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I. Wissenschaftliche Arbeit und ihre Organisation am Institut - ein Überblick

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* als Gründungsdirektor berufen. Der Beschluss basierte auf einer Empfehlung der Chemisch-Physikalisch-Technischen Sektion, die in einer Kommission der Sektion erarbeitet worden war. 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 weiten 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* unter 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 und mehrere hundert Wissenschaftler waren bis dahin bereits am Institut zu Gast.

1999-2002 • *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 wird in modifizierter Form von *Dr. H. Schomerus* (Leiden) weiter gepflegt, der im November 2000 mit dem Aufbau einer Nachwuchsgruppe *Wellen in komplexen Medien* begann.

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.

Seither forschen ständig etwa 10-150 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.

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* mit Mitteln der statistischen Physik biologischen Themen.

Darüber hinaus verstärken von den gegenwärtig acht Arbeitsgruppen fünf die jeweilige Arbeit an den Schwerpunkten (siehe Graphik auf S. 23).

Drei Gruppen, darunter zwei Nachwuchsgruppen, interpolieren und ergänzen die Schwerpunkte.

- Die Nachwuchsgruppe von *Dr. Schomerus* schlägt mit ihrem Forschungsinteresse *Wellen in komplexen Medien und mesoskopische Phänomene* inhaltlich eine Brücke zwischen den Abteilungen *Korrelierte Elektronen* und *Endliche Systeme*.
- Die Nachwuchsgruppe *Strukturbildung* von *Dr. Bär* war Ausgangspunkt und Brückenkopf für biologisch orientierte Arbeit am Institut, bevor die Abteilung *Biologische Physik* gegründet wurde (siehe z.B. die *Initiative Biologie,* S. 147).
- 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. Die gemeinsame Ausrichtung der Tagung *Dynamics Days Europe* (siehe S. 152) durch *Prof. Kantz* und *Dr. Richter* ist hierfür ein Beleg.

Mit der *Initiative Biologie* (S. 147) hat das Institut einen neuen Weg beschritten, einer Gruppe von Wissenschaftlern, die an einem innovativen Thema interessiert sind, für begrenzte Zeit eine Organisations- und damit auch Begegnungsplattform zu bieten. Damit haben auch neue Gastwissenschaftler am Institut die Möglichkeit einer raschen Information und Teilnahme an den Aktivitäten der Initiative. *Dr. A. Deutsch* schuf ein neuartiges landesweites Netzwerk *MTBio-modelling and theory in the biosciences*, das neben der Unterstützung durch das mpi**pks** auch von der Tschira-Stiftung gefördert wurde (S. 172).
Für zwei der Initiatoren war die *Initiative Biologie* ein Sprungbrett, sich erfolgreich um eine Nachwuchsgruppe der Volkswagenstiftung an Universitäten zu bewerben: *Dr. Or-Guil* forscht mit ihrer Gruppe nun in Berlin in Zusammenarbeit mit der Charité, *Dr. Cuniberti* siedelte seine Gruppe an der Universität Regensburg an.

3. Workshop- und Gästeprogramm

Eine zentrale Aufgabe des Instituts ist die Durchführung von internationalen *Workshops und Seminaren* (S. 151). Hinsichtlich dieser Funktion nimmt das mpi**pks** eine Sonderstellung innerhalb der MPG ein. Ein kleiner, aber effektiver 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. 142) 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. 190).

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.
Für die in den letzten Jahren zunehmende Raumknappheit, der übergangsweise mit der Umwandlung von Fläche im Gästewohnhaus in Büros begegnet wurde, zeichnet sich eine erfreuliche Lösung ab.
Zur weiteren Strukturierung des Gästeprogramms vergibt das mpi**pks** seit 2000 jährlich an einen international angesehenen erfahrenen Wissenschaftler das *Martin-Gutzwiller-Fellowship*. Mit ihm forschten bisher *Prof. D. Delande* (Paris), *Prof. E. Prange* (Maryland) und *Prof. A. Ozorio de Almeida* (Rio) jeweils bis zu einem akademischen Jahr am Institut (S. 145).
Ferner schreibt das mpi**pks** jedes Jahr ein *PKS-Distinguished Postdoctoral-Fellowship* aus. Hiermit sollen hervorragende Nachwuchswissenschaftler mit einiger Forschungserfahrung angesprochen werden. Die beiden *distinguished fellows*, die bisher das Institut verlassen haben, taten dies vor Ablauf ihres Fellowships, um dem Ruf auf eine Assistenzprofessur bzw. dem Angebot einer C2-Stelle zu folgen (S. 176).

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. 174). 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. 178), zu sammeln.
Forschungsorganisation • Durch unser großes Workshop-/Seminarprogramm haben wir die einmalige Chance, auch Training im Organisieren von Tagungen bieten zu können. Von 57 Veranstaltungen in den Jahren 2000-2003 (S. 151) waren bei knapp der Hälfte (26) junge Wissenschaftler des mpi**pks** 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. Über die Tagungsorganisation hinaus bieten die offenen Strukturen des Instituts viel Raum für Eigeninitiative, wie z.B. die Realisierung einer dreisemestrigen Ringvorlesung im Studium Generale der TU Dresden durch *Dr. Morawetz* (S. 174).

5. Öffentlichkeitsarbeit

Das Institut versteht seinen Auftrag im weitesten Sinn 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 haut-

nah zu erleben. Für diese Aktivitäten erhielt das mpi**pks** den *Max-Planck-Preis für öffentliche Wissenschaft 2000*.
Für die interessierte Bevölkerung organisiert das Institut seit 1999 im Dresdner Rathaus zusammen mit der Universität und der Stadt die Reihe *Wissenschaft im Rathaus*, in der prominente Wissenschaftler aktuelle Forschung bürgernah erläutern (S. 177). Außerdem ermutigen wir die Organisatoren von Workshops, einen öffentlichen Abendvortrag im mpi**pks** anzubieten.

6. Vernetzung der Forschung

Lokal • Das mpi**pks** 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. Außerdem sind Wissenschaftler des Instituts an mehreren Sonderforschungsbereichen und einer Forschergruppe beteiligt (S. 170). Eine Zusammenarbeit besteht weiterhin durch die Abteilung *Elektronische Korrelationen* mit dem IFW und dem benachbarten MPI für Chemische Physik fester Stoffe, sowie mit dem MPI für Zellbiologie durch die Abteilung *Biologische Physik*.
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. 150).

7. Kurzdarstellung der Arbeitsgruppen

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

Die Arbeiten in der Abteilung befassen sich überwiegend, aber nicht ausschließlich mit elektronischen Korrelationen oder Vielteilchentheorie. Daneben wird auch auf dem Gebiet kalter Gläser, von Systemen mit großem Spin sowie nichtlinearen Gittern und deren Anregungen (breather etc.) gearbeitet.

Das Verständnis elektronischer Korrelationen ist eines der wichtigsten Probleme in der Theorie der kondensierten Materie. Dazu zählt man all die physikalischen Effekte, die sich nicht im Rahmen einer Molekularfeld- oder Hartree-Fock-Näherung beschreiben lassen. Besonders stark korrelierte Elektronensysteme werden weltweit stark untersucht. Die Arbeiten in der Abteilung zu diesem Themenkreis teilen sich grob in zwei Richtungen auf. Eine Richtung befasst sich mit ab initio Berechnungen von Vielteilchenwellenfunktionen und deren Anregungsenergien mit Hilfe der Greenfunktionsmethode. Hierzu bietet die Dichtefunktionalmethode keinen Zugang, denn sie vermeidet ja gerade die Berechnung von Vielteilchenwellenfunktionen. Man ist deshalb auf Verfahren ähnlich denen in der Quantenchemie angewiesen, die für Festkörper geeignet modifiziert werden müssen. Bisher wurden die Grundzustandswellenfunktionen einer

großen Anzahl von Festkörpern berechnet, deren Genauigkeit vergleichbar ist mit derjenigen kleiner Moleküle. Gegenwärtig geht es um die Berechnung von Energiebändern in Festkörpern. Diese Arbeiten geschehen in enger Wechselbeziehung mit der Arbeitsgruppe *Quantenchemie* und sind dort ausführlicher beschrieben (siehe S. 8f). Sie erlauben ein detailliertes Studium der Größe und des Einflusses elektronischer Korrelationen. Die zweite Richtung, die wir zum Studium insbesondere stark korrelierter Elektronensysteme eingeschlagen haben, ist phänomenologischer Natur. Hier geht es um die Frage, welche physikalischen Mechanismen zu schweren Quasiteilchenanregungen (heavy fermion systems) in stark korrelierten Metallen führen können. Ursprünglich wurde der Kondo-Effekt als alleinige Ursache dieser Anregungen angesehen. In der Zwischenzeit wurden von uns jedoch eine Reihe anderer Mechanismen aufgefunden und entdeckt. So konnten wir in den vergangenen zwei Jahren zeigen, dass in Uran-Verbindungen die 5f-Elektronen einen dualen Charakter haben, der für die Bildung der schweren Quasiteilchen verantwortlich ist. Es stellt sich nämlich heraus und lässt sich theoretisch begründen, dass in einigen Orbitalen die 5f-Elektronen lokalisiert sind, während sie in anderen delokalisiert sind (Zusammenarbeit mit Frau Prof. Zwicknagl, Univ. Braunschweig). Auch für LiV_2O_4 konnte ein neuer Mechanismus aufgezeigt werden, der zu schweren Quasiteilchen führt und auf der magnetischen Frustration in Pyrochlor-Gittern zurückzuführen ist. Überraschend hat sich herausgestellt, dass in diesen Gittern auch Anregungen mit halbzahliger Elektronenladung auftreten können. So etwas war bisher nur für das eindimensionale, hoch dotierte Polyacetylen und für den gebrochenzahligen Quanten-Hall-Effekt in zwei Dimensionen bekannt. Ein dreidimensionales System war bisher noch nicht gefunden worden.

Mit diesen Arbeiten sind wir u.a. am Sonderforschungsbereich 463 der TU Dresden beteiligt. Die Arbeiten über kalte Gläser konzentrieren sich auf das Verständnis von deren Verhalten im Magnetfeld, wo völlig unerwartete Effekte gefunden wurden. Hierzu gibt es eine enge Zusammenarbeit mit Herrn Dr. Strehlow von der Physikalisch-Technischen Bundesanstalt in Berlin.

Arbeitsgruppe: Nichtlineare Dynamik und Zeitreihenanalyse
(Leiter: Prof. H. Kantz)

Nichtlineare dynamische Systeme besitzen eine große Vielfalt an möglichen Verhaltensweisen, von denen deterministisches Chaos einer der faszinierendsten Aspekte ist. Wir konzentrieren uns auf ausgewählte offene Probleme im Verständnis von Nichtlinearität, insbesondere in der Wechselwirkung von Rauschen und Chaos, dem Übergang von Chaos zu Rauschen, Chaos mit vielen aktiven Freiheitsgraden, und Dynamik mit zeitverzögerter Rückkopplung. Zurückliegende Arbeiten zum Verständnis stochastischer Aspekte deterministischen Chaos ermöglichten uns, das sehr wichtige und weitgehend unerforschte Gebiet der stochastischen Modellierung zu betreten. In vielen numerischen Langzeitsimulationen (beispielsweise von Klimamodellen) ist die Integration schneller chaotischer Freiheitsgrade sehr aufwendig. Eine geeignete Ersetzung dieser Dynamik durch weißes Rauschen könnte die Numerik beträchtlich beschleunigen. Deshalb haben wir Arbeiten begonnen, die unter Einsatz von Operatorprojektionsmethoden eine rigorose Ersetzung schneller chaotischer Freiheitsgrade ermöglicht. Näheres findet sich im Kapitel II des Berichtes ab Seite 77.

Zeigt eine Zeitreihe einer experimentellen Messgröße komplexes, aperiodisches Verhalten, so kann man darüber spekulieren, ob ein relativ einfaches deterministisches Systemverhalten die Ursache dafür ist. Dieser inverse Ansatz wird seit den Achtzigern verfolgt. Allerdings ist es offensichtlich, dass die meisten interessanten dynamischen Phänomene kein niedrigdimensionales Chaos widerspiegeln. Deshalb wird gegenwärtig daran gearbeitet, die zu behandelnde Systemklasse zu erweitern. Ein Schwerpunkt der letzten zwei Jahre lag in Analysemethoden für nichtstationäre deterministische Systeme, für Markov-Modelle, und für die Verbindung von Nichtstationarität und stochastischer Modellierung. Methoden für Zeitreihenanalysen werden von uns in verschiedenen Anwendungen eingesetzt und getestet, wobei diese Projekte oft in enger Zusammenarbeit mit Experimentatoren oder Industriepartnern durchgeführt werden. Erwähnenswert ist unser patentiertes Verfahren zur Vorhersage von Bodenwindgeschwindigkeiten, das für Windkraftanlagen von großem Interesse ist (siehe den Bericht auf Seite 81). In einem anderen Projekt wird Faltenbildung bei der Blechumformung als dynamische Instabilität untersucht, in enger Zusammenarbeit mit Maschinenbau-Ingenieuren der Uni Dortmund.

Unsere zwei Hauptarbeitsgebiete, nichtlineare Dynamik und Zeitreihenanalyse, sind eng verzahnt. Anwendungen stellen Herausforderungen an Zeitreihenmethoden, die wiederum auf Grundlage theoretischer Überlegungen weiterentwickelt werden. Gleichzeitig erfordern die in den Zeitreihen sichtbaren dynamischen Verhaltensweisen ein theoretisches Verständnis. Ein gutes Beispiel für dieses Wechselspiel ist die Vorhersagbarkeit von Bodenwindgeschwindigkeiten. Gleichzeitig bringen uns Zeitreihen in engen Kontakt mit anderen Arbeitsgruppen und Abteilungen am Institut, insbesondere mit der *Strukturbildung, Biologischen Physik und Endlichen Systemen*. In Seminaren und Diskussionen ergibt sich somit ein guter Kontakt über die Grenzen der Arbeitsgruppen hinaus.

Zukunftsperspektiven

Auch zukünftige Arbeit wird in die zwei Hauptarbeitsrichtungen zerfallen, also Verbesserung des grundlegenden Verständnisses komplexer dynamischer Vorgänge und Entwicklung und Anwendung von Zeitreihenmethoden. Im ersten Bereich werden wir stärker an der Verbindung von Dynamik und statistischer Physik arbeiten, insbesondere im Hinblick auf Nichtgleichgewichtsstatistik. Im Zeitreihenbereich geht es zum einen darum, nichtlineare Methoden enger in Bezug zu bestehenden Methoden für stochastische Prozesse zu setzen (Hidden Markov, extended Kalman filters). In Bezug auf Nichtstationarität vergrößern wir gerade unser mathematisches und physikalisches Verständnis für Anzeichen der Nähe von Bifurkationen, um eine datengetriebene prädiktive Bifurkationsanalyse durchführen zu können. In Anwendungen beabsichtigen wir, biologischen Systemen mehr Aufmerksamkeit zu widmen.

Alles zusammen zielt unsere Arbeit auf Fortschritte in Bereichen, die von großer allgemeiner Relevanz sind und unsere anerkannte Expertise in nichtlinearer Dynamik und Zeitreihenanalyse aus der relativ schmalen Nische "deterministisches Chaos" herausführen sollen. Gleichzeitig suchen wir eine umfassende Sicht von Dynamik, Stochastik und Nichtstationarität. Die zunächst nebeneinanderstehenden Aspekte haben einen tiefen inneren Zusammenhang: Weißes Rauschen und driftende Parameter sind vergleichbare Phänomene von nicht-autonomem Systemverhalten mit unterschiedlichen Korrelationszeiten, und Nichtstationarität eines linearen Prozesses lässt

sich in speziellen Situationen als Nichtlinearität interpretieren. Schließlich erscheinen langsame Freiheitsgrade in nichtlinearen Systemen mit Zeitskalentrennung in den schnellen Subsystemen wie fluktuierende Parameter. Diese Zusammenhänge rufen nach einem vereinheitlichenden Zugang.

Kooperationen

- Prof. C. Grebogi, Univ. Sao Paolo, Brasilien: Einfluß von Rauschen auf Attraktoren mit variabler Dimension der instabilen Mannigfaltigkeit.
- PD Dr. Wolfram Just, Theoretische Physik, Technische Universität Chemnitz: Modellierung schneller Freiheitsgrade durch stochastische Prozesse.
- Prof. Dr. M. Kleiner, Maschinenbau, Universität Dortmund: Analyse von dynamischen Instabilitäten bei der Blechumformung.
- Prof. Dr. Bernhard Mehlig, Universität Göteborg: Gemeinsame Arbeit am Lehrbuch "Complex Systems in Classical and Quantum Physics - Statistics versus Dynamics".
- Prof. Dr. J. Parisi, Universität Oldenburg: Datenanalyse, Modellverifikation, Bifurkationsprädiktion eines Nd:YAG-Lasers, gemeinsame Betreuung eines Doktoranden (Tobias Letz, Abschluss Dezember 2001).
- Prof. Dr. J. Peinke, Universität Oldenburg: Charakterisierung von Oberflächenrauigkeiten durch Fokker-Planck-Gleichungen, Austausch eines Doktoranden (Matthias Wächter).
- Prof. Dr. A. Vulpiani, Universität Rom I, Italien: Skalenabhängige Analyse von Prozessen mit getrennten Zeit- und Längenskalen.
- Vielfältige Kontakte der Gastwissenschaftler zu ihren Heimatinstituten.

Arbeitsgruppe: Quantenchemie
(Leiter: Dr. U. Birkenheuer (ab 3/2000))

Die neue Quantenchemiegruppe besteht seit März 2000. Sie hat eine durchschnittliche Personalstärke von 2-3 promovierten Mitarbeitern und einem Doktoranden. Hauptarbeitsgebiet der Quantenchemiegruppe sind wellenfunktionsbasierte 'first-principles'-Rechnungen zur elektronischen Korrelation in Festkörpern und Polymeren. Mit diesem Forschungsschwerpunkt werden die bereits in der vorherigen Quantenchemiegruppe begonnenen Arbeiten über die Korrelationbeiträge zu Gesamtenergie und Ionisierungspotentialen ausgedehnter Systeme fortgesetzt.

Unser Hauptanliegen ist die Entwicklung und Umsetzung eines Konzepts, das auch die Berechnung von Elektronaffinitäten erlaubt, um so schlussendlich u.a. die Bandlücke von periodischen Systemen zu bestimmen.

Dem anionischen Charakter der Elektroneinfangzustände angemessen Rechnung tragend, musste das für kationische Lochzustände entwickelte Inkrementenschema in mehrfacher Weise modifiziert werden: Um ein Weglaufen des zusätzlichen Elektrons zu verhindern, muss die Wirkung der umgebenden Kristallelektronen auf die im Inkrementenschema verwendeten lokalen Clusterausschnitte explizit berücksichtigt werden.

Zu diesem Zweck wurde ein spezielles Einbettungsverfahren entwickelt. Es basiert auf den Hartree-Fock-Daten aus einer Schnittstelle zum CRYSTAL-Programm, die eigens dazu von uns in enger Zusammenarbeit mit der Arbeitsgruppe in Turin geschaffen wurde. Ferner bedarf das Inkrementenschema für Einfangzustände möglichst niederenergetischer, lokalisierter virtueller Orbitale. Verschiedene Konzepte zur Generierung solcher Orbitale wurden entwickelt. Sie greifen entweder auf entsprechend präparierte Clusterorbitale zurück oder nutzen die im CRYSTAL-Programm implementierte Erzeugung von Wannier-Orbitalen. Ähnliches gilt für die externen Orbitale, in die die Elektronen während einer Korrelationsrechnung angeregt werden. Auch sie müssen lokal sein, um den lokalen Charakter des Inkrementenschemas bei der Einbettung zu bewahren. Und auch hier waren neue Konzepte gefragt, da die in der Literatur diskutierten Verfahren sich als unzureichend herausgestellt haben.

Die Implementierung der hier beschriebenen CRYSTAL-MOLPRO-Schnittstelle ist abgeschlossen und umfangreiche Untersuchungen zur Leistungsfähigkeit des Einbettungsformalismus und der Konvergenz des Inkrementenschemas für Elektroneneinfangzustände wurden durchgeführt. Zusätzlich ist ein allgemein einsetzbarer Prä- und Postprozessor für das verwendete Korrelationsprogramm MOLPRO entstanden, welcher die Durchführung von Inkrementenrechnungen weitestgehend automatisiert und somit den Eingabe- und Auswertungsaufwand auf ein Minimum reduziert.

Korrelierte Valenz- und Leitungsbandstrukturen von Diamant und Polyacetylen (berechnet auf 'MRCI(SD)+Q'-Niveau mit einer VTZ-Basis) liegen inzwischen vor. Kollaborationen mit Prof. V. Staemmler (Bochum) zur Durchführung solcher Rechnungen mit der größenkonsistenteren CEPA-Methode bestehen ebenfalls.

Neben Bandstrukturen werden in der Quantenchemiegruppe auch weiterhin Korrelationsenergien periodischer Systeme untersucht. Hier sind Arbeiten an Polymeren mit konjugiertem π-System (Poly-para-Phenylen) und Studien zur Leistungsfähigkeit nichtorthogonaler lokalisierter Orbitale bei der inkrementellen Bestimmung der Gesamtenergie von Silizium zu nennen.

Zukunftsperspektiven

Die Quantenchemiegruppe wird sich auch weiterhin hauptsächlich mit der wellenfunktionsbasierten Beschreibung von Korrelationseffekten in ausgedehnten Systemen beschäftigen. Mit der Entwicklung der CRYSTAL-MOLPRO-Schnittstelle steht ihr dazu erstmals ein Einbettungsformalismus zur Verfügung, der es gestattet, Grundzustandsenergien, Ionisierungspotentiale (Elektronlochzustände) und Elektronaffinitäten (Elektroneinfangzustände) gleichermaßen zu erfassen.

Vorrangiges Ziel der Quantenchemiegruppe wird sein, die in den ersten Anwendungen aufgedeckten Schwachstellen der derzeitigen Umsetzung des Inkrementenschemas zu beseitigen.

Bei einer Inkrementenrechnung hat man es typischerweise nur mit einem relativ kleinen Variationsraum zu tun (10-100 Molekülorbitale), obwohl die zugrunde liegenden Cluster bereits recht groß sind (10-50 schwere Atome). Dieser Umstand kann bei den im MOLPRO-Programm implementierten Multireferenz-Methoden nicht zu unserem Vorteil genutzt werden. Deshalb soll versucht werden, auch andere in dieser Hinsicht flexiblere Korrelationsprogramme für Inkrementrechnungen einzusetzen.

Durch direkte Auswertung der benötigten Mehr-Zentrenintegrale in der Basis der lokalisierten Molekül- bzw. Kristallorbitale wäre es dann möglich, ganz auf die Einführung eines lokalen, alle relevanten Orbitale aufnehmenden Clusters zu verzichten. Der Aufwand für eine Korrelationsrechnung würde sich dadurch erheblich reduzieren. Ein solches Integraltransformationsprogramm ist von der Quantenchemiegruppe bereits entwickelt und ausgetestet worden. Die Anbindung an ein geeignetes Korrelationsprogramm steht jedoch noch aus.

Das Konvergenzverhalten des Inkrementenschemas hängt ganz wesentlich von der Ausdehnung der lokalisierten Loch- bzw. Einfangorbitale ab. Eine Trennung der für Leitungsbandrechnungen relevanten virtuellen Orbitale von den restlichen Orbitalen ist schwierig. Daher glauben wir, dass mit den bisher in der Quantenchemiegruppe entwickelten Konzepten die Möglichkeiten zur Generierung hochkompakter virtueller Orbitale noch nicht ausgeschöpft sind. Es sollen deshalb in Zusammenarbeit mit Prof. C. Zicovich-Wilson (Morelos, Mexico) Algorithmen zur optimalen Lokalisierung virtueller Wannier-Orbitale erarbeitet und in das CRYSTAL-Programm integriert werden.

Größenkonsistenz der Korrelationsmethode spielt beim Inkrementenschema eine wichtige Rolle. Viele der üblichen quantenchemischen Multireferenz-Methoden (z.B. MRCI(SD)+Q) sind aber nur näherungsweise größenkonsistent. Eine vielversprechende Alternative ist die für Ionisierungspotentiale (und Elektronaffinitäten) adaptierte "equation-of-motion"-CCSD-Methode von R. Bartlett. Die Verwendbarkeit dieses "coupled cluster"-Ansatzes im Rahmen einer Inkrementenrechnung zu evaluieren, ist ein weiteres Anliegen der Quantenchemiegruppe.

Kurz erwähnt werden sollen noch unsere Pläne in Richtung Exzitonen. Erste Untersuchungen, in welchem Umfang das Inkrementenschema auch direkt zur Beschreibung von vertikalen optischen Anregungen verwendet werden kann, laufen bereits.

Kooperationen

- Prof. Roberto Dovesi, Dipartimento di Chimica IFM, Università degli Studi di Torino, Italien: Kooperation im Aufbau der CRYSTAL-MOLPRO-Schnittstelle zur Durchführung von Inkrementrechnungen an eingebetteten Clustern.
- Prof. Claudio Zicovich-Wilson, Facultad de Ciencias, Universidad Autonoma del Estado de Morelos: Kooperation bei der Lokalisierung virtueller Wannier-Orbitale mit dem CRYSTAL-Programm
- Prof. Hermann Stoll, Institut für Theoretische Chemie, Universität Stuttgart: Kooperation in der Durchführung von Inkrementrechnungen von Festkörpern und Polymeren
- Prof. Volker Staemmler, Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum: Inkrementrechnungen zur Bandstruktur mit der "Multireferenz CEPA-0"-Methode

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

Unsere Gruppe interessiert sich für die nichtlineare Dynamik angeregter Quantensysteme mit einer endlichen Anzahl von Teilchen. Der Schwerpunkt liegt hierbei

auf Atomen und Clustern. Wir haben auch begonnen, uns mit Wenig-Elektronen-Quantendots zu beschäftigen, sowie mit hoch angeregten kalten Atomen ('Rydbergmaterie'). Mit dem letztgenannten Projekt beteiligen wir uns an dem kürzlich gegründeten DFG-Schwerpunkt SPP 1116 "Wechselwirkung in ultrakalten Atom- und Molekülgasen".

Die Energie für die angeregten Systeme kann von geladenen Projektilen oder Photonen kommen. Vor allem die Wechselwirkung mit Laserlicht spielt eine wichtige Rolle in unserer Forschung - hierin liegt auch ein gemeinsames Interesse der Gruppen von *Prof. Rost* und *Dr. Buchleitner*, wobei erstere sich auf starke Laserpulse im nahen Infrarot konzentriert, während letztere sich mit schwachen Mikrowellenpulsen beschäftigt.

Spezielle Themen betreffen Muster in partiellen Photoionisationsquerschnitten sowie Zerfallsbreiten von doppelt angeregten Zwei-Elektron-Zuständen, dynamische Symmetrien in Wenig-Elektronen-Quantendots, Umstände, die zu einer nichtlinearen Verstärkung höherer Harmonischer führen, wenn ein Atom von einem starken Laserpuls bestrahlt wird, sowie quasiklassische Formulierungen wesentlicher Streuprozesse (Vielfach-Photoionisation und Elektronenstoßionisation, siehe S. 88).

Themen, die sich auf viele Teilchen beziehen, schließen geometrieinduzierte Oszillationen in Photoionisationsquerschnitten von Targets mit delokalisierten Elektronen ein, Ladungstransfer in Kollisionen von schweren Ionen mit Molekülen und Clustern, Wechselwirkungen von Clustern mit kurzen und intensiven Laserpulsen (siehe S. 90), sowie die Zerstörung der Phasenkohärenz einfacher, gebundener Bewegung unter externem Rauschen.

Schließlich war *Dr. Porto* ein sehr aktives Mitglied der Gruppe. Seine Arbeit, unter anderem zu molekularen Motoren, random walk Problemen und der Evolution von Proteinen (siehe S. 85), war in der Gruppe zwar eher randständig, sie bot aber einen Kristallisationspunkt für mehrere Projekte am Institut und wird sich mühelos in die neugegründete Abteilung von *Prof. Jülicher* einfügen.

Zukunftsperspektiven

Unsere Arbeit zur Dynamik von Wenig-Elektronen-Systemen werden wir fortsetzen. Neue Initiativen sind in folgende Richtungen geplant: Die Konstruktion der ersten Lichtquelle der 4. Generation, eines X-ray free electron lasers bei DESY in Hamburg, wird ein neues Regime in der Wechselwirkung von Licht mit Materie eröffnen. Grundlegende atomare Prozesse, deren detaillierte Kenntnis Voraussetzung für zukünftige Anwendungen in anderen Gebieten ist, sind für die hohen Intensitäten (10^{18}W/cm^2), die großen Photonfrequenzen (bis zu 2 keV), und die kurzen Pulslängen (100-200 fs) des XFEL noch nicht erforscht. Dies ist speziell für Wechselwirkung mit Clustern von Interesse. Technisch, da die Brillanz der Lichtquelle den niedrigen Cluster-Fluss kompensiert und eine akzeptable Ereignisrate erwarten lässt. Physikalisch, da sich in diesem neuen Regime das Licht anders auf Cluster auswirken wird als bisher gewohnt. Anstelle eines Abschälens der Elektronen von aussen wird es zu einer Ionisation von innen durch das Leeren der inneren Schalen kommen. *Dr. Ulf Saalmann* wird die Clusteraktivitäten koordinieren.

Das Verhalten von Materie unter XFEL-Licht wird von wachsender Bedeutung für unsere Abteilung sein, nicht nur in Clustern, sondern auch in Atomen und Molekülen. Diese Aktivitäten werden von einem neuen Gruppenleiter, *Dr. Andreas Becker*, gebündelt werden.

Wir planen auch, unser Studium der Licht-Materie-Wechselwirkung in entgegengesetzter Richtung auszudehnen, auf schwache Mikrowellenstrahlung, die mit Quantendots wechselwirkt. Da der typische Niveauabstand meV beträgt, die ponderomotive Energie $I/4\omega^2$ aber durch das kleine ω sehr groß ist, wird ein ähnliches Regime mit nichtlinearer Antwort auf das Licht erreicht wie für Atome mit starken Lasern im nahen Infrarot.

Schließlich werden wir die Forschung auf dem Gebiet kalter Atome intensivieren. Hierbei sind wir primär an kalten Plasmen interessiert, die in einem Gas aus kalten Rydbergatomen entstehen. Diese Aktivitäten, und allgemein der Bereich der Atomphysik, wird von *Dr. Thomas Pattard* koordiniert. Ein enger Austausch mit unserem PKS-Fellow, *Dr. Joachim Brand*, ist ebenfalls zum Thema kalter Atome geplant.

Kollaborationen

Mit experimentellen Gruppen
Wir arbeiten mit Prof. Beckers Gruppe am Fritz-Haber-Institut in Berlin bezüglich der Abbildung delokalisierter Elektronen mit Hilfe von Photonen aus Synchrotronstrahlung zusammen. C_{60} Photoionisationsdaten wurden aufgenommen, ausgewertet und gemeinsam publiziert. In Zukunft planen wir die Universalität dieser Abbildungstechnik anhand von Metallclustern zu demonstrieren. Hierzu soll eine Gruppe der Universität Freiburg mit einer guten Quelle für Metallcluster in das Team integriert werden.

Des Weiteren besteht eine Zusammenarbeit mit der Gruppe von Prof. Schmidt-Böcking (Frankfurt). Hier geht es um die experimentelle Verifizierung des Übergangs von Regularität zu Chaos bei der Photoionisation durch die Besetzung hoher, doppelt angeregter Zustände in Atomen. Nach dem Bau neuer Detektoren mit der nötigen hohen Auflösung wurde kürzlich am HASYLAB in Hamburg eine Strahlzeit mit guter Datenausbeute abgeschlossen.

Mit theoretischen Gruppen (einige Beispiele)

- zu *random walks* mit H. E. Roman (Milano, Italy)
- zur Photoionisation in komplexen Atomen mit S. T. Manson (Atlanta, USA)
- zur Frage der Zeit in der Quantenmechanik mit J. S. Briggs (Freiburg)
- für das Buch *Komplexe Systeme* mit K. Richter (Regensburg)

Lokale Kooperationen
Die Zusammenarbeit mit Prof. Schmidts Gruppe von der TU Dresden wurde fortgesetzt, ihre Basis ist das gemeinsame, wöchentliche Seminar *Quantum Dynamics*. Es findet am **mpipks** mit externen Sprechern statt, die beide Gruppen einladen. Gemeinsame Forschungsaktivitäten umfassen *quantum adiabatic molecular dynamics* direkt

mit Prof. Schmidt und *Ladungstransport in ungeordneten und mesoskopischen Systemen* mit Dr. Großmann und Dr. Gutierrez von der TU Dresden.

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

"Nichtlineare Dynamik in Quantensystemen" 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 Anregungs- und Ionisationsdynamik von Einelektronen-Rydbergatomen bei hohen spektralen Dichten (s. Beitrag "Chaotic Ionization of non-classical alkali Rydberg states", A. Krug);
- die spektrale Charakterisierung der magnetischen Randzustände ebener Billards (s. Beitrag "Spectral cross correlations of magnetic edge states", K. Hornberger);
- die Theorie der kohärenten Rückstreuung polarisierten Lichts an einem Gas kalter Atome mit Spinfreiheitsgraden (C. Müller);
- die Zustandskontrolle einfacher Quantensysteme mittels Verschränkung und unter Vermeidung von Meßrauschen (s. Beitrag "Quantum state preparation via asymptotic completeness", T. Wellens),

mit meist 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 Hitachi SR8000-F1 des Leibniz-Rechenzentrums der Bayerischen Akademie der Wissenschaften, zum Einsatz.

Bis zum Abschluss von vier Promotionen während des vergangenen Jahres setzte die Arbeitsgruppe sich – mit einer Ausnahme – aus Diplomanden und Doktoranden zusammen. Dank enger Kontakte zu Arbeitsgruppen in Frankreich, Italien, Israel und Polen gingen sämtliche Promotionen mit ausgedehnten Auslandsaufenthalten der Doktoranden einher, was in zwei Fällen zum Abschluss einer binationalen Promotion führte (C. Müller, Nizza/München) bzw. führen wird (S. Wimberger, Como/München). Das Gästeprogramm des Instituts ermöglichte umgekehrt mehrwöchige Gastaufenthalte renommierter Kollegen (D. Delande, S. Fishman, I. Guarneri, B. Kümmerer, R. N. Mantegna, U. Smilansky, K. Taylor, J. Zakrzewski), was zu fruchtbaren Zusammenarbeiten führte. Zwei neue Doktoranden (J. Madroñero, F. Mintert) und der erste PostDoc (V. Shatokhin) wurden 2001 über ein von unserer Arbeitsgruppe am Institut organisiertes, zweimonatiges Seminar ("Coherent Evolution in Noisy Environments")

mit siebenwöchigem Vorlesungsprogramm und einwöchigem internationalen Workshop gewonnen. Ein im Rahmen dieser Veranstaltung am Institut erstmals durchgeführter öffentlicher Abendvortrag (A. Zeilinger), ebenso wie ein für Schüler und Studenten aller Fachrichtungen konzipiertes Wochenendseminar (in Zusammenarbeit mit der Evangelischen Akademie Tutzing in Heilsbronn) unter Mitwirkung von Rednern des Workshops (H. Walther, G. Leuchs, B. Kümmerer) erfreuten sich unerwartet regen Interesses.

Die Forschungsaktivitäten der nächsten Jahre werden durch folgende Schwerpunkte unserer aktuellen Arbeit definiert:

I die exakte quantenmechanische Beschreibung zunehmend komplexerer, atomarer Coulomb-Systeme, insbesondere hinsichtlich ihrer spektralen Charakteristika und ihrer Zerfallseigenschaften;

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

III die Transporteigenschaften von Materiewellen in optischen Potentialen mit Unordnung und Dissipation.

Während wir in (I) mit der Entwicklung eines allgemeinen theoretischen Apparats zur näherungsfreien Beschreibung der Fragmentationsdynamik des periodisch getriebenen Dreikörper-Coulombproblems die nächste große Herausforderung im Bereich der modernen, rechnergestützten Atomphysik ins Auge fassen, zielt (II) auf die fundamentale Ressource jeder zukünftigen Quanteninformationstechnologie und insbesondere auf deren Robustheit bei gleichzeitiger Forderung der Skalierbarkeit. Dank eines von der Volkswagenstiftung für drei Jahre bewilligten Kooperationsprojektes mit der Polnischen Akademie der Wissenschaften (K. Życzkowski, M. Kuś) werden wir letzteres Projekt im Rahmen einer intensiven bilateralen Zusammenarbeit, getragen durch den weitgehend kontinuierlichen Austausch von Doktoranden oder PostDocs in beiden Richtungen, verfolgen. Zu guter Letzt widmet sich (III) grundlegenden Szenarien des kohärenten Quantentransports (Anderson- oder dynamische Lokalisierung, Mott-Hubbard-Übergang), die dank spektakulärer Fortschritte in der experimentellen Quantenoptik nun mit ungekannter Genauigkeit überprüft werden können.

