Elektronen-Atomen und Molekülen in intensiven Laserfeldern* , Dr. A. Becker, together with Dr. L. Plaja, Universidad Salamanca
- Ministerio de Educacion y Cienca, Spanien, *Efectos no lineales con laseres de femtosegundo intensos*, Dr. A. Becker
- DAAD, *Spin excitations in the strongly correlated systems with competing orders*, Prof. I. Eremin
- DAAD (PROCOPE), *Spektrale Eigenschaften von Mehrelektronenatomen im elektromagnetischen Feld*, Dr. A. Buchleitner, together with Dr. D. Delande, Universite Pierre et Marie Curie, Paris

4.4.5 Stipends

- *Ricardo Pinto*, DFG stipend
- *Anrey Kolovski*, DFG stipend
- *Victor Bezugly*, DFG stipend
- *Elena Voloshina*, DFG stipend
- *Maxim Korshunov*, INTAS stipend
- *Karol Zyczkowski*, VW stipend
- *Rafal Demkowicz-Dobransky*, VW stipend
- *Marek Kus*, VW stipend
- *Valerio Cappelini*, VW stipend
- *Igor Pasichnyk*, VW stipend
- *Ioan Vancea*, EU stipend
- *Madruga Sanchez*, EU stipend
- *Anatole Kenfack*, Reimar-Lüst stipend
- *Grzegorz Urbanik*, Klaus-Tschira stipend
- *Pawel Pasciak*, Klaus-Tschira stipend
- *Pawel Wielgus*, Klaus-Tschira stipend
- *Wojciech Miiller*, Klaus-Tschira stipend
- *Vardan Apinyian*, Klaus-Tschira stipend

4.4.6 Cooperations With Industry

Prof. Holger Kantz: Wind speed predictions and more specifically the prediction of turbulent gusts is of high potential use for wind energy conversion. With the help of Garching Innovation, the technology transfer branch of the Max Planck Society, we have established contacts to the spanish manufacturer GAMESA in Pamplona in order to explore the technological usefulness of our patented gust prediction algorithm.
Automatic speech recognition suffers strongly from environmental noises superimposed to the recording of human voice. Together with LINGUATEC in Munich we are exploring how far the recognition rate of human speech, using commercial speech recognition systems, can be enhanced by our noise reduction technique.

4.4.7 Patents and Licences

- *Dr. Mario Ragwitz, Prof. Holger Kantz*
  Verfahren und Vorrichtung zur Steuerung von Windenergieanlagen, since 2000
- *Prof. Holger Kantz*
  Verfahren und Vorrichtung zur Vorhersage von Strömungsparametern turbulenter Medien, since 2002

4.5 Teaching and Education

4.5.1 Lectures at Universities

Wintersemester 04/05

Physikochemische Hydrodynamik - Dr. U. Thiele, BTU Cottbus

Physik der Bose-Einstein Kondensate - Dr. J. Brand, TU Dresden

Grundlagen der Laserkühlung - Dr. Th. Pattard, TU Dresden

Introduction au chaos quantique - Dr. A. Buchleitner, Universite de Louvain

Sommersemester 05

Theoretische Biophysik - Prof. Frank Jülicher,Prof. Karsten Kruse, TU Dresden

Ultrakurz und extrem intensiv: Laserlicht und seine Anwendungen - Dr. A. Becker, TU Dresden

Atome, Moleküle, Festkörper - Prof. S. Kümmel, Uni Bayreuth

Biologische Physik - Prof. R. Everaers, Uni Mainz

Wintersemester 05/06

Control of quantum mechanical processes - Dr. A. Becker, Uni Bielefeld

Special chapters from Quantum Mechanics - Prof. I. Eremin, TU Braunschweig

Stochastic Processes and the Fokker Planck Equation - Prof. H. Kantz, Uni Wuppertal

Photo Ionization Mechanisms in Extended Systems , Minerva Winter School on Photo Induced Dynamics and Charge - Prof. J.M. Rost, Technion Haifa

Sommersemester 06

Gruppen-Theorie - Prof. I. Eremin, TU Braunschweig

Physical Implementations of Quantum Information - Dr. A. Buchleitner, ICTP Trieste

Theoretische Biophysik - Prof. Frank Jülicher, Prof. Karsten Kruse, TU Dresden

Quantum Information - Dr. A. Buchleitner, National Center for Theoretical Sciences, Hsinchu

Quantum Chaos - Dr. A. Buchleitner, National Center for Theoretical Sciences, Hsinchu

Stochastik Processes - Dr. B. Lindner, TU Dresden

Physik der weichen Materie - Prof. R. Everaers, ENS de Lyon

Semiclassical theory of electronic processes, Summer School on Few-body Dynamics in Atomic and Molecular Systems - Prof. J. M. Rost, Uni Wittenberg

Wintersemester 06/07

Modern Topics in Quantum Physics - Dr. M. Hentschel, TU Dresden

Gruppen-Theorie - Prof. I. Eremin, TU Braunschweig

Quantum Electrodynamics - Prof. I. Eremin, TU Braunschweig

Simulationsmethoden in der Physik kondensierter Materie - Prof. R. Everaers, ENS de Lyon

4.5.2 Degrees

Habilitations

- *Paulus, B.: The methods of increments - a wavefunction-based ab-initio correlation method for solids.* Regensburg 2005
- *Kruse, K.: Physical aspects of pattern formation and force generation in the cytoskeleton.* Dresden 2006
- *Pattard, T.: Coulomb correlation in atomic systems: from single atoms to large plasmas.* Dresden 2006

Dissertations

- *Baba, N: Elimination schneller chaotischer Freiheitsgrade in Hamiltonschen Systemen.* Wuppertal 2005
- *Bollenbach, T.: Formation of morpogen gradients.* Dresden 2005

- *Buth, C.: Advanced electronic structure theory: from molecules to crystals.* Dresden 2005
- *John, K.: Self-organization in biology and chemistry.* Dresden 2005
- *Pohl, T.: Relaxationsdynamik ultrakalter Plasmen.* Dresden 2005
- *Zumdick, A.: Dynamics of active filament systems.* Dresden 2005
- *Borowski, P.: Stochastic dynamics in olfactory signal transduction and development.* Dresden 2006
- *Hilfinger, A.: Dynamics of cilia and flagella.* Dresden 2006
- *Jurgk, M.: Numerische Simulation von Erstarrungsprozessen: Wege zur mehrskaligen Modellierung ausgehend von Mikrostrukturmodellen.* Aachen 2006
- *Klein, G.: Theoretical aspects of motor protein inducced filament depolymerisation.* Dresden 2006
- *Meacci, G.: Physical aspects of min oscillations in escherichia coli.* Dresden 2006
- *Pollmann, F.: Charge degrees of freedom on frustrated lattices.* Ilmenau 2006

4.5.3 Appointments and Awards

Appointments

- *Prof. Henning Schomerus* accepted the offer for a Reader in Physics at the University Lancaster.
- *Prof. Stephan Kümmel* accepted the offer for a Professorship in Physics at the University Bayreuth.
- *Prof. Ralf Everaers* accepted the offer for a Professorship at the Ecole Normale Superieure, Lyon.
- *Prof. Karsten Kruse* accepted the offer for a Professorship at the University Saarland
- *Dr. Joachim Brand* accepted the offer for a lecturer at the Massey University Auckland

Awards

- *Jülicher, F.:* Robert-Wichard-Pohl-Preis der DPG 2006
- *Shabat, M.:* Galileo Galilei Award 2006
- *Pohl, T:* Otto-Hahn Medaille 2006
- *Fulde, P.:* Sächsischer Verdienstorden 2007

4.6 Public Relations

4.6.1 Long Night of Sciences

On 1st of July, 2005 and June 30, 2006 the institute participated in the *Long Night of Sciences* jointly with the Technische Universität Dresden and many other research institutes in Dresden. We opened the doors for everyone interested in visiting our institute from 6pm to 12pm. The members of our institute conveyed the importance and fascination of their research to a broad audience with various talks, video shows, a physics show, a physics quiz, a science cinema and poster presentations. The resonance was very good with about 4000 visitors counted at each event.