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

Im Februar 2002 hat die Abteilung die Arbeit am Institut aufgenommen und ist in der Aufbauphase. Kernthemen sind die Beschäftigung mit aktiven und dynamischen Phänomenen der Zellbiophysik und Zellbiologie. Dabei werden vorwiegend Ansätze und Konzepte aus der statistischen, Vielteilchen- und Nichtgleichgewichtsphysik verwendet. Ziel ist es, physikalische Eigenschaften und grundlegende Prinzipien, die eine wichtige Rolle in molekularen und zellulären Vorgängen spielen, zu charakterisieren. Beispiele für aktuelle und geplante Forschungsthemen sind:

Molekulare Motoren: Motorproteine sind die Prototypen aktiver molekularer Vorgänge, die in tierischen und pflanzlichen Zellen für Vorgänge wie Bewegungserzeugung, Materialtransport und Zellteilung eine herausragende Bedeutung haben. Unsere

Abteilung untersucht die physikalische Natur dieser Vorgänge auf molekularer Ebene und analysiert Situationen, in denen eine große Zahl solcher aktiven Moleküle zusammenwirken und durch Selbstorganisationsphänomene und kollektives Verhalten neuartige Eigenschaften hervorbringen.

Physik von Membranen und dem Zytoskelett: Membranen und Zytoskelett repräsentieren Materialien, die die Form und die Materialeigenschaften von Zellen festlegen und das Umfeld für viele zelluläre Vorgänge schaffen. Diese Materialien sind dynamisch und haben aktive Eigenschaften. Sie werden von der Zelle ständig neu gestaltet. Dabei können sich Materialeigenschaften drastisch ändern, Kräfte und Bewegungen sowie räumliche Muster erzeugt werden. Wir entwickeln physikalische Beschreibungen solcher aktiven polymerischen Materialien und deren Wechselwirkung mit Membranstrukturen.

Physik der Wahrnehmung und Sinneszellen: Sinneszellen sind spezialisierte Zellen, die physikalische Reize aufnehmen und in elektrische und Nervensignale umsetzen. Wir untersuchen insbesondere die Funktionsprinzipien von mechanosensitiven Sinneszellen, die z.B. im Innenohr für die Schallwahrnehmung verantwortlich sind. Diese Zellen sind in der Lage, über einen dynamischen Bereich von 6 Größenordnungen zu arbeiten und schon extrem schwache Schallsignale zu erkennen. Dabei werden von der Zelle aktive und nichtlineare Verstärkungsmechanismen verwendet. Wichtig ist dabei insbesondere das Verständnis der sowohl hilfreichen als auch limitierenden Rolle von Fluktuationen, und die Frage, wie aus biologischen Materialien solche Systeme in einer Größenordnung von Mikrometern realisiert werden.

Der Kontakt mit Experimentatoren, Biophysikern und Zellbiologen ist für diese Forschungsthemen sehr wichtig. Unsere Abteilung unterhält rege Kontakte zu Gruppen dieser Disziplinen, insbesondere ist eine Zusammenarbeit mit dem Max-Planck-Institut für molekulare Zellbiologie und Genetik (MPICBG) geplant. Die Abteilung ist auch an das internationale PhD Programm "Cell Biology, Bioengineering, Biophysics" angeschlossen, welches vom MPICBG initiiert wurde. Seit November 2002 haben zwei Arbeitsgruppen die Arbeit aufgenommen. Die Gruppe von Dr. Martin Zapotocky beschäftigt sich mit der Biophysik des Geruchssinnes und ergänzt damit Aktivitäten zur Physik der Sinneszellen. Dr. Ralf Everaers arbeitet insbesondere mit nummerischen Methoden und Computersimulationen an der Physik weicher und biologischer Materie.

Zukunftsperspektiven

Biologische Systeme sind außerordentlich komplex und vielschichtig strukturiert. Die großen Fortschritte der Molekular- und Zellbiologie der vergangenen Jahrzehnte haben viele neue Fragen aufgeworfen und dabei die Komplexität und die Bedeutung aktiver Vorgänge in Zellen sehr deutlich gemacht. Diese Entdeckungen haben neue Forschungslinien angeregt, in denen die Physik wichtige Beiträge leisten kann. Aus der Sicht der theoretischen Physik gilt es, grundlegende Konzepte, die z.B. zur Beschreibung fluktuierender Nichtgleichgewichtsprozesse, nichtlinearer Systeme oder für das Verständnis komplexer Materialien entwickelt wurden, so anzupassen und zu vertiefen, um der Realität biologischer Prozesse und Funktionen gerecht zu werden und dabei allgemeine Prinzipien und Organisationsmuster herauszuarbeiten. Die Abteilung biologische Physik deckt gemeinsam mit den neu eingerichteten Arbeitsgruppen Themenbereiche ab, die von den Eigenschaften biologischer Materialien, bis hin zu der Frage reichen,

wie die Funktionsweisen von Sinneszellen organisiert und reguliert sind. Dieses sind Gebiete, die sich sehr schnell entwickeln auf Grund neuer Erkenntnisse, insbesondere der Zellbiologie. Zellbiologische Vorgänge finden auf Größenordnungen von 10-1000 nm statt und sind oft Vorbild für Realisierungen, wie sie in der Nanotechnologie angestrebt werden. Alle diese Entwicklungen stehen erst am Anfang und werden begleitet von verwandten Aktivitäten in den Computer- und Ingenieurwissenschaften (Bioinformatik, Biotechnologie).

Das Max-Planck-Institut für Physik komplexer Systeme bietet ein besonderes Umfeld für theoretische Arbeiten in biologischer Physik und hat schon in den vergangenen Jahren Forschungsinitiativen auf diesem Gebiet gezeigt ("Initiative Biologie"). Das breite Spektrum an Forschungskompetenz im Bereich komplexer Phänomene erlaubt den Austausch und die Zusammenarbeit mit anderen Gruppen, die sich z.B. mit Musterbildung und nichtlinearer Dynamik beschäftigen. Die Nähe zur TU, dem zu gründenden Biotechnologiezentrum, sowie dem Max-Planck-Institut für molekulare Zellbiologie und Genetik (MPICBG), ermöglichen einen Austausch mit vielfältigen Forschungsaktivitäten unterschiedlicher Disziplinen. Angestrebt sind insbesondere eine enge Zusammenarbeit mit Prof. Jonathon Howard am MPICBG in Dresden und mit Prof. Albrecht Ott an der Universität von Bayreuth. Es ist auch geplant, im Gebäude des MPICBG einen Laborraum einzurichten, in dem Experimente, die in unmittelbarem Zusammenhang mit theoretischen Projekten stehen, durchgeführt werden können. Das Gäste- und Workshopprogramm des Instituts bietet weiterhin die Möglichkeit zur Zusammenarbeit und dem Ideenaustausch mit Wissenschaftlern aus aller Welt. Dies ermöglicht jungen Wissenschaftlern, neue Entwicklungen frühzeitig wahrzunehmen und aufzugreifen.

Kooperationen

- Max-Planck-Institut für molekulare Zellbiologie und Genetik, Dresden
  - Zusammenarbeit mit Jonathon Howard zur Dynamik von Cilia und Flagella und zur Physik des Zytoskeletts und molekularer Motoren
  - Zusammenarbeit mit Markos Gonzalez-Gaitan zur Entstehung von Morphogen Gradienten
- Universität Bayreuth
  - Zusammenarbeit mit Albrecht Ott zur Entwicklung und Strukturbildung einfacher Organismen.
- Cavendish Laboratory, Cambridge, UK
  - Zusammenarbeit mit Thomas Duke zur Physik des Gehörs.
- Institute Curie, Paris
  - Zusammenarbeit mit Jacques Prost zur Physik molekularer Motoren und zur Dynamik des Zytoskeletts
  - Zusammenarbeit mit Pascal Martin zur Physik mechanosensibler Sinneszellen.

- Rockefeller University, New York
  - Zusammenarbeit mit J. A. Hudspeth zur Biophysik mechanosensibler Sinneszellen
- AMOLF, Amsterdam
  - Zusammenarbeit mit Marileen Dogterom und Bela Mulder zur Dynamik des Zytoskeletts in Pflanzenzellen

Nachwuchsgruppe: Strukturbildung in Reaktions-Diffusions-Systemen
(Leiter: Dr. M. Bär)

Die Nachwuchsgruppe "Musterbildung" am mpipks existiert seit November 1995 und erreichte ihre heutige Stärke von ca. zehn Mitarbeitern Anfang 1999. Unsere Forschung konzentrierte sich zunächst auf komplexe Strukturen und Raum-Zeit-Chaos in chemischen und physikalischen Reaktions-Diffusions-Systemen. Im Laufe der Zeit bildete sich die Modellierung biologischer Prozesse als zweiter, gleichwertiger Schwerpunkt heraus.

Komplexe Strukturen
Strukturbildung wird in vielen physikalischen, chemischen und biologischen Systemen beobachtet. Übergänge zwischen einfachen (Fronten, Pulse, periodische Muster, Spiralen) und komplexen Strukturen (Raum-Zeit-Chaos, modulierte Strukturen, Musterdomänen) werden mit Hilfe von numerischen Simulationen, Störungstheorien sowie numerischer Bifurkations- und Stabilitätsanalyse untersucht. Kürzlich ist uns eine nichtlineare Analyse sekundärer Instabilitäten periodischer Wellen gelungen, die neue Erkenntnisse über raumzeitlich chaotische Muster und modulierte Wellen, z.B. die Superspiralen im Bericht von *Brusch et al.* auf S. 111, liefert. Weitere Themen sind die Strukturbildung in anisotropen und heterogenen Medien sowie die externe Steuerung von Mustern (siehe den Bericht von *Kühne et al.* auf S. 115). Anwendungen schließen dabei chemische Reaktionen in Gelen und auf Oberflächen sowie hydrodynamische Systeme (dünne Filme, Oberflächenwellen und Konvektion) sowie Wachstum von Nanostrukturen mit ein.

Biophysik und Theoretische Biologie
Insbesondere Modelle aus der Physiologie (intrazelluläre Dynamik, Kalziumwellen) und Morphogenese (Aggregation von Bakterien und Schleimpilzen) wurden hier betrachtet. Methodisch wurde dabei insbesondere der Übergang von kontinuierlichen, deterministischen auf diskrete, stochastische Modelle betrachtet. Hervorzuheben sind stochastische Modelle für intrazelluläre Kalziumdynamik und Dichtewellen in Myxobakterien ("Rippling"), die auf Migration und Kollision basieren (siehe den Bericht von *Börner et al.* auf S. 118). Einige Probleme aus der Immunologie wurden modelliert, z.B. die Dynamik des Keimzentrums sowie die Entwicklung von Antikörpern und Antigenen im Zustandsraum. Neuere Projekte beschäftigen sich mit der Beschreibung biochemischer Netzwerke, z.B. bei metabolischen Prozessen, und der Clusterbildung von Rezeptoren in Membranen.

Zukunftsperspektiven

Ausgangspunkt: Strukturbildung ist ein relativ junges Forschungsgebiet. Am Anfang standen die Untersuchung hydrodynamischer Instabilitäten sowie die Analyse dissipativer Strukturen in chemischen Reaktionen. Das Interesse an nichtlinearer Dynamik und Chaos führte zu einer Ausweitung der Aktivitäten seit 1985. Ein Katalog von Mechanismen der Musterbildung wurde dann in dem klassischen Übersichtsartikel von Cross und Hohenberg 1993 gegeben. Dabei wurden universelle Szenarien mit Hilfe von Amplitudengleichungen nahe der Schwelle zwischen räumlich homogenen und periodischen Mustern zusammengefasst. Am mpi**pks** haben wir uns seit 1995 mit der Analyse sekundärer Instabilitäten periodischer Wellen und Szenarien zum Auftreten von Raum-Zeit-Chaos befasst. Dazu wurde der Einfluss von Symmetriebrechungen (Anisotropie, Heterogenitäten, Randgeometrie, internes Rauschen) untersucht.

Zukunftspläne: Besonders vielversprechend ist im Moment die *Modellierung biologischer Prozesse* auf intra- und interzellulärer Ebene. Modellsysteme wie Kalziumwellen und Schleimpilzaggregation sind bis zu einem gewissen Grade verstanden, aber die rapide Zunahme des Wissens über biochemische Reaktionen, metabolische und Signalnetzwerke sowie Transportprozesse aus Experimenten bietet viele Möglichkeiten für quantitative mathematische Modelle. Neben direkten Simulationen wird auch die numerische Bifurkationsanalyse für eine effiziente Analyse benötigt werden. Internes Rauschen spielt eine große Rolle in vielen biologischen Systemen. Daher sollten die Methoden für kontinuierliche, deterministische Modelle auf *stochastische diskrete Modelle* übertragen und entsprechend erweitert werden. Zusammenfassend ist insbesondere der Frage nach dem Verhältnis von genetischem Determinismus zu Selbstorganisationsprozessen in Lebewesen zu klären. Diese Betrachtungen werden eine wichtige Rolle in der Zellbiologie, Mikrobiologie, Immunologie und Neurobiologie spielen.

In physikalischen und chemischen Systemen wird die Forschung sich weiterhin mit Effekten weit weg von der Primärschwelle befassen. Ziele für Theoretiker sind hier die Ausdehnung numerischer Methoden auf zwei und drei Dimensionen sowie die *Charakterisierung irregulärer, chaotischer Muster*. Insgesamt erwarten wir einen zunehmenden Übergang von einfachen qualitativen Modellen zu komplizierteren quantitativen Modellen. Eine weitere Herausforderung für Experimentatoren und Theoretiker stellt die Beschreibung *strukturbildender Prozesse auf der Nanoskala* dar.

Kooperationspartner

Wir verfügen über vielfältige nationale und internationale Kooperationsprojekte. Unter anderem waren wir an der DFG-Forschergruppe "Nanostrukturierte Funktionselemente in makroskopischen Systemen" der TU Dresden beteiligt. Gegenwärtig wird die Kooperation mit Prof. Meron (Beer-Sheva) und Prof. Pismen (Technion Haifa) durch die Deutsch-Israelische Gesellschaft zum Thema "Strukturbildung in der Katalyse: Von der Mikro- zur Nanoskala" unterstützt. Auf Zusammenarbeiten mit experimentellen Gruppen legen wir besonderen Wert; hier sind Projekte zur chemischen Strukturbildung (Prof. Müller (Magdeburg), Prof. Engel (TU Berlin)), zum Wachstum von Nanostrukturen (Dr. Mertig, Prof. Pompe (TU Dresden)) und zur Oberflächenkatalyse (Prof. Imbihl (Hannover)) zu nennen. Auf dem Gebiet der biologischen Systeme existieren Projekte zur räumlichen Organisation von Bakterien (Dr. Reichenbach (GBF Braun-

schweig), Prof. Sogaard-Andersen (Odense)) sowie zu Biotransformationen (Dr. Bertau (TU Dresden)). Weitere theoretische Kooperationen finden statt mit Dr. Torcini und Prof. Ruffo (Florenz), Dr. Provenzale (Turin) und Prof. Kevrekidis (Princeton).

Was wird aus Gruppenmitgliedern nach ihrer Zeit am mpipks?

Dr. Thomas Boeck (Gastwissenschaftler 2000-2002) erhielt ein Emmy-Noether-Stipendium und arbeitet jetzt in Paris. *Dr. Andreas Deutsch* (Gastwissenschaftler 1999-2001) ist jetzt am Hochleistungsrechenzentrum der TU Dresden als wissenschaftlicher Mitarbeiter fest angestellt und leitet eine Gruppe zur Bioinformatik. *Dr. Martin Falcke* (Gastwissenschaftler 1997-1998, 2000-2001) erhielt eine längerfristige Stelle als Leiter einer Gruppe zur Calcium-Dynamik in der neuen Theorieabteilung am Hahn-Meitner-Institut in Berlin unter der Leitung von Prof. Frey. *Dr. Haye Hinrichsen* (Gastwissenschaftler 1997-1999) vertritt Prof. P. Grassberger an der Universität Wuppertal für sechs Jahre. *Dr. Thomas Höfer* (Gastwissenschaftler 1996-1997) war wissenschaftlicher Assistent an der Humboldt-Universität Berlin (1997-2001) und wurde vor kurzem zum "Junior Professor" an der Humboldt-Universität ernannt. *Dr. Michal Or-Guil* (Wissenschaftliche Mitarbeiterin 1997-2002) wurde 2001 mit einer Nachwuchsgruppe der Volkswagenstiftung ausgezeichnet und hat diese mit dem Thema "Theoretische Immunologie" am Institut für Theoretische Biologie der Humboldt Universität Berlin angesiedelt.

Nachwuchsgruppe: Wellen in komplexen Medien und mesoskopische Phänomene

(Leiter: Dr. H. Schomerus)

Die Nachwuchsgruppe besteht seit November 2000. Neben dem Leiter und einem Assistenten (M. Titov) betreiben hier zur Zeit fünf Postdocs und ein Doktorand theoretische Grundlagenforschung zu Problemen und Phänomenen von Elektronen und Licht in kleinen Strukturen, in denen Phasenkohärenz eine besondere Rolle spielt. Dies geschieht in Zusammenarbeit mit einem guten Dutzend weiterer Wissenschaftler im mpi**pks** und an auswärtigen Einrichtungen.

Es lassen sich drei Hauptforschungsrichtungen ausmachen:

- Mesoskopische Effekte in Quantenpunkten und Quantendrähten, einschließlich Hybridstrukturen mit supraleitenden Komponenten. Das Interesse gilt etwa der Leitfähigkeit, dem Schrotrauschen und der lokalen und globalen Zustandsdichte. Der Zerstörung von Phasenkohärenz durch äußere Einflüsse und interne Wechselwirkungen wird nachgegangen, auch unter den Aspekten der Quanteninformatik. Eine neue Zielrichtung ist die Molekular- und Nanoelektronik. H. Schomerus, M. Titov, A. Nemes-Salgueiro; Zusammenarbeit mit H. S. Sim, S. W. Kim, I. Rotter, R. Nazmitdinov (alle mpi**pks**), Gruppen von C. W. J. Beenakker (Leiden), M. Büttiker (Genf), P. Brouwer (Cornell), Y. Blanter (Delft), K. Richter (Regensburg), J. Dalibard (Paris).

- Elektromagnetische Welleninterferenz innerhalb unregelmäßig geformter dielektrischer Streukörper oder in ungeordneten Wellenleitern; intensive Laser-Atom Wechselwirkung. Als Aspekte treten hier Verstärkung in aktiven Medien und

Absorption in passiven Medien hinzu, inklusive quantenoptischer Effekte etwa in Lasern, in denen Rückkopplung durch Mehrfachstreuung an Unordnung oder dielektrischen Grenzflächen realisiert wird. H. Schomerus, J. Wiersig, M. Hentschel; mit C. W. J. Beenakker (Leiden), F. Laeri (Darmstadt), J. Noeckel (Oregon), W. Becker (MBI Berlin), C. Faria (mpi**pks**, MBI Berlin).

- Quantendynamik für klassisch nichtintegrable Systeme. Neben dem herkömmlichen Feld des Quantenchaos liegt ein besonderes Augenmerk auf dem erheblich komplexeren Feld der nicht völlig chaotischen Systeme (mit gemischtem Phasenraum), sowie auf quasiintegrablen Systemen. Dazu wird auch auf ein vertieftes Verständnis der nichtlinearen klassischen Dynamik abgezielt. H. Schomerus, J. Wiersig, G. Carlo, M. Sczyrba; H. S. Sim (mpi**pks**), F. Haake (Essen), M. Saraceno (Buenos Aires), J. Keating, M. Berry, M. Sieber (alle Bristol), R. Schubert (Paris), A. Bäcker (Ulm).

In all diesen Problemfeldern steht die Bestimmung von universellen Phänomenen im Vordergrund. Dies geschieht anhand flexibler und exakter mathematischer Methoden, die zu quantitativen Ergebnissen führen und zugleich die Schlüsselmechanismen zu identifizieren helfen. Es kommen Methoden der Zufallsmatrixtheorie, feldtheoretische Methoden, Fokker-Planck-Gleichungen und semiklassische bzw. quasiklassische Ansätze zur Anwendung. Die Ergebnisse lassen sich in der Regel mit den Resultaten exakter Numerik oder von Experimenten vergleichen.

Zukunftsperspektiven

Langfristige Perspektive:

Neue vorgesehene Zielrichtungen sind die Schnittstelle von Mesoskopik und Quantenoptik, Molekular- und Nanoelektronik sowie mesoskopische Aspekte der Quanteninformationsverarbeitung. Der generelle Wissensstand in diesen jungen Gebieten ist noch sehr gering, Grundlagenforschung kann hier viel bewegen. Die Methoden und Konzepte, die in den aktuellen Projekten der Gruppe zum Tragen kommen, die angesammelte Kompetenz und das Umfeld definieren einen geeigneten Ausgangspunkt, um sich diesen Themenkreisen erfolgversprechend zuzuwenden.

Die Forschung in der mesoskopischen Physik, der Wellenpropagation in ungeordneten Medien und der Quantendynamik nichtlinearer Systeme soll fortgeführt werden, zunächst im Rahmen der Punkte, die in der kurzfristigen Perspektive aufgeführt sind.

Der heutige grundlegende Erkenntnisstand über passive dielektrische Resonatoren ist recht umfangreich. Sehr wenig ist über Resonatoren mit aktiven Medien bekannt, insbesondere wenn quantenoptische Prozesse eine Rolle spielen.

Kurzfristige Aussichten:

Eine Anzahl von ins Auge gefassten Projekten zielt auf die Eingrenzung und Erforschung von Phänomenen sowie die Etablierung konzeptioneller Herangehensweisen, die neulich in der Gruppe entwickelt wurden. Phänomene sind etwa dynamische und statische Signaturen von Wellenlokalisierung, systematische aber nichtuniverselle Unterdrückung von Schrotrauschen in generisch geformten Strukturen, und ein Quanteninterferenzeffekt an einem Streuer mit internem Freiheitsgrad. Mit den kürzlich ent-

wickelten Methoden lassen sich einige Probleme in Angriff nehmen, die vorher gar nicht, oder nicht in diesem Umfang, zugänglich waren. Dies betrifft einen Streuzugang zur lokalen Zustandsdichte für eine Vielzahl mesoskopischer Systeme, eine Innen–Außen–Dualität an dielektrischen Grenzflächen, eine gleichförmige semiklassische Näherung für starke Laser-Atom-Wechselwirkung, eine Methode, Dynamik in mesoskopischen Strukturen über das Schrotrauschen zu testen, und eine Familie von Quantenabbildungen, die eine völlige Analogie zu Quantenpunkten aufweisen. Es ist ein Ziel, diese Phänomene und Methoden auszuweiten und zu etablieren.

Personal und Ressourcen:

Die Nachwuchsgruppe ist auf fünf Jahre angelegt, wobei die generelle Forschungsrichtung mit großer Wahrscheinlichkeit auch über diesen Zeitrahmen hinaus am Institut vertreten sein wird, da sie sich auch zum Teil in anderen Gruppen, im Gästeprogramm, in den Seminaren und in den Workshops wiederfindet. Der Zeitrahmen für Fluktuationen in der Gruppenzusammensetzung beträgt ein bis zwei Jahre, wobei Kontinuität durch den Leiter und den Assistenten erzeugt wird. Die Fluktuationen können genutzt werden, um zusätzliche Themen und Kompetenz zuzuführen und weitere Verknüpfungspunkte nach Außen zu schaffen, indem die Kontakte zu ehemaligen Mitgliedern gepflegt werden. Die jetzige Gruppenstärke und laufende Kooperationen sollen beibehalten werden.

Kooperationen im Institut

H. S. Sim, S. W. Kim, I. Rotter, R. Nazmitdinov

Gemeinsame Interessen im Institut auch mit G. Cuniberti, Gutzwillerfellow A. Ozorio de Almeida, allgemein mit den Gruppen Rost, Fulde, Buchleitner.

Kooperationen außerhalb des Instituts

- C. W. J. Beenakker, P. Jacquod (Uni Leiden)
- J. Nöckel (Oregon)
- M. Büttiker, P. Samuelsson, S. Pilgram (Uni Genf)
- P. Brouwer (Cornell)
- Y. Blanter (Delft)
- F. Haake (Essen)
- M. Saraceno (Buenos Aires)
- J. Keating, M. Berry, M. Sieber (alle Bristol)
- R. Schubert (Paris/zuvor mpi**pks**)
- A. Bäcker (Ulm/TU Dresden)
- F. Laeri (Darmstadt)
- W. Becker (MBI Berlin), C. Faria (MBI Berlin/zuvor mpi**pks**)
- J. Dalibard (Paris)

Nachwuchsgruppe: Quantenchaos und mesoskopische Systeme
(Leiter: Dr. K. Richter (bis 4/2001))

Mesoskopische Physik bezieht sich auf Systeme, die im interessanten Grenzbereich zwischen der Mikro- und Makrowelt angesiedelt sind, typischerweise kleine leitende Strukturen mit reduzierter räumlicher Dimensionalität. Das komplexe Verhalten mesoskopischer Systeme beruht darauf, dass sie sowohl Quantenkohärenzeffekte (auf Mikrometerskala) als auch klassisch chaotische Dynamik aufweisen. Von uns verwendete moderne semiklassische Methoden und Quantenchaos stellen eine geeignete theoretische Basis dar, um das Wechselspiel zwischen klassischer und Quantenphysik im mesoskopischen Regime zu untersuchen. Darüber hinaus kommen rein quantenmechanische, teils numerische Verfahren zum Einsatz. Die untersuchten Systeme sind Quantenpunkte, Halbleiterübergitter, Halbleiter-Supraleiter-Hybride, molekulare Leiter, photonische Kavitäten und nanomechanische Systeme.

Nach der Berufung von Klaus Richter im April 2001 auf einen Lehrstuhl für Theoretische Physik an der Universität Regensburg haben die letzten Mitglieder die Nachwuchsgruppe Ende 2001 verlassen. Die Forschung der Gruppe umfasste von 1999 bis 2001 drei Hauptrichtungen:

- Die Untersuchung spektraler Statistik in komplexen Quantensystemen. Hierzu gehören insbesondere die grundlegende Frage nach dem Zusammenhang zwischen semiklassischen Näherungen für spektrale Korrelationsfunktionen und Vorhersagen der Zufallsmatrixtheorie. Wir konnten in einem wichtigen Schritt Vorhersagen der Zufallsmatrixtheorie jenseits der sogenannten Diagonalnäherung direkt aus der chaotischen Dynamik herleiten (siehe Bericht: *Sieber und Richter*, S. 122).

- Quantentransport in mesoskopischen Systemen wurde insbesondere in Hinblick auf die Rolle des Elektronenspins untersucht (Spintronik). In zwei Doktorarbeiten wurden Spin-Effekte aufgrund von Berry-Phasen berechnet und ein auf Interferenz beruhender Schalteffekt für die Richtung spinpolarisierter Elektronen entdeckt (siehe Bericht: *Hentschel, Frustaglia und Richter*, S. 131).

- Einen neuen Forschungsschwerpunkt der Gruppe bildete die molekulare Elektronik: Wir untersuchten Quanteneffekte im Transport durch molekulare "Drähte" und Kohlenstoff-Nanoröhren. In Zusammenarbeit mit der Gruppe von Prof. R. Schmidt an der TU Dresden wurde ein C_{60}-Molekül zwischen Nanoröhren als molekularer Schalter vorgeschlagen (siehe Bericht: *Cuniberti* S. 126).

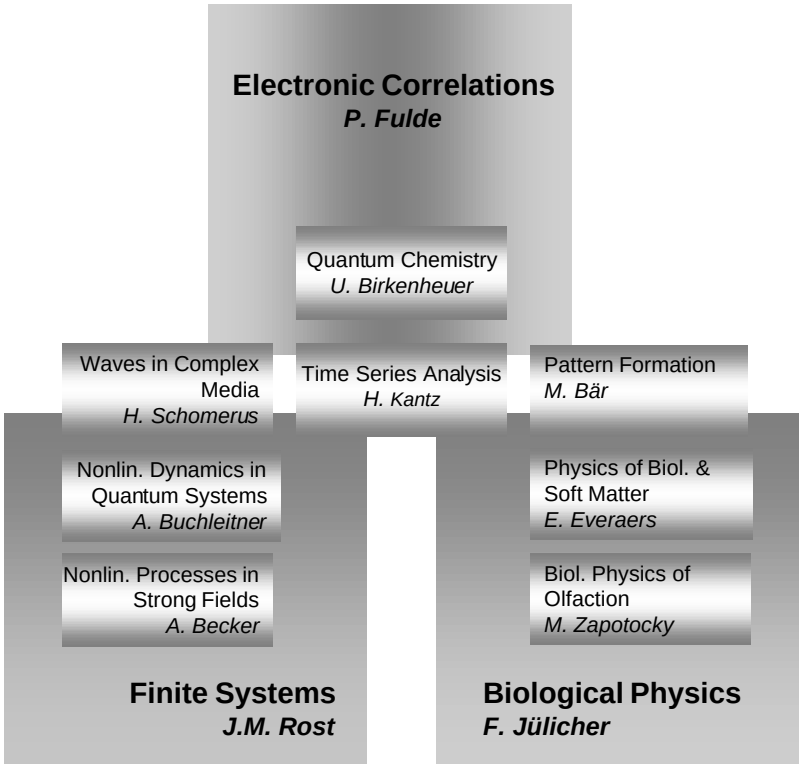

Figure 1: *Verzahnung der drei wissenschaftlichen Abteilungen und der acht Arbeitsgruppen am mpi**pks** • Links among the three scientific departments and the eight research groups at mpi**pks**.*

I. Scientific Work and its Organisation at the Institute - an Overview

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 Senate followed a recommendation which had been worked out by a Committee of the Chemisch-Physikalisch-Technische Sektion. 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 barrack in the Bayreuther Straße, close to the university campus, as a temporary location for the institute. 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.

1999-2002 • 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. Since that time there have been approximately 100-150 long-term guest scientists at the institute at a given time, together with 1200-1500 short-term guests who annually participate in the workshop and seminar program.

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.

The Board of Trustees supports 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 are accompanied by the work of the Scientific Advisory Board since June 1996.

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 classical statistical physics.

Furthermore, five of the currently eight research groups are broadening and strengthening the work of the corresponding divisions (see figure on p. 23).

Three more groups, among them two junior research groups, interpolate between and add to the above listed research topics.

- The research of the junior research group *Waves in Complex Media and Mesoscopic Phenomena* headed by *Dr. Schomerus* bridges the work of the divisions *Electronic Correlations* and *Finite Systems*.
- The junior research group *Pattern Formation in Reaction-Diffusion Systems* headed by *Dr. Bär* was a nucleation center for - and a link to - research in biological physics before the division *Biological Physics* started its activities (see also *Initiative Biology*, p. 147).
- 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. The joint organization of the international conference *Dynamics Days Europe* (see p. 152) by *Prof. Kantz* and *Dr. Richter* is one of the fruitful results of these research efforts.

With the *Initiative Biology* the institute has taken a new route to provide scientists working on new emerging topics with a temporary organizational and meeting structure. It has turned out to be very useful also for new guest scientists at the institute to quickly gain information and access to the activities of the initiative. *Dr. A. Deutsch* also directed a novel German-wide network *MTBio-Modelling and theory in the Biosciences*, which was supported by mpi**pks** and the Tschira-Foundation (p. 172).

Two of the co-initiators of the *Initiative Biology* successfully applied for heading junior research groups at universities funded by the Volkswagen Foundation: *Dr. Or-Guil* now conducts now research in Berlin, in collaboration with the Charité, and *Dr. Cuniberti* set up his group at the University of Regensburg.

3. Workshop and Visitors Program

A central task of the institute is to conduct international *Workshops and Seminars* (p. 151), 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. 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. 142) 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. 190).
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.
The success of the Visitors Program led to dramatic shortage in free office space. As a consequence, parts of the guest house apartments have temporarily been converted into offices. In the meantime, a satisfactory solution of this problem within the next

years has appeared on the horizon.
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. D. Delande* (Paris), *Prof. E. Prange* (Maryland) and *Prof. A. Ozorio de Almeida* (Rio de Janeiro) have spent up to one academic year at mpi**pks** (p. 145).
The mpi**pks** also offers one *Distinguished PKS Postdoctoral fellowship* annually. It aims at excellent young researchers, shortly before accepting a tenure track position. The two *distinguished fellows* who already left our institute accepted assistant professorships (p. 176).

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. 174). 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. 178).
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 57 events during 2000-2003, young scientists of the institute took part in the coordination of 26. This has a positive educational effect for young scientists, and helps the external coordinators through the permanent contact with a local scientific coordinator. The flexible structure of the institute permits and encourages individual initiatives, e.g., a three semester ring lecture in the Studium Generale of the TU Dresden initiated by *Dr. Morawetz* (p. 174).

5. Public Relations

The institute understands its mission in the broadest sense to provide 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. The mpi**pks** has been awarded the *Max-Planck-Preis für öffentliche Wissenschaft 2000* for its efforts in this area of public relations.
Since 1999, mpi**pks** coordinates, 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. 177).
Furthermore, coordinators of workshops are encouraged to offer one public evening lecture at mpi**pks**, in the course of the workshop.

6. Research Networking

Local • The mpipks 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). Institute members are involved in several Sonderforschungsbereiche and one Forschergruppe (p. 170). 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.
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. 150).

7. Reports by the Research Groups

Division: Electronic Correlations
(Prof. P. Fulde)

The research of the department is focusing mainly, but not exclusively, on electronic correlations and many-body theory. Further topics include cold glasses, large spin systems and nonlinear lattice dynamics (breathers etc).

The understanding of effects of electronic correlations is one of the main topics of the theory of condensed matter. It includes all those effects which can not be explained within the framework of molecular-field or Hartree-Fock approximations. Strongly correlated electronic systems are currently intensively studied world-wide. The department research in this field can be roughly split into two parts. The first direction follows ab initio calculations of many-body wavefunctions and excited energy spectra using Green-function methods. While density functional methods are not of much use here (because they do not allow to compute the many-body wavefunctions), we use quantum-chemical methods, which are modified and optimized for being applied to solid-state problems. Main results have been so far the calculation of the ground state wavefunction of a large number of solids, with precision as good as is common for small molecules. Presently we focus on the computation of energy bands in solids. This particular research is done in close collaboration with the *Quantum Chemistry* group (cf. p. 31). It allows for a detailed study of the qualitative and quantitative impact of electronic correlations on solid state properties. The second part of our research in the field of electronic correlations is of phenomenological nature. A main goal is to understand the physical mechanisms leading to heavy quasiparticle excitations (heavy fermion systems) in strongly correlated metals. While the Kondo effect was initially considered as the only source of heavy fermions, we have discovered in the meantime a number of other mechanisms leading to the same result. During the past two years we have shown that Uranium compounds contain 5f electrons of dual nature, leading to the formation of heavy quasiparticles. Our theoretical studies in cooperation with

Prof. Zwicknagl (Universität Braunschweig) result in a mix of localized and delocalized 5f electrons in different orbitals. For LiV_2O_4 we found another new mechanism leading to the formation of heavy quasiparticles. It is based on magnetic frustration in pyrochlore lattices. Excitations in such lattices may have, surprisingly, a fractional charge of one-half of an electron.

Similar effects have been known so far only for one-dimensional, highly doped polyacetylene, and for the fractional Quantum Hall effect in two-dimensional systems. Our results provide for the first time an example of a three-dimensional solid having such excitations. With these studies we are participating also in the research work of the Sonderforschungsbereich 463 of the Technische Universität Dresden.

Our research on cold glasses is focusing on the understanding of the impact of magnetic fields on the low-energy excitations in such systems, which led to a number of unexpected surprising results. This research is done in close collaboration with Dr. Strehlow from the Physikalisch-Technische Bundesanstalt in Berlin. Studies of nonlinear lattice dynamics are mainly focusing on the role of localized excitations in various systems, such as lattice dynamics of solids, bond excitations in molecules, coupled Josephson junction arrays, and coupled optical waveguides. These studies are embedded in a TMR network of the European Union, and are done in close collaboration with Prof. Ustinov from Universität Erlangen-Nürnberg.

Group: Nonlinear Dynamics and Time Series Analysis
(Prof. H. Kantz)

Nonlinear dynamical systems exhibit a diversity of complex behaviours, among which deterministic chaos is one of the most fascinating aspects. We focus on selected open problems in the understanding of nonlinearity, such as the interaction between chaos and noise, the transition from chaos to noise, chaos with many degrees of freedom, and the dynamics of systems with time delayed feedback. Earlier work devoted to the understanding of stochastic aspects of deterministic chaos enabled us to enter the highly relevant and largely unexplored field of stochastic modelling. In many long-time numerical simulations (e.g., of climate models), the integration of the dynamics of fast chaotic variables consumes a huge amount of computation power. A suitable replacement of such dynamics by white noise would speed up computations by one or more orders of magnitude. We are working on rigorous approaches for the replacement of fast chaos by noise, employing projection operator techniques (see report on p. 77).