4.6.2 Science in the City Hall

The mpi**pks**, the Technische Universität Dresden and the City of Dresden are running a series of public lectures (about 3 per year) called *Wissenschaft im Rathaus*. The following lectures were delivered during the period 2005-2006:

- 16. März 2005, Prof. Dr. Heckl, *Chancen und Risiken der Nanotechnologie*, about 400 participants
- 13. Oktober 2005, Prof. Dr. Christensen, *Die ungleichen Geschwister der Erde - Planetenforschung heute*, about 300 participants
- 8. März 2006, Prof. Dr. Hofmann, *Vom Elementarteilchen zum Universum - Verbindungen zwischen den Welten des ganz Kleinen und des ganz Grossen*, about 250 participants
- 25. September 2006, Prof. Dr. Emmermann, *Das deutsche Tsunamifrühwarnsystem im Indischen Ozean*, about 300 participants
- 15. November 2006, Prof. Dr. Vogel, *Nanomedizin: die Wissenschaft vom Kleinsten und unsere Gesundheit*, about 250 participants

4.6.3 mpipks School Contact Program

On the 27th of April 2006 we hosted the fourth *Girls Day - Mädchenzukunftstag* at mpi**pks**. It was aimed at young female high school students to get information on the spot about career opportunities and challenges when pursuing a scientific career. About 35 female students participated in that event.
In addition mpi**pks** offers lecturing at high schools on a permanent basis. High school teachers receive updated lists of available lecture topics offered. About twenty five lectures are given annually.

4.6.4 Workshops for Teachers in Saxony

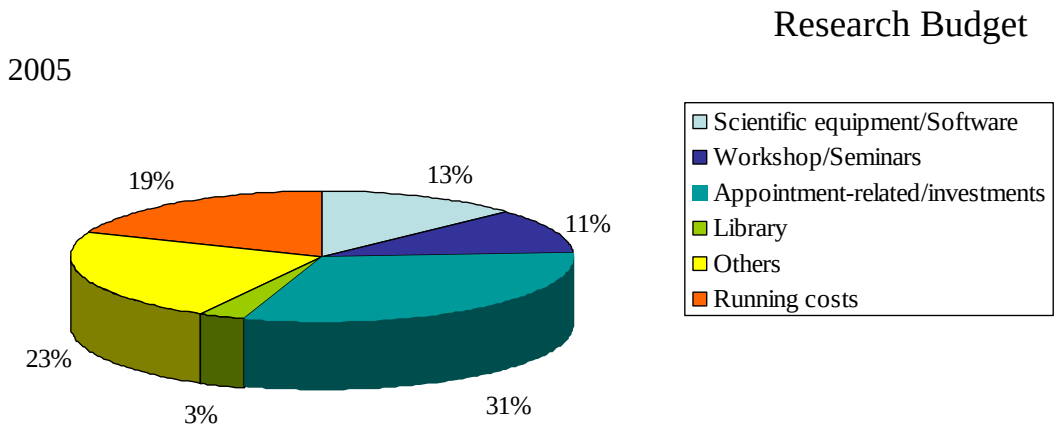
Together with the Technical University in Chemnitz, we have applied for and obtained funding from the Robert Bosch foundation within a program *NatWorking*. This program aims at establishing links between academia and high schools. Our joint project

consists in a series of three workshops for about 40-60 teachers. We arranged an entertaining and educating mixture of scientific talks. Our schools were extremely well received by the participating teachers.

- 9. November 2005, *Kosmologie heute*, 42 participants
- 9. Mai 2006, *Wie vermittelt man Naturwissenschaften unterhaltsam und lehrreich?*, 65 participants
- 5. Oktober 2006, *Chaos und Vorhersagbarkeit*, 45 participants

4.7 Budget of the Institute

Figures 1 and 2 show a breaking down of the budget for personnel and for research for the years 2005 and 2006



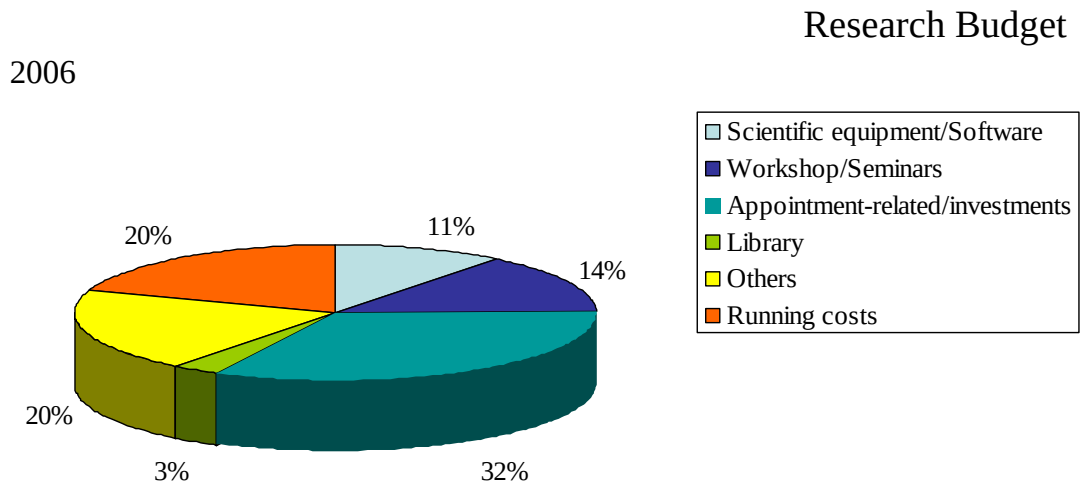
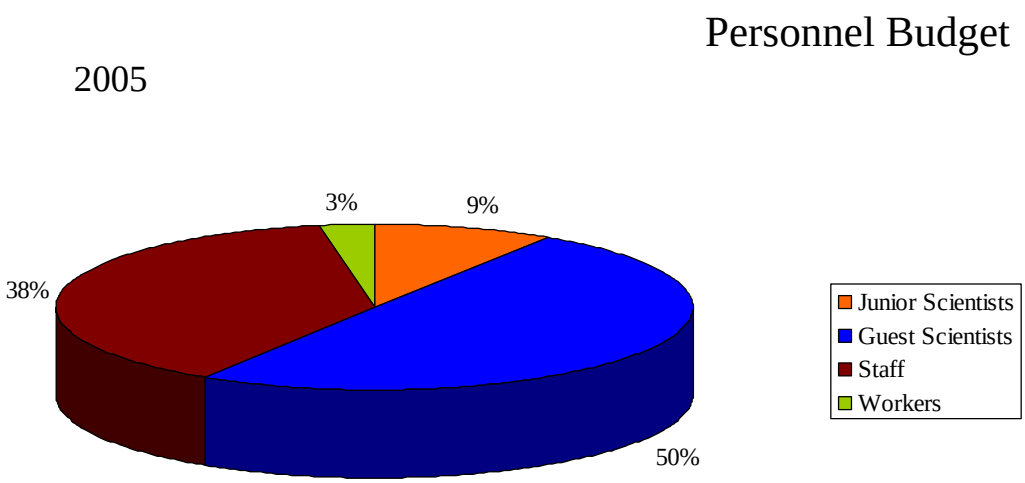