When a time series derived from an experiment or from field measurements shows complex, aperiodic oscillations, one can speculate to which extent this can be modelled by a rather simple but chaotic deterministic system. This inverse approach has been studied since the early eighties, but it is meanwhile evident that most phenomena of interest are not due to low-dimensional deterministic chaos. Therefore, effort is taken not only to extend the understanding of nonlinear time series methods, but to enlarge the class of systems which can be treated with these methods. A particular focus of the last two years is non-stationarity, the analysis of nonlinear stochastic systems, and combinations of nonstationarity and stochasticity. In addition to the development of methods we apply them to real-world problems in different projects, which are partly conducted jointly with experimental groups, with industrial partners, or with third

party funding. One recent example is the prediction of surface wind velocities (see p. 81), a method for which we filed a patent. In a project with mechanical engineers, dynamical instabilities of metal sheet forming are investigated, where wrinkles and buckling express themselves as a pattern forming process.

The two branches of our research are closely linked, since applications confront us with dynamical phenomena which call for theoretical understanding, and they call for improved data analysis methods due to precise questions which have to be answered. Analysis schemes themselves are again based on theoretical understanding. These links will be illustrated by the wind speed prediction project (p. 81). Due to the variety of systems and phenomena contained in time series problems, the work of this group has various links to other groups' interests, such as biological physics, pattern formation, and nonlinear aspects in finite systems. In seminars and discussions members of the different groups therefore have frequent exchange.

Perspectives for the future

Also future work will be split into the main two directions, namely improving the fundamental understanding of complex dynamical and statistical behaviour, and designing and applying time series methods for complex signals. In the former field, we aim at merging dynamics with statistical physics, in particular non-equilibrium statistics. In the latter we are working on a link to known methods for stochastic processes (hidden Markov models, extended Kalman filters). In terms of nonstationarity, we are currently increasing our mathematical and physical understanding of precursors of bifurcations with the goal of data driven, predictive bifurcation analysis. In terms of systems and data, we intend to pay increasing attention to issues risen by biological physics.

Alltogether, we are aiming at progress in issues which will lead our recognized expertise in nonlinear dynamics and time series analysis out of the rather narrow niche of deterministic chaos. At the same time, the three aspects nonlinearity, nonstationarity, and stochasticity will be seen from a unifying point of view: Only seemingly unrelated, nonstationarity and stochasticity are non-autonomous extensions of dynamical systems, with the essential difference lying in correlation times. Nonstationarity in a linear stochastic process, on the other hand, can sometimes be modelled as nonlinearity. Finally, in deterministic systems with time scale separation, slow variables in fast subsystems might look like slowly time dependent parameters. Hence, these three aspects call for a common approach.

Cooperations

- Prof. C. Grebogi, Univ. Sao Paolo, Brasil: Influence of noise on attractors with variable dimension of the unstable manifolds.
- PD Dr. Wolfram Just, Theoretische Physik, Technische Universität Chemnitz: Modelling of fast degrees of freedom through stochastic processes.
- Prof. Dr. M. Kleiner, Maschinenbau, Universität Dortmund: Analysis of dynamical instabilities during metal sheet forming.
- Prof. Dr. Bernhard Mehlig, Universität Göteborg: Common work for the textbook *Complex Systems in Classical and Quantum Physics - Statistics versus Dynamics*.

- Prof. Dr. J. Parisi, Universität Oldenburg: data analysis, model verification, and prediction of bifurcation for a Nd:YAG laser, joint supervision of the PhD work by *T. Letz,* PhD December 2001).
- Prof. Dr. J. Peinke, Universität Oldenburg: Characterization of surface roughness through Fokker Planck equations, exchange of a PhD student (*M. Wächter*).
- Prof. Dr. A. Vulpiani, Universität Rom I, Italy: Scale dependent analysis of processes with separated time and length scales.
- Various contacts of the guest scientists with their home institutions.

Group: Quantum Chemistry
(Dr. U. Birkenheuer (since 3/2000))

The new Quantum Chemistry group started its activities in March 2000. On average, it hosts 2-3 scientific members and one Ph.D. student. The main research area of the Quantum Chemistry group are wavefunction-based first-principles calculations on electron correlation in solids and polymers. With this focus we proceed the work of the former Quantum Chemistry group on the correlation contributions to ground state energy and ionization potentials of extended systems.

Our main emphasis is to develop and implement a concept which also allows the determination of electron affinities. Among other things this would ultimately give access to the band gap of periodic systems.

Properly accounting for the anionic character of the electron attachment states the incremental scheme for the cationic electron hole states had to be modified in several ways: To avoid a spilling away of the additional electron, the effect of the surrounding crystal electrons on the local cluster used in the incremental scheme had to be included explicitly. To this end, a special embedding formalism was developed. It is based on the Hartree-Fock data from an interface to the CRYSTAL program which was established by us especially for that purpose, in close collaboration with the research group in Torino. Furthermore, the incremental scheme for electron attachment states requires localized virtual orbitals with one-particle energies as low as possible. Different concepts to generate such orbitals were developed. They either refer to particularly designed cluster orbitals or they take advantage of the ability of the new CRYSTAL program to determine Wannier orbitals. Similar things hold for the external orbitals into which the electrons are excited during a correlation calculation. They also must be local to preserve the local character of the incremental scheme for the embedding. Again, new concepts had to be worked out, because the schemes discussed in the literature turned out to be insufficient.

The implementation of the CRYSTAL-MOLPRO interface described above is completed and extensive tests on the performance of the embedding formalism and the convergence on the incremental scheme for electron attachment states have been performed. In addition, a general purpose pre- and post-processor for the employed correlation program MOLPRO could be established. It automizes to a large extent the execution of incremental calculations, and thereby reduces the effort for input and data analyses to a minimum.

Correlated valence and conduction band structures of diamond and poly-acetylene (calculated on the MRCI(SD)+Q level with a VTZ basis) could be produced by now. Collaborations with Prof. V. Staemmler (Bochum) to perform such calculations with the more size-consistent CEPA method also exist.

In addition to band structures, the Quantum Chemistry group also carries on investigating the correlation energies of periodic systems. Studies on polymers with a conjugated π system (poly-para-phenylene) and research into the performance of non-orthogonal localized orbitals for the incremental determination of the total energy of silicon have to be mentioned here.

Perspectives for the future

The Quantum Chemistry group will keep on dealing mostly with the wavefunctions-based description of correlation effects in extended systems. Having developed the CRYSTAL-MOLPRO interface, for the first time an embedding formalism is at hand which allows to tackle ground state energies, ionization potentials, and electron affinities on the same footing.

A major aim of the Quantum Chemistry group will be to remove the weak points of the current implementation of the incremental scheme, which have shown up in the first applications.

For an incremental calculation typically only a relatively small variational space is used (10-100 molecular orbitals), even though the underlying clusters are already quite big (10-50 heavy atoms). The multi-reference methods implemented in the MOLPRO program package are not able to take advantage of this fact. Hence, we will try to also employ other correlation programs for our incremental calculations which are more flexible in this respect.

By a direct evaluation of the required multi-center integrals in the basis of the localized molecular or crystal orbitals it would be possible to entirely avoid the introduction of a local cluster which contains all the relevant orbitals. In this way, the effort for a correlation calculation could be reduced substantially. Such an integral transformation program has already been developed and tested by the Quantum Chemistry group. The linkage to a suitable correlation program must still be established.

The convergence of the incremental scheme strongly depends on the spatial extent of the localized, hole or electron carrying orbitals. Separating the relevant virtual orbitals for a conduction band calculation from the remaining ones is difficult. Therefore, we believe that the concepts developed so far in the Quantum Chemistry group do not fully exhaust the possibilities of generating highly localized virtual orbitals. Thus, in collaboration with Prof. C. Zicovich-Wilson (Morelos, Mexico), algorithms for an optimal localization of virtual Wannier orbitals should be developed and incorporated into the CRYSTAL program.

Size-consistence of the correlation method plays an important role in the incremental scheme. Many of the commonly used quantum chemical multi-reference methods (e.g. MRCI(SD)+Q), however, are only approximately size-consistent. The equation-of-motion CCSD method for ionization potentials (and electron affinities) developed by R. Bartlett is a promising alternative. To evaluate the usability of this coupled cluster ansatz in the context of an incremental calculation is another aim of the Quantum Chemistry group.

Briefly to be mentioned are also our plans concerning excitons. First investigations to which extent the incremental scheme could also be used to directly describe vertical optical excitations are already going on.

Collaborations

- Prof. Roberto Dovesi, Dipartimento di Chimica IFM, Università degli Studi di Torino, Italy: Cooperation on the development of the CRYSTAL-MOLPRO interface for incremental calculations on embedded clusters.
- Prof. Claudio Zicovich-Wilson, Facultad de Ciencias, Universidad Autonoma del Estado de Morelos, Mexico: Cooperation on the localization of virtual Wannier orbitals with the CRYSTAL program.
- Prof. Hermann Stoll, Institut für Theoretische Chemie, Universität Stuttgart: Cooperation on the use of incremental calculations for solids and polymers.
- Prof. Volker Staemmler, Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum: Incremental calculations for band structures with the multireference CEPA-0 method.

Division: Finite Systems
(Prof. 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 also started to work on few-electron quantum dots and on highly excited cold atoms ("Rydberg matter"). With the latter project, headed by *Dr. Thomas Pattard*, we participate in the recently founded DFG-Priority Program SPP 1116 "Wechselwirkung in ultrakalten Atom- und Molekülgasen".

The energy to excite these systems can come either from charged particles or photon impact. Particularly, the interaction with laser light has been an important element in our research - this is also a common interest between the *Rost* and the *Buchleitner* group, with the first one concentrating on strong laser pulses in the near infrared, the latter one being interested in weak pulses in the microwave regime.

Our techniques range from full quantum approaches and density functional theory (TDLDA) over semiclassical approximations to a full classical treatment of microscopic phenomena.

Specific topics include patterns of partial photo cross sections and decay widths of two-electron doubly-excited states, dynamical symmetries of few-electron quantum dots, special situations under which the high harmonic yield of a laser-irradiated atom is nonlinearly amplified, and quasiclassical formulations of basic scattering processes such as multiple photoionization and electron impact ionization (see p. 88).

Topics which refer to systems with more than a few particles include geometry-induced oscillations in photo cross sections of systems with delocalized electrons, charge transfer in collisions of heavy ions with molecules and clusters, cluster interaction with short and

intense laser pulses (see p. 90), and Saalmann and Christian Siedschlag), destruction of phase coherence of simple bound motion under external noise.

Finally, *Dr. Porto* has been a very active group member working among other things on molecular motors and the evolution of proteins (p. 85). His work, although not in the center of the group activities, has been a crystallization point for several projects at the institute and will fit nicely into the recently founded new department headed by *Prof. Jülicher*.

Perspectives for the future

Our work on the dynamics of few-electron systems will continue. New initiatives are planned in the following directions. The construction of the fourth-generation light source, an X-ray free electron laser at DESY, Hamburg, will realize a new regime in light-matter interaction. Basic atomic physics processes, whose detailed knowledge is the basis for future application in other fields, are still unknown for the high intensities (10^{18}W/cm^2), the large photon frequencies (up to 2 keV) and the short pulse lengths (100-200 fs) which will be possible with the XFEL. This is particularly attractive for clusters as a target: Technically, because the brilliance of the light source will compensate the low flux of clusters allowing for an acceptable event rate. Physically, because in the new regime the light will act completely differently on the cluster by ionizing it from within instead of boiling off electrons from the outside as it has been so far with near-infrared laser light. *Dr. Ulf Saalmann* will coordinate the cluster activities.

Matter exposed to XFEL radiation will be an important issue in the department, not only in clusters but also in atoms and molecules. These activities will be coordinated by a new group leader, *Dr. Andreas Becker*.

We also plan to extend our study of light-matter interactions into the opposite regime: Low-intensity microwave radiation interacting with quantum dots. Since the dots have a typical level spacing of meV and the ponderomotive energy $I/4\omega^2$ is very large for small ω, a non-perturbative regime with non-linear response to the light can be reached, much alike to atoms/molecules exposed to strong lasers in the near infrared.

Finally, we will intensify our research in the field of cold atoms. We are primarily interested in ultracold plasmas which are formed from a gas of Rydberg atoms. These activities, and, more generally, the atomic physics activities, are coordinated by *Dr. Thomas Pattard*. A close exchange with the PKS-distinguished fellow, *Dr. Joachim Brand*, is also planned.

Collaborations

With experimental groups
We collaborate with Uwe Becker's group at the Fritz Haber Institute in Berlin on imaging of delocalized electrons by photoionization with synchrotron radiation. Data on C_{60} photoionization have been taken, evaluated, and published jointly. Future plans include the demonstration of the universality of the proposed imaging with metal

clusters, integrating a group from the University of Freiburg with a good source for metal clusters into the team.

Furthermore, a collaboration with Horst Schmidt-Böcking's group, University of Frankfurt, exists, concerning experimental traces of the transition from regularity to chaos in the photoionization via highly doubly-excited atoms. New detectors have been built and tested in a first beam-time for this experiment, and a good set of data has been collected.

With theoretical groups (some examples)

- on random walks with H. E. Roman (Milano, Italy)
- on photoionization in complex atoms with S. T. Manson (Atlanta, USA)
- on time in quantum mechanics with J. S. Briggs (Freiburg)
- on the book *Komplexe Systeme* with K. Richter (Regensburg)

Local cooperations
The interaction with Prof. Rüdiger Schmidt's group from the TU Dresden has continued - the basis is the weekly 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 *charge transport in disordered and mesoscopic systems* with F. Großmann and R. Gutierrez from the TU Dresden.

Group : Nonlinear Dynamics in Quantum Systems
(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 excitation and ionization dynamics of one-electron Rydberg states at high spectral densities (see "Chaotic ionization of non-classical alkali Rydberg states", A. Krug);
- the spectral characterization of magnetic edge states of plane billiards (see "Spectral cross correlations of magnetic edge states", K. Hornberger);
- the theory of coherent backscattering of polarized light off a gas of cold atoms with spin degrees of freedom (C. Müller);
- the state control of simple quantum systems through entanglement, avoiding measurement noise (see "Quantum state preparation via asymptotic completeness", T. Wellens),

mostly 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 Hitachi SR8000-F1 at the Leibniz-Rechenzentrum of the Bavarian Academy of Sciences.

Before the defence of four PhD theses during the past year, our research group was – with one single exception – composed of diploma and PhD students. Thanks to close contacts with research groups in France, Italy, Israel, and Poland, all PhD students could spend extended research periods abroad, leading to a binational PhD in two cases (C. Müller, Nice/Munich, 2001, and S. Wimberger, Como/Munich, scheduled for 2003). In turn, the visitors program of the institute allowed us to host renowned colleagues (D. Delande, S. Fishman, I. Guarneri, B. Kümmerer, R. N. Mantegna, U. Smilansky, K. Taylor, J. Zakrzewski) for several weeks, initiating fruitful collaborations. Two fresh PhD students (J. Madroñero, F. Mintert) and the first PostDoc of the group (V. Shatokhin) were recruited during a two-months seminar ("Coherent Evolution in Noisy Environments") which we organized, comprising a seven weeks lecture program and a one week international workshop. During the latter, a public evening lecture (A. Zeilinger) was organized (for the first time) at the institute, as well as a week-end seminar involving invited speakers (H. Walther, G. Leuchs, B. Kümmerer) of the workshop, addressing high school and university students (in collaboration with the Evangelische Akademie Tutzing, at Heilsbronn). Both events met overwhelming interest from a broad public audience.

The research activities of the next years are defined by the following principal subjects of our current work:

I the accurate quantum mechanical description of increasingly complex, atomic Coulomb systems, with a particular focus on their spectral characteristics and decay properties;

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

III the transport properties of matter waves in optical potentials with disorder and dissipation.

Whilst striving at the next grand challenge in modern computational atomic physics in (I), with the development of a general theoretical framework for the approximation-free description of the fragmentation dynamics of the periodically driven three body Coulomb problem, we focus on the fundamental resource of any future quantum information technology in (II), and particularly on its robustness under the requirement of scalability. Thanks to a cooperation with the Polish Academy of Sciences (K. Życzkowski, M. Kuś), which is funded by the Volkswagen-Stiftung for three years, we shall realize this project in the framework of an intense bilateral cooperation, underpinned by the essentially continuous exchange of PhD students and PostDocs in both directions. Last but not least, (III) addresses fundamental scenarios of coherent quantum transport (Anderson- or dynamical localization, Mott-Hubbard transition) which – thanks to spectacular advances in experimental quantum optics – are now amenable to experimental tests of unprecedented accuracy.

Division: Biological Physics
(Prof. F. Jülicher)

The division started work in February 2002 and is being built up. Central research areas are active and dynamic phenomena from single molecules to cellular biophysics. Approaches and concepts from statistical physics, many particle physics and non-equilibrium systems are used in order to describe physical properties and principles, which play an important role in molecular and cellular processes. Examples for ongoing and future research activities are:

Molecular motors: Protein motors are the prototype systems for active molecular phenomena in cells of animals and plants. They play a key role for the generation of motion, material transport and cell division. Our group studies the physical nature of force generation on the molecular scale, and in particular discusses situations where a large number of such active molecules act together and new types of behavior emerge as collective effects and self-organization of many elements.

Physics of membranes and the cytoskeleton: Membranes and cytoskeleton represent biomaterials which define the morphologies and the mechanical properties of cells, and which provide a scaffold for many cellular processes. These systems are very dynamic, the cell is constantly reorganizing and rebuilding them. The material properties can change in dramatic ways, forces, motion and spatio-temporal patterns can occur. We develop physical descriptions of such active polymeric materials and their interaction with membrane structures.

Physics of sensation and sensory cells: Sensory cells are highly specialized in order to detect physical stimuli and to transduce them to electrical and nervous signals. We study in particular the underlying principles of mechano-sensitive hair cells, which in the inner ear detect sounds. These cells are capable to operate over a dynamic range of 6 orders of magnitude and to detect extremely weak sound signals. The ear uses active and nonlinear amplification mechanisms. Important hereby is the role of fluctuations which are both limiting and helpful for detection, and the question how such nonlinear active systems can be realized with biological materials on scales of micrometers.

For these research activities, the interaction with experimentalists, biophysicists and cell biologists is important. Our group has stimulating contacts with groups of these disciplines and plans to interact with groups of the Max Planck Institute for molecular cell biology and genetics (MPICBG). The group is affiliated with the International PhD Program "Cell Biology, Biotechnology, Biophysics" which was initiated by the MPICBG.

Since November 2002, two groups have started as part of the division biological physics. Dr. Martin Zapotocky works on the biophysics of olfaction, thus complementing our activities on the physics of sensory cells. Dr. Ralf Everaers works on physical properties of soft and biological matter with a focus on numerical and simulation techniques.

Perspectives for the future

Biological systems are of extraordinary complexity. The advances in molecular and cell biology in recent decades have opened new lines of research where physics can make important contributions. From the point of view of theoretical physics, the aim is to adapt general concepts developed for the description of fluctuating, non-equilibrium

phenomena, nonlinear systems or complex materials to biological situations and to develop new concepts and methods to study such systems. The division biological physics, together with the new groups, covers subjects ranging from the properties of biological materials to the analysis of function and organization of sensory cells. These areas are in a process of rapid development due to new discoveries particularly in cell biology. Cellular processes occur on scales of 10-1000nm and often also stimulate possible realizations of artificial systems on such scales. These developments are only beginning and are accompanied by related activities in the computer sciences and engineering.

The Max Planck Institute for the Physics of Complex Systems provides a special environment for theoretical work in biological physics and has already in recent years shown initiatives in this field. The wide range of research in the area of complex systems allows for stimulating interactions and exchanges with other groups in order to apply techniques used in other areas to biological phenomena. Examples are time-series analysis and the study of nonlinear systems. The vicinity to the Technical University Dresden, to the Biotechnology Center, which is in the process of development, as well as to the Max Planck Institute of Molecular Cell Biology and Genetics (MPICBG), allows for a stimulating exchange with a wide range of research activities of different disciplines which work on related problems. A close collaboration with Prof. Jonathon Howard, MPICBG, Dresden and Prof. Albrecht Ott at the University of Bayreuth are planned. Furthermore, we plan to build a laboratory which will be located in the MPICBG in order to realize experiments, which are closely related to ongoing projects in theory. The guest and workshop program at the institute provides an environment for exchange and collaborations with scientists from many countries. This also allows young researchers of universities and other research institutions to take up new developments at an early stage.

Cooperations

- Max Planck Institute for Molecular Cell Biology und Genetics, Dresden
  - Collaboration with Jonathon Howard on the dynamics of Cilia and Flagella and on the physics of the cytoskeleton and molecular motors
  - Collaboration with Marcos Gonzalez-Gaitan on the formation of morphogen gradients
- Universität Bayreuth
  - Collaboration with Albrecht Ott on the development and structural formation of simple organisms
- Cavendish Laboratory, Cambridge, UK
  - Collaboration with Thomas Duke on the physics of the sense of hearing
- Institut Curie, Paris
  - Collaboration with Jacques Prost on molecular motors and the dynamics of the cytoskeleton

  - Collaboration with Pascal Martin on the physics of mechanosensitive sensory cells.

- Rockefeller University, New York
  - Collaboration with J. A. Hudspeth on the biophysics of mechanosensitive sensory cells

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

Junior Research Group: Pattern Formation in Reaction-Diffusion Systems
(Dr. M. Bär)

The junior research group "Pattern formation" started its activity in November 1995 and reached its present size of around ten members in early 1999. Our research has initially focussed on complex pattern formation and spatiotemporal chaos in chemical and physical reaction-diffusion media. In the course of time, modelling of biological systems became an equally important second topic.

Complex Pattern Formation: Pattern formation occurs in a wide variety of physical, chemical and biological systems. Transitions between simple patterns (fronts, pulses, periodic patterns, spirals) and complex patterns (spatiotemporal chaos, modulated structures, pattern domains and bound states) are investigated by numerical simulations, numerical bifurcation and stability analysis, and perturbation theoretical approaches in reaction-diffusion models. We have carried out a nonlinear analysis of secondary instabilities of periodic waves leading to spatiotemporal chaos and modulated waves, e.g., superspirals discussed in the report by *Brusch et al.* on p. 111. Other aspects include anisotropic pattern formation, impact of heterogeneities and spatiotemporal forcing as well as the control of pattern formation (see report by *Kühne et al.* on p. 115). Applications range from chemical reactions in gels and surface catalysis to hydrodynamical systems (thin films, surface waves, Marangoni convection).

Biophysics and Theoretical Biology: Here, mostly models from physiology (intracellular dynamics, calcium waves) and morphogenesis (bacterial growth, aggregation and pattern formation) have been considered. Emphasis has been put on the transition from continuous deterministic models (differential equations) to discrete stochastic models. A stochastic model has been developed to reproduce abortive calcium waves known as sparks and puffs. A discrete stochastic model of myxobacterial aggregation allows predictions for density patterns and dynamics of individual cells at the same time. Rippling, a standing wave pattern, has been shown to arise from cell migration and interaction alone (see report by Börner *et al.* on p. 118). Various models in immunology have been considered, e.g., for the dynamics of the germinal center and the evolution of antibodies and antigens in shape space. New projects address biochemical networks in cell metabolism and signalling and receptor clustering in membranes.

Where do we stand ? Pattern formation is a relatively young field, it originated from the study of hydrodynamic instabilities and the investigation of dissipative structures in chemical reactions. The growing interest in nonlinear dynamics and chaos in the late 1970s led to an extensive study of patterns in hydrodynamical systems and chemical reactions in particular after 1985. This culminated in the classification of basic pattern forming instabilities by a catalogue of appropriate amplitude equations in the classic 1993 review paper by Cross and Hohenberg. Such universal scenarios apply to transitions from spatially homogeneous to periodic scenarios. Since 1995, we have studied secondary instabilities and described scenarios for the emergence of spatiotemporal chaos as well as the impact of symmetry breaking (anisotropy, heterogeneities, boundaries, forcing, internal noise) in reaction-diffusion systems and amplitude equations.

Where will we go ? A very promising direction is the **modelling of biological processes** both on the intra- and intercellular level. Model systems like calcium waves and the aggregation of slime molds have been explored to a certain extent, but a rapid growth in knowledge about biochemical reactions, signalling and metabolic networks and transport processes from biological experiments will call for quantitative mathematical models. Apart from direct simulations, numerical bifurcation and stability analysis will allow for an efficient analysis of complicated models. The role of internal noise has to be considered in many biological situations and calls for an extension of the methods already developed for continuous deterministic models to **stochastic and discrete models**. Overall, the importance of self-organisation processes in relation to the impact of genetic determinism in biological systems is unclear and offers an exciting field of study. Such considerations will be important in many fields like cell biology, microbiology, immunology and neurobiology. In physical and chemical systems, research will continue on effects far from the primary pattern formation threshold, as experimental equipment and computer power continue to improve and numerical methods become more sophisticated. Prospective goals for modellers include numerical stability analysis in two and three dimensions as well as a **characterisation of irregular patterns**. In many areas we will see a transition from the use of simplified qualitative models to more elaborate quantitative models. Finally, the understanding of **pattern formation on the nanoscale** will require a substantial experimental and theoretical effort.

Collaborations

We maintain numerous national and international collaborations. Among other things, we have been a part of the "DFG-Forschergruppe" on "Nanostructured Functions in Macroscopic Systems" (TU Dresden) and hold a German-Israeli Foundation (GIF) grant on "Pattern Formation in Catalysis" with Profs. Meron (Ben-Gurion) and Pismen (Technion). Collaborations with experimentalists cover chemical pattern formation (Profs. Müller (Magdeburg), Engel (TU Berlin)), growth of nanoclusters (Dr. Mertig, Prof. Pompe (TU Dresden)) and surface catalysis (Prof. Imbihl (Hannover)), as well as myxobacteria (Profs. Reichenbach (GBF Braunschweig) and Sogaard-Andersen (USD Odense)) and biotransformations (Dr. Bertau (TU Dresden)). Theoretical collaborations exist with groups in Firenze and Torino (Drs. Torcini and Provenzale, Prof. Ruffo) as well as Princeton (Prof. Kevrekidis).

Some "Careers"

Dr. Thomas Boeck (Guest Scientist, 2000 - 2002) was awarded an Emmy Noether Fellowship and currently works in Paris. *Dr. Andreas Deutsch* (Guest Scientist, 1999 - 2001) moved to the Hochleistungsrechenzentrum (High Performance Computer Center) of the Technical University of Dresden, where he is employed as a permanent staff scientist and directs a group on bioinformatics. *Dr. Martin Falcke* (Guest Scientist, 1997 - 1998, 2000 - 2001) is a staff scientist in the Theory Department of the Hahn Meitner Institute in Berlin, where he leads a group working on calcium dynamics. *Dr. Haye Hinrichsen* (Guest Scientist,1997 - 1999) holds a temporary professorship for Theoretical Physics at the Wuppertal University. *Dr. Thomas Höfer* (Guest Scientist, 1996 - 1997) was a research assistant at the Humboldt University in Berlin (1997 - 2001) and has recently been appointed as "Junior Professor" at the Humboldt University. *Dr. Michal Or-Guil* (Staff Scientist, 1997 - 2002) won a grant for a Volkswagen Foundation junior research group in "Theoretical Immunology" in 2001, and works as a group leader in the Institute for Theoretical Biology at the Humboldt University in Berlin.

Junior Research Group: Waves in Complex Media and Mesoscopic Phenomena
(Dr. H. Schomerus)

The junior research group exists since November 2000. Besides the head of the group and a staff member (M. Titov), there are currently five postdocs and a PhD student conducting theoretical fundamental research on problems and phenomena of electrons and light in small structures, in which phase coherence plays a decisive role. Close cooperation exists with more than a dozen of researchers at the mpi**pks** and at other facilities. Three main lines of research can be singled out:

- Mesoscopic effects in quantum dots and quantum wires, also including hybrid structures with superconducting components. The research addresses, e.g., the conductance and impedance, the shot noise, and the local and global density of states. The destruction of phase coherence by external influences and internal interactions is considered, also concerning quantum IT. Another emerging subject is molecular and nano electronics. *H. Schomerus, M. Titov, A. Nemes-Salgueiro; with H. S. Sim, S. W. Kim, I. Rotter, R. Nazmitdinov* (all mpi**pks**), groups of C. W. J. Beenakker (Leiden), M. Büttiker (Genf), P. Brouwer (Cornell), Y. Blanter (Delft), K. Richter (Regensburg), J. Dalibard (Paris).

- Electromagnetic wave interference in irregularly shaped dielectrics and disordered wave guides; intense laser-atom interaction. Additional features arise by amplification in active media and absorption in passive media, also including quantum-optical effects, like in lasers with feedback by multiple scattering at disorder or dielectric interfaces. H. Schomerus, J. Wiersig, M. Hentschel; C. W. J. Beenakker (Leiden), K. Richter (Regensburg), F. Laeri (Darmstadt), J. Noeckel (Oregon), W. Becker (MBI Berlin), C. Faria (mpi**pks**/MBI Berlin).

- Quantum dynamics for classically nonintegrable systems. Besides conventional quantum chaos we turn the attention to the much more complex realm of not

completely chaotic systems (with a mixed phase space), as well as to quasi-integrable systems. This requires also a deeper understanding of the classical dynamics. *H. Schomerus, J. Wiersig, G. Carlo, M. Sczyrba; H. S. Sim* (mpi**pks**), F. Haake (Essen), M. Saraceno (Buenos Aires), J. Keating, M. Berry, M. Sieber (all Bristol), R. Schubert (Paris), A. Bäcker (Ulm).

In all of these areas of expertise the focus is on the identification of universal phenomena. This is accomplished by the means of flexible and exact mathematical approaches which give quantitative results and allow to tag the key mechanisms. Approaches encompass random matrix theory, field-theoretical methods, Fokker-Planck equations, and semiclassical or quasiclassical methods. In many cases results are directly compared to numerical computations or to experiments.

Perspectives for the future

Long-term perspective:

Emerging fields of interest intended to be intensified are the intersection of mesoscopic physics and quantum optics, molecular and nano-electronics, and also mesoscopic aspects in quantum IT. General knowledge in those subject areas is still at the early stages and fundamental research has much to contribute here. The methods and concepts of the previous research and the expertise in the group and in its environment define a suitable starting point to venture into these fields.

The research in mesoscopic physics, wave propagation in random media, and quantum dynamics of nonlinear systems will be continued, initially along the lines indicated in the short-term perspectives.

The current knowledge on passive dielectric resonators is quite exhaustive, although two running projects still promise a considerable deepening of the understanding. The arena of active media in such resonators is wide open, especially when it comes to quantum-optical processes, and will be considered if suitable expertise can be imported into the group.

Short-term perspective:

Several current and emerging projects address the identification of phenomena, and the exploration of phenomena and approaches which have been recently developed in the group. Phenomena include dynamical and static signatures of wave localization, systematic but nonuniversal shot noise suppression in generic quantum devices, and a quantum interference effect at scatterers with internal degrees of freedom. Recently developed approaches allow to solve some problems which have not been accessible (or even considered) before. Specifically, this concerns a scattering approach to the local density of states in a wide range of mesoscopic systems, an inside-outside duality at dielectric interfaces, a uniform semiclassical approximation for intense atom-field interaction, a method to analyze the dynamics of transport in quantum dots from the shot noise, and a family of open quantum maps which are completely identical to quantum dots (including their energy dependence). The goal is to explore and establish these phenomena and tools in a broad range of contexts.

Personnel and resources:

The junior research group is designed for a duration of five years, but the general direction of research is very likely to be continued at this institution, since it is also represented in other groups, the visitors program, and the seminars and workshops. The time scale for fluctuations in the constitution of the group is one to two years, where continuity is generated by the head and the staff member. The fluctuations can be used to import additional ideas and expertise and to generate further links by retaining the contacts to former members. The current size of the group and interactions with other groups are intended to be maintained.

Cooperations at the mpipks

H. S. Sim, S. W. Kim, I. Rotter, R. Nazmitdinov

Common interests at the institute also with G. Cuniberti, Gutzwiller-fellow *A. Ozorio de Almeida*, and in general with the *Rost, Fulde, and Buchleitner* group.

External Cooperations

- C .W. J. Beenakker, P. Jacquod (University of Leiden)
- J. Noeckel (Oregon)
- M. Buettiker, P. Samuelsson, S. Pilgram (University of Geneva)
- P. Brouwer (Cornell)
- Y. Blanter (Delft)
- F. Haake (Essen)
- M. Saraceno (Buenos Aires)
- J. Keating, M. Berry, M. Sieber (all Bristol)
- R. Schubert (Paris/formerly mpi**pks**)
- A. Bäcker (Ulm/TU Dresden)
- F. Laeri (Darmstadt)
- W.Becker (MBI Berlin), C. Faria (MBI Berlin/formerly mpi**pks**)
- J.Dalibard (Paris)

Junior Research Group: Quantum Chaos and Mesoscopic Systems
(Dr. K. Richter (until 4/2001))

Mesoscopic physics refers to systems in between the micro and the macro world; typically small objects of reduced spatial dimensionality. Their complexity arises from the fact that they exhibit both quantum coherence effects on micronscales and classically chaotic dynamics. Modern semiclassical methods and quantum chaos provide the appropriate framework to study the relation between quantum and classical physics in the mesoscopic regime. Besides we used (numerical) quantum mechanical methods. Systems under consideration are quantum dots, semiconductor-superlattices, semiconductor-superconductor hybrids, molecular conductors, photonic cavities, and nanomechanical devices.

After Klaus Richter received a full professorship in Theoretical Physics at the University of Regensburg in April 2001 the last members left the group at mpi**pks** at the end of 2001.

Research in our group comprised three main directions:

- Spectral statistics of complex quantum systems, in particular the open link between semiclassical approaches and random matrix theory for spectral correlation functions. In an important step we could deduce random matrix predictions directly from the classical chaotic dynamics (see report by *Sieber and Richter*, p. 122).

- We studied mesoscopic quantum transport with particular emphasis on the role of electron spin (spintronics). In two PhD works spin effects due to Berry phases were computed and a spin switch effect for spin-polarized electrons was found. (see report by *Hentschel, Frustaglia and Richter*, p. 131).

- Molecular electronics represents a new research focus of the group. We studied quantum effects in charge transport through molecular wires and carbon nanotubes. In collaboration with the group of Prof. R. Schmidt at TU Dresden we proposed a junction formed by a C_{60} molecule in between nanotubes, as an all-carbon molecular switch (see report by *Cuniberti et al.*, p. 126).

II. Details and Data

1 Selection of Research Results

1.1 Optical Manifestations of disorder-induced Wavefunction Localization in Semiconductor Nanostructures

Erich Runge, Vincenzo Savona, and Roland Zimmermann

Semiconductor nanostructures have the potential to serve as test ground for many quantum mechanical aspects of chaos, order and disorder. They combine two desirable features: On the one hand, modern technology permits fabrication of structures with a tailored design, and, on the other hand, those structures can easily be studied with optical techniques in a convenient frequency and time regime with extraordinary spectral ($\approx 25\,\mu$eV), temporal (≈ 1 ps), and often spatial (≈ 150 nm) resolution. Furthermore, large ensembles are easily available providing enough data for a statistical analysis. Many effects familiar from textbook quantum mechanics can thus conveniently be studied in semiconductor nanostructures. The realization of the Sinai billiard as electrostatically defined quantum dots can serve as a well-known illustrative example.

Compared to, e.g., experiments measuring the weak localization correction to the resistance of disordered metallic wires at low temperatures, optical laser experiments have the additional advantage that it is rather easy to generate coherent excitations and to detect the excitonic quantum coherence via the optical coherence of the emitted light. This allows experiments which have no equivalent in other disordered quantum systems. Another important difference is that the properties of only a subset of wavefunctions, those which are optically active, are tested.

Optical properties of semiconductor structures are at low temperatures dominated by excitons. These are electron-hole bound states. Their wavefunction can directly be interpreted as optical polarization. In an ideal quasi-2D semiconductor film, a so-called quantum well (QW), the quantum mechanical exciton states are products of a plane-wave factor describing the center-of-mass (COM) motion and a part involving the relative motion and the atomic Bloch parts.[1] For the COM motion, a Schrödinger equation

$$\Big(-\frac{\hbar^2}{2M_X}\nabla^2 + v_{\text{eff}}(\vec{R})\Big)\,\psi_\alpha(\vec{R}) \;=\; \varepsilon_\alpha\,\psi_\alpha(\vec{R}) \tag{1}$$

can be derived. The exciton mass is denoted M_X, and v_{eff} is an effective disorder potential which is correlated over distances of the order of the exciton radius (≈ 10 nm) and characterized by its strength $\sigma = \langle v_{\text{eff}}^2\rangle^{1/2}$ ($\approx$1-10 meV). It depends, of course, on the materials involved and the interface quality and other parameters of the heterostructure under consideration. The theory can be developed analogously for quasi-1D structures (quantum wires). The COM wavefunctions enter the optical spectra via the optical matrix element

$$M_\alpha = \int d\vec{R}\, e^{-i\vec{k}\cdot\vec{R}}\,\psi_\alpha(\vec{R})\ ,\ k\approx 0\ , \tag{2}$$

describing the overlap of the exciton with the light wave of in-plane momentum $\vec{k}$. Results for the radiative rates (inverse life time) $r_\alpha \sim |M_\alpha|^2$ are summarized in Fig. 1.