Figure 1: *Research budgets during the past two years*



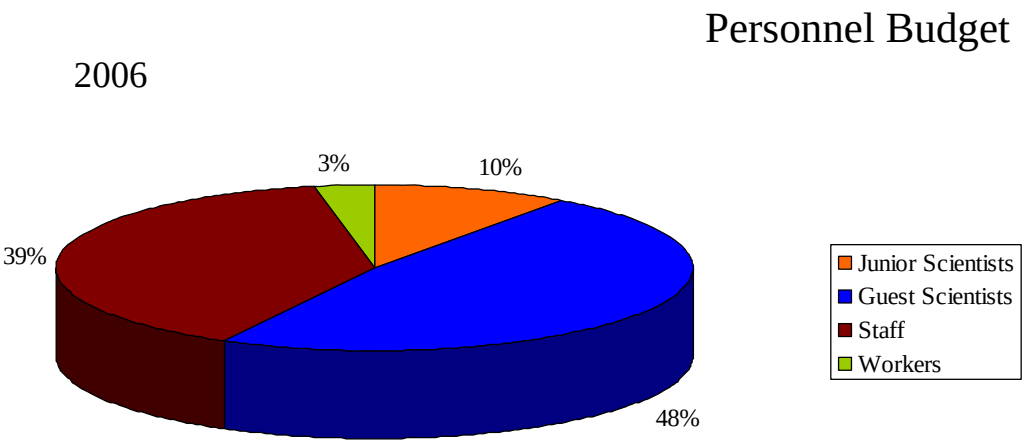


Figure 2: *Budgets for personnel*

4.8 Equipment and Premises

4.8.1 Computer Facilities

Since many of our scientists perform extensive numerical calculations, the main focus of the computer ressources in our institute is on the computational throughput, whereas the request for graphics is still rather moderate on average. This implies that most offices are equipped with X-Terminals while nearly all the compute servers are located in server rooms. At present the institute has approximately 340 computers with a total of 1000 CPU cores.
Our computers offer from one to 16 CPU cores and a maximum of 128 Gigabytes of main memory and twelve Terabytes of local disk space. We use both Gigabit and Fast Ethernet as a local area network interconnect. By the end of 2006 about 95 % of the computing power available was based on Linux systems, 5 % on computers running Tru64 Unix. In order to maximize the computational throughput in our computing cluster, we run a network queuing system which achieves an overall average utilization of more than 90 % of the available CPU time. Besides the unix cluster there are about 20 PC's in our institute, running a Windows operating system, mainly for office applications. We also offer about 30 Laptops for our scientists in order to give them the possibility to continue their work while they are abroad. Furthermore we are running a Windows Terminalserver in our network in order to offer access to a Windows environment from every desktop. For numerical and analytical calculations there are various software packages available for our scientists. During the last years we noticed a tendency towards integrated software environments while fewer people are writing their own programs using programming languages like C or Fortran.
For our short-term guests that participate in seminars and workshops we run a separate small cluster. We offer those guests the possibility to connect their own laptops to our network or use X-Terminals to access that cluster. The separation was introduced for both greater convenience and higher security.
We are connected to the Internet using a bandwidth of 75 MBit/s which we share with our neighboring institute.
The computer department is run by four employees with their respective main tasks being unix and networks, web and windows, hardware and general user support. In addition to those four people we employ one trainee and three students of the Berufsakademie Dresden. Smaller to medium programming tasks are done by our staff and two students who are working part-time in the computer department. Larger programming tasks have to be given to external companies.

Future

Linux will continue to be the main operating system for our number crunchers in the near future, running mainly on AMD Opteron based hardware. By 2007 we will have to decide which way to go with our main servers. If Linux has become mature by then, it will be tempting to leave the proprietary operating system - Tru64 Unix from HP (formerly Compaq, formerly Digital) - in order to become independent from hardware vendors and still having the option to run the same flavor of operating system on all hardware.

History

In 1996 the institute occupied three buildings in Dresden and an outpost in Stuttgart. Before we moved to our new building, a further office in Dresden was needed. This implied that the interconnection of the offices and running the distributed infrastructure made up the biggest part of the work of the two employees in the computer department at that time. Moving to the new building in 1997 implied a boost in local network bandwidth from shared ethernet to ATM and an increased bandwidth of our internet connection from 128 kBit/s to 2 MBit/s. While during the first years nearly all the computing power was covered by workstations, starting from 2000 we switched to small and medium sized servers. 2002 was the first year to see an inhomogeneous unix cluster in our institute when we introduced linux on standard PC systems. By the end of 2002 we even decided to give away our 16 processor server in favor of a Linux based PC cluster that delivers several times the cpu performance of that server. The new extension building which was finished late 2005 added several new offices and also an excellent new server room for our computers. The following table shows the development of the computer resources at our institute over time.

year	computers	GFlops	main memory (GB)	disk space (TB)
1996	33	15	13	0.5
1997	49	30	30	1.0
1998	66	60	60	2.0
1999	68	100	190	5
2000	95	140	310	8
2001	138	220	420	10
2002	162	400	590	22
2003	261	1200	1150	32
2004	327	2100	2600	90
2005	357	3100	3600	140
2006	345	5400	5500	190

4.8.2 Library

The library is a specialised library offering services firstly to scientists working at the institute. Scientists from outside the institute are welcome and may use the library. The library is permanently accessible for members of the institute including guests and provides the scientists with media and scientific information in many forms.
The annual growth rate in 2005/2006 of the library holdings increased in line with the budget and our holdings list consists of 3.953 monographs, 14.061 bound journal volumes and 55 scientific journals subscriptions. The online access to journals is covered by the Grundversorgung, i.e., the Max Planck Society secured a permanent right to full text access for currently 21.117 journal titles (number increasing). The search in online databases (Web of Knowledge, INSPEC, Current Contents, PubMed etc.) is also part of the Grundversorgung and offered by the library. Books or references, which are not available in the library can be ordered through document delivery (2005/2006 - 1462 documents). The scientists receive articles within 24 hours as email files (this service might be strongly affected by the new German law on intellectual property and copyright, Urheberrecht). With an automatic lending system all users can borrow

literature themselves 24 hours a day. In February 2007 we switched to a new library catalogue and booking system - ALEPH from Ex Libris. For making copies of printed material there are two special scanners available for books and journals only. In the library steering committee scientists representing the departments and research groups of the mpi**pks** discuss new developments in quarterly meetings.

Since 2006 there is a reading room in the new D-wing of the institute. Copies of the most important books and journals for each research group are available there for easy access.

The library supports the electronic document server (eDoc) of the Max Planck Society. Via eDoc scientists can make their work openly accessible online, but it is also used as a documentation system for our reporting tasks (in particular, for the production of the yearbook). Meta-data, full texts, or links to full texts in other preprint servers of 1156 documents have been so far registered in the eDoc system. The mpi**pks** is also a pilot institute contributing to the development of a new institutional repository system called eSciDoc within the MPDL (Max Planck Digital Library). The eSciDoc system will provide a sustainable infrastructure for scientific information, communication and dissemination of research results via Open Access with persistent identifiers to make documents citable.
Our as well as other libraries are in a transition phase where the classical services continue to be indispensable but where new media and new services receive increased relevance. It is foreseeable that print issues of journals might be fully replaced by online access in a few years, where the online access is guaranteed by the centralised MPDL. Instead, the library will be more and more involved in the dissemination of publications created by mpi**pks** members through Open Access and an institutional repository.

4.8.3 Guest Houses

To accommodate the large number of short- and long-term visitors, the Max Planck Institute for the Physics of Complex Systems provides three guest houses with different apartment types for up to 75 guests in total.
Guest house 1 comprises 20 single and 5 double rooms (with two separate bedrooms). All of them have a bathroom, a telephone and a terrace or a balcony. The guests are able to use the fully equipped communal kitchen and two meeting rooms, one of them with a small library, the other one with a TV set.
Guest house 2 offers ten apartments with kitchen for up to two persons and three large apartments with two bedrooms, a living room, bathroom and kitchen for up to three persons (e.g. families). One of these apartments is suited for disabled persons. All apartments have TV connection ports, telephones and a balcony or a terrace. In the basement of guest house 2, two washing machines and a tumble dryer are available. They are accessible from all three guest houses.
Guest house 3 allows to accommodate guests in five large apartments similar to the ones in guest house 2. They are situated on the second floor. On the first floor, two additional apartments have been transformed into offices. Like in the two other guest houses, guest house 3 offers TV connection ports, telephones and balconies.
The guest house rooms and apartments are regularly cleaned and towels and bed linen exchanged. Additionally, the institute provides free of charge rental service for cots and TV sets.
Since September 2006 the institute has provided a special apartment for scientists with children. It can be used by institute members and workshop participants under certain conditions and upon consultation with the visitors program. Also daycare can be arranged.

4.9 Committees

4.9.1 Scientific Advisory Board

According to the statutes of the Max Planck Society the mpi**pks** has a Scientific Advisory Board. The members of the Board advise the board of directors concerning the research at the institute. The Board assesses the research direction of the institute, the scientific relevance and chances for success of the research projects, as well as the collaborations among members of the institute, with universities, other research institutions and with industry. The Scientific Advisory Board evaluates the results of the research work presented by the board of directors in the biannual research report and prepares, usually every two years, a report for the President of the Max Planck Society on the research of the institute.
Currently the Scientific Advisory Board has the following members:

Bensimon, D.
Professor Dr.