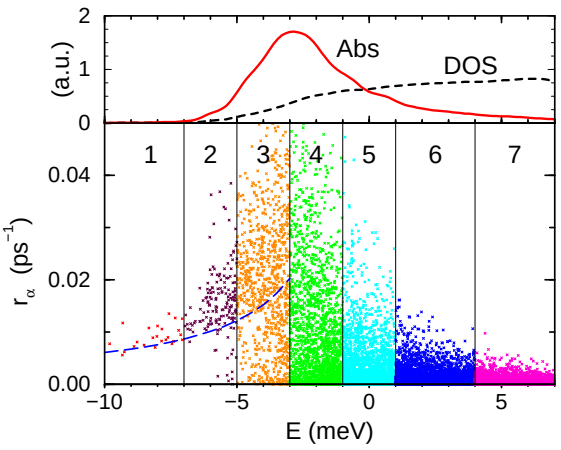

Fig. 1: Distribution of radiative rates, lower panel, with resulting absorption (Abs) and excitonic density of states (DOS), upper panel. Simulation for a 5-nm-wide GaAs/AlGaAs QW with $\sigma = 8$meV, $r_\alpha = 1.7 \cdot 10^{-5}\mathrm{ps}^{-1}\mathrm{nm}^{-2}\,|\mathrm{M}_\alpha|^2$. Numbers mark energy intervals analyzed in Fig. 2. The dashed line is the optimum fluctuation result (Lifshitz-Halperin-Lax-Zittarz-Langer theory) in the white-noise limit.

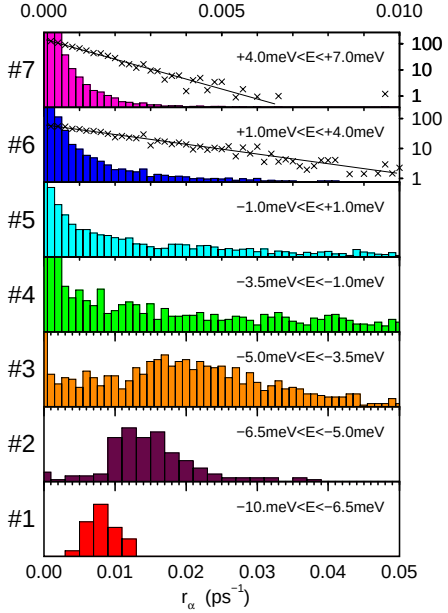

Fig. 2: Histogram for radiative decay rates of Fig. 2 for different energy intervals. Note the different scaling of the x-axis in panels 1-3 and 4-7. Symbols in panels 6,7 show $\sqrt{r_\alpha}\mathcal{P}(r_\alpha)$ on a logarithmic scale (rhs coordinate). For a Porter-Thomas distribution, they should lie on a straight line (solid).

These determine, e.g., the inhomogeneously broadenend absorption profile

$$I_{\mathrm{ABS}}(\hbar\omega) \sim \sum_\alpha r_\alpha \delta(\hbar\omega - \varepsilon_\alpha)\ . \tag{3}$$

Eqs. (1,2) supplemented by a microscopic expression for the electron-phonon interaction [2] can be used for quantitative predictions for new experiments and analysis of current ones. The Schrödinger equation is then solved numerically for many realizations of the v_{eff} and ensemble averages are obtained. Theoretical results include: (i) A strongly asymmetric line shape of the optical density (absorption) with a tail towards higher energies is found, see upper panel of Fig. 1. (ii) A non-monotonic Stokes shift of the temperature-dependent luminescence peak position was predicted by us a while ago and confirmed experimentally. (iii) A dramatic cut-off of the low-energy part in photoluminescence excitation spectroscopy and, thus, an apparent blue-shift relative to absorption, can be interpreted as manifestation of an effective mobility edge for exciton relaxation — which in turn can be related to properties of the disorder wavefunctions.

While these results are of some practical importance, from a more fundamental point of view it is more important that optical experiments – if carefully analyzed – exhibit remarkable manifestations of quantum mechanical phenomena associated with disorder-induced localization. Several examples are discussed in the following.

Enhanced back-scattering from localized states

An astonishing feature observed for wave propagation in many systems, both classical and quantum mechanical, is an enhanced (coherent) back-scattering (EBS) into a narrow angular region around the incoming beam [3]. Well known examples include light scattering in suspensions of micro spheres in water, radar reflection in clouds, and acoustic waves in crystals. For these systems, considerable effort has been made to produce samples of dense, strong scattering centers in order to localize, e.g., the light as much as possible. Closely related to EBS is a negative magneto resistance in disordered metallic wires at low temperature (weak localization). Here the disorder can be increased and localization lengths less than the sample size can be achieved. Unfortunately, this implies that the wavefunction looses the contact to the leads.

We studied whether EBS is to be expected for the excitonic Rayleigh signals from quantum wells and quantum wires [4]. Enhanced back-scattering was found in our calculations indeed, however strongly modified compared to the other EBS systems. A fundamental difference is that QW excitons are localized. Another one, the different role of the electromagnetic light field, was mentioned already in the introduction. The scattering geometry and the dependence of the intensity on time and direction (parametrized by the in-plane momentum) are illustrated in Fig. 3.

Different temporal regimes can be identified in Fig. 3(c): Instantaneously after the energetically broad excitation at $t = 0$, the reflected beam in direction $\vec{k}_{\rm in}$ is present and lasts for a time span given by the inverse inhomogeneous line width. In all other directions, intensity grows $\sim t^2$. The EBS features around $-\vec{k}_{\rm in}$ starts broad in reciprocal space and narrows to a finite width. This corresponds to the exciton wave packet spreading in real space until it reaches its localization size. Thus, time-dependent Rayleigh scattering allows the observation of wavepacket localization. At even later times, an enhanced forward scattering (EFS) is seen. Its angular profile is identical to that of the EBS peak, and it has, to the best of our knowledge, no correspondence in the usual EBS systems.

Level Repulsion in spatially resolved spectra

Any reasonable analysis of spatially resolved spectra must be of statistical nature. Based on experiences in other fields of quantum physics, it seemed natural to look for energy-level correlations, i.e. correlations of the energetic positions of the individual peaks in the spectra. Recent experiments showed clear signs of level repulsion in quantitative agreement with our predictions [6]. The amount of level repulsion at a given spatial resolution permits derivation of a characteristic size of the wavefunctions. This constitutes a rather direct approach to a quantity related to the widely discussed localization length.

Wave function statistics and radiative life times

The $\vec{k} = 0$ component of the COM wavefunction in Fourier space is directly observable: It determines according to Eq. (3) the radiative lifetime and weight of the individual narrow peaks in spatially resolved spectra. Our simulations and theoretical arguments clearly show a transition within the inhomogeneous exciton line from Lifshitz tails with well-localized wavefunctions describable by Lifshitz-Halperin-Lax-Zittarz-Langer optimum fluctuation theory to Anderson-localized states at the high-energy side, which

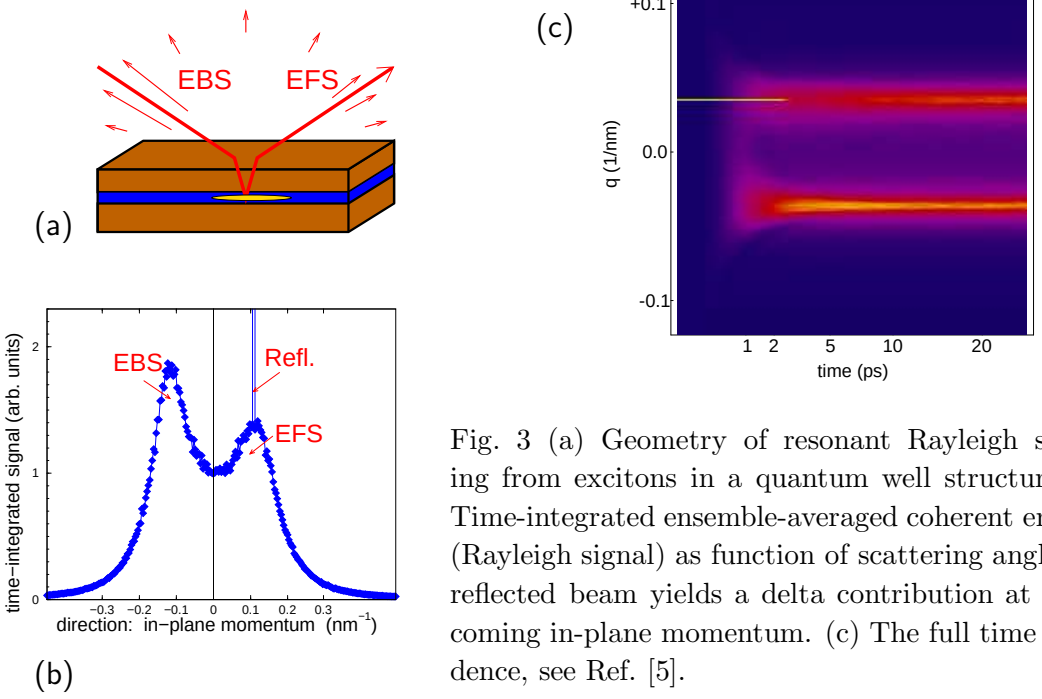

Fig. 3 (a) Geometry of resonant Rayleigh scattering from excitons in a quantum well structure. (b) Time-integrated ensemble-averaged coherent emission (Rayleigh signal) as function of scattering angle. The reflected beam yields a delta contribution at the incoming in-plane momentum. (c) The full time dependence, see Ref. [5].

show a Porter-Thomas distribution in agreement with Berry's conjecture. The distributions of wavefunction values or, equivalently, radiative life times, as shown in Fig. 2 can, in principle, be obtained experimentally. One can also expect to see in the near future studies of energy-levels and their correlation as function of external parameters and in response to local perturbations by, e.g., presence of a free carrier or another exciton (spatially resolved non-linear optics). "Level-correlation spectroscopy" will allow new experiments finding interesting physics which otherwise is hidden in what seems to be "random data"[6, 7].

The theoretical results presented here were obtained in close collaboration with various experimental groups. We would like to thank particularly Wolfgang Langbein and Christoph Lienau and their coworkers.

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1.2 UPt_3: dual character of $5f$ electrons

P. Fulde, G. Zwicknagl and A. Yaresko

The compound UPt_3 is one of the most studied heavy-fermion systems [1, 2]. The γ coefficient of the low-temperature specific heat C=γT is γ=420 mJ (mole·K^2)$^{-1}$ and the Pauli susceptibility is similarly enhanced as compared with the one of ordinary metals like sodium. Heavy quasiparticles have been observed in de Haas-van Alphen (dH-vA) experiments [3, 4] but the observed masses are by a factor of 20 larger than the calculated band masses based on the local-density approximation (LDA) to density functional theory [5]. The dH-vA frequencies are rather well reproduced within that approximation. This failure of LDA in predicting the observed masses indicates that the correlations are strong and raises the question for their adequate description.

We have recently suggested that in UPt_3 one is dealing with localized as well as delocalized $5f$ electrons [6]. This proposal was motivated by accurate quantum chemical calculations on $U(C_8H_8)_2$. Thereby both types of $5f$ electrons were found to exist, giving rise to low-lying excitations. They correspond to intraatomic rearrangements of the localized $5f$ electrons. The mass enhancement of the quasiparticles results then from virtual excitations of the internal degrees of freedom of the localized $5f$ electrons by the delocalized ones, which are part of the conduction electron system. Note the similarity of this source of the mass enhancement of conduction electrons to the one in Pr metal [7].

We consider two $5f$ electrons as being localized and put them into $j_z = \pm\frac{1}{2}$ and $\pm\frac{5}{2}$ orbitals. This is consistent with the ground state of UPd_2Al_3, a different but closely related U compound. Electrons with $j_z = \pm\frac{3}{2}$ are treated as being delocalized. Performing a LDA band-structure calculation, thereby keeping the localized $5f$ electrons as fixed yields the measured dH-vA frequencies for the heavy quasiparticles, a satisfying feature of the proposed theory (see Fig 1). This agreement is not obtained when $5f$ electrons with $j_z = \pm\frac{5}{2}$ or $\pm\frac{1}{2}$ are delocalized instead. We want to point out that this result is obtained without any adjustments of the bands. The band mass is found to be twice as large as in the conventional LDA calculation where all $5f$ electrons are treated as itinerant. Thus a discrepancy to the observed quasiparticle mass by a factor of 10 remains to be explained. The Fermi surface is formed by two bands which are doubly degenerate and have partially $5f$ $(j, j_z) = (\frac{5}{2}, \pm\frac{3}{2})$ character. One band gives rise to open orbits for a magnetic field along the c-axis in agreement with magnetoresistance measurements. The other one gives rise to a cylindrical surface with six arms in the $a-b$ plane. Inside that surface is a Γ-centered hole surface in form of an ellipsoid. In addition, there are ellipsoids centered at H points.

The missing factor of 10 in the quasiparticle mass is explained by the all important excitation of internal degrees of freedom of the localized $5f$ electrons by the delocalized ones. It is given by

$$m^*/m = 1 + 4a^2 N(0)\ 2|\ M\ |^2/\delta \quad . \tag{1}$$

Here a denotes the weight of the delocalized $5f$ orbital in the conduction-electron states near the Fermi energy, and N(0) is the density of states per spin direction of the latter.

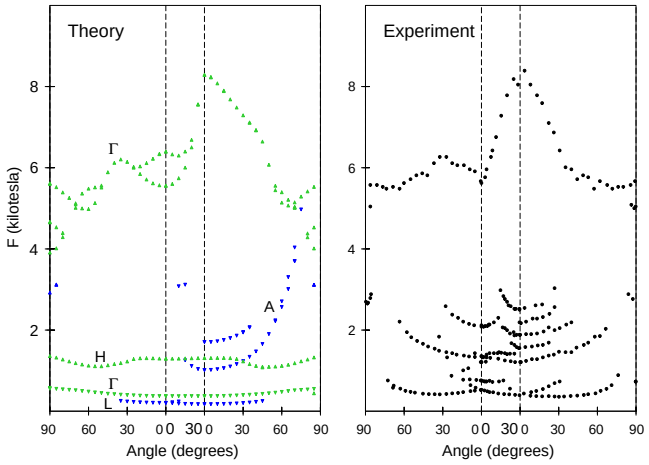

Figure 1: *DeHaas-vanAlphen cross sections as calculated within the present theory and from experiment. Green and blue triangles correspond to the first and second band, respectively. The labelling indicates the origin of the orbit. Branches without labels are derived from those extremal areas of the lower band which are not centered on symmetry points. The upper green branch describes the heavy quasiparticles.*

The transition-matrix element between the ground state of the localized $5f$ electrons and the low-energy excited state is denoted by M and δ is that excitation energy. In order to determine the multiplet structure of the localized f^2 states we diagonalize a 6 x 6 Coulomb matrix based on the six two-particle states which can be built from $|j = \frac{5}{2}; j_z = \pm\frac{5}{2}\rangle$ and $|j = \frac{5}{2}; J_z = \pm\frac{1}{2}\rangle$ states. The matrix elements are determined according to Condon-Shortley. It is found that the ground state is doubly degenerate with total angular momentum $J = 4$ and $J_z = \pm 3$. The degeneracy is lifted by the crystal field giving rise to two singlets

$$| \Gamma_{3,4}\rangle = \frac{1}{\sqrt{2}}(| J = 4; J_z = 3\rangle \pm | J = 4; J_z = -3\rangle) \quad . \tag{2}$$

We assume that the center of gravity of the broadened energy splitting is of order δ=20 meV. This is the same order of magnitude as the splitting which has been assumed for UPd_2Al_3 [8] or UBe_{13}. More recently, for UPd_2Al_3 a smaller splitting of 7 meV has been proposed based on a fit of the susceptibility and other physical properties [9]. For URu_2Si_2 a splitting of the lowest CEF states of 6.5 meV was suggested. Note that in all these cases no crystalline field splitting has been directly observed by inelastic neutron scattering. Instead, the above values were derived indirectly. In the present theory the next-higher states are 0.2 eV above the two singlets and can be neglected. This way we find for the transition matrix element

$$M = \langle f'; \frac{5}{2}, \frac{3}{2} \mid \otimes\langle \Gamma_4 \mid U_{\rm coul} \mid \Gamma_3\rangle\otimes \mid f'; \frac{5}{2}, \frac{3}{2}\rangle = 0.19\text{eV} \quad . \tag{3}$$

For more details we refer to [6]. With N(0) $\simeq$ 15.5 states/(eV cell), $|M|^2 = 36 \cdot 10^{-3}$ eV^2, 4a^2=0.13 and δ=20 meV we find that m*/m$_b$=8.3 which is close to the missing enhancement factor. Note that all parameters appearing in (1) have been *calculated* except δ which we have estimated as explained above. When a smaller value is chosen instead the quasiparticle mass increases according to (1). We believe that the above theory supplies a satisfactory explanation of the physical origin of the heavy quasiparticle mass in UPt_3. But it is seemingly much more general. In the meantime also the quasiparticle masses of UPd_2Al_3 have been explained by the same approach.

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1.3 Fractional charges and heavy fermions in pyrochlore lattices

P. Fulde, K. Penc, N. Shannon, A. Yaresko and A. Zvyagin

The experimental observation of heavy-fermion behaviour of LiV_2O_4 [1] has drawn attention to pyrochlore lattice systems with half–integer valency of the involved ions. For example, the average valency of V in LiV_2O_4 is +3.5, and the same is true for Ti in $LiTi_2O_4$. Therefore, the average 3d electron number is $d^{1.5}$ in the first case, and $d^{0.5}$ in the second one. From LDA band–structure calculations [2, 3] it is known that the conduction bands have 3d-t_{2g} character, and are well separated from higher energy valence electron states. However, the LDA effective electron mass found for LiV_2O_4 is by a factor of twenty–five smaller than the quasiparticle mass inferred from specific heat and spin susceptibility data. This is a sign of strong electronic correlations. On–site Hubbard U interactions alone are not sufficient to explain the large measured quasiparticle mass. They merely reduce the atomic configurations of the V ions to $3d^1$ and $3d^2$, i.e., they exclude $3d^0$, $3d^3$ configurations, etc. In order to obtain a sufficiently high density of low–energy excitations one must therefore include correlations between neighbouring sites. The nearest–neighbour interactions are minimised if for each of the corner-sharing tetrahedra which make up the pyrochlore lattice, there are two $3d^1$ and two $3d^2$ configurations. This so–called "tetrahedron rule", which is implicit in Verwey's

treatment of the metal–insulator transition in the spinel Fe_3O_4 [4], was first stated explicitly by Anderson [1]. The number of configurations which obey the tetrahedron rule grows exponentially with the number of tetrahedra, so in the absence of any perturbation (such as the electrons' kinetic energy) which selects between these states, the ground state of pyrochlore systems with nearest–neighbour interactions and half–integer valency is extremely degenerate. An important property of these degenerate ground–state configurations is that each of them consists of chains of $3d^1$ and $3d^2$ sites in the case of LiV_2O_4 [6], and of empty $3d^0$ and $3d^1$ sites in the case of $LiTi_2O_4$. Spin excitations in those chains can give rise to a linear low temperature specific heat $C(T)=\gamma T$ with a large γ coefficient and to a large spin susceptibility as experimentally observed [6]. Because of the special features of one–dimensional systems, these spin excitations can be described by either bosons or fermions.

Fractional charges appear when the effects of a small kinetic energy term on a pyrochlore lattice obeying the tetrahedron rule are considered. For simplicity consider the case of an average $d^{0.5}$ count per site. Furthermore, for a better visualization consider a checkerboard lattice instead of the original three-dimensional pyrochlore lattice. All results which we discuss for the checkerboard lattice also apply to the pyrochlore lattice.

In order to first discuss excitations associated with charge degrees of freedom, we begin by considering the reduced Hamiltonian

$$\mathcal{H}_0 = -t \sum_{\langle ij \rangle} \left\{ f^\dagger(i) f(j) + h.c. \right\} + V \sum_{\langle ij \rangle} n^f(i) n^f(j) \tag{1}$$

where $n^f(i) = f^\dagger(i) f(i)$ and $\langle ij \rangle$ denotes nearest neighbor sites with an interaction V. This refers to a system with an average d-electron count of 0.5 and one orbital per site. Because of the assumed large value of U, only empty (d^0) and singly occupied (d^1) sites are considered. Spinless fermions are assumed, which corresponds to a full spin polarisation of the electrons. Charge conservation requires the subsidiary condition

$$\sum_i n^f(i) = N/2 \tag{2}$$

for a system with N lattice sites, while in the limit $V \to \infty$ the tetrahedron rule requires that

$$\sum_{\nu=1}^{4} \left(n^f(i_\nu) - \frac{1}{2} \right) = 0 \tag{3}$$

where ν denotes the four different sites within *any* given tetrahedron i.

When a charge $-e$ is added to an empty site j we are left with two corner–sharing squares with three d^1 sites each. This is illustrated in Fig. 1b. The corresponding state is $\mid j\rangle = f^\dagger(j) \mid \Phi_I\rangle$ where $\mid \Phi_I\rangle$ denotes the chosen ground-state configuration. The kinetic energy term now permits the five electrons within these two squares to move. However, the motion has to occur in such a way that the number of squares with three d^1 sites is conserved.

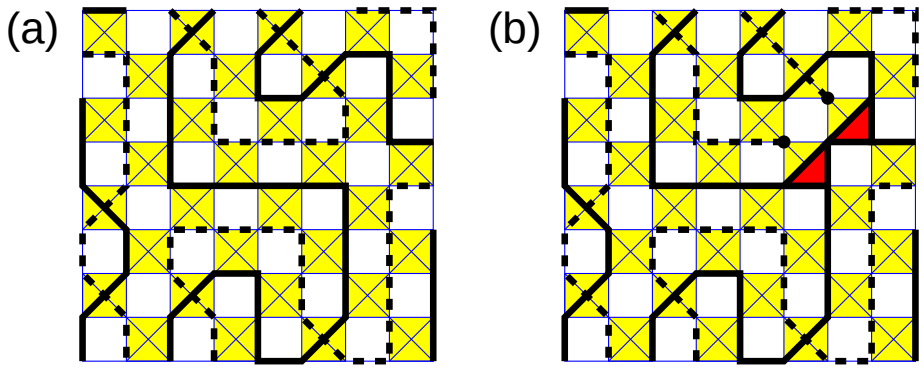

Figure 1: *Checkerboard lattice, the thin lines indicate hopping and interactions connecting sites. Thick lines connect sites in a d^1 configuration while dotted lines connect empty (d^0) sites. (a) example of a fraction of the lattice in which the tetrahedron rule is obeyed. (b) the sample as (a) but with an electron added ($d^0 \rightarrow d^1$). Dots indicate the end of the chain.*

If the added electron moves along the chain of empty sites in which it was inserted, it retains its integrity and the state $\mid j\rangle$ transforms successively into states $\mid n\rangle = f^\dagger(n)f(j) \mid j\rangle$. However, if we instead allow one of the four neighbouring electrons belonging to chains of occupied sites to move, the electron immediately breaks up into two disjoint pieces. These carry fractional electric charge $-e/2$ (note that every electron is shared by two squares and so contributes a charge $-e/2$ to each of them). These two cases are indicated in Figs. 2a,b.

Energy and momentum (as well as topological charge) must be conserved by these decay processes. Therefore if we were to associate a momentum $\mathbf{k}$ and energy $E(\mathbf{k})$ with the electron which we inserted, this must now be shared between the fractionally charged particles into which it has decayed

$$E(\mathbf{k}) = 4V + \epsilon(\mathbf{k}_1) + \epsilon(\mathbf{k}_2) \tag{4}$$

where $\epsilon(\mathbf{k})$ is the dispersion of the fractional charge and $\mathbf{k}_1 + \mathbf{k}_2 = \mathbf{k}$. Clearly, a metal which has a charge excitation spectrum with low energy contributions of the form of Eq. (4) *cannot* be a conventional Fermi liquid.

When an electron is added to an empty site, a spin 1/2 is added to the system. In order to gain some insight into how this spin is distributed when the electron decays into two fractional charges, one must introduce spin degrees of freedom in Eq. (2) and also add a spin-spin interaction term between neighbouring sites as soon as the electron decays into two fractional charges, its spin is no longer localised at one point. In most cases, the insertion of an electron will connect two different spin chains. The decay of the electron converts a single spin 1/2 site into a spin chain with an odd number of spin 1/2 sites coupled symmetrically to two Heisenberg chains with an even number of sites. Since the total number of sites involved is odd, the ground state remains a Kramers doublet, as required. But it is no longer possible to uniquely assign this spin 1/2 degree of freedom to a single site.

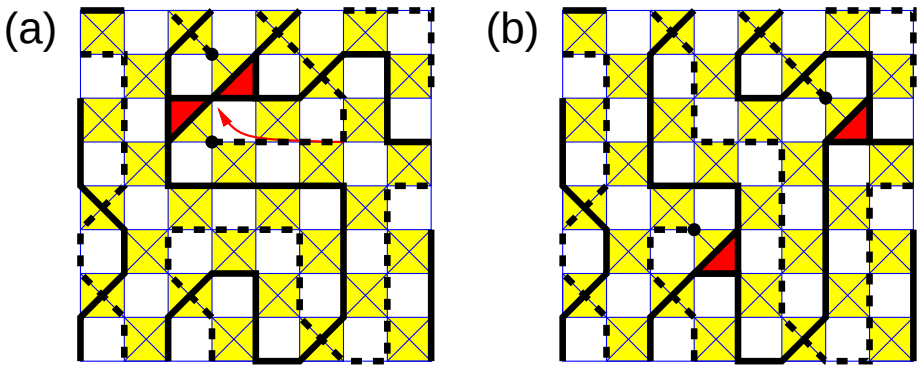

Figure 2: *(a) The added electron has moved in four steps along a chain of empty sites. It remains an entity. (b) An electron from lower triangle in Fig. 1b has moved along the diagonal. As a consequence the excitation has decayed into two with a fractional charge of* $-e/2$ *each.*

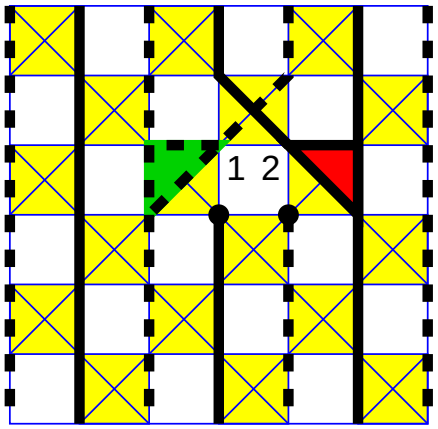

Figure 3: *Vacuum fluctuation due to an electron hopping from 1 to 2. Two charges* $\pm e$ *are generated which can propagate freely. Note that the Heisenberg chains involve even numbers of sites.*

In the arguments presented so far we have considered the limit $t/V \to 0$ for which repulsive interaction between electrons on neighbouring sites can be replaced with a simple "tetrahedron rule". If we relax this constraint to the extent of considering finite (but very large) V, quantum fluctuations about the many degenerate states obeying the tetrahedron rule can themselves single out a ground state. We start from one of the degenerate ground states $\mid \Phi_I \rangle$ which obey the tetrahedron rule, and consider to lowest order the effect of the kinetic energy. At $\mathcal{O}(t/V)$ this mixes into the wavefunction virtual states in which two squares (tetrahedra) violate the tetrahedron rule at the net cost of an interaction energy of V. However overall charge must be conserved, so in this case one square contains three d^1 sites, while the other has three d^0 sites. This is illustrated for the checkerboard lattice in Fig. 3. If this virtual excitation lives long enough for the contributing electrons to hop to neighbouring sites it, just like an added electron, will decay into two fractional charges. In this case the two pieces of the excitation must carry the opposite sign of electrical charge.

Importantly, the $+e/2$ "tail" of the vacuum fluctuation (the tetrahedron with only

one d^1 site), can annihilate with one of the fractional charges $-e/2$ produced by the fragmentation of an added electron. This makes it possible to locally reassemble the added electron anywhere in the lattice. Furthermore, fluctuations can recombine in such a way that they create the objects associated with an extra electron and one hole (the latter being an open chain of spins). Therefore we expect a balance between fractional charges $\pm e/2$ and full charges $\pm e$ when electrons (holes) are added to the system, or even in the metallic state.

Fractionally charged excitations were first proposed in the context of heavily doped trans–polyacetylene by Su and Schrieffer [7], where they are linked to a commensurate superstructure of the polymer chain. They have also famously been invoked in a ground–breaking paper by Laughlin [8], in connection with the fractional quantum Hall effect. However, polyacetylene is a one–dimensional system, and the quantum Hall effect is a phenomenon occurring in two dimensions and high magnetic field. To the best of our knowledge the present case provides the first example of a microscopic model supporting fractional charge in three dimensions [9].

The above considerations apply primarily to pyrochlore insulators, when doped with electrons or holes. An example of such a system is magnetite (Fe_3O_4), an insulating spinel oxide, whose B sites form a pyrochlore lattice of Fe^{2+} and Fe^{2+} ions.

Obviously, many unsolved problems remain. For example, the calculation of thermodynamic and transport properties of the model, or the effect of an applied magnetic field, have yet to be attempted. It would also be worthwhile to search for other lattice geometries in which fractional charges could occur. The present communication can only point to these problems and does not pretend to provide an answer. It should, however, be considered as a first step in that direction.

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1.4 Electric fields in superconductors

Ernst Helmut Brandt, Jan Koláček, Pavel Lipavský, Klaus Morawetz

In 1968 Bok and Klein [1] first observed a non-zero Hall voltage in the Meissner state of a type-I superconductor. The highest accuracy has been achieved by Morris and Brown

[2]. They found a perfect agreement with the prediction of van Vijfeijken and Staas [3] in which the original Bernoulli potential is extended by the fountain term of the two-fluid model. In particular, this measurement shows no traces of effects predicted later within more sophisticated thermodynamical approaches [4, 5, 6]. Since that time this theoretical puzzle has remained unsolved.

We have shown now that, indeed, the electrostatic Bernoulli potential measured at the surface of a superconductor via Kelvin capacitive coupling is independent of the pairing mechanism [7, 8]. This contrasts with the Bernoulli potential in the bulk where contributions due to pairing dominate close to T_c. The surface potential is influenced by the surface dipole which brings a step-like contribution to the electrostatic potential [8]. With the surface dipole included, we have shown that the measured surface potential agrees with the prediction of the thermodynamic approaches. Therefore the Hall voltage measurements cannot serve as a tool to determine material parameters. Instead, more intrinsic observables are necessary to measure quantities like the nuclear magnetic resonance spectra.

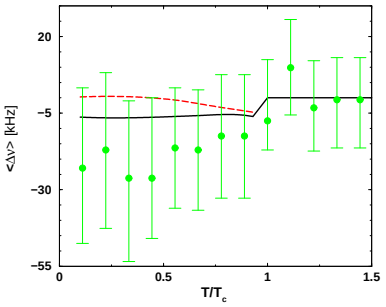

Figure 1: *The difference of NMR and QMR shifts, which is a direct measure for the charge transfer, versus temperature. The theoretical results of a single crystal (red) and after averaging over grain orientation (black) are compared to the experimental values [9].*

Recently, an unexpected temperature dependence of NMR spectra in high temperature superconductors has been reported [9]. Subtracting frequencies of the NMR and NQR spectra, Kumagai *et al* observed a redistribution of charge in the Abrikosov lattice in CuO_2 planes of YBCO. In contrast to simple BCS predictions for bulk superconductors, the observed charge transfer is more than two orders of magnitude larger and shows moreover a different sign. We show that the observed sign and the large magnitude of vortex charge can be explained by a phenomenological theory of the Ginzburg-Landau type, if the screening by holes in CuO chains is included [10], see figure 1.

In order to describe the above experiment, Bardeen's extension of the Ginzburg-Landau theory to low temperatures by the two-fluid model of Gorter-Casimir is used to derive three Ginzburg-Landau equations, the Maxwell equation for the vector potential, the Schrödinger equation for the wave function and the Poisson equation for the electrostatic potential [11]. The electrostatic and the thermodynamic potential compensate each other to a great extent resulting in an effective potential acting on the superconducting condensate. For the Abrikosov vortex lattice numerical solutions are presented in figure 2 and the different contributions to the effective potential are seen in figure 3.

Sometimes there are electric fields applied as in field effect transistor structures. Then the pairing mechanism is changed by this external field itself. An enhancement of pairing temperature has been observed due to field effects as well as a suppression of

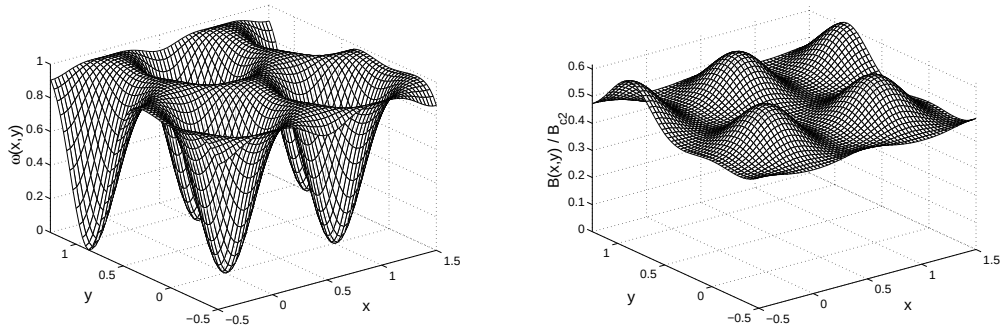

Figure 2: *Left: The condensate density (plotted as $\omega(x,y)$) in the triangular lattice of Nb for temperature $t = T/T_c = 0.5$, magnetic induction $\bar{B}/B_{c2} = 0.5$, and GL parameter $\kappa_0 = 1.5$. In the vortex centers the condensate density $n_s(x,y)/n = (1-t^4)\omega(x,y)$ goes to zero. Between the vortices $\omega(x,y)$ approaches its equilibrium value 1 (which would be constant in the absence of a magnetic field) yielding $n_s^{\rm eq}/n = 1 - t^4 = 0.94$. Right :The magnetic field in units of the upper critical field B_{c2}. $B(x,y)$ reaches its maximum $B_{\rm max}$ at the vortex centers.*

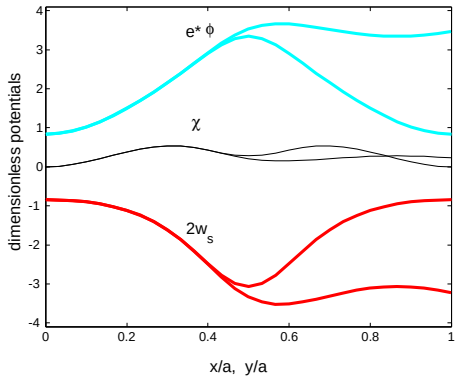

Figure 3: *The effective potential $\chi = e^*\varphi + 2w_s$ (black), the electrostatic potential $e^*\varphi$ (blue) acting on the Cooper pair and the thermodynamic potential $2w_s$ (red).*

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1.5 From classical to nonlocal quantum transport

Pavel Lipavský, Klaus Morawetz, Václav Špička

Since the foundation of Ludwig Boltzmann's famous kinetic equation in 1872 there has been a tremendous development to understand nonequilibrium processes in classical and quantum systems. In absence of the time operator, there are many definitions of characteristic times one can associate with collisions. Regardless of a definition one uses, if the finite duration of collisions is included in a kinetic equation, this equation is non-Markovian since the initial and final states of the collision are at distinct times. The family of non-Markovian kinetic equations also includes retarded equations of Levinson type in which the collision is expressed in terms of the time integral describing the whole process of the two-particle interaction.