Laboratoire de Physique Statistique
Ecole Normale Superieure
24, rue Lhomond, 75231 Paris cedex 05
Frankreich

Efetov, K.
Professor Dr.
Institut für Theoretische Physik III
Ruhr-Universität Bochum
Universitätsstraße 150, 44801 Bochum

Frey, E.
Professor Dr.
Ludwig-Maximilians-Universität
Theresienstraße 37
80333 München

Haake, F.
Professor Dr.
Fachbereich Physik
Universität Duisburg-Essen
Universitätsstraße 2, 45141 Essen

Heller, E. J.
Professor Dr.
Lyman Laboratory of Physics
Harvard University
Cambridge, MA 02138
USA

Ketzmerick, R.
Professor Dr.
Technische Universität Dresden
Helmholtzstr. 10
01069 Dresden

Lhuillier, C., J. C.
Professor Dr.
Physique Theoretique des Liquides
Université Pierre & Marie Curie
4, Place Jussieu, 75252 Paris Cedex 05
Frankreich

Pietronero, L.
Professor Dr.
Dipartimento di Fisica
Universita degli Studi di Roma
La Sapienza
Piazzale Aldo Moro 2, 00185 Roma
Italien

van Saarloos, W.
Professor Dr.
Instituut-Lorentz LION
Postbus 9506
2300 RA Leiden
Niederlande

Starace, A.
Professor Dr.
Department of Physics and Astronomy
The University of Nebraska
116 Brace Laboratory
Lincoln NE 68588-0111
USA

Stark, J.
Professor Dr.

Department of Mathematics
University College London
Gower Street, WC1E 6BT, London
Grossbritannien

Sznajd, J.
Professor Dr.

Institute of Low Temperature and
Structure Research
Polish Academy of Sciences
ul. Okolna 2,
50-422 Wroclaw
Polen

4.9.2 Board of Trustees

In accord with the statutes of the Max Planck Society the mpi**pks** has formed a Board of Trustees. The board members discuss and consult the proposed budget, the annual report, and the budget of the last year of mpi**pks** together with the directors. The Board of Trustees advises the institute on important issues and promotes the connection of the institute to research oriented circles in the society. The Board of Trustees had the following members during the period of this report (current membership is until December 31 2012):

Birgel, D.

Chefredakteur
Dresdner Neueste Nachrichten
Hauptstraße 21, 01097 Dresden

Eschelbacher, H. C.
Dr.-Ing.

Ministerialdirigent a. D.
Hauptstraße 124, 53604 Bad Honnef

Junker, F.
Dr.-Ing.

Mitglied des Vorstandes
König & Bauer AG
Friedrich-König-Straße 4, 97080 Würzburg

Kokenge, H.
Professor

Rektor der
Technischen Universität Dresden
Mommsenstraße 13, 01069 Dresden

Kretschmer, M.
Dipl.-Ing., MdB

Mitglied des Deutschen Bundestages
Wahlkreisbüro
Dresdener Straße 6, 02826 Görlitz

Laubschat , C. Professor, Dr.	Prodekan der Fachrichtung Physik Fakultät für Mathematik und Naturwissenschaften Technische Universität Dresden Helmholtzstraße 10, 01069 Dresden
Sauerbrey, R. Professor, Dr.	Wissenschaftlicher Direktor des Forschungszentrums Dresden-Rossendorf e.V. Bautzner Landstraße 128, 01328 Dresden
Schmidt, F. Dr.-Ing.	Staatssekretär a.D. Birkenstraße 18, 01328 Dresden
Stange, E.-M. Dr.	Sächsische Staatsministerin für Wissenschaft und Kunst Wigardstraße 17, 01097 Dresden
Tschira, K. Dr. h.c.	Geschäftsführender Gesellschafter Klaus Tschira Stiftung gGmbH Schloss Wolfsbrunnenweg 33, 69118 Heidelberg
Vogel, L. Dr.	Erster Bürgermeister der Landeshauptstadt Dresden, Dr.-Külz-Ring 19, 01067 Dresden
Weber, S.	Vorsitzender des Vorstandes Sächsische Aufbaubank Pirnaische Straße 9, 01069 Dresden

4.10 Members of the mpipks

(as of December 2006)

1.	**mpipks positions**	**47**
1.1	Scientific personnel	
	Scientific members	3
	Research staff (including four junior research groups)	14
1.2	Technical staff	5
1.3	Administration and infrastructure staff	25
2.	**Externally funded research staff**	**5**
3.	**PhD students**	**45**
3.1	German PhD students	23
3.2	Foreign PhD students	22
3.3	PhD students with external funding	5
3.4	IMPRS PhD students with external supervision	13
4.	**Guest scientists**	**82**
4.1	German guest scientists	5
4.2	Foreign guest scientists	77

The research positions are generally limited in time. Only *Prof. H. Kantz*, head of the group "Time Series Analysis" is employed on a permanent position. Furthermore, *Priv. Doz. Dr. S. Flach*, head of the Visitors and Workshop Program, is a permanent staff member of the scientific service.