For slowly varying systems, we have shown that one half of the Levinson-type retardation describes the off-shell motion and corresponding renormalizations of single-particle functions. The second half compensates the decay of propagators during the integration and can be eliminated leaving the pole contribution to the scattering integral identical to the one obtained from the quasiparticle approximation. The kinetic equation which unifies the achievements of transport in dense gases with the quantum transport of dense Fermi systems can be derived and is presented in a monography [1]. The quasiparticle drift of Landau's equation is connected with a dissipation governed by a nonlocal and non-instant scattering integral in the spirit of Enskog corrections.

$$\begin{aligned}&\frac{\partial f_a}{\partial t}+\frac{\partial \varepsilon_a}{\partial k}\frac{\partial f_a}{\partial r}-\frac{\partial \varepsilon_a}{\partial r}\frac{\partial f_a}{\partial k}\\&=\sum_b\int\mathcal{P}\Big\{f'_af'_b(1-f_a)(1-f_b)-f_af_b(1-f'_a)(1-f'_b)\Big\}\end{aligned}\tag{1}$$

with $f'_a=f_a(k-q-\Delta_K,r-\Delta_3,t-\Delta_t)$, $f'_b=f_b(p+q-\Delta_K,r-\Delta_4,t-\Delta_t)$, $f_a=f_a(k,r,t)$ and $f_b=f_b(p,r-\Delta_2,t)$. The differential cross section $\mathcal{P}\sim|t^R|^2$ is proportional to the square of the amplitude of the T-matrix. All non-local corrections are given by derivatives of the scattering phase shift $\phi=\mathrm{Im}\,\ln t^R(\omega,k,p,q,t,r)$,

$$\begin{aligned}\Delta_t &= \frac{\partial\phi}{\partial\omega},\quad \Delta_E=-\frac{1}{2}\frac{\partial\phi}{\partial t},\quad \Delta_K=\frac{1}{2}\frac{\partial\phi}{\partial r},\quad \Delta_3=-\frac{\partial\phi}{\partial k},\\ \Delta_2 &= \frac{\partial\phi}{\partial p}-\frac{\partial\phi}{\partial q}-\frac{\partial\phi}{\partial k},\qquad \Delta_4=-\frac{\partial\phi}{\partial k}-\frac{\partial\phi}{\partial q}.\end{aligned}\tag{2}$$

These corrections are expressed in terms of shifts in space and time that characterize non-locality of the scattering process. In this way quantum transport is possible to recast into a quasiclassical picture [2]. The non-instant and non-local corrections given by the Δ's do not change the structure and the overall interpretation of the scattering integral but only slightly renormalize its ingredients. The exclusive dependence of the non-local and non-instant corrections on the scattering phase shift confirms results from the theory of gases [3, 4] obtained by very different technical tools.

The balance equations for the density, momentum and energy include quasiparticle contributions and the second order quantum virial corrections beyond the Landau theory. The medium effects on binary collisions are shown to mediate the latent heat, i.e.,

an energy conversion between correlation and thermal energy. The kinetic equation is now a time delayed one showing an interplay between continuous differential equations and discrete mapping such that a chaotic time dependence of the distribution function can occur under certain circumstances [5].

This collision delay resulting from the energy dependence of the scattering phase shift is what remains as a genuine non-Markovian correction. We have separated individual contributions included in the so called memory effect resulting in (i) off-shell tails of the Wigner distribution, (ii) renormalization of scattering rates and (iii) of the single-particle energy, (iv) collision delay and (v) related non-local corrections to the scattering integral. The physical quantity sensitive to the actual choice of the collision delay is the density of quasiparticles, or its complementary quantity, the density of correlated particles. The method presented in this paper, and at the same time the choice of the collision delay, reproduces the correlated density obtained within the generalized Beth-Uhlenbeck approach.

Compared to the Boltzmann equation, the presented form of virial corrections only slightly increases the numerical demands in implementations [6]. Applications range from impurity systems in solid state physics to heavy ion collisions in nuclear physics where recent experimental puzzles could be solved. The enhancement of mid-rapidity matter in heavy ion reactions around the Fermi energy shows the necessity to include correlations beyond the Boltzmann equation which was performed in the framework of nonlocal kinetic theory. Anomalous expansion velocities appear due to the included correlations which can be interpreted in terms of Tsallis statistics and which is a signal of phase transition [7].

The virial corrections to the balance equations appear from intrinsic gradients instead of correlation parts in the equation of the reduced density matrix. The balance equations for the density, momentum and energy include quasiparticle contributions and the second order quantum virial corrections beyond the Landau theory. The medium effects on binary collisions are shown to mediate the latent heat, i.e., an energy conversion between correlation and thermal energy.

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1.6 Ab-initio calculation of ground-state properties of rare-gas crystals

Krzysztof Rościszewski and Beate Paulus

Introduction

The *ab-initio* description of rare-gas crystals is a challenging problem of computational physics. Due to the weak van-der-Waals interaction very accurate correlated *ab-initio* methods are necessary for a reliable calculation of the ground-state properties of such crystals. Density-functional methods with different functionals yield results for rare gas dimers which range from purely repulsive to severe over-binding [1]. Wavefunction-based correlation methods have been mainly applied to dimers so far [2] and very rarely to crystals [3]. We want to apply a coupled-cluster approach with single and double excitations and perturbative treatment of triples (CCSD(T)) [4] for the rare-gas crystals neon, argon, krypton and xenon, using an incremental scheme [5] for the electronic part of the cohesive energy. With this approach we want to gain more insight into factors governing the relative stability of the fcc and hcp structures of the rare-gas solids Ne through Xe. Most theoretical predictions of the lattice structure favoured the hexagonal close-packed (hcp) structure whereas experimentally only the face-centered cubic (fcc) one was observed [6].

Methodology

Interaction energies per atom are calculated, as functions of the lattice constant a, according to

$$E(a) = E^{(2)}(a) + E^{(3)}(a) + E^{(4)}(a) + E_{\mathrm{ZPE}}(a). \tag{1}$$

Here, the $E^{(n)}$ are static electronic n-body contributions and E_{ZPE} is the zero-point energy.

The two-body contributions $E^{(2)}$, which are derived from dimer data, cover the main part of the cohesive energy of the rare-gas solids. We have them calculated at the CCSD(T) level using scalar-relativistic pseudopotentials and $[7s7p]6d5f4g$ valence basis sets (for details see [7]). On the other hand model potentials [8] have been fitted to experimental data. Our calculation yields between 92% and 95% of the two-body contributions calculated with the model potentials to the cohesive energy, where the main error source is the limited basis set.

The three-body contributions are divided into two parts: $E^{(3)} = E^{(3)}_{\mathrm{s.r.}} + E^{(3)}_{\mathrm{l.r.}}$. In the short range part $E^{(3)}_{\mathrm{s.r.}}$ both Pauli repulsion and van-der-Waals-type interactions are important. Therefore accurate *ab-initio* calculations are required. The long-range three-body contributions $E^{(3)}_{\mathrm{l.r.}}$ are calculated by using a multipole expansion [9]. In order to get an indication of the magnitude of four-body contributions $E^{(4)}$ to the cohesion of the rare gas solids, we calculated the four-body increment of the most compact four-atom cluster occurring in the lattice.

The rare-gas solids are weakly bound systems where the zero-point vibrational energy (ZPE) cannot be neglected. In the harmonic approximation, it is easy to define the zero-point crystal energy (per rare-gas atom) as sum of the individual frequencies of the independent oscillators: $E_{\mathrm{ZPE}} = \frac{1}{2rN}\sum_{\mathbf{k},j}\hbar\omega_j(\mathbf{k})$. We calculate the ZPE only on the level of two-body interactions yielding from the model potentials.

	Ne	Ar	Kr	Xe
$E^{(2)}_{\mathrm{m.p.}}$	-993.4	-3464.2	-4840.6	-6799.1
$E^{(3)}_{\mathrm{s.r.}}$	18.9	148.6	230.1	343.0
$E^{(3)}_{\mathrm{l.r.}}$	7.7	59.4	93.0	145.1
$E^{(4)}$	3.2	24.9	38.9	58.9
E_{ZPE}	212.7	288.3	214.7	200.1
E_{coh}	-750.9	-2943.0	-4263.9	-6052.0
E_{exp}	-752.2	-2943.9	-4264.3	-6051.2

Table 1: *The influence of different contributions to the cohesive energy (in μHartree) for the fcc structure at the experimental lattice constant.*

	Ne	Ar	Kr	Xe
2-body	+0.13	+0.43	+0.61	+0.85
3-body s.r.	-0.08	-0.35	-0.53	-1.03
3-body l.r.	+0.03	+0.32	+0.54	+0.56
ZPE	-1.08	-3.24	-2.64	-2.72
total	-1.00	-2.84	-2.02	-2.34

Table 2: *The energy difference between the fcc and hcp structures (in μHartree) evaluated at equilibrium lattice constants optimized for the various levels of approximation.*

Results and Discussion

For the experimentally observed fcc structure, we determined the cohesive energy, the lattice constant and the bulk modulus. In Table 1 we present different contributions to the cohesive energy evaluated at the experimental lattice constant. It is seen that the static two-body contribution overestimates the binding energy by between 12% for xenon and 30% for neon. Including the (repulsive) three-body contributions, this overbinding is reduced. While for neon the effect is small (only 3% of the cohesive energy), its importance rises for the heavier rare-gas solids to $\sim$8% (for xenon). The short-range part amounts to about 70% of the three-body contribution. The four-body contribution is small (between 0.4% for neon and 1.0% for xenon), but its importance increases for the heavier rare gases. The zero-point energy is repulsive, too, of course. It amounts to 30% of the cohesive energy for neon, 10% for argon, 5% for krypton, and 3% for xenon. Comparing our results with experiment, we find very small deviations ($\pm$0.5%). The calculated fcc lattice constants [10] agree well with the experimental ones (deviation $<$0.7%). The calculated bulk moduli [10] agree within $\pm$10% with the experimental data, which by themselves have uncertainties of the same magnitude.
Table 2 shows energy differences between the fcc and hcp structures calculated at the different levels of approximation for the equilibrium lattice constants. (The optimization of the hcp lattice constants always yields the same nearest-neigbor distances as for the corresponding fcc ones, to $< 1 \cdot 10^{-3}$ Å). The two-body contribution slightly favours the hcp structure. The short-range three-body contributions favour the fcc structure, but would render it stable only for xenon. Taking into account the long-range contributions, too, which favour hcp again, the net effect of the three-body contributions is almost zero. The largest contribution to the hcp-fcc difference comes from the zero-point energy which favours the fcc structure by about 1 to 3μH. We have tested the influence of the three-body contributions and anharmonic effects. They increase the ZPE by at most 10%, but have no significant influence on the fcc-hcp-energy difference [11].

Conclusion

We have calculated some ground-state properties of the rare-gas solids Ne through Xe and investigated the origin of the relative stability of the lattice structure. For the two-body contributions, $E^{(2)}$, we applied accurate empirical model potentials derived from dimer data. Three-body contributions, $E^{(3)}$, were treated separately, with respect to short-range and long-range terms. For the short-range part we performed *ab-initio* calculations at the CCSD(T) level, while the long-range part was evaluated using a multipole expansion. In addition, a first estimate has been obtained for the four-body contributions, which turned out to be non-negligible for the heavier rare-gas solids. Finally, the zero-point energy, E^{ZPE}, has been calculated via the harmonic phonon spectrum derived from the two-body model potential. The influence of the three-body contributions and anharmonic effects on the ZPE have been found negligible for the fcc-hcp-energy difference. All these contributions are essential for the accurate determination of the cohesive energy, E_{coh}, the lattice constant, a, and the bulk modulus, B. For the (experimental) fcc structure we achieve agreement with experiment to $\sim$2 μH for E_{coh}, 0.04 Å (0.7%) for a, and 3 kBar (10%) for B. The fcc structure is favoured energetically over the hcp one mainly by the ZPE.

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1.7 Development of a Green's function approach based on a local scheme.

Martin Albrecht

Framework of the project

The project put forth here is part of a broad activity to develop explicitly wave function based correlation methods for solids. While such methods are conceptually clear and

systematically improvable, they tend to be tedious from a computational point of view. The present approach combines a general Green's function approach with an efficient incremental scheme to cope with the problem of numerical cost. The aim is to calculate the band structure of ionic crystals, semiconductors and polymers in an *ab initio* way with full account of correlation effects.

Up to the present such calculations are still subject to immense numerical efforts. A very efficient scheme is density–functional theory (DFT) [1, 2], which focuses on the electron density in order to obtain ground state properties. In several cases the interpretation of the single orbital energies as quasi–particle energies also turns out to be successful. Particular attention has been paid to the local density approximation (LDA)DFT. However, it is found that in insulating materials the LDA results tend to underestimate the band gap [3]. Improvements like the GW–approximation [4], the optimized effective potential method [5] or an exact exchange potential [6] are available. Yet all these procedures rely on special functionals which might not be improvable in a systematic way.

On the other hand, explicitly wave function–based approaches use a correlation interaction scheme to incorporate correlation effects. Naturally, first applications to infinite periodic systems focussed on one–dimensional problems, i. e. polymers [7]–[10].

Early proposals for three–dimensional applications date back to the use of local operators by Horsch et al. [11]. An *ab initio* approach based on local HF orbitals was introduced by Stoll [12] who set up an incremental scheme for the ground state energy. Gräfenstein et al. [13, 14] were able to extend this scheme to excitation energies, but using a finite cluster approximation this attempt was restricted to the valence bands only [15]. In order to obtain genuine local HF orbitals for gap materials, taking into account the entire infinite system, A. Shukla et al. developed the program package WANNIER [17]–[19]. We proposed to construct an *ab initio* effective Hamiltonian perturbatively using such local HF orbitals [10, 20]. Igarashi et al. conceived a local Green's function approach [21] to a model Hamiltonian, and applied this procedure to various open shell crystals [22, 23]. This procedure has now been transferred to the *ab initio* case, where the use of the aforementioned incremental scheme allowed for the necessary boost in numerical efficiency for applications in three dimensions [24, 25].

The Green's function

HF calculations are used as a starting point. The correlation hole around a quasi–particle can be considered to have a fairly local nature [27]. In order to exploit this feature it is advantageous to formulate the correlation corrections in terms of localized rather than extended HF orbitals. The program package WANNIER is employed to provide localized HF orbitals [17, 18, 19].

In the localized orbital basis an incremental scheme is applied to the self energy in real space. The use of local HF orbitals allows to define separate regions characterized by strong, weak and very weak individual correlation contributions to the self energy. For the strong contributions an exact diagonalization method will be used, while further approximations are adequate for the weak parts. This approach is guided by the general idea of employing methods of different accuracy for different classes of correlation contributions as it is efficiently done already for molecules [28].

At the HF level, a hole can be represented as:

$$\big|\mathbf{R}n\big\rangle = c_{\mathbf{R}n}\big|\Phi_{\mathrm{HF}}\big\rangle, \tag{1}$$

where $c_{\mathbf{R}n}$ destroys one electron in a local occupied HF orbital which is characterized by its unit cell $\mathbf{R}$ and its cell orbital index n.

The Hamiltonian is partitioned into a zeroth order Hamiltonian and a residual interaction introducing compound indices $i = \mathbf{0}n, j = \mathbf{R}m$:

$$\begin{aligned} H &= H_0 + W & (2)\\ H_0 &= \sum_{ij} F_{ij} a_i^\dagger a_j & (3)\\ W &= \sum_{ijkl} W_{ijkl} a_i^\dagger a_j^\dagger a_l a_k - \sum_{ij} \sum_{l}^{\mathrm{occ}} (W_{lilj} - W_{lijl}) a_i^\dagger a_j, & (4) \end{aligned}$$

where F is the Fock operator and the residual interaction comprises the two–body part of the Coulomb interaction.

The Green's function is defined as

$$G_{\mathrm{nm}}(\mathbf{R}, t) = -i\langle T[a_{\mathrm{n}}(\mathbf{0}, 0) a_{\mathrm{m}}^\dagger(\mathbf{R}, t)]\rangle, \tag{5}$$

where T is the time–ordering operator and the brackets denote the average over the exact ground state. In reciprocal and frequency space the Green's function obeys the Dyson equation:

$$G_{\mathrm{nm}}(\mathbf{k}, \omega) = G^0_{\mathrm{nm}}(\mathbf{k}, \omega) + \sum_{\mathrm{kl}} G^0_{\mathrm{nk}}(\mathbf{k}, \omega) \Sigma_{\mathrm{kl}}(\mathbf{k}, \omega) G_{\mathrm{lm}}(\mathbf{k}, \omega). \tag{6}$$

The Dyson equation (6) introduces the self energy $\Sigma_{\mathrm{kl}}(\mathbf{k}, \omega)$ which contains the correlation effects. $G^0_{\mathrm{nm}}(\mathbf{k}, \omega)$ is the HF propagator

$$\big[G^0(\mathbf{k}, \omega)\big]^{-1}_{\mathrm{nm}} = \omega - F_{\mathrm{nm}}(\mathbf{k}). \tag{7}$$

As a result of Dyson's equation the Green's function is then calculated from

$$G_{nm}(\mathbf{k}, \omega) = \left[\omega - F(\mathbf{k}) - \Sigma(\mathbf{k}, \omega)\right]^{-1}_{\mathrm{nm}}. \tag{8}$$

The correlated band structure is given by the poles of the Green's function which are numerically iteratively retrieved as the zeros of the denominator in Eq. (8).

The self energy is approximated by decomposition into a retarded and an advanced part

$$\Sigma_{\mathrm{kl}}(\mathbf{k}, \omega) = \Sigma^{(\mathrm{r})}_{\mathrm{kl}}(\mathbf{k}, \omega) + \Sigma^{(\mathrm{a})}_{\mathrm{kl}}(\mathbf{k}, \omega). \tag{9}$$

Furthermore, the configuration space will be restricted to single excitations, i. e. three–body interactions.

In the following, only the construction of the retarded self energy part is described. Let a, b, c, d and r, s, t, u represent occupied and virtual orbitals, respectively. The space of 2–particle 1–hole states (2p1h) is spanned by

$$\big|r, s, a\big\rangle = a_{\mathrm{r}}^\dagger a_{\mathrm{s}}^\dagger a_{\mathrm{a}} \big|\Phi_{\mathrm{HF}}\big\rangle. \tag{10}$$

The Hamiltonian H^{R} is set up in this basis, i. e.

$$[H^{\mathrm{R}}]_{\mathrm{rsa,r's'a'}} \;=\; \langle r,s,a\big|H-E_0\big|r',s',a'\rangle.$$

The superscript 'R' is used to refer to the 2–particle–1–hole space (2p1h). There is a similar matrix for the 2h1p space. Here E_0 is the ground state energy while the brackets indicate the HF average.

Diagonalizing the matrix H^{R} results in the eigenvectors S^{R} and eigenvalues λ^{R}. The retarded part of the self energy is then constructed as

$$\begin{aligned}\Sigma^{(\mathrm{r})}_{\mathrm{nm}}(\mathbf{R},\omega) &= \sum_{\mathrm{rsa;r's'a'}} \Gamma(\mathrm{rs;na})\big[\omega - H^{\mathrm{R}} + i\delta\big]^{-1}_{\mathrm{rsa;r's'a'}}\Gamma(\mathrm{r's';ma'}) \\ &= \sum_{\mathrm{rsa;r's'a'}} \Gamma(\mathrm{rs;na}) \sum_{\mathrm{q}} S^{\mathrm{R}}_{rsa;q}\frac{1}{\big(\omega-\lambda^{\mathrm{R}}_{\mathrm{q}}+i\delta\big)}S^{\mathrm{R}}_{q;r's'a'}\Gamma(\mathrm{r's';ma'}). \quad (11)\end{aligned}$$

The self energy in reciprocal space, as it appears in Eq. (8), can then be obtained as:

$$\Sigma^{(\mathrm{r})}_{nm}(\mathbf{k},\omega) = \sum_{\mathbf{R}} \mathrm{e}^{\mathbf{ikR}}\Sigma^{(\mathrm{r})}_{nm}(\mathbf{R},\omega). \quad (12)$$

The incremental scheme

In principle the three–body excitations $\big|r,s,a\big\rangle, \big|r',s',a'\big\rangle$ taken into account while performing the calculation, should run over the entire solid. Secondly, the expression (11) ought to be evaluated for each lattice vector $\mathbf{R}$ as all these terms are needed in Eq. (12). However, since the correlation hole around a quasi particle is for its major part a rather local quantity, it turns out that only excitations in the neighborhood of the central unit cell will considerably contribute to the self energy, so that the number of relevant three–body excitations is finite. Secondly, by the same token the parts of the self energy with $\mathbf{R} \neq \mathbf{0}$ will be found to decay rapidly with increasing distance of $\mathbf{R}$, so that again only a finite number of calculations needs to be performed. To further enhance the performance and to focus on the important contributions, an incremental scheme was introduced by Stoll [12] and Gräfenstein [13, 14]. The idea amounts to breaking up the task of diagonalizing the Hamiltonian in the full space of configuration interaction into a series of smaller tasks arranged in a controlled and well–defined way.

For example, a first simple approximation for the matrix element $\Sigma_{\mathrm{ii'}}$ of the self energy from Eq. (11) can be obtained by restricting all excitations to the central unit cell $\mathbf{0}$. This is sketched in the left panel of Fig. 1, labelled 'intra'. The figure shows a certain finite environment of the solid around the central unit cell and displays by continuous shading the active cells where excitations are taken into account. The result $\Sigma_{\mathrm{ii'};\mathbf{0}}$ of this simple procedure defines the first of a series of approximations to the exact result denoted as *intra* increment:

$$\Delta\Sigma^{\mathrm{intra}}_{\mathrm{ii'}} \;=\; \Sigma_{\mathrm{ii'};\mathbf{0}}. \quad (13)$$

The next step is to perform a calculation of the self energy where now excitations are allowed in the central cell *and* one additional cell denoted K in the middle panel of

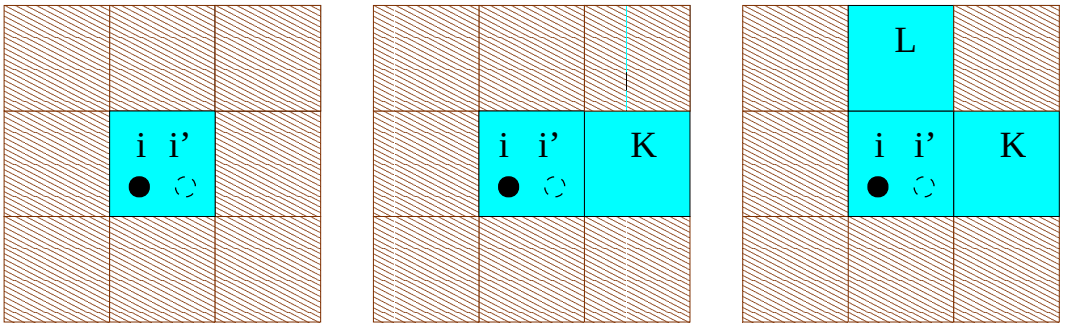

Figure 1: *Each of the three pannels shows the same finite nine–cell–part of an infinite solid. The active cells are schematically displayed for an intra cell ('intra'), a one–cell and a two–cell increment.*

Fig. 1. Denoting the result of this calculation as $\Sigma_{\mathrm{ii'};\mathbf{R}_\mathrm{K}}$, the corresponding one–cell increment, labelled 'I' to mark the use of *one* additional cell, is defined to be:

$$\Delta\Sigma^{\mathrm{I}}_{\mathrm{ii'};\mathbf{R}_\mathrm{K}} \;=\; \Sigma_{\mathrm{ii'};\mathbf{R}_\mathrm{K}} - \Delta\Sigma^{\mathrm{intra}}_{\mathrm{ii'}}. \tag{14}$$

Obviously this procedure can be continued to include more and more cells. The two–cell increment, labelled 'II', indicated on the right of Fig. 1, is given by:

$$\Delta\Sigma^{\mathrm{II}}_{\mathrm{ii'};\mathbf{R}_\mathrm{K}\mathbf{R}_\mathrm{L}} \;=\; \Sigma_{\mathrm{ii'};\mathbf{R}_\mathrm{K}\mathbf{R}_\mathrm{L}} - \Delta\Sigma^{\mathrm{I}}_{\mathrm{ii'};\mathbf{R}_\mathrm{K}} - \Delta\Sigma^{\mathrm{I}}_{\mathrm{ii'};\mathbf{R}_\mathrm{L}} - \Delta\Sigma^{\mathrm{intra}}_{\mathrm{ii'}}. \tag{15}$$

The self energy is finally obtained from:

$$\Sigma_{ii'} \;=\; \Delta\Sigma^{\mathrm{intra}}_{\mathrm{ii'}} + \sum_{\mathbf{R}_\mathrm{K}} \Delta\Sigma^{\mathrm{I}}_{\mathrm{ii'};\mathbf{R}_\mathrm{K}} + \frac{1}{2!} \sum_{\mathbf{R}_\mathrm{K}\neq\mathbf{R}_\mathrm{L}} \Delta\Sigma^{\mathrm{II}}_{\mathrm{ii'};\mathbf{R}_\mathrm{K}\mathbf{R}_\mathrm{L}} + \;\ldots\;\; . \tag{16}$$

Of course, there is an infinite number of one–cell, two–cell and higher–order increments. However, only a limited number of them needs actually to be calculated since with increasing number of active cells and the distance between them the respective increments rapidly decay to zero. As the decrease of the increments can be monitored, the truncation of the summation (16) can be explicitly controlled.

To be specific, increments with cells arranged approximately as a sphere in a certain range R_c will be calculated explicitly. Beyond R_c individual contributions are found to basically vanish and only the sum of local excitations up to infinity would give a noticeable contribution, known as the long–range polarization cloud. As has been demonstrated in earlier works [13, 14, 15, 24], this part can be well approximated by a continuum correction.

As described in Ref. [24], the self energy matrices with $\mathbf{R} \neq \mathbf{0}$ (non–local part) can be obtained in the same way.

The coupling of the doubles to the singles is at least fourth order and can thus be expected to be rather small, yet to include them approximately, a diagonal dressing technique is adopted. If the single excitation space is indexed with S and the double one with D, the eigenvalue problem takes the form

$$\begin{pmatrix} H_{\mathrm{SS}} & H_{\mathrm{SD}} \\ H_{\mathrm{DS}} & H_{\mathrm{DD}} \end{pmatrix} \begin{pmatrix} C_\mathrm{S} \\ C_\mathrm{D} \end{pmatrix} = \lambda \begin{pmatrix} C_\mathrm{S} \\ C_\mathrm{D} \end{pmatrix}. \tag{17}$$

Table 1: *Energy values (in eV) of the valence band (v) and the lower two conduction bands (c_1, c_2) at selected points in reciprocal space for LiH. The amount of correlations recovered is given in percent.*

	L		Γ		X		W		K	
	HF	$Corr$	HF	$Corr$	HF	$Corr$	HF	$Corr$	HF	$Corr$
v	−6.28	−1.97	−10.72	−5.97	−3.03	1.01	−3.41	0.62	−3.71	0.36
c_1	12.44	9.54	23.65	19.92	10.05	7.09	13.69	10.79	12.00	9.03
c_2	23.49	20.11	25.90	22.19	18.48	15.31	13.69	10.63	16.50	13.40
gap	18.72	11.51			13.08	6.08			20.21[a]	13.04[a]
gap[b]	(74%)	≈9.0			(87%)	4.99			(107%)	≈13.5

[a] the dipole allowed transition is to c_2. [b] experimental values from Ref. [**?**, 29]

This yields an effective Hamiltonian $H_{\rm SS}^{\rm eff}$ which operates entirely in the space of the single excitations but incorporates the effects of the double excitations as well:

$$\underbrace{\left[H_{\rm SS} - H_{\rm SD}\left[H_{\rm DD} - \lambda\right]^{-1} H_{\rm DS}\right]}_{H_{\rm SS}^{\rm eff}} C_{\rm S} = \lambda C_{\rm S}. \tag{18}$$

$H_{\rm SS}^{\rm eff}$ depends on the sought eigenvalue λ. A perturbative solution is readily constructed by iteration.

Results and Discussion

The method has been applied to LiH and LiF [24, 25]. In the correlation calculation, the first three shells around the central unit cell, i. e. up to third nearest neighbors or 43 unit cells, have been taken into account.

Test application and satellites: LiH

For LiH test calculations were performed in a medium–size basis set to demonstrate the applicability of the method, i. e. a [3s,1p] basis is given on the hydrogen and a [2s,1p] one on the lithium [24]. Correlations lead to a significant narrowing of the gaps with respect to the HF results. In particular, at the X–point, the fundamental gap is changed by an amount of 7.00 eV from its HF value of 13.08 eV to 6.08 eV. The experimental gap is reported to be 4.99 eV [29] together with some indication for somewhat weaker transitions at about 9 eV and 13.5 eV. On the ground of the present calculation the latter two transitions might be ascribed to the gap at the L–point and to the dipole allowed transition to the second conduction band (c_2 in Tab. 1) at the K–point, respectively, as is indicated in Tab. 1.

So, experiments indicate for the gap a correlation contribution of 13.08 eV−4.99 eV= 8.09 eV. Our correlation calculation recovers 7.00 eV or 87% of this amount. This result seems rather satisfactory given the basis set limitation investigated carefully by Shukla et al. [19].

Another typical effect of electron correlations on the band structure, the flattening of the bands, can be understood in principle in the real space picture developed above.

Intra	5.654
S_1	0.190
S_2	0.032
S_3	0.007
D_1	0.002

Table 2: *Individual increments in eV for LiH.*

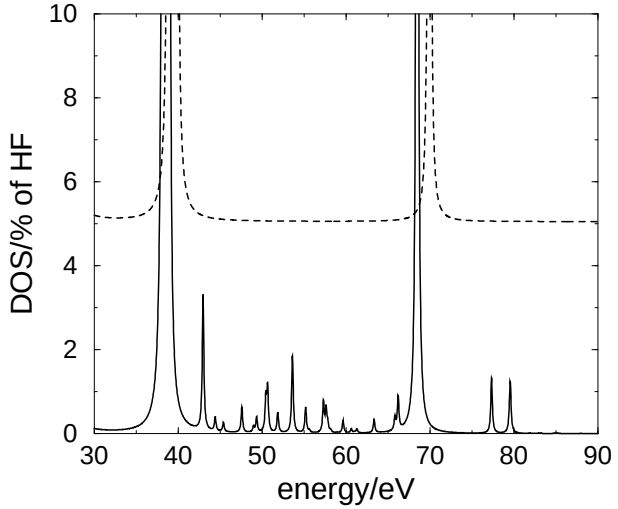

Figure 2: *DOS of LiH at a single point in reciprocal space (Γ). The dashed line gives the (shifted) HF DOS, the solid line shows the correlated one obtained from diagonalization of the central unit cell. The units at the DOS axis are in percent of the hight of the HF peaks.*

Correlations allow the quasi particles to arrange themselves better within their local environment, so they become less itinerant which is expressed by a flattened band structure. The HF valence band width is calculated to be 7.69 eV, while the correlated band width is obtained as 6.98 eV, which corresponds to a reduction of 9%. This has to be compared to experimental measurements which yield 6.3±1.1 eV [30] . So, while the HF band width is definitely too large, the correlated result is well in the range of experimental errors.

The Green's function method has the potential to describe satellite bands, which appear because of the strong mixing of energetically high–lying states of the model space, the one–particle states (1p), with low–lying 2p1h states. Fig. 2 gives the contribution of only one individual point in reciprocal space, the Γ–point, to the overall density of states (DOS) in the upper part of the conduction bands. The (upward shifted) dashed line shows two HF peaks, while the solid line displays the correlated result. The HF lines are pushed towards the gap due to correlations. Moreover in the correlated DOS a lot of satellite peaks have appeared which were clearly absent in the HF calculation.

LiF

For this system a [4s3p1d] basis set was given on the fluorine anion, while a [2s1p] basis set was used for the lithium cation. For the lithium cation this constitutes a polarized double zeta basis. This point has been carefully studied by Tatewaki [16]. All calculations were done at the experimental fcc lattice constant a=3.990 $\mathring{A}$.

As an analysis of the mechanism of the incremental scheme, the importance of different increments is considered. In Tab. 2 the contribution of various increments to the correlation correction of the fundamental gap at the Γ–point is presented. The intra increment gives by far the largest individual contribution, reducing the HF gap by 5.65 eV. The one–cell increments are denoted as S_{n}, where n indicates that the additional

Table 3: *Comparison of values for the band gap and the valence band width from various calculations for LiF. All values are in eV.*

	This work			From ref. [16]		From ref. [26]			Exp	
	HF	$Heff$	$Corr$	LDF	$Cluster$	HF	LDA	GW		
gap	22.40	17.30	13.50	13.9	13.9	21.29	8.82	14.30	13.5[a]	14.2[b]
$width$	3.37		3.40	2.8	2.7	3.31	3.12	3.61	3.5[c]	

[a] from ref. [31, 32]; [b] from ref. [33]; [c] from ref. [34] y

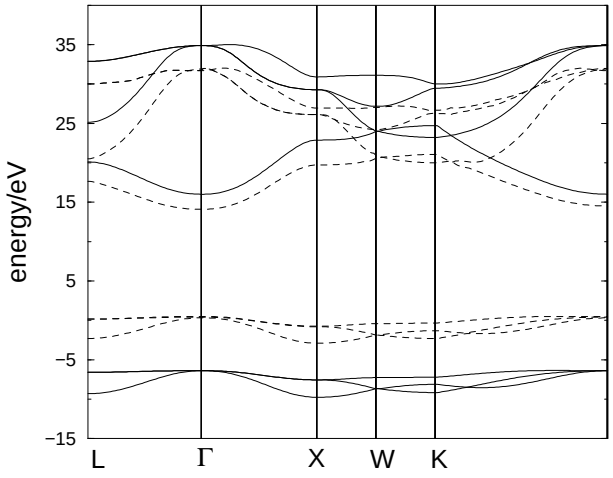

Figure 3: *Band structure of LiF for selected directions in the first Brillouin zone between L[b($\frac{1}{2},\frac{1}{2},\frac{1}{2}$)], Γ[(0,0,0)], X[b(1,0,0)], W[b(1,$\frac{1}{2}$,0)] and K[b($\frac{3}{4},\frac{3}{4}$,0)] (cartesian coordinates, b=$\frac{2\pi}{a}$). The upper three valence bands together with the lowest four conduction bands are shown as solid and dashed lines for the HF and the correlated results, respectively.*

cell is chosen from the nth coordination sphere. Shifting the additional cell from a first nearest neighbor position (S_1) to a third nearest one (S_3) decreases the one–cell contribution from 0.190 eV to 0.007 eV. Even the largest two–cell increment D_1 amounts to only 0.002 eV. The rapid decrease of increment contributions is a consequence of the fairly local character of a correlation hole around a quasi particle. It allows to efficiently calculate the band structure including major correlation effects.

For the band structure calculation the final result is shown in Fig. 3. Solid lines represent the HF result while dashed lines give the result of the correlation calculation. The HF gap of 22.40 eV is reduced to a correlated value of 13.50 eV. This result compares well with the experimental value of 13.6 eV [31, 32] or 14.2 eV [33]. A comparison with other *ab initio* calculations is shown in Tab. 3. The correlated results are in a narrow range from the 13.5 eV of this work to 14.3 eV given by the GW calculation of ref. [26], (except LDA), and are close to experiment.

Secondly, the width of the valence bands is compared. While the usual tendency to be expected is a flattening of the bands, in the case of the LiF valence bands this effect is not pronounced. In the present calculation the HF band width of 3.37 eV does basically not change, displaying a minute broadening to 3.40 eV. This finding is mirrored in the experimental width of 3.5 eV [34]. The other works cited in Tab. 3 consistently show the same tendency.

Conclusion

In conclusion, a localized–orbital–based ab initio scheme for band structure calculations has been presented which is designed to include correlation effects on top of HF results.

The procedure starts from localized HF orbitals and strives to calculate the self energy matrix. This task was efficiently split into the calculation of individual increments arranged in a series of rapidly decaying contributions. The scheme is flexible and allows for a different treatment for different contributions, depending on their relative weight. Being explicitly orbital–based, the presented scheme is amenable to systematic improvements in a clear manner.

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1.8 Wavefunction-based Correlation Calculations for Hole and Electron Attachment States in Solids and Polymers

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Wavefunction-based correlation methods such as truncated CI (configuration interaction) or coupled cluster are widely used in quantum chemistry and have proven to provide an accurate and systematic approach to electron correlation in atoms and molecules. Yet, until now, these techniques have not found their way to standard *ab initio* electronic structure calculations in solid-state physics. They are still commonly considered to be computationally too demanding for being applicable to large or even infinite periodic systems, although it has been demonstrated for more than a decade, by now, that a systematic exploitation of the predominantly local character of electron correlations allows to perform such wavefunction-based calculations in a reasonably efficient way (e.g. [1, 2, 3]).

In fact, an incremental scheme based on localized Hartree-Fock orbitals and series of constraint correlation calculations, where only the electrons from a limited number of localized orbitals are allowed to respond to each other, could successfully be established to determine the ground-state correlation energies of solids, polymers, and clusters (see for example Ref. [4, 5, 6, 7, 8, 9]). Essentially any standard quantum-chemical correlation code (with a frozen core orbital option) can be used for that purpose, and hence, the full variety of quantum-chemical post-SCF correlation methods is available.

An extension of this ansatz to excited (N+1)- and (N-1)-particle states of periodic systems is possible as demonstrated in the pioneering studies [10, 11, 12] where the correlation contributions to the *valence* bands, i.e., the energies of the electron hole states, of diamond, silicon, and germanium were investigated. The basic concept employed there is the introduction of an effective Hamiltonian which maps — very much in the spirit of one-particle Green's functions — the first relevant excited states Ψ_n of a given (N-1)-particle system to a set of Hartree-Fock hole configurations Φ_a (single-determinant $(N-1)$-particle wavefunctions built from Hartree-Fock orbitals) such that the energetic and dynamical properties of the correlated wavefunctions are fully maintained,

$$\widetilde{\Psi}(t) := P\Psi(t) \quad \text{with} \quad \Psi(0) = \sum_n c_n \Psi_n \qquad \Rightarrow \qquad i\hbar \frac{\partial}{\partial t} \widetilde{\Psi}(t) = H_{\text{eff}} \widetilde{\Psi}(t) \quad . \qquad (1)$$

Here P is the projector onto the space spanned by the model configurations Φ_a and $\widetilde{\Psi}(t)$ is the "shadow" thrown by the propagating true wavefunction into that model space. Having the eigenstates (E_n, Ψ_n) and their projections $\widetilde{\Psi}_n = P\Psi_n$ at hand (which

is the case for constraint correlation calculations) the effective Hamiltonian $H_{\rm eff}$ and the back-mapping wave operator $\Psi = \Omega\widetilde{\Psi}$ are easily accessible,

$$H_{\rm eff} = \sum_n |\widetilde{\Psi}_n\rangle E_n \langle\widetilde{\Psi}^*_n| \quad \text{and} \quad \Omega = \sum_n |\Psi_n\rangle\langle\widetilde{\Psi}^*_n| \tag{2}$$

with

$$\widetilde{\Psi}^*_n = \sum_m \widetilde{\Psi}_m (S^{-1})_{mn} \quad \text{where} \quad S_{nm} = \langle\widetilde{\Psi}_n|\widetilde{\Psi}_m\rangle \quad . \tag{3}$$

The crucial point now is that after switching to a basis of *local* model configurations

$$\Phi_a = \hat{c}_a \Phi_{\rm HF} = \tfrac{(-1)^{N-a}}{\sqrt{(N-1)!}} \det(\varphi_1, \ldots, \varphi_{a-1}, \varphi_{a+1}, \ldots, \varphi_N) \tag{4}$$

with φ_n being *localized* occupied Hartree-Fock orbitals of the neutral N-particle system (with correlated ground-state energy E_0^N), the matrix elements

$$H^{\rm eff}_{ab} = \langle\Phi_a|H_{\rm eff} - E_0^N|\Phi_b\rangle \tag{5}$$

turn out i) to decay fast with increasing distance of the associated orbitals φ_a and φ_b, and ii) to be highly transferable from one model cluster to another. Hence, extrapolation of $H^{\rm eff}_{ab}$ to the infinite system is straightforward. Introducing multi-indices $a = (\alpha, R)$ with α denoting localized orbitals in the reference unit cell of the periodic system and R being lattice displacements, the matrix of the effective Hamiltonian can be transformed into k-space, which is its translational-symmetry-adapted form,

$$H^{\rm eff}_{\alpha\beta}(k) = \sum_R e^{ikR} H^{\rm eff}_{(\alpha,0)(\beta,R)} \quad \text{with} \quad k \in 1^{\rm st}\ \text{Brillouin zone} \quad , \tag{6}$$

and, after diagonalization, the (projected) correlated hole states $\widetilde{\Psi}_n(k)$ of the solid (which are delocalized Bloch waves carrying a crystal momentum k) and the corresponding energy bands $E_n(k)$ are obtained.

In a completely analog way, the matrix elements of the effective Hamiltonian for electron attachment states are set up. Note, however, that localized *virtual* orbitals φ_r are required for that purpose to be able to construct local model configurations

$$\Phi^r = \hat{c}^\dagger_r \Phi_{\rm HF} = \tfrac{1}{\sqrt{(N+1)!}} \det(\varphi_1, \ldots, \varphi_N, \varphi_r) \tag{7}$$

for the electron attachment states.

The correlation contributions to the effective Hamiltonian matrix elements $H^{\rm eff}_{ab}$ are extracted from individual model clusters arranged around the respective local orbitals φ_a and φ_b. Because of the predominantly local character of the correlation hole around moving hole states, reliable information on the matrix elements of a solid can be retrieved from the inner part of such model clusters once the clusters are sufficiently large. The incremental scheme is used to make these correlation calculations feasible in essentially the same way as it has been done for the ground-state energy,

$$H^{\rm eff}_{ab} = H^{\rm eff}_{ab}() \ + \ \sum_c \Delta H^{\rm eff}_{ab}(c) \ + \ \sum_{c,d} \Delta H^{\rm eff}_{ab}(c,d) \ + \ \ldots \tag{8}$$

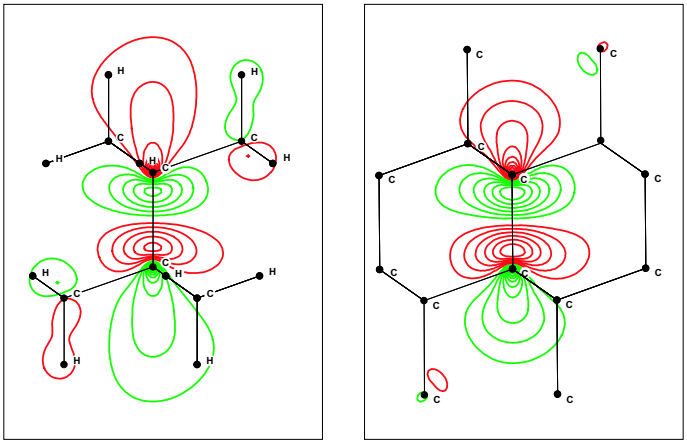

Figure 1: *Localized virtual orbitals of diamond from a C_8H_{18} model cluster surrounded by a potential wall (left), and from the infinite periodic crystal shown after projection onto a C_{26} cluster (right). The contours are ± 0.05, ± 0.10, ± 0.15, ± 0.20, ..., ± 0.55 au.*

with $H_{ab}^{\rm eff}(c,\ldots)$ being the matrix elements of the effective Hamiltonian resulting from a constrained correlation calculation where only electrons from the α-spin orbitals $\varphi_a, \varphi_b, \varphi_c, \ldots$ and the corresponding β-spin orbitals are correlated, and

$$\begin{aligned} \Delta H_{ab}^{\rm eff}(c) &= H_{ab}^{\rm eff}(c) - H_{ab}^{\rm eff}() \\ \Delta H_{ab}^{\rm eff}(c,d) &= H_{ab}^{\rm eff}(c,d) - H_{ab}^{\rm eff}() - \Delta H_{ab}^{\rm eff}(c) - \Delta H_{ab}^{\rm eff}(d) \\ &\ldots \end{aligned} \tag{9}$$

being the corresponding incremental corrections of increasing order. While convergence of the incremental series (8) with respect to the number of correlated electrons is fast — usually, only the first and second order increments shown explicitly in eq. (9) have to be considered — convergence with respect to the spatial distance of the involved local orbitals is less pronounced than for the ground-state energies. But, algebraic tail corrections [11, 12] can be applied to account for that circumstance.

Hole states are cationic states and no severe problems arise when simple hydrogen or pseudopotential terminated clusters are used to model the moving hole. Electron attachment states, however, are anionic states and due to the negative extra charge the added electron is at best loosely bound to such a cluster. In cases like diamond, where the saturated model clusters don't even exhibit positive electron affinities, the added electron simply leaves the cluster if no special means are taken to avoid this. Potential walls put up by using minimal basis sets on the atoms which saturate the dangling bonds couldn't stabilize the anionic clusters sufficiently, even if they are augmented by shift (or penalty) operators on the bonding and anti-bonding orbitals of the dangling bonds, as can be seen from Fig. 1 where the central Foster-Boys-localized virtual orbital from a C_8H_{18} cluster subject to such a potential wall is compared to the localized Wannier orbitals generated by the most recent version of the CRYSTAL code [13, 14].

Hence, we decide for a strict incorporation of the infinite crystal environment in the constrained correlation calculations. Exploiting the fact that only very few orbitals have to be correlated explicitly in an incremental calculation, while all other Hartree-Fock orbitals are kept frozen, an embedding formalism was derived in which the effect of the crystal environment on the region where the correlated electrons reside can be entirely subsumed in an external one-particle potential $V_{\rm emb}$ whose matrix elements

with respect to the orbital basis functions χ_i read

$$\langle\chi_i|V_{\rm emb}|\chi_j\rangle = \langle\chi_i|V_{\rm ion}^{\rm env}|\chi_j\rangle + \sum_a^{\rm env}\langle\chi_i\varphi_a||\chi_j\varphi_a\rangle \tag{10}$$

with $\langle\varphi\widetilde{\varphi}||\psi\widetilde{\psi}\rangle := \langle\varphi\widetilde{\varphi}|\frac{1}{r_{12}}|\psi\widetilde{\psi}\rangle - \langle\varphi\widetilde{\varphi}|\frac{1}{r_{12}}|\widetilde{\psi}\psi\rangle$ as the usual bi-electronic contributions in Hartree-Fock theory. The summation in the last term runs over all *localized* occupied Hartree-Fock orbitals φ_a of the host crystal which are *not* attributed to the embedded region. In addition, a constant (and in principle infinite) energy contribution

$$E_{\rm emb} = \sum_a^{\rm env}\langle\varphi_a|T + V_{\rm ion}^{\rm clus} + V_{\rm ion}^{\rm env}|\varphi_a\rangle + \tfrac{1}{2}\sum_{a,b}^{\rm env}\langle\varphi_a,\varphi_b||\varphi_a,\varphi_b\rangle \tag{11}$$

arises from the embedding, which, however, does not affect the explicitly correlated electrons. It only enters the chemical potential of the removed or added electron and thus finally drops out, once it comes to the correlation contributions to the ionization potentials or electron affinities. Evidently, it is essential for the above embedding scheme that one is able to localize the occupied Hartree-Fock orbitals of the periodic N-particle system.

Direct evaluation of the embedding potential $V_{\rm emb}$ would require infinite lattice summations over slowly decaying Coulomb and exchange integrals, but having the crystalline Hartree-Fock operator $F_{\rm host}$ at hand, the embedding potential can simply be obtained via

$$V_{\rm emb} = F_{\rm host} - F_{\rm clus}[P_{\rm host}({\rm clus})] \quad \text{with} \quad P_{\rm host}({\rm clus}) = \sum_a^{\rm clus}|\varphi_a\rangle\langle\varphi_a| \quad . \tag{12}$$

Here the summation in the last term runs over all *localized* occupied orbitals of the host crystal which *are* attributed to the embedded region. To perform such embedded cluster correlation calculations an interface between the CRYSTAL code (for periodic Hartree-Fock calculations) [15] and the MOLPRO code (for correlation calculations in finite systems) [16] has been implemented in collaboration with the developers of CRYSTAL which provides i) the required Hartree-Fock matrix elements and ii) the relevant localized Wannier orbitals (which are only available in the not yet public version 200x of CRYSTAL).

Despite the strong formal analogy between electron hole and electron attachment states, the requirements for such calculations are quite different. An embedding scheme is necessary for the anionic $(N+1)$-particle states, and energetically low-lying local *virtual* orbitals must be generated to set up the model space. Straightforward Foster-Boys localization [17] (as routinely employed for the hole states) usually fails, because it is hard to separate the relevant canonical virtual orbitals from the remaining ones. In the two sample systems studied so far (diamond and *trans*-polyacetylene) a small (indirect) band gap exists between the conduction bands of interest and the energetically higher states, and thus the Wannier orbitals resulting from the first low-lying conduction band complex of the infinite host system turned out to be sufficiently localized to serve as model space orbitals. In general, however, one cannot rely on such a feature. Hence, more sophisticated schemes to properly disentangle the virtual orbitals

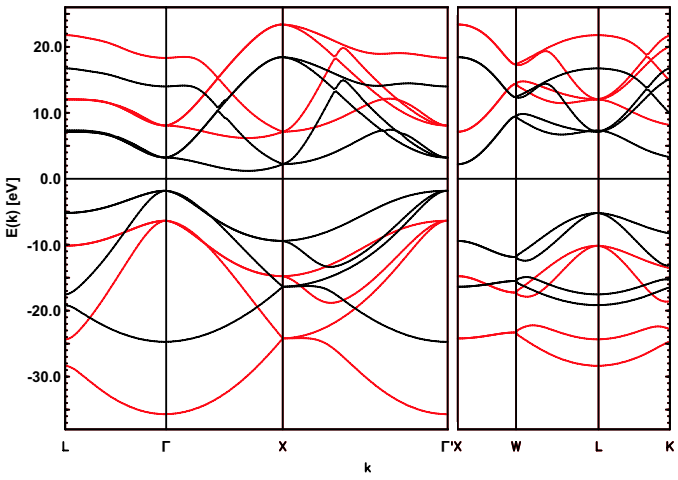

Figure 2: *SCF (red) and correlated (black) band structure of diamond calculated on the MR-ACPF(SD) level using an spd cc-pVTZ basis set.*

before localization (very much like the disentanglement procedure recently described by Marzari and Vanderbilt [18]) are currently tested.

Two further subtle, but important differences arise which will briefly be mentioned but not discussed in detail here. First, the external space of a periodic system (i.e., the space spanned by all those virtual orbitals which do *not* belong to the virtual model space) is infinite, and hence, has to be partitioned into "atomic" contributions to be able to select proper subspaces for a given constrained correlation calculation. A modified version of the concepts introduced by Hampel and Werner [19] is used for that purpose. Second, all the local orbitals constructed so far still exhibit fast decaying but nevertheless infinite tails. For the final correlation calculation they are projected onto the basis set of the embedded cluster, and special means must be taken to ensure that during this projection the virtual model space orbitals stay orthogonal, not only to the occupied space of the cluster, but also to the occupied space of the surrounding host system. Otherwise, the Pauli exclusion principle would be violated and "ghost states" could easily arise. Similar considerations hold for the external orbitals which must be orthogonal on the occupied and the virtual model space. All these have been built into the MOLPRO-CRYSTAL interface which now allows to perform embedded cluster correlation calculations with the MOLPRO program package for essentially any of the correlation methods available in that package.

Since there is no substantial energy gap between the most stable hole or electron attachment state and the first excited states, which are necessary to describe *complete* valence or conduction bands, multi-reference correlation methods have to be used. To keep the computational effort low, a minimal active space treatment is adopted where only the model space configurations are taken as reference configurations. Two standard correlation methods have been chosen which are believed to be reasonably size-consistent even with a minimal active space (an important prerequisite for the incremental scheme to converge properly): single-double CI with Davidson corrections and averaged coupled pair functions (ACPF) together with standard quantum-chemical cc-pVDZ and cc-pVTZ basis sets.

In Fig. 2 the correlated valence *and* conduction bands of diamond are shown as resulting from the above described setup of the embedding scheme using the MR-ACPF(SD)

method and a cc-pVTZ basis set (without f-functions). As expected, a significant upwards shift (4.54 eV) of the Hartree-Fock valence bands of diamond is observed upon inclusion of the electron correlation. In addition, the band width is reduced substantially (by 10.97 eV) and even more subtle features such as the coupling strength of the avoided crossing on the Σ line (from X to Γ') is affected quite strongly by electron correlation. In accordance, the four sp^3-dominated Hartree-Fock *conduction* bands of diamond are shifted downwards (4.86 eV) by electron correlation leading to a direct band gap at the Γ point of 5.03 eV, just 35% of the original Hartree-Fock gap of 14.43 eV. Besides that shift, no further pronounced correlation effects could be detected for the low-lying conduction bands. Compared to the experimental direct band gap of diamond of 7.3 eV [20] the correlation corrected band gap is too small by about 2.3 eV. This is most probably due to a general tendency of the ACPF methods to overestimate the correlation effects in $(N-1)$- and $(N+1)$-particle systems. In all constrained correlation calculations which have been performed for different correlation methods, the ACPF ansatz was found to yield noticeably larger correlation effects than all the other methods, although for the neutral N-particle system it gave results in good accordance with the coupled cluster (CCSD) method. It has been demonstrated here that it is possible to extract correlated band structures from wavefunction-based correlation calculations of embedded clusters by means of the effective Hamiltonian approach in combination with the incremental scheme. Diamond served as a sample compound here, but, in a quite similar way, the band structure of *trans*-polyacetylene could be calculated. Yet, according to our experience there are two major physical effects that limit the applicability of the above scheme in its present form. If excitation energies much higher than the band gap of a system are considered (to deep-lying hole states, for example) quite a lot of three- (and more)-particle states show up in the *ab initio* calculations which are hard to suppress, and thus increase the computational cost tremendously. Similarly, for 1- or 2-dimensionally extended systems (such as surfaces and polymers) with large band gaps, many scattering states with energies lower than the relevant one-particle resonances are found, and it becomes difficult to reach and identify the desired states. An equation-of-motion ansatz for the $(N-1)$- or $(N+1)$-particle states starting from an (approximate) correlated N-particle ground-state wavefunction (as the one used in the IP-EOM-CCSD method described in Ref. [21]) could be more suitable in these cases.

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1.9 Replacement of fast chaotic degrees of freedom by white noise

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The issue of whether observed aperiodic time series data represent chaos or noise is as old as nonlinear time series analysis itself. During the years, the difficulties of this distinction have been explored well. Our group was able to show that high entropic deterministic signals are indistinguishable from noise on the large length scales [2], such that it is plausible that fast chaos can be modeled by noise processes in the limit of time scale separation.

The elimination of fast degrees of freedom is one of the classical and central issues of non-equilibrium statistical physics. There exist numerous concepts to model the influence of a deterministic thermodynamic heat bath by effective stochastic forces or noise, resulting either in Langevin equations or stochastic differential equations, in Fokker–Planck equations or in Master equations and so on. Time scale separation and elimination of fast variables is of course also a central issue in quite different contexts, e.g. for the investigation of instabilities or the treatment of quantum mechanical systems on a mesoscopic level. Here one typically has a finite number of fast degrees of freedom and time scale separation is mediated by parameters of the system. For the case that fast variables have a relaxatory dynamics or for purely periodic fast degrees of motion several elimination schemes of fast variables have been developed (e.g. adiabatic elimination or slaving and averaging). In these cases the effective equation of motion for slow degrees of freedom reduces to a deterministic evolution equation and no stochastic features of the fast motion is visible on that level.

In our investigation we assume that slow degrees of freedom are coupled to a *finite number of fast chaotic modes*, hence, we do not involve any thermodynamic limit. Such problems arise for instance in climate research [1] and in molecular dynamics, where long time simulations are severely limited by the time needed to integrate the fastest modes in the system. Fast chaotic modes share with thermodynamic heat baths the exponential decay of correlations, and additional comparisons to noise processes suggest [2] that fast chaotic degrees of freedom can be modelled by suitable stochastic

processes. The goal of this project is to derive rigorously effective equations of motion for the slow degrees of freedom which contain the effect of the fast ones through a stochastic process.

We study a general model system with two time scales, where the slow degrees of freedom $\underline{x}$ are coupled to fast variables $\underline{y}$

$$\frac{d\underline{x}}{dt} = \underline{f}(\underline{x}, \underline{y}) \tag{1a}$$

$$\frac{d\underline{y}}{dt} = \frac{1}{\varepsilon}\underline{g}(\underline{x}, \underline{y}) \tag{1b}$$

Here the small parameter $0 < \varepsilon \ll 1$ mediates the separation of time scales, where $\underline{f}$ and $\underline{g}$ are assumed to be of the order of unity. We assume that the dynamics of the fast variables is exponentially mixing. We are aiming to approximate the motion of the slow variables $\underline{x}$ by an effective equation of motion where the fast variables $\underline{y}$ are replaced by a suitable stochastic process.

Therefore, we switch from a trajectory–wise description of solutions of equations (1) to the evolution in time of some time dependent phase space density ρ_t which is governed by the Liouville equation

$$\frac{\partial \rho_t}{\partial t} = -\mathcal{L}\rho_t\,, \quad \rho_0 = \rho\,, \tag{2}$$

where the generator $\mathcal{L}$ is given by

$$\begin{aligned} \mathcal{L}\rho &= -\left(\frac{1}{\varepsilon}\mathcal{L}_0 + \mathcal{L}_1\right)\rho\,, \text{ with} \qquad (3)\\ \mathcal{L}_0\rho(\underline{x}, \underline{y}) &= \sum_\nu \frac{\partial}{\partial y_\nu} g_\nu(\underline{x}, \underline{y})\rho(\underline{x}, \underline{y}) \\ \mathcal{L}_1\rho(\underline{x}, \underline{y}) &= \sum_\mu \frac{\partial}{\partial x_\mu} f_\mu(\underline{x}, \underline{y})\rho(\underline{x}, \underline{y})\,. \end{aligned}$$

Eq. (3) displays a natural splitting of the generator which we use in our perturbation scheme. The reduction to the slow degrees of freedom can be performed on the level of densities in a straightforward way by considering the reduced density

$$\bar{\rho}_t(\underline{x}) = \int d\underline{y}\rho_t(\underline{x}, \underline{y}) =: \mathrm{Tr}_{\underline{y}}[\rho_t]\,. \tag{4}$$

If we model the fast degrees of freedom by a fixed distribution $\rho_{\mathrm{ad}}(y|x)$ then the reduction can be achieved by the projection operator

$$\mathcal{P}\rho(\underline{x}, \underline{y}) = \rho_{\mathrm{ad}}(y|x)\mathrm{Tr}_{\underline{y}}\rho = \rho_{\mathrm{ad}}(y|x)\bar{\rho}(\underline{x}). \tag{5}$$

This operator is employed in a Mori-Zwanzig reduction technique which is well known in the context of non-equilibrium statistical physics [3]. Here it yields a formally exact and closed equation of motion for the reduced density, involving a memory term. By expansion of this memory term and approximation in lowest order perturbation theory this equation reduces to the Fokker-Planck equation for $\bar{\rho}_t$

$$\frac{\partial \bar{\rho}_t}{\partial t} = -\sum_\mu \frac{\partial}{\partial x_\mu} D_\mu^{(1,\mathrm{eff})}(\underline{x})\bar{\rho}_t(\underline{x}) + \sum_{\mu,\lambda} \frac{\partial^2}{\partial x_\mu \partial x_\lambda} D_{\mu\lambda}^{(2,\mathrm{eff})}(\underline{x})\bar{\rho}_t(\underline{x})\,, \tag{6}$$

where we obtain effective drift and diffusion coefficients which are given in terms of time averages of the fast dynamics. The drift consists of the adiabatic average of the slow vector field and a renormalisation by chaotic fluctuations[1]

$$D_\mu^{(1,\mathrm{eff})}(\underline{x}) = \langle f_\mu \rangle_{\mathrm{ad}} + \sum_\lambda \int_0^\infty dt' \left\langle f_\lambda(\underline{x},\underline{y}) \frac{\partial}{\partial x_\lambda} \delta f_\mu(\underline{x}, \underline{\eta}[t'/\varepsilon, \underline{y}; \underline{x}]) \right\rangle_{\mathrm{ad}} . \tag{7}$$

The diffusion is given by the autocorrelation of the fluctuation of the slow vector field

$$D_{\mu\lambda}^{(2,\mathrm{eff})}(\underline{x}) = \int_0^\infty dt' \langle \delta f_\mu(\underline{x}, \underline{\eta}[t'/\varepsilon, \underline{y}; \underline{x}]) \delta f_\lambda(\underline{x},\underline{y}) \rangle_{\mathrm{ad}} . \tag{8}$$

Since by assumption the correlation functions of the fast chaotic dynamics decay, the integrals in Eq. (7) and (8) converge if we impose some regularity assumptions. The Fokker-Planck equation may now be converted into the corresponding Langevin equation for the slow degrees of freedom, such that typical sample paths can be generated. Hence, fast chaotic degrees of freedom are replaced by Gaussian white noise. The fact that the approximate model is stochastic does not change the nature of the slow motion, since even the full model is stochastic in the sense that in many practical applications the initial conditions of the fast degrees of freedom are unknown and hence have to be chosen randomly, where due to chaos the slow solution sensitively also depends on the fast initial conditions.

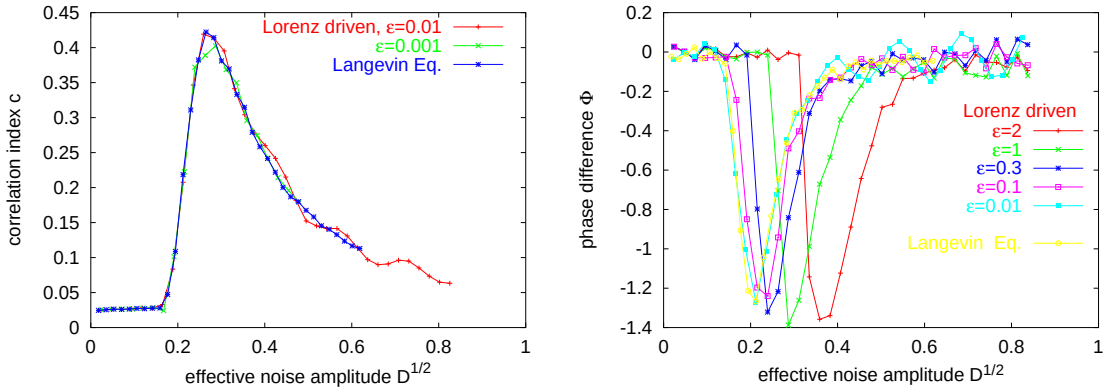
While the accuracy of our perturbation expansion has been analysed in detail by the discussion of an exactly solvable model (e.g. [4]) several systems have been investigated numerically (e.g. [5]). We briefly present the following investigation of the damped motion in a double well potential which is driven by small periodic forcing and the fast Lorenz system ($\sigma = 10, r = 28, b = 8/3$ and $\omega = 0.001, a = 0.1, \varepsilon > 0$)

$$\dot{x} = x - x^3 + a\cos(\omega t) + \kappa y_1 \qquad \begin{aligned} \dot{y}_1 &= \tfrac{\sigma}{\epsilon}(y_2 - y_1) \\ \dot{y}_2 &= \tfrac{1}{\epsilon}(r y_1 - y_1 y_3 - y_2) \\ \dot{y}_3 &= \tfrac{1}{\epsilon}(y_1 y_2 - b y_3) . \end{aligned} \tag{9}$$

For $0 < a \ll 1$ the periodic forcing is so weak that it cannot induce any transition between the two wells, nevertheless for $\kappa > 0$ one expects a finite probability for a jump from one well to the other. If the variable y_1 were white noise instead of fast chaos, this would be the classical stochastic resonance scenario. The maximal synchronisation between the jumps and the periodic forcing occurs at certain nonzero noise amplitude. The effective description of our deterministic "chaotic resonance" scenario in terms of the Fokker-Planck equation (6) for $D^{(1,\mathrm{eff})}$ and $D^{(2,\mathrm{eff})}$ given by

$$D^{(2,\mathrm{eff})} = \epsilon\kappa^2 \int_0^\infty \langle y_1(\tau) y_1(\tau + t) \rangle_\tau \, dt, \quad D^{(1,\mathrm{eff})}(x) = x - x^3 + a\cos(\omega t) \tag{10}$$

($\langle \cdot, \cdot \rangle_\tau$ denotes the auto-correlation function) is identical to the stochastic resonance scenario, where the noise amplitude is given by the properties of the fast deterministic subsytem. Using these predicted noise amplitude, the stochastic model generates correctly the hopping rates and phase relation obtained from the deterministic model (see



(a) (b)

Figure 1: *Chaotic and stochastic resonance: (a) Correlation c between the coordinate $x(t)$ and the periodic driving, and (b) the phase shift ϕ between the periodic driving force and the response $x(t)$, both a comparison of the numerical integration of the equation (6) and the approximate Langevin dynamics. The 'effective noise amplitude' for the deterministic simulation is obtained according to $D = D^{(2,\mathrm{eff})}$. In the simulation we fix ε and tune κ to produce the curves shown above.*

Eq. (1)). This example shows impressively the benefits of stochastic modelling. The *ad hoc* complete elimination of the fast degrees of freedom, which here is equivalent to zeroth order approximation in ε, would destroy the relevant dynamical feature of hopping between the wells. In contrast to that, our derived noise process which is of first order in $\sqrt{\varepsilon}$ produces quantitatively correct hopping rates and synchronization effects. We remark that due to the one-dimensional nature of the slow dynamics, no deterministic reduced model would be capable of producing these phenomena.

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[1]Here, by $\langle h\rangle_{\mathrm{ad}}(\underline{x}) := \int d\underline{y} h(\underline{x},\underline{y})\rho_{\mathrm{ad}}(\underline{y}|\underline{x})$ we denote the adiabatic average and by $\delta\underline{f}(\underline{x},\underline{y}) = \underline{f}(\underline{x},\underline{y}) - \langle\underline{f}\rangle_{\mathrm{ad}}(\underline{x})$ we denote the static fluctuation. Further, $\underline{\eta}[t,\underline{y};\underline{x}]$ denotes the solution of the equation of motion (b) for $\varepsilon = 1$ with initial condition $\underline{y}$.

1.10 Markov chain models from data - prediction of turbulent gusts in surface wind

Holger Kantz, Mario Ragwitz, Detlef Holstein

Time series analysis in reconstructed state spaces [1] has proven its usefulness in the analysis of a huge number of physical laboratory experiments. Starting from the paradigm of low dimensional deterministic chaos, scalar time series data obtained by typical physical measurements are embedded in the time delay embedding space. As it is guaranteed by the theorems of Takens and Sauer et al. [2], this space is equivalent to the unobserved (and most often unobservable) phase space of the system, so that it serves as a valid basis for all successive analysis steps. Among them and most strikingly is the possibility of prediction: In the reconstructed space, successive delay vectors as images of the underlying state vectors of the system are related to each other by a unique deterministic map. This map can be extracted from observed data on different levels of sophistication and can be used for modelling and for the prediction of future measurements [3].

Unfortunately, the class of deterministic low dimensional systems is extremely small – outside the physics laboratory it is almost absent. Hence, we have devoted considerable effort during the last years to extend the above mentioned methods towards more realistic situations. Two directions have been pursued: First, it is evident that a more natural class of systems is represented by nonlinear stochastic processes generated by Langevin equations of the form

$$\dot{\vec{x}} = \vec{f}(\vec{x}) + \mathbf{G}(\vec{x})\vec{\eta}(t) \tag{1}$$

where $\vec{x}$ describes the state of the system and $\vec{\eta}$ is a vector valued Gaussian white noise process. Hence, we assume a small number of degrees of freedom to be driven by random forces. As it is well known, the Langevin dynamics represents a vector valued Markov process.

The second complication which we encounter in practice is non-stationarity. Almost all time series tools require stationarity, which implies that all system parameters should be constant during the time of observation. Exactly this is violated in almost all field measurements and also in many laboratory systems. As we could verify in previous work together with Hegger, Schreiber, Matassini [4], the concept of over-embedding is a suitable approach towards non-stationary deterministic data, if the non-stationarity is induced by slow parameter drifts with rare sudden jumps. Over-embedding means that the identification of the current state vector is given by a time delay vector of higher dimensionality than needed for the same system with fixed parameter values. More precisely, the reconstructed space is designed to be equivalent to the *extended state space* of the system given by the direct product of the state space and the space spanned by the time dependent parameters. Following Whitney's embedding theorem, k extra dimensions of the extended state space require additional $2k$ dimensions in the time delay embedding.

For the analysis of time series data from a nonlinear stochastic process, let us for a moment assume that this process is a time discrete Markov chain of order m in the single variable s. This means that the full knowledge of this process is represented by the set of all m dimensional transition probability densities $p(s_{n+1}|s_n, \ldots, s_{n-m+1})$.

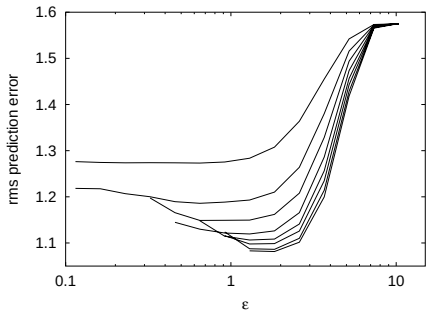

Figure 1: *The average prediction error for independent Gaussian random numbers with a time dependent mean as a function of the neighbourhood diameter ϵ in Eq. 4, and for Markov chain orders m=1,...,8 from top to bottom. For stationary data, m=1 and $\epsilon = 1$ would be perfect. In the non-stationary case, over-embedding ($m > 1$) and locality ($\epsilon < 1$) improve the predictions, since implicitly the actual value of the time variant mean of the Gaussian distribution is identified.*

If we possess a single long time series $\{s_n\}$, $n = 1, \ldots, N$, we can estimate these transition probabilities in a straightforward way from the data by the relative frequencies of occurrences, under the additional assumption of a smooth dependence of $p(s_{n+1}|s_n, \ldots, s_{n-m+1})$ on all of its arguments (maximum likelihood estimate).

As mentioned above, a sample path generated by a Langevin equation represents a vector valued Markov process. The observable s of our time series data is, as in the deterministic case, assumed to be obtained by applying a measurement function $o(\vec{x})$ to the state vectors, $s_n = o(\vec{x}(t = n\Delta t))$, where Δt is the sampling interval. It is tempting but wrong [5] to assume that the observable s_n itself represents a scalar Markov process, or more precisely, that the discrete time sampling converts it into a Markov chain of finite order. Instead, an infinite memory has to be expected.

The concept of coarse grained dynamical entropies [6] in the sense of the Kolmogorov Sinai entropy can be used to investigate this memory. It turns out that typically the amount of information stored in the past decays fast with the time lag, so that an approximate description in terms of a Markov chain is appropriate for most data sets. This is true even more, since modelling errors introduced by statistical fluctuations due to the finiteness of the time series become the larger the higher the order of the chosen Markov chain model, such that the optimal model where the truncation error and the modelling error are of the same smallness is definitely of finite order. However, an ongoing PhD thesis (D. Holstein) is devoted to the issue of determining the decay of memory through coarse grained dynamical entropies and to derive criteria for the accuracy of finite approximations to non Markovian processes.

Once we accept that a given stationary multivariate Markov process can be approximated in some accuracy by a Markov chain of order m in a scalar observable s, the issue of non-stationarity can be solved as before [7]: We assume that the transition probabilities are smooth functions of some few slowly time dependent parameters. Hence, we have to include the desired values of the time dependent parameters into the conditioning, i.e., $p(s_{n+1}|s_n, \ldots, s_{n-m+1}, t) = p(s_{n+1}|s_n, \ldots, s_{n-m+1}, p_1(t), \ldots, p_k(t))$. Since the parameters $p(t)$ are unobserved, we have to estimate them implicitly from the data, which is again done by a kind of over-embedding. Hence, $p(s_{n+1}|s_n, \ldots, s_{n-m+1}, p_1(t), \ldots, p_k(t)) \approx p(s_{n+1}|s_n, \ldots, s_{n-m+1}, s_{n-m}, \ldots, s_{n-l})$. However, in contrast to the deterministic case, again the lack of a Markovian structure in the time delay embedding space prevents us from setting $l - m = 2k$ (as above), but instead the identification of the actual values of the parameters becomes the better the larger m. This is illustrated in Fig.1, where we demonstrate the ability to model non-stationary stochastic data by Markov chains by predictions [8].

Prediction means to derive an estimate for a future observation which minimises a certain cost function. If we assume uncorrelated Gaussian errors, the maximum likelihood principle yields as a cost function the mean squared prediction error,

$$e^2 = \langle (\hat{s}_{n+1} - s_{n+1})^2 \rangle \stackrel{!}{=} \min \tag{2}$$

where $\hat{s}_{n+1}$ is the prediction of the observation s_{n+1} exclusively based on information from the past. In view of our Markov chain approximation for the observed data, the solution of this minimisation problem is given by

$$\hat{s}_{n+1} = \int s' p(s'|\vec{s}_n) ds' \ , \tag{3}$$

which is the mean value of the transition probability conditioned to the actual m-dimensional delay vector $\vec{s}_n$ which represents the actual state of our mth order Markov chain. This expression can be easily turned into a statistical estimator to be applied to data when we assume that the transition probability is smooth in all its arguments:

$$\hat{s}_{n+1} = \frac{1}{||\mathcal{U}_\epsilon(\vec{s}_n)||} \sum_{k:\vec{s}_k \in \mathcal{U}_\epsilon(\vec{s}_n)} s_{k+1} \ . \tag{4}$$

Here, $\mathcal{U}_\epsilon(\vec{s}_n)$, the ϵ-neighbourhood of $\vec{s}_n$, is the set of all delay vectors from the past whose distance to $\vec{s}_n$ is smaller than ϵ in some suitable norm. Their futures are supposed to represent a random sample according to $p(s'|\vec{s}_n)$, since the fact that $\vec{s}_k \in \mathcal{U}_\epsilon(\vec{s}_n)$ serves as the correct conditioning. The order of the Markov chain model is implicitly contained in Eq. (4) through the dimension m in which neighbours are sought.