Chapter 5

Publication List 2005-2006

5.1 Light-Matter Interaction

2005

Aközbek, N., A. Becker and S.L. Chin: Propagation and filamentation of femtosecond laser pulses in optical media. Laser Physics **15**, 607 - 615 (2005).

Arévalo, E. and A. Becker: Theoretical analysis of fluorescence signals in filamentation of femtosecond laser pulses in nitrogen molecular gas. Physical Review A **72**, 043807 (2005).

Arévalo, E. and A. Becker: Variational analysis of self-focusing of intense ultrashort pulses in gases. Physical Review E **72**, 026605 (2005).

Becker, A., R. Dörner and R. Moshammer: Multiple fragmentation of atoms in femtosecond laser pulses. Journal of Physics B **38**, S753 - S772 (2005).

Becker, A. and F.H.M. Faisal: Intense-field many-body S-matrix theory. Journal of Physics B **38**, R1 - R56 (2005).

Chin, S.L., S.A. Hosseini, W. Li, Q. Luo, F. Théberge, N. Aközbek, A. Becker, V.P. Kandidov, O.G. Kosareva and H. Schroeder: The propagation of powerful femtosecond laser pulses in optical media: physics, applications, and new challenges. Canadian Journal of Physics **83**, 863 - 905 (2005).

Chin, S.L., W. Liu, S.A. Hosseini, Q. Luo, F. Théberge, N. Aközbek, A. Becker, V.P. Kandidov, O.G. Kosareva and H. Schroeder: Intense femtosecond laser filamentation: physics and applications. Jurnal Fizik Malaysia **26**, 125 -133 (2005).

Czasch, A., M. Schöffler, M. Hattass, S. Schössler, T. Jahnke, T. Weber, A. Staudte, J. Titze, C. Wimmer, S. Kammer, M. Weckenbrock, S. Voss, R.E. Grisenti, O. Jagutzki, L.P.H. Schmidt, H. Schmidt-Böcking, R. Dörner, J.M. Rost, T. Schneider, C.N. Liu, I. Bray, A.S. Kheifets and K. Bartschat: Partial photoionization cross sections and angular distributions for double excitation of helium up to the N=13 threshold. Physical Review Letters **95**, 243003 (2005).

Dundas, D. and J.M. Rost: Molecular effects in the ionization of N_2, O_2, and F_2 by intense laser fields. Physical Review A **71**, 013421 (2005).

Flach, S., V. Fleurov, A.V. Gorbach and A.E. Miroshnichenko: Resonant light scattering by optical solitons. Physical Review Letters **95**, 023901 (2005).

Gaier, L.N., M. Lein, M.I. Stockman, G.L. Yudin, P.B. Corkum, M.Y. Ivanov and P.L. Knight: Hole-assisted energy deposition in dielectrics and clusters in the multiphoton regime. Journal of Modern Optics **52**, 1019 - 1030 (2005).

Gryzlova, E.V., A.I. Magunov, I. Rotter and S.I. Strakhova: Laser polarization control

of autoionization in the Helium atom. Laser Physics **15**, 1568 - 1575 (2005).

Gryzlova, E.V., A.I. Magunov, I. Rotter and S.I. Strakhova: Photoionisation of a helium atom involving autoionisation states coupled by a circularly polarised laser field. Quantum Electronics **35**, 43 - 47 (2005).

Hemmers, O., R. Guillemin, D. Rolles, A. Wolska, D.W. Lindle, E.P. Kanter, B. Krässig, S.H. Southworth, R. Wehlitz, P.W. Langhoff, V. McKoy and B. Zimmermann: Nondipole effects in molecular nitrogen valence shell photoionization. Journal of Electron Spectroscopy **144-147**, 155 - 156 (2005).

Jaroń-Becker, A., A. Becker and F.H. Faisal: Erratum to "Ionization of N_2, O_2, and linear carbon clusters in a strong laser pulse [Phys. Rev. A 69, 023410 (2004)]". Physical Review A **72**, 069907 (2005).

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