Wind speeds measured at the surface of the earth represent an immense reduction of information about the turbulent wind field. Our data are from the research centre in Lammefjord in Denmark. The absolute wind speeds measured by cup anemometers are recorded with a sampling rate of 8 Hz. The optimisation of parameters such as embedding dimension and neighbourhood sizes was performed for prediction horizons of up to three seconds, since the goal of these short term predictions is a forecast of turbulent gusts. Since turbulent gusts are a major danger for the save operation of wind energy turbines, their prediction is of high technological and economical relevance. A predicted gust could be made harmless by a simple change of the pitch angle of the rotor blades, which uncouples them from the wind field. For this purpose, a prediction horizon of up to a few seconds is sufficient. Evidently, the longer into the future predictions are to be made, the less accurate they are.

Several benchmarks for predictions exist in this case: persistence, which means that on average, the future wind speed is identical to the actual one, supplies a trivial but rather good predictor for the absolute speed, but it is evidently worthless for the prediction of gusts, which are characterised by a sudden increase of the wind speed. The trend extrapolation from the last two measurements $\hat{s}_{n+1} = 2s_n - s_{n-1}$ yields good short time predictions for smooth data but is worse than persistence for our turbulent data. Beyond that, linear auto-regressive models can exploit linear correlations in the data. The quality of the predictions is measured by the root mean squared prediction errors Eq. (2). The comparison of the prediction errors as a function of the prediction

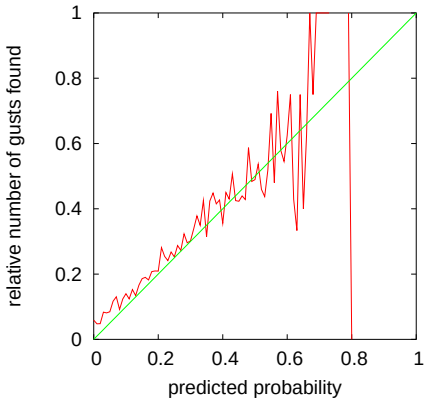

Figure 2: *The reliability plot for 20000 predictions during 24 h of Lammefjord data "tag191.dat" containing wind speeds between 2.8 and 18.8 m/s. The curve is truncated where for large predicted probabilities no events occurred. If the predictions were perfect, the empirical line should coincide with the diagonal (8Hz data, prediction 1.5s ahead, m=6 with a time lag 2).*

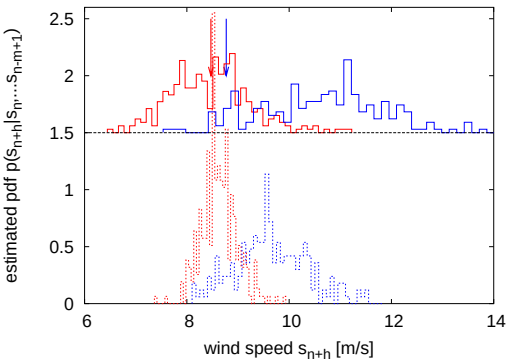

Figure 3: *Estimated conditional probability density functions: Red in a situation where prob(gust > 1)= 0.09, blue for prob(gust > 1)=0.7. The arrows indicate the wind speeds s_n at the moment when the prediction was performed. The lower histograms show the pdfs after 3/8s (h=3), the ones shifted by 1.5 are for 1.5s ahead (h=12). Evidently, the conditioning on the $m-1$ past components which are not shown introduces the very difference of the two situations (data and parameters as in Fig. 2).*

horizon obtained by the different prediction schemes shows an about 10% superiority of the locally constant scheme Eq. (4). This by itself would not be a relevant result.

Since within our treatment turbulent gusts appear randomly according to a rather broad distribution, where our prediction represents its mean value, it is not surprising that the predicted wind speed typically does not predict a gust. It is more appropriate to predict how probable it is that during the next h samples the wind speed increases by more than g m/s with respect to its present value. This probability can be computed from the conditional probability by

$$prob(\text{gust} > g) = \frac{1}{h}\sum_{k=1}^{h}\int_{s_n+g}^{\infty} ds_{n+k}\; p(s_{n+k}|\vec{s}_n)\;, \tag{5}$$

where the conditional probability density is again obtained from the data as described above. Since by construction for every prediction we have a single realisation only, one might ask how to check the correctness of the predicted probabilities. This is done by the *reliability plot* known from weather forecasting. One gathers all those events among the predictions where the predicted probability *prob*(gust) in Eq. (5) is inside $[r, r+dr]$ and counts in how many of these cases actually a gust followed. If our predicted probabilities were perfect and the sample were large enough, we would expect that a fraction of exactly r of these events were gust events. As we show in Fig. 2, we are pretty close to such a situation, where, however, the large predicted probabilities occur too rarely for a meaningful statistical test. Finally, we show in Fig.3 two transition probabilities. The last observation s_n has almost the same value in both cases, but the $m-1$ past values are very different, so that the conditioning

onto a delay vector (i.e., assuming a Markov chain of order $m > 1$) is essential for a meaningful prediction.

The results together with a more general investigation of two and three dimensional turbulent data are described in detail in [9]. A few words on the supposed origin of predictability in a turbulent wind field are in order. Our measurements are local in space. For nonzero mean wind speeds, the wind field drifts across our measurement locations. Hence, what we want to predict is not a result of the local dynamics, but it is spatially remote in the moment when the prediction is to be made. Hence, predictability can only be possible due to spatio-temporal correlations. Such correlations are known as eddies or coherent structures in turbulence research. It seems that a typical source of a sudden increase of the wind speed is the backward border of a coherent structure drifting across the measurement device, and that the approach of this border can be partly predicted from the data.

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1.11 Neutral Evolution of Proteins

Markus Porto

The neutral theory of molecular evolution was formulated in the late 1960's to explain the high substitution rate of amino acids observed in proteins of many vertebrates and the large intra-specific genetic variations between most species [1]. The theory assumes that most of the amino acid substitutions occurring in an evolving population do not bring any selective advantage to the individual but are selectively neutral, as they maintain the biological activity of the protein at the original level. Such neutral

mutations are assumed to occur at random at a rate μx, where μ represents the genomic mutation rate and x is the fraction of mutations which happen to be neutral. The theory predicts that (i) the rate of substitutions (mutations which become fixed in the population) equals the neutral mutation rate μx and depends only on the protein considered, independent of the size of the population and its ecology, and that (ii) the number of amino acid substitutions taking place in a time t follows a Poisson distribution with mean value $\mu x t$, thus giving an explanation to the 'molecular clock' observed in the early 1960's [2]. Later studies in the 1970's and 1980's have shown, however, that the variance of the substitution process is larger than its mean value [3], pointing to an underlying non-Poissonian process. Since then, different alternatives have been suggested to explain these observations. Some authors have extended the neutral theory by including into it slightly deleterious mutations [4], others have rejected the neutral theory completely and have suggested that most mutations are fixed by positive selection [5]. An interesting proposal within the realm of neutral theory is its modification in terms of a fluctuating neutral space model [6], which can account for the non-Poissonian statistics.

In recent years a lot of progress in the understanding of protein folding and the thermodynamics of biomolecules has been made. These achievements have opened the way to assess the thermodynamical stability of biomolecules involved in evolution through computational methods, thus providing powerful tools to complement the traditional population genetic approach. This structural approach has been introduced in the study of neutral networks (i.e., the set of sequences connected by structure conserving mutations) of RNA secondary structures [7], and has found fruitful applications in the study of protein evolution [8]. Following this structural approach, we have investigated seven of the most studied protein folds using a model of neutral evolution, which we have called *structurally constrained neutral model* (SCN model), in which conservation of the thermodynamic stability of the native structure is imposed [9, 10]. This assumption relies on the empirical observation that protein structures are much more conserved than amino acid sequences. Within the SCN model, well-established empirical methods which are able to estimate the thermodynamic stability of a test sequence in the target structure provide a realistic genotype to phenotype mapping. Based on these methods, the simulations yield evolutionary trajectories consisting of sequences connected through neutral point mutations. For each visited sequence, we determine all neutral neighbor sequences accessible by a point mutation (one of which is randomly chosen to become the next visited sequence), and measure the number of these possible neutral mutations, the latter being proportional to the local connectivity of the neutral network. We find that this quantity fluctuates strongly along an evolutionary trajectory [9], and consequently the SCN model produces a non-Poissonian substitution process, consistent with a fluctuating neutral network scenario [6] and with the statistics of protein evolution [3].

One interesting application of the SCN model is the possibility to distinguish between functional and structural conservation using a comparison with actual evolution data extracted from protein databases [9]. The simulated neutral evolution yields the positions being more difficult to mutate, which we identify as structurally conserved residues. On the other hand, the positions which are conserved in actual evolution but not in the SCN model are the functionally conserved ones, and practically all residues

whose functional role is known belong to this class. Most positions are not conserved in the SCN model, as similarly observed in actual evolution data. Those are the neutrally evolving positions, and their preeminence is an evidence of the importance of neutral evolution. Finally, a very small number of residues appear structurally important in the SCN model but are not significantly conserved in empirical data. This could be due to a limitation either of the SCN model or of the protein databases, but it could also be a hint of structural changes, possibly positively selected.

We have also established that the number of neutral neighbors along the evolutionary trajectories generated by the SCN model, besides being broadly distributed, displays strong auto-correlations [10]. This feature should have very general consequences. For example, one might expect that more densely populated folds possess a larger average value of neutral neighbors, since this makes it more likely that a fold develops new functions through gene duplication and subsequent substitutions conserving its stability. However, the observed correlations could increase the importance of 'frozen accidents' in the evolution of new functions and hence reduce the extent to which the number of sequences per fold is correlated to the average value of neutral neighbors. Moreover, we have shown that the found correlations cause the breakdown of self-averaging of the resulting evolutionary substitution process, which can drastically influence the patterns of protein evolution. For instance, the correlations might overshadow lineage effects such as the generation time effect [5, 11], or mimic patterns that resemble those that may result from positive selection. The best current bioinformatic method to identify such cases of positive selection [12] assumes a neutral substitution process with constant number of neutral neighbors. The broad distribution and the correlations that we observe might serve to improve the performance of such methods.

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1.12 Double photoionization: Mechanisms and their separation

Tobias Schneider, Peter L. Chocian and Jan M. Rost

In an effort to understand correlation in excited electron dynamics one often resorts to simple pictures and speaks of different "mechanisms", e.g., "shake-off"[1, 2] and "TS1"("two-step-one") [3]. If justified at all such pictures are mostly based on a perturbative approach. In the specific situation of double photoionization, this refers to a perturbative treatment of the photon-electron interaction *and* the electron-electron interaction. While the first approximation is clearly justified, the second approximation comes from a traditional diagrammatic perturbation theory (e.g., many-body perturbation theory) whose first terms were used in the early days to theoretically predict double photoionization. Present day theory has reached much more accuracy and excellent agreement with experiment by solving the problem fully numerically [4]. This can be accomplished by expanding the Schrödinger equation into a system of first order close coupling equations. However, the familiar "pictures"of how to understand the process are lost in this accurate treatment.

Is it possible to preserve these mechanisms, yet obtain accurate results which are approximate but not in the electron-electron interaction? This would require to justify the mechanisms on a completely different basis. Indeed, this can be done if one makes use of an $\hbar$-expansion, i.e., views the mechanisms in terms of their quantum nature [5]. It turns out that "shake-off"(SO) is a pure quantum effect. This means, on the other hand, that a quasi-classical description of double-photoionization will not contain any SO-contribution. From a classical perspective, one could say that one needs SO as a quantum correction to the classical result to adequately describe the experiment. It also implies (since it is claimed that the TS1 process and SO together explain the experiments) that the classical description should correspond to TS1. The latter means in the double photoionization context that in a first step one electron absorbs the photon taking all its energy and in the next step this fast electron collides on its ionizing path with the other bound electron transferring enough energy to set it free as well. This scenario one can indeed see in the classical ionizing electron trajectories in Fig. 1 where at a certain time there is a strong interaction between the electrons (large e-e interaction energy). This encounter transfers enough energy to free the electron which was bound before. Hence, TS1 indeed occurs even in a classical but fully correlated description of e-e interaction. The details of our classical photoionization model are described elsewhere [5]. We make use of a Wigner transform of the initial wavefunction to translate it to phase space and propagate the electrons classically.

It remains to describe the shake-off. This has been done many times in the literature,

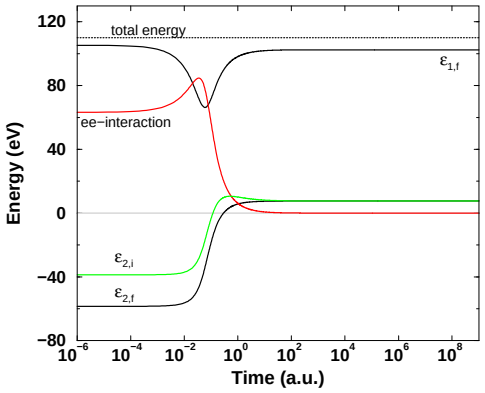

Figure 1: *Energy of the two electrons in helium after photoabsorption along a classical double-ionizing trajectory. One electron ($\mathcal{E}_{Z,1}$) has absorbed the photon, the energy of the other one is measured with respect to the screened $\mathcal{E}_{(Z_{\rm eff},2)}$ and unscreened ($\mathcal{E}_{Z,2}$) nucleus. The electron-electron repulsion has a maximum indicating the single collision between the electrons. The total energy is E.*

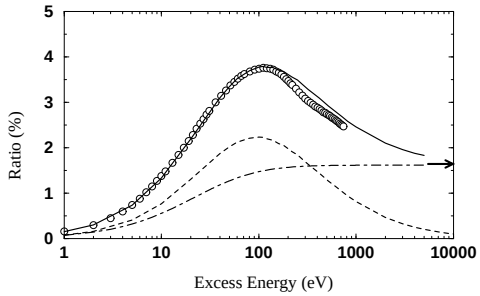

Figure 2: *Contribution of shake-off (dashed-dotted) and knock-out (TS1, dashed) and their sum (solid) to the experimental double-to-single photoionization ratio (circles, [7]). The arrow indicates the asymptotic ratio for large energies.*

what is less known is an energy dependent SO since SO is traditionally an approximation for high energies or short interaction times: One assumes that one electron leaves the atom so fast that the other electron remains at its position, or, in other words, the initial wavefunction is unchanged but taken at the position $\vec{r} = 0$ for the electron which escaped. (This would be its position in the wavefunction for infinitely high energy). The extent to what the remaining electron has been shaken off or up can be quantified further in a sudden approximation by projecting the wavefunction onto final states of the *ion*. Integrating over the continuum part of the shaken electron distribution provides the shake-off probability for double ionization $P_{\rm SO}^{++}$. This probability becomes energy dependent if one takes into account that the shake electron acquires energy only up to the total energy E since the other electron is in the continuum as well and its minimum energy is therefore zero. Figure 2 shows the contributions of shake-off and TS1 to the double-to-single photoionization ratio, a quantity directly accessible in the experiment. As one can see the agreement is good and only achieved if both contributions are added. Thereby, one sees again that SO is a high energy phenomenon, with zero weight at threshold ($E = 0$), and a finite value for $E \to \infty$. On the other hand, TS1 vanishes near threshold and it also vanishes for high energies.

The classical/quantum approach provides an alternative to justify the separation into TS1 and SO. So far, it has been the only way to describe double photoionization accurately in terms of these two mechanisms. Furthermore, SO may be interpreted as a quantum correction to the classical photoionization.

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1.13 Electron release in rare gas atom clusters

Christian Siedschlag and Jan M. Rost

Exposing a rare gas atom cluster of some ten atoms to an intense and short laser pulse results in a violent and complete disintegration of the cluster into multiply charged ions and many electrons.

The electron release depends on a number of parameters, e.g., the peak intensity of the laser, the pulse length, the atomic element, and, last not least, the number of atoms in the cluster, i.e., the cluster size.

Is there a way to predict quantitatively the electron release? Or, more precisely, does one of the aforementioned parameters influence the electron release dominantly, and if so, what is the mechanism behind it?

At least four time scales are involved in this problem: the orbital time of the bound electron ($\sim$ 1 a.u.), the optical period ($\sim$ 100 a.u. for 780 nm light), the pulse length (some 10-1000 optical cycles), and finally the motion of the ions, depending on the atomic mass from 10^3 to 10^5a.u.. Since ionic motion and pulse length share roughly the same time scale, one might gain insight into the dynamics of electron release by recording it as a function of pulse length T. We have formulated a mixed quantum-classical description to follow the cluster dynamics in time [1]. A typical result is shown in Fig. 1 for a Xe_{16} cluster in comparison with an atom. Indeed, a behavior very different from the decreasing atomic electron release is observed. A characteristic maximum occurs at some pulse length T^* - this hallmark we have also found for other rare gas clusters and for different cluster sizes, from 8 to 30 atoms.

The degree of freedom which the atom lacks is the cluster's ability to expand, at a different speed depending on the degree of ionization and the mass of the cluster atoms. Hence, one could suspect that a critical cluster radius R^* exists for maximum electron release, which the cluster may or may not reach during expansion. This can be easily checked by subjecting the cluster to the laser pulse with fixed atoms. Changing the size of the cluster without changing its shape by a scaling $R_i^\lambda = \lambda R_i^0$, where R_i^0 are the equilibrium distances of the cluster atoms, confirms the existence of a critical radius R^* for maximum electron release (Fig. 2.). We have identified the mechanism leading to the critical radius to be the same as in diatomic and triatomic molecules, namely enhanced ionization (ENIO), first discovered in diatoms [3]. Resonance driven mechanisms, as recently proposed for metal clusters [4], can be excluded based on the behavior for different laser frequencies. While resonance mechanisms naturally are very sensitive to the laser frequency to which some internal frequency must be in resonance,

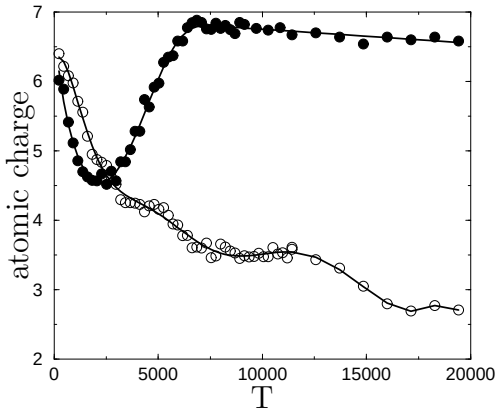

Figure 1: *Average atomic charge of Xe_{16} (•) and Xe (∘) as a function of pulse length. The lines are to guide the eye.*

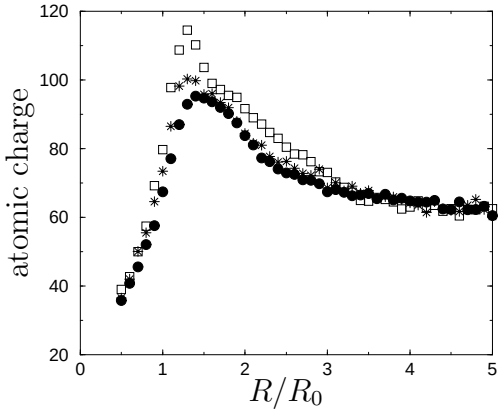

Figure 2: *Electron release of Xe_{16} for fixed nuclei. Results are shown for a pulse length of $T = 55$ fs and the frequencies $\omega = 0.055$ a.u. (•), $\omega = 0.075$ a.u. (⋆), and $\omega = 0.11$ a.u. (□).*

the ENIO mechanism is insensitive to change of the frequency and this is what we find (Fig. 2).

We can even quantitatively relate the maximum electron release to the critical pulse length T^* [2]. This requires a careful analysis of the different processes which happen during the laser pulse. In a first "atomic phase", a few electrons are boiled off the cluster, purely by the laser field. This phase lasts until time T_0, determined (somewhat arbitrarily) by the condition that every second atom of the cluster is ionized, or, equivalently, that each atom is ionized with 50 % probability. Now the cluster begins to expand, and the second "molecular phase", which is the important one, lasts until the critical radius R^* has been reached. Finally, in phase III the relaxation and complete disintegration of the cluster proceeds. Maximum electron release should occur if R^* is reached roughly at the maximum intensity of the pulse, i.e., after $T^*/2$. Hence, phase II lasts for $\tau^* = T^*/2 - T_0^*$. Using a simple Coulomb explosion scenario with a time-dependent scaling parameter $\lambda(t)$ one can motivate that τ^* is proportional to the ratio $r = (K_0/V_0)^{1/2} f(\lambda)$ where V_0 is the potential energy of the ions at time T_0^*. K_0 has form and units of a moment of inertia and represents the influence of the shape of the cluster (at time T_0^*) on its expansion [1]. The function $f(\lambda)$ is the analytical solution of the time-dependent Coulomb explosion in λ.

Hence, the seemingly complicated dynamics of a rare gas atom cluster in an intense laser pulse exhibits a remarkably simple and characteristic behavior when approached in a time-dependent fashion by changing the laser pulse length.

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1.14 Chaotic ionization of non-classical alkali Rydberg states

Andreas Krug and Andreas Buchleitner

Rydberg states of atomic hydrogen are the perfect quantum analog of classical planetary motion. They incarnate the correspondence principle via the equivalence of the classical principal action and the principal quantum number n_0, as well as of the classical Kepler frequency and the local energy spacing in the Rydberg progression. Also under strong periodic driving they exhibit the essential features of the underlying classical dynamics [1, 2], which go chaotic as the driving field amplitude F is increased. However, classically chaotic motion is tantamount to the destruction of symmetries and, hence, of good quantum numbers in the quantum system. Therefore, a large number of quantum states, i.e. a large spectral density is needed as a prerequisite for quantum dynamics to resolve the intricate phase space structures of classically chaotic dynamics [1]. Furthermore, the periodic driving induces multiphoton transitions of variable order between atomic bound and continuum states, which finally gives rise to the ionization of the atom [3]. Indeed, it is the resulting ionization yield which is typically used as the experimental probe of the chaotic bound-state dynamics [2].

In laboratory experiments, it is state of the art to produce atomic Rydberg states with principal quantum numbers n_0 between 20 and 120 [2, 4, 5]. Employing typical laboratory microwave frequencies, chaotic ionization is mediated by multiphoton transitions of the order $k \geq 29$ (simply given by the ratio of the initial state ionization potential to the photon energy), and an exact theoretical/numerical treatment of the corresponding quantum mechanical eigenvalue problem remained untractable so far, simply due to its dimension [3]. Furthermore, for reasons of experimental convenience, a considerable part of experiments was performed using Rydberg states of alkali [5, 6] rather than of hydrogen atoms [2], starting from the hypothesis that the driven dynamics of the highly excited Rydberg electron should not undergo any relevant changes due to the presence of a multielectron core localized in the immediate vicinity of the nucleus. All available data prove, however, the opposite: nonhydrogenic alkali Rydberg states appear to ionize at considerably lower driving field amplitudes than Rydberg states of atomic hydrogen [2, 5, 6].

Yet, the alkali ionization problem is even more complex than the one of atomic hydrogen above, since it additionally involves quantum mechanical scattering of the Rydberg electron off the multielectron core [7, 8]. Given the unavailability of a rigorous theoretical treatment, the above puzzling experimental observations were therefore unexplained for more than one decade [2, 9].

Only now, with the advances in high-performance, massively parallel computing, and the availability of large scale supercomputing facilities (like the CRAY T3E Garching, and the HITACHI SR8000-F1 Munich) we are able to tackle this challenging problem, i.e. to treat the described atomic ionization process in its full complexity, without any essential approximations nor adjustable parameters. Combining group theoretical methods for the description of the atomic degrees of freedom (including the continuum), R-matrix theory to include the non-vanishing quantum defects induced by the multielectron core [7], the Floquet theorem to account for the periodic driving, complex dilation to extract the energies and decay rates of the atomic eigenstates in the field [3], and an intelligent, parallel implementation of the Lanczos algorithm with excellent scalability, we have been able to perform the first numerical experiment on the microwave ionization of nonhydrogenic $\ell = 0$ angular momentum Rydberg states of lithium [10]. We precisely chose the experimental parameters employed in laboratory experiments on atomic hydrogen [11] (i.e., driving field frequency $\omega/2\pi = 36$ GHz, atom-field interaction time $t = 327\times 2\pi/\omega$, and principal quantum numbers in the range $n_0 = 28, \ldots, 80$), with the *only exception* of a finite quantum defect of the lithium $\ell = 0, 1, 2, 3$ angular momentum states (i.e., $\delta_{\ell=0} = 0.39947$, $\delta_{\ell=1} = 0.04726$, $\delta_{\ell=2} = 0.00213$, $\delta_{\ell=3} = -8\cdot 10^{-5}$ [12]), and a well-defined atomic initial state $\mid n_0,\ \ell_0 = m_0 = 0\rangle$, with m_0 the angular momentum projection along the fixed field polarization axis. Furthermore, we assumed a constant microwave amplitude F experienced by the atoms, thereby neglecting pulse-induced switching effects. These, however, are of minor importance in this kind of experiments [2, 3]. Consequently, the order of the multiphoton process that finally leads to the disintegration of the atom extends from $k \geq 15$ (for $n_0 = 80$) to $k \geq 120$ (for $n_0 = 28$).

Figure 1 compares our numerical experiment on lithium to laboratory data on atomic hydrogen [2, 11]. The plot uses "scaled variables" [1] F_0 and ω_0, i.e. the driving amplitude F and the driving frequency ω are measured in units of the Coulomb force ($\sim n_0^{-4}$) and of the Kepler frequency ($\sim n_0^{-3}$) along the unperturbed classical two-body Coulomb trajectory. It shows the ionization threshold field $F_0(10\%)$, i.e. the field amplitude needed to induce an ionization probability of 10% at given interaction time t and frequency ω, for different principal quantum numbers n_0 [1, 2, 4, 5]. In a classical description of the driven two-body Coulomb problem, F_0 and ω_0 completely determine the classical phase space structure, what allows for an immediate interpretation of the experimental hydrogen data in Fig. 1 in terms of the underlying classical dynamics [2]. Most prominently, the hydrogen ionization threshold decreases almost monotonously in the frequency windows (II) and (III), and exhibits local maxima around $\omega_0 \simeq 1.0 \ldots 1.3$ and $\omega_0 \simeq 2.0 \ldots 2.5$, on top of a global increase in the frequency window (I). The decrease in (III) and (II) essentially follows the classical ionization threshold which can be extracted, e.g., from classical 3D Monte Carlo simulations of the hydrogen experiments [2], whereas the global increase in (I) is a signature of dynamical localization [5, 11], the analog of Anderson localization in the quantum transport of driven, chaotic, low-dimensional Hamiltonian systems [13]. The local maxima around $\omega_0 \simeq 1.0$ and $\omega_0 \simeq 2.0$ are a quantum signature of locally integrable [2] or "sticky" [14] classical dynamics, within or in the vicinity of nonlinear resonance islands in classical phase space.

Comparison of the laboratory to the numerical experiment immediately leads to the following observations:

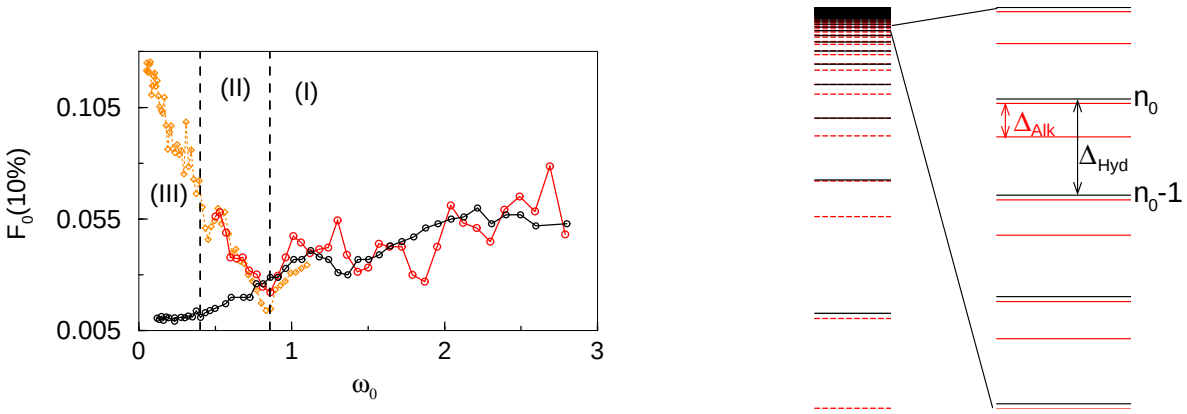

Figure 1: *Left: Laboratory ionization threshold* $F_0(10\%) = F(10\%)n_0^4$ *of atomic hydrogen (orange [11] and red [2]), compared to our numerical experiment on the* $|\, n_0,\ \ell_0 = m_0 = 0\rangle$ *state of lithium (black), as a function of the scaled frequency* $\omega_0 = \omega n_0^3$. *Laboratory and numerical data were obtained under* precisely *the same conditions, i.e. at* $\omega/2\pi = 36$ GHz, *interaction time* $t = 327 \times 2\pi/\omega$, *and principal quantum numbers* $n_0 = 28 \ldots 80$. *Finite switching times of the microwave pulse are responsible for the more pronounced structures of the laboratory data as compared to the lithium results (obtained for constant microwave amplitude), but do not affect the globally very good agreement in the* ω_0*-interval (I). We also reproduce the experimental results obtained with* $\omega/2\pi = 9.923$ GHz *[2], to cover the low-*ω_0 *regime for hydrogen. (I), (II), and (III) distinguish the scaled frequency ranges where* $\omega > \Delta_{\rm Hyd}^{(n_0)}$, $\Delta_{\rm Alk}^{(n_0)} < \omega < \Delta_{\rm Hyd}^{(n_0)}$, *and* $\omega < \Delta_{\rm Alk}^{(n_0)}$, *as illustrated by the level scheme on the right. Here, the black and the red lines distinguish the hydrogenic and nonhydrogenic energy levels of the lithium Rydberg progression. The detail on the right identifies the relevant frequency scales.*

1. In the frequency window (I), the ionization thresholds of nonhydrogenic Rydberg states of lithium follow the global trend of the hydrogen data, in particular with the *same* absolute values of the driving field amplitude. Furthermore, the lithium data exhibit local maxima at $\omega_0 \simeq 1.1$ and $\omega_0 \simeq 2.2$, very much as the hydrogen data.

2. There is a dramatic difference between hydrogen and lithium thresholds in the frequency window (II), where the lithium thresholds continue to increase with ω_0, whereas the hydrogen thresholds decrease from rather high values, in accordance with classical results [1, 2].

3. The scaled lithium thresholds are essentially n_0-independent at very low values in the interval (III), whereas hydrogen exhibits (classical) thresholds approx. 10 to 20 times as large as for lithium, in this low-frequency regime.

The clue for understanding these features lies in the level structure of the unperturbed alkali spectrum which is illustrated in Fig. 2: For driving frequencies ω larger than or comparable to the energy difference $\Delta_{\rm Hyd}^{(n_0)} \sim n_0^{-3}$ between neighbouring hydrogen manifolds, and this is precisely in the regime (I), the driving field can efficiently mix hydrogenic and nonhydrogenic levels of the lithium atom, even for initial atomic states with nonvanishing quantum defect. Since in this frequency domain the essential symmetry properties of the driven two-body Coulomb problem below the ionization threshold prevail in the alkalis [7], also the transition to chaotic transport in the classical dynamics (i.e., the destruction of these symmetries) dominates the ω_0- or n_0-dependence

of the ionization threshold of nonhydrogenic alkali Rydberg states, *despite* their manifestly non-classical character due to the scattering of the Rydberg electron off the multielectron core [8].

For driving frequencies ω larger than the closest energy-gaining dipole transition frequency $\Delta_{\rm Alk}^{(n_0)}$ starting out from the nonhydrogenic initial state, but smaller than $\Delta_{\rm Hyd}^{(n_0)}$ (regime (II)), the driving field is still capable to efficiently couple different hydrogenic and nonhydrogenic states, whereas no comparable excitation mechanism is available in the hydrogen atom. Consequently, the general dependence of $F_0(10\%)$ on ω_0 is unaltered for lithium in this regime, whereas the hydrogen threshold is now determined by the classical ionization process in the absence of near-resonant quantum mechanical transition amplitudes [1]. Accordingly, the alkali data display the general trend of increasing threshold with ω_0, i.e. the signature of dynamical localization [11], over both frequency intervals (I) and (II), where only the former has a classical counterpart, not the latter. As a matter of fact, all currently available experimental data which exhibit dynamical localization in the ionization of nonhydrogenic alkali Rydberg [5, 6, 9] states have been obtained in regime (II) and (III), what explains the apparent discrepancy (reaching a factor 10) between hydrogen and alkali thresholds to the largest extent. (A second, though secondary, reason are the systematically longer atom-field interaction times in the alkali as compared to the hydrogen experiments, which account for a correction of the observed threshold value which depends algebraically on t [5].)

Finally, at driving frequencies $\omega < \Delta_{\rm Alk}^{(n_0)}$, even the alkali spectrum doesn't offer any atomic transition which allows for an efficient one-photon-coupling of the initial atomic state to any other Rydberg level. This is clearly reflected by the transition from decreasing to essentially constant scaled threshold fields, which defines the border line between (II) and the low-frequency range (III) in Fig. 1. Only higher-order processes can induce efficient depletion of the initial state population, with subsequent ionization, which results in a change of the slope of $F_0(10\%)$ as a function of ω_0.

In summary, we performed an exact numerical experiment which allows – for the first time, in the experimentalist's as well as in the numerical laboratory – for the direct and accurate comparison of complex energy transport in decaying Rydberg states of atomic hydrogen and of nonhydrogenic alkali atoms, under *precisely identical* experimental conditions. Not only do our results resolve the long-standing puzzle of an apparently enhanced ionization yield of strongly driven alkali Rydberg states, but they also identify a *general scaling law* for the ionization process of one electron Rydberg states, and predict a *universal ionization threshold* of atomic hydrogen and alkali atoms in an experimentally (for alkali atoms) yet unexplored regime. This quantitative prediction is immediately amenable to laboratory tests [4].

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1.15 Spectral cross correlations of magnetic edge states

Klaus Hornberger, Uzy Smilansky, and Andreas Buchleitner

One of the main goals in the field of "quantum chaos" is to link the auto-correlations found in a quantum spectrum to the periodic orbits of the classical problem [1]. Here, we extend this study and investigate whether *cross*-correlations exist between quantum systems which are different but related by their classical dynamics. We develop this idea for magnetic quantum billiards [2] which often serve to model semiconductor quantum dots [3].

Magnetic billiards consist of a charged particle moving ballistically in a compact domain in the plane subject to a homogeneous magnetic field. The quantum wave function is required to vanish at the billiard boundary while the impinging classical particle is reflected specularly [4]. The boundary defines also a complementary problem – an anti-dot – where the particle is confined to the exterior, and is scattered at the billiard boundary. Although the exterior domain is unbounded, its spectrum is *discrete* [5] and it is a natural question to ask whether it is possible to relate the energy levels of the dot to those of the anti-dot. We show that there exists indeed an intimate, non-trivial connection between the spectra of the interior and the exterior problem. It is the quantum manifestation of a duality in the classical dynamics.

The classical *interior-exterior duality* is illustrated in Fig. 1(a): Since a (periodic) orbit consists of arcs of constant curvature, one can construct a *dual* orbit in the complementary domain by completing the arcs to circles. Any skipping trajectory meets with a dual one under rather general conditions – if every circle of cyclotron radius ρ intersects the boundary at most twice. Pairs of dual periodic orbits have the same stability and their actions add up to an integer multiple of the action of a cyclotron orbit. On semiclassical grounds one may therefore expect the correlation between the interior and the exterior motion to carry over to the quantum spectrum. This is also corroborated by the existence of pairs of interior and exterior quantum eigenstates which match up well, cf. Fig. 1(b), although their energies differ.

The semiclassical analysis of the spectra is complicated by the fact that in the exterior each Landau level is an accumulation point for an infinite series of energies. The respective states – the *bulk states* – correspond to unperturbed cyclotron motion. Also in the interior one may find (a finite number of) bulk states if ρ permits complete cyclotron orbits to fit into the domain. The eigenfunctions which correspond to the

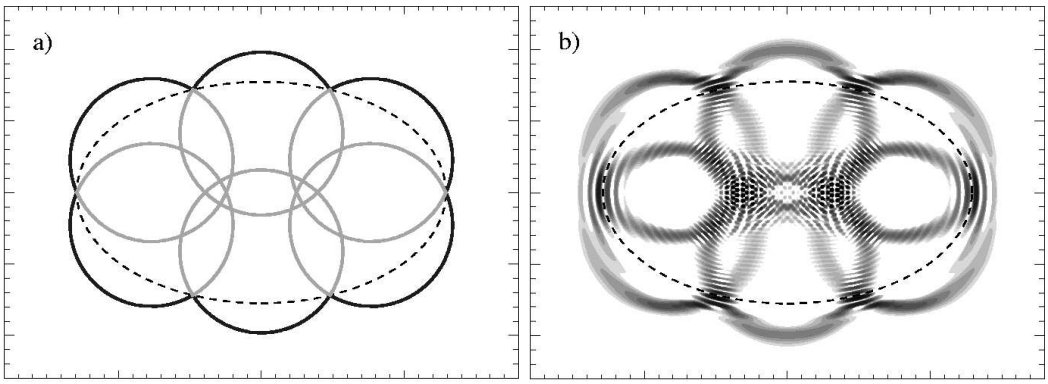

Figure 1: *(a) A pair of dual periodic trajectories, and (b) a pair of correlated eigenfunctions, found in the interior and the exterior ellipse billiard (superimposed). The billiard boundary is indicated by a dashed line.*

skipping trajectories, on the other hand, are called *edge states*. Clearly, a possible correlation is to be expected only between these non-trivial exterior and interior states.

Although the notion of edge states is intuitively clear and often used (e.g. in the context of the quantum Hall effect [6]), we are not aware of a general quantitative definition in the literature. Therefore, the purpose of our contribution is twofold. First, we propose a definition for the spectral density of edge states, which provides a meaningful characterization, and applies in the quantum and in the semiclassical regime. Only with this can we then establish the existence of a pairwise relation between the edge states of the interior and the exterior [16, 8].

A definition for edge states should take into account that a clear separation into edge and bulk occurs only in the semiclassical limit $b \to 0$. Here, we express the quantum scale in terms of the magnetic length $b = \sqrt{2\hbar/(m\omega_c)}$. At finite values of b, states of intermediate type may exist. We propose to quantify their "edginess" by attributing a weight $w_i > 0$ to each eigenstate ψ_i (of energy ν_i), which gives a measure of the degree to which ψ_i has the character of an edge state. The spectral density of edge states in either the interior or the exterior is then defined as

$$d_{\mathrm{edge}}(\nu) = \sum_{i=1}^{\infty} w_i \, \delta(\nu - \nu_i) \ . \tag{1}$$

Here, we scale the energy E by the spacing between Landau levels, $\nu = E/(\hbar\omega_c) = \rho^2/b^2$. Any reasonable definition of the weights w_i must suppress the bulk states by exponentially small values, such that the mean edge density $\overline{d}_{\mathrm{edge}}$ is well-defined in the exterior and equal to the interior one, to leading order. In the semiclassical limit it should match our notion of edge states admitting a trace formula which involves only the skipping trajectories. Moreover, we shall demand $\overline{d}_{\mathrm{edge}}$ to coincide with the unweighted interior mean density if the cyclotron radius is large enough to prevent bulk states.

To motivate our definition of the weights w_i, consider the *scaled* magnetization $\mathcal{M}$ of the interior billiard, a sum over the scaled magnetic moments

$$\mathcal{M}(\nu;b) = \sum_{\nu_i \le \nu} \frac{\langle\psi_i|\mathbf{r}\times\mathbf{v}|\psi_i\rangle}{\omega_c b^2} = \int_0^\nu \mathrm{m}(\nu';b)\,\mathrm{d}\nu' \ . \tag{2}$$

The scaled magnetization density $\mathrm{m}(\nu)$ can be expressed by the derivatives of the spectral counting function $\mathrm{N}(\nu;b) = \sum_i \Theta(\nu-\nu_i(b))$ with respect to b^2 and ν, $\mathrm{m}(\nu) = -b^2\partial_{b^2}\mathrm{N} - \nu\partial_\nu \mathrm{N}$. It exhibits a natural partitioning into a bulk part and an edge part since it complies with the scaling properties of the system: The scaled magnetic moment of a Landau state is $-\nu$. Hence, the second part of the magnetization density, $\mathrm{m}_{\mathrm{bulk}}(\nu) = -\nu\,\partial_\nu \mathrm{N} = \sum_i(-\nu_i)\,\delta(\nu-\nu_i)$ attributes the full diamagnetic response of a Landau state to each state ψ_i. We call it the bulk magnetization density. It follows that the remaining part, the *edge magnetization* density, $\mathrm{m}_{\mathrm{edge}}(\nu) = -b^2\partial_{b^2}\mathrm{N} = \sum_i b^2 \frac{\mathrm{d}\nu_i}{\mathrm{d}b^2}\,\delta(\nu-\nu_i)$, assigns the positive excess magnetic moments induced by the presence of a billiard boundary. Its mean value, $\overline{\mathrm{m}}_{\mathrm{edge}}(\nu)$, follows from the mean number of states in a magnetic billiard with area $\mathcal{A}$ and circumference $\mathcal{L}$ [9]. We note that $\overline{\mathrm{m}}_{\mathrm{edge}}$ cancels the mean bulk magnetization density exactly, $\overline{\mathrm{m}}_{\mathrm{edge}} = -\overline{\mathrm{m}}_{\mathrm{bulk}}(\nu)$: There is no orbital magnetism apart from the quantum fluctuations. Hence, $\mathrm{m}_{\mathrm{edge}}$ characterizes those few (edge) states which carry a finite current along the boundary, balancing the bulk magnetization due to their large positive magnetic moments.

The edge magnetization is well defined in the exterior as well. There, it is negative with the mean like in the interior but for a minus sign. This suggests to define the edge state density as $d_{\mathrm{edge}}(\nu) = \pm\mathrm{m}_{\mathrm{edge}}(\nu)/\nu$, with the lower sign for the exterior problem. The corresponding weights

$$w_i = \pm\frac{b^2}{\nu_i}\,\frac{\mathrm{d}\nu_i}{\mathrm{d}b^2} = \pm\frac{1}{\nu}\left(\frac{\langle\psi_i|\mathbf{r}\times\mathbf{v}|\psi_i\rangle}{\omega_c b^2} + \nu\right) > 0 \tag{3}$$

are easily obtained as the derivative of the eigenenergies taken at fixed ρ. This definition satisfies the conditions formulated above. In particular, the weights are exponentially small for bulk states since the Landau energies $\nu = N + \frac{1}{2}$ are independent of b [8].

The semiclassical edge state density is derived by inserting the trace formula for $\mathrm{N}(\nu)$ into the differential expression for $\mathrm{m}_{\mathrm{edge}}$. For the fluctuating part $d_{\mathrm{edge}} - \overline{d}_{\mathrm{edge}}$ one obtains a sum over all skipping periodic orbits. It differs from the semiclassical expression of the unweighted spectral density only by a factor $w_\gamma = (2\mathcal{A}_\gamma \pm \rho\mathcal{L}_\gamma)/(\rho\mathcal{L}_\gamma)$ attributed individually to each periodic orbit contribution. This *classical weight* is determined by the area $\mathcal{A}_\gamma$ enclosed by the trajectory γ and by its length $\mathcal{L}_\gamma$. The weights approach zero as the skipping orbits are further detached from the boundary. Hence, the classical weights w_γ smoothly suppress the bulk contributions to the semiclassical spectral density.

In order to unravel the relation between the interior and the exterior spectra we consider the cross-correlation function

$$C(\nu_0) \ = \ \sum_{i,j=1}^{\infty} \frac{w_i w'_j}{w_i + w'_j}\, g\left(\frac{\frac{\nu_i-\nu_0}{w_i} - \frac{\nu_0-\nu'_j}{w'_j}}{\frac{1}{w_i}+\frac{1}{w'_j}}\right) h\left(\frac{\nu_i-\nu'_j}{w_i+w'_j}\right) - C_{\mathrm{background}} \ . \tag{4}$$

The primes label the exterior energies and weights, and g and h are normalized Gaussians. Since the width of g is taken small, $\sigma_g \ll (\overline{d}_{\mathrm{edge}})^{-1}$, only those pairs of interior

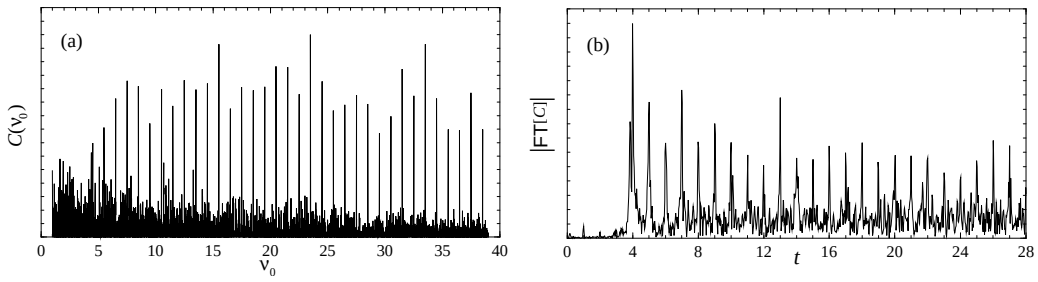

Figure 2: *(a) Cross-correlation function (4) for the elliptic billiard (eccentricity* 0.8*). The pronounced spikes indicate the existence of pairwise correlations between interior and exterior edge states. (b) Fourier transform of (4). The peaks at integers starting from* 4 *prove the classical origin of the correlations.*

and exterior energies contribute whose distances to ν_0, *scaled* by the respective quantum weights, are approximately equal. The prefactor in (4) ensures that only pairs of edge energies contribute.

When evaluating $C(\nu_0)$ semiclassically, those pairs in the sum over interior and exterior orbits γ and γ' are selected which satisfy $w_\gamma \mathcal{L}_\gamma \simeq w_{\gamma'} \mathcal{L}_{\gamma'}$, a relation fulfilled by the *dual* pairs. Restricting the summation to the latter is tantamount to the "diagonal approximation" [11]. The actions complement each other to $2\pi\nu_0 n_\gamma$, where $2\pi\nu_0$ is the scaled action of a cyclotron orbit, and n_γ is the number of reflections. We obtain $C(\nu_0) = \sum_n f(n)\, \hat{g}(n) \cos(2\pi n(\nu_0 - \frac{1}{2}))$ with $\hat{g}$ the Fourier transform of g. The sum starts at $n_{\min}$, the minimal number of reflections needed for a periodic orbit at given ρ, and $f(n) = \frac{2}{\pi} \sum a_\gamma^2 w_\gamma^2$ is a sum over the set of dual orbits with n reflections. It involves the classical weights w_γ and the stability amplitudes a_γ of the unweighted spectral density.

¿From its semiclassical form the correlator is expected to be appreciably different from zero only at energies where the cosine terms are stationary. Hence, $C(\nu_0)$ must exhibit peaks at $\nu_0 = N + \frac{1}{2}$. Its Fourier transform, on the other hand, should be peaked at the integer values starting from $n_{\min}$. A numerical verification of these predictions is presented in Fig. 2 for the spectra of an ellipse billiard at $b = 0.1$ [5]. In Fig. 2(a) one observes that the cross correlation function is strongly fluctuating but displays pronounced spikes at the expected energies. They are a clear signature of a non-trivial correlation between the interior and exterior edge states. The peaks in the Fourier transform, Fig. 2(b), are positioned at integer values of t which start at $n_{\min} = 4$, as expected for the (desymmetrized) ellipse. They clearly expose the classical duality as the origin of the cross-correlations.

Moreover, the spikes of $C(\nu_0)$ imply the existence of a *pairwise* relation between the interior and exterior edge states: For each correlated pair of interior and exterior edge energies, ν_i and ν'_j, there exists a Landau level $\nu_0 = N + \frac{1}{2}$ such that the distances – scaled individually by the quantum weights w_i and w'_j – are approximately equal,

$$\frac{\nu_i - (N - \frac{1}{2})}{w_i} \simeq \frac{(N - \frac{1}{2}) - \nu'_j}{w'_j} \ . \tag{5}$$

This follows immediately from (4), where we took the width of g to be small on the quantum scale. The relation (5) shows that the interior and exterior edge spectra are

intimately connected in the semiclassical limit. Note in particular the vital role played by the quantum weights (3) without which the correlations would not be observable.

Equation (5) allows to spot single pairs of correlated states in the spectrum, and Fig. 1(b) gives an outstanding illustration (with the shade proportional to $|\psi|^2$): The wave functions are clearly localized along the stable dual periodic orbits drawn in Fig. 1(a). Although the respective energies are separated by 20 mean edge state spacings, the difference between the two sides of (5) is approximately one tenth of the mean level spacing scaled by the mean weight. The correlation of pairs of *chaotic* wave functions cannot be verified as easily by visual inspection, but also in these cases their normal derivatives at the boundary are very similar.

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1.16 Quantum state preparation via asymptotic completeness

Thomas Wellens and Andreas Buchleitner

In order to encode or process quantum information, the ability to prepare quantum systems in arbitrary states is a necessary prerequisite. In principle, this goal can be achieved by application of suitable classical control fields (e.g., laser pulses), such that the unitary evolution induced by the corresponding time-dependent Hamiltonian transfers the system from a well-defined initial state to the desired target state $|\chi\rangle$. While this idea of coherent control by external classical fields covers a great variety of different preparation schemes [1, 2, 3], it may in some cases also be of advantage to replace the classical control field by another quantum system. Most methods of preparing quantum states of the electromagnetic field [4, 5, 6], for example, rely on the interaction with atoms – which themselves have an internal quantum structure. Then a fundamental problem arises, since field and atoms will in general be in an entangled state after their mutual interaction. One possible way to create the desired, pure target state of the field consists in a sequence of final state measurements on the atoms [4]. However, this procedure only succeeds with finite probability much less than one, due to measurement noise. Therefore, if we strive for a *deterministic* state preparation, we have to avoid any entanglement between atom and field. In other words, the final

state has to be a product of the desired target state $|\chi\rangle$ and some final state $|\psi\rangle$ of the control system.

Here, we shall show that, under relatively general conditions, a final state $U|\chi_0\rangle\otimes|\psi_0\rangle = |\chi\rangle \otimes |\psi\rangle$ of the interacting quantum system can indeed be prepared, by choosing an appropriate initial state $|\psi_0\rangle$ of the control system, under a simple, *time-independent* interaction U, and *independently* of the initial state $|\chi_0\rangle$ of the target system. Specifically, we choose the latter to be a quantized harmonic oscillator (experimentally realized as a single mode radiation field in cavity QED experiments [7]), interacting with a sequence of N two-level atoms. A necessary condition for the success of our control scheme is the experimentalist's ability to entangle a small number N of atoms prior to the atom-field interaction [8, 9]. The larger N, the better the fidelity of the target state preparation, which approaches 100% exponentially fast in N.

To accomplish our ambitious task, we make use of a recent mathematical result [10], which states that the atoms-field interaction $U_N = U^{(N)} \dots U^{(1)}$ (where $U^{(i)}$ denotes the resonant Jaynes-Cummings interaction of the field with the i-th atom, with constant interaction time for subsequent atoms) fulfills the property of *asymptotic completeness*, in the following sense: every observable A of the photon field develops (in the Heisenberg picture) into an observable M_A of the atoms, i.e.

$$\lim_{N\to\infty} U_N^\dagger (A \otimes \mathbb{1}) U_N \;=\; \mathbb{1} \otimes M_A. \tag{1}$$

In a more physical language, Eq. (1) tells us that the field – after the interaction with infinitely many atoms – loses the memory about its initial state: the final field state ρ, i.e., the expectation value $\langle A\rangle = \mathrm{tr}\{A\rho\}$ of any photon field observable A after the atoms-field interaction, is completely determined by the initial state of the atoms injected into the cavity, irrespective of its initial state. Furthermore, if we take advantage of the interaction U_N being unitary, asymptotic completeness ensures that any field state can be prepared by choosing an appropriate initial atomic state: according to Eq. (1), any projection $A = |\chi\rangle\langle\chi|$ onto a field state $|\chi\rangle$ develops into an projection M in the atomic space, and, consequently, any state $|\psi_0\rangle$ from the range of M yields the desired expectation value 1. Note that, since M acts in the total atomic Hilbert space, the required initial atomic states will in general exhibit entanglement between different atoms.

In order to verify that our atoms-field interaction U_N fulfills property (1), we examine the following two conditions, which can be shown [10] to be sufficient for asymptotic completeness: The first one is the existence of an invariant field state $|\tilde{\chi}\rangle$ with the following property: there exists a single-atom state $|\tilde{\psi}\rangle$, such that the field converges into the uniquely determined *pure* state $|\tilde{\chi}\rangle$ under the interaction with infinitely many atoms in the initial state $|\tilde{\psi}\rangle \otimes |\tilde{\psi}\rangle \otimes \dots$, independently of the initial field state. In the case of the Jaynes-Cummings interaction U_N, a sufficiently long sequence of ground state atoms forces the field into the vacuum state $|\tilde{\chi}\rangle = |0\rangle$. The second condition states that if the field state $|\chi_2\rangle$ can be prepared from $|\chi_1\rangle$, also the reverse process is possible. Also this time-reversal symmetry is fulfilled by the Jaynes-Cummings interaction U_N [12].

Both these sufficient conditions immediately suggest a recipe to prepare the target state $|\chi\rangle$, in two steps: first, the field vacuum is prepared by a sufficiently long sequence of

ground state atoms, thereby erasing the memory of the initial field state. In the second step, we exploit time reversal symmetry, in order to prepare $|\chi\rangle$ from $|0\rangle$, since the reverse process is possible due to the first of the above conditions.

Note, however, that such procedure requires an infinite number of atoms interacting with the cavity field, and, in addition, that these have to be entangled prior to the atoms-field interaction. Therefore, the crucial question for the experimentalist is whether the state preparation can – at least approximately – also be accomplished with a finite number of atoms. In order to quantify the accuracy of the field state preparation for finite N, we use the *fidelity* F of the final state with respect to the desired field state $|\chi\rangle$, that is, the probability of finding $|\chi\rangle$ when performing a measurement. A simple calculation shows [11] that F is given in terms of the initial N-atom state $|\psi_0\rangle$, as the expectation value

$$F \;=\; \langle\psi_0|M^{(\rho_0)}|\psi_0\rangle \tag{2}$$

of the following (Hermitian) atomic operator, which depends on the (possibly mixed) initial field state ρ_0:

$$M^{(\rho_0)} = \mathrm{tr}_f\left\{(\rho_0\otimes\mathbb{1})\;U_N^\dagger(|\chi\rangle\langle\chi|\otimes\mathbb{1})U_N\right\}. \tag{3}$$

Here, tr_f denotes the partial trace over the field. According to Eq. (2), the maximum fidelity F is obtained as the largest eigenvalue of $M^{(\rho_0)}$, and the associated eigenvector $|\psi_0\rangle$ is the optimal initial atomic state. From asymptotic completeness, Eq. (1), we know that, in the limit $N\to\infty$, the operator $M^{(\rho_0)}$ does not depend on the initial field state ρ_0, and converges to a projection on the atomic space, with largest eigenvalue 1. For a finite N, however, the fidelity will be smaller than 1. In order to see how fast F increases with N, we can also derive an analytical lower bound for the maximum fidelity. For this purpose, we exploit the time reversal symmetry of the atoms-field interaction, making use of the fact that the cavity vacuum can be prepared by a sequence of ground state atoms. Thereby, we arrive at the following expression for the fidelity F of preparing the target field state $|\chi\rangle=\sum_n c_n|n\rangle$ from the vacuum, with $|\chi\rangle$ an arbitrary superposition of the n photon Fock states $|n\rangle$ [11]:

$$F \;\geq\; \sum_n |c_n|^2 F'(n), \tag{4}$$

$$F'(n) \;=\; 1-\sum_{k=1}^{n}(1-B_k)^N\prod_{\substack{i=1\\ i\neq k}}^{n}\frac{B_i}{B_i-B_k}. \tag{5}$$

Here, the coefficients $B_i=\sin^2(\phi\sqrt{i})$, which reflect the Rabi dynamics of the atom-field interaction, depend on the vacuum Rabi angle ϕ, i.e., the interaction time of a single atom with the field. Evidently, the appearance of N in the exponent of Eq. (5) points at an exponentially fast convergence of the fidelity towards the ideal value 100%, as a function of N. This prediction is confirmed by Fig. 1, which shows the maximum fidelity F for the preparation of two different target field states, the Fock state $|5\rangle$ (filled circles) and a superposition $|\chi_5\rangle=\sum_{i=0}^{5}|i\rangle/\sqrt{6}$ of Fock states (open circles), as a function of the number N of atoms. To highlight the very high fidelities we can

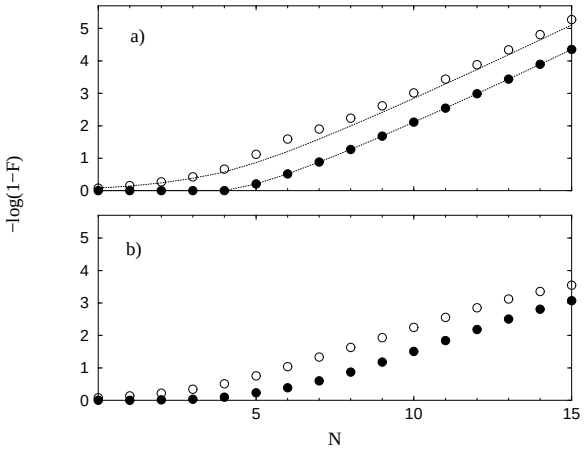

Figure 1: *Maximum fidelity F for the preparation of the 5-photon state $|\chi\rangle = |5\rangle$ (filled circles), and of the truncated phase state $|\chi\rangle = \sum_{i=0}^{5} |i\rangle/\sqrt{6}$ (open circles) of the cavity field, respectively, as a function of the number N of atoms injected into the resonator. Vacuum Rabi angle $\phi = 0.91$. Initial field state: a) vacuum $|0\rangle$, b) thermal equilibrium with average photon number $\langle n\rangle = 0.55$ (corresponding to a temperature of $T \simeq 1$ K in the microwave regime). The dotted lines display the analytical lower bound, Eqs. (4,5). In case (a), F approaches the ideal value* 1 exponentially *fast, whereas the convergence towards $F = 1$ is slower for the mixed initial field state (b).*

achieve, we choose a logarithmic scale $-\log(1 - F)$ for its deviation from 1. Two distinct initial states of the cavity field are considered, the vacuum, Fig. 1(a), and the thermal equilibrium with average photon number $\langle n\rangle = 0.55$, Fig. 1(b). The dotted lines in Fig. 1(a) display the above analytical lower bound, Eqs. (4,5), which agrees exactly with the maximum fidelity, Eq. (2), in the case of the Fock state $|5\rangle$ as target state, and gives a quite good approximation also for the other target state $|\chi_5\rangle$. As predicted by Eq. (5), the linear increase in the semilogarithmic plot demonstrates that the optimum fidelity 1 is approached *exponentially* fast when increasing N. Not surprisingly, convergence towards $F = 1$ is slightly slower for the thermal initial field state (where population of high n values has to be transferred to $n \leq 5$ during the preparation process), Fig. 1(b), than for the vacuum. Furthermore, let us note that the optimal initial atomic states $|\psi_0\rangle$ are almost identical in cases (a) and (b), what demonstrates the independence of our preparation scheme from the initial field state.

Finally, Fig. 1(a) shows that $N = 10$ atoms are sufficient to prepare the 5 photon Fock state with fidelity $F > 99\%$. We have found that, for the preparation of other Fock states $|n\rangle$, the required number of atoms scales approx. linearly with n, provided that also the vacuum Rabi angle ϕ is appropriately scaled. [From Eq. (5), an estimation for the optimal value of ϕ gives $\phi \simeq \pi/(1 + \sqrt{n})$ [12].] By virtue of Eq. (4), this implies that, to prepare any field state including at most n photons with fidelity $F > 99\%$, not more than $N = 2n$ atoms are needed.

Since the entanglement of a larger number of atoms remains an experimentally formidable task, let us conclude with some remarks on a finite fidelity $F_0 = \langle\psi_0|\rho_a|\psi_0\rangle$ of the initial state preparation - with ρ_a describing the imperfect atomic initial state. Eq. (2) is then generalized by $\tilde{F} = \mathrm{tr}\{\mathrm{M}^{(\rho_0)}\rho_\mathrm{a}\}$, and, consequently, $\tilde{F} \geq FF_0$, with the above estimations on F unaffected. Given the recent experimental result on the entanglement of four particles [8], and entangling procedures that should operate on

even larger particle numbers [9], we are therefore confident that our novel approach to quantum state preparation opens an experimentally practicable perspective.

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1.17 Motor-filament systems - Self-organisation and mechanical properties

Karsten Kruse and Frank Jülicher

Living cells have remarkable mechanical properties. In addition to a passive response to mechanical stresses, eucaryotic cells are able to actively change their shapes, to generate motion and forces [1] as well as to react to externally imposed mechanical conditions [2]. The cytoskeleton, which is a complex network of elastic protein filaments such as actin filaments and microtubules, plays a key role in these processes. These filaments are rod-like and polar structures, where the polarity is resulting from the two ends being structurally different. A large number of specific cytoskeletal proteins interacting with the filaments makes the cytoskeleton a highly dynamic system. Examples are cross-linkers which induce formation of a gel-like filament network and bundling proteins which lead to filaments aligned in parallel. In addition, motor proteins are able to use the chemical energy of the hydrolysis of Adenosinetriphosphate (ATP) to generate forces and motion along filaments [1, 3]. In contrast to passive filament solutions, filament systems which interact with molecular motors and other enzymes are thus intrinsically active and exhibit rich types of behaviour. Our aim is to develop general tools for describing the dynamics and the mechanical properties of such active biopolymer liquids and gels.

In order to reach this aim, we have started by analysing a model system, which still represents essential features of the cytoskeleton. It consists of filaments that are actively displaced with respect to each other. We take the filaments to be arranged in

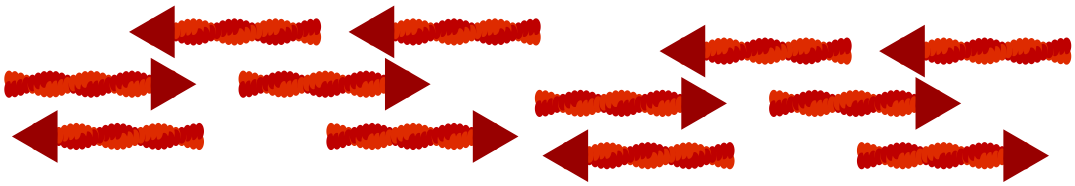

Figure 1: *Schematic representation of a bundle of aligned filaments. Arrowheads indicate the direction of motion of motors attached to the filaments.*

Figure 2: *Schematic representation of interacting filament pairs and their associated coupling constants. The black figure-eight symbols indicate cross-linking motors.*

a bundle, see Fig. 1, such that we arrive at an essentially one-dimensional system. In cells such linear structures exist in the form of stress fibres or contractile rings, which appear towards the end of cell division. There, active displacements are, for example, a consequence of small aggregates of motors which contain two or more active domains, that can bind at the same time to two filaments. Hydrolysing ATP, they exert relative forces and thus motion between the filaments. Purified motor-filament systems have been studied in recent years experimentally *in vitro* and revealed in particular self-organisation [4, 5, 6, 7], a subject which has also been addressed theoretically [8, 9].

The crucial property of filaments with respect to their interaction with motors is their polarity. Indeed, the direction of motion of motor molecules is uniquely determined by the orientation of the filaments they move on. Thus, when restricting attention to filament *pairs*, only the relative orientation between the cross-linked filaments is of importance. We denote the corresponding coupling parameters by α and β, see Fig. 2.

Due to the finite length of the filaments our description of the bundle dynamics is given by a non-linear integro-differential equation [10]. This description does not depend on any particular mechanism of the motor-filament interaction. It does, however, respect the symmetries displayed by this interaction and can therefore be expected to describe

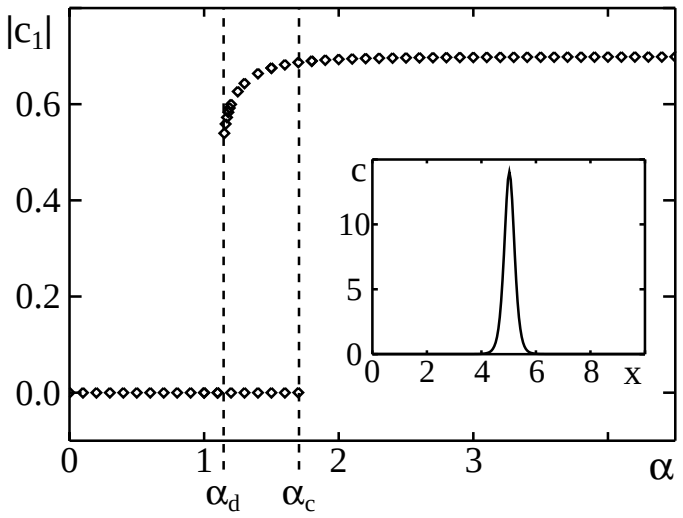

Figure 3: *The modulus of the first Fourier-component of stable stationary solutions of our model [10] in the presence of filaments of one orientation only. Periodic boundary conditions apply. The inset presents the non-homogeneous stationary solution for* $\alpha = 1.5$

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the generic behaviour of active filament bundles.

The study of our model system has revealed the importance of dynamic instabilities for the behaviour presented by active motor-filament systems. Furthermore, the relevant control parameter could be identified to be the interaction strength between filaments of the same orientation. A linear stability analysis of the homogeneous state shows that if α exceeds some positive critical value, a bundle consisting of filaments of only one orientation will contract, see Fig. 3 for the corresponding phase-diagram. But also in the general case, when filaments of both orientations are present, interesting dynamics follows from α being larger than a positive critical value. In this case we have found travelling waves [11]. These waves either advance as a solitary wave, i.e., without changing their form, or by oscillating around some mean profile. Remarkably, taking filament adhesion into account, these waves are associated with a persistent net filament transport. This observation suggests a role for self-organisation in the context of cell locomotion. Experimental evidence for this had been obtained by studying fragments of fish keratocytes [12].

Momentum exchange of the filament bundle with a substrate leads to the mechanical properties of filament-motor systems. As the filaments are of finite length and may interact whenever they overlap, the relation describing the momentum exchange in the bundle is rather subtle. Within our model, which concentrates on the essential properties of the filament-motor interactions, we are able to extract from this relation the actively created tension Σ at any point in the bundle. For a homogeneous bundle it becomes particularly simple and reads

$$\Sigma = \alpha\eta\ell^3(c_0^{+2} + c_0^{-2}).$$

In this expression c_0^+ and c_0^- are the densities of one and the other orientation, respec-

tively, ℓ is the length common to all filaments, and η an effective friction constant. If α is positive, this tension is contractile, and could be used to contract a stress fibre or a contractile ring in the course of cell division.

Ongoing work is aimed at generalising our description in order to treat two- and three-dimensional systems. In addition, the effects of polymerisation and depolymerisation of filaments will be taken into account. Furthermore, we are developing a description of active gels rather than the active fluids presented here. Together, this will bring us closer to a more realistic description of cellular phenomena.

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1.18 Active amplification by self-tuned critical oscillators in the ear

Frank Jülicher

Detecting the sounds of the outside world imposes stringent demands on the design of the inner ear, where the transduction of acoustic stimuli to electrical signals takes place [1]. In the cochlea of the inner ear, about 16000 highly specialized hair cells act as mechanosensors that are at the origin of sound detection. They must each be responsive to a particular frequency component of the auditory input. Moreover, these sensors need the utmost sensitivity, since the weakest audible sounds impart an energy, per cycle of oscillation, which is no greater than that of thermal noise [2]. At the same time, they must operate over a wide range of volumes, responding and adapting to intensities which vary by many orders of magnitude. It was pointed out as early as 1948 that the familiar resonant gain of a passive elastic system is far from sufficient for the required demands, because of the heavy viscous damping at microscopic scales [3]. Clearly, some form of non-linear amplification is necessary in sound detection. There is now a lot of evidence that the cochlea has developed active amplificatory processes, whose precise nature remains to be discovered [4, 5]. The most striking evidence for active behaviors in the ear are so-called otoacoustic emissions which are sounds emitted from the ears of mammals, birds and amphibians [6].

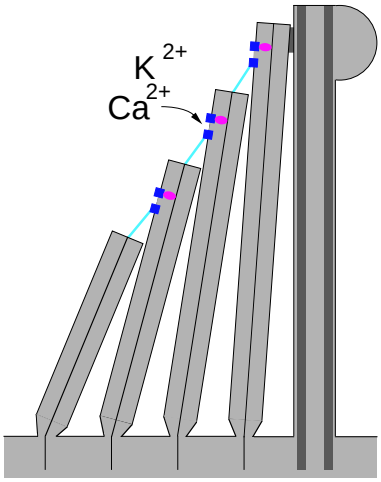

Figure 1: Schematic representation of the hair bundle, the sensitive element of mechanosensory hair cells. It consists of 10-50 rod-like stereocilia which have a length of 1-10 μm and are connected by fine filaments. The stereocilia contain ion channels which open as a result of mechanical stimulation.

It has recently been proposed that the ears of all vertebrates achieve frequency selectivity and the operation over a large dynamic range by employing the generic nonlinearities in the vicinity of an oscillatory instability or Hopf bifurcation [7, 8]. The idea is that the inner ears of these animals contain a large number of active dynamical systems, each of which is close to the critical point of a Hopf bifurcation. The oscillation frequencies of these oscillators cover the whole audible range. Proximity to the bifurcation point required for high sensitivity and the detection of weak stimuli can in general and in a robust way be achieved by a self-tuning mechanism [7]. An incoming sound wave excites motion of the basilar membrane in the cochlea which is the elastic structure in which the mechanosensory cells are embedded. This motion which is the response of the system to sounds is driven partly by the dynamic oscillators. The hair-cells detect this response and send nerve signals to the brain.

The principles of such a detector can be described as follows. We denote the basilar membrane deformation in the vicinity of an oscillator of frequency ω_0 by $x(t)$, and the sound pressure exciting this oscillator by $p(t)$. We assume for simplicity that only one frequency ω is present in the sound stimulus, the response however contains all harmonics of the base frequency:

$$p(t) = p_1 e^{-i\omega t} + p_{-1} e^{i\omega t} \quad (1)$$

$$x(t) = \sum_n x_n e^{-in\omega t} \quad (2)$$

In the vicinity of a Hopf bifurcation, the properties of the oscillator in response to external stimuli can be expressed in a general power expansion up to third order as

$$p_1 = A(\omega, C)x_1 + B|x_1|^2 x_1 \quad (3)$$

Here, A and B are complex coefficients which depend on frequency ω and a control parameter C which has to be adjusted to a critical value to tune the system to its

critical point. If $C = C_c$, the linear response vanishes for the oscillation frequency ω_0:

$$A(\omega) \simeq \alpha(\omega - \omega_0) \tag{4}$$

As a result, the system exhibits for $\omega = \omega_0$ a compressive nonlinearity

$$x_1 \sim p_1^{1/3} \tag{5}$$

mapping 6 orders of magnitude in sound pressure on only 2 orders of magnitude in deformations. This nonlinearity can explain the large dynamic range of the ear. This nonlinear response leads to a diverging gain $|x_1|/|p_1| \sim p^{-2/3}$ for small stimuli. If the stimulus frequency does not match the oscillation frequency, the response becomes linear for small stimuli:

$$x_1 \sim 1/(\omega - \omega_0) \tag{6}$$

The nonlinear response at resonance as well as the linear response for nonmatching frequencies have been observed experimentally in the cochleas of animals [9]. Since the dynamic oscillator is an active system, it can generate motion in the basilar membrane using a metabolic energy source and therefore generate amplitudes for weak signals that are much larger than those generated by a passive resonance.

In order to be close to the Hopf bifurcation, the control parameter has to be tuned to its critical value C_c. This tuning can be achieved in a robust and reliable way by a feedback mechanism using the detection apparatus of hair cells. Any basilar membrane deflection x gives rise to an influx of ions into the hair cell. If we assume that for example Ca-ions are related to the control parameter, the latter behaves as

$$\frac{dC}{dt} = -\frac{1}{\tau}C + JP_o(x) \tag{7}$$

Here τ is a relaxation time of the ions and P_o the opening probability of mechano-sensitive ion channels. This self-tuning mechanism brings the oscillator to an operating point $C = C^*$ very close to the bifurcation:

$$\frac{C^* - C_c}{C_c} \simeq \frac{\delta^2}{\Delta^2} \simeq 10^{-5} \tag{8}$$

where the detection threshold $\delta < 1$ nm and the saturated amplitude $\Delta \simeq 100$ nm.

Sound detection based on self-tuned critical oscillators provides a general operating principle of the inner ear which can explain a number of seemingly unrelated properties of hearing. In addition to the large dynamic range and the frequency discrimination capabilities of the ear, it can explain adaptation and fatigue, the observation that sensitivity is reduced when the ear was subjected to stronger sounds and needs a short time to recover. This behavior follows naturally from a self-tuning feedback. In our picture, spontaneous oto acoustic emissions are a natural consequence if active oscillators are not perfectly tuned to the bifurcation. This could happen transiently or as a result of a local pathology. That the ear is a nonlinear detector has been known for a long time. More than 250 years ago, the musician Tartini noted that the ear detects so-called combination tones [10]. These are frequencies that result from nonlinear interferences of input frequencies. For example, the frequency $2f_1 - f_2$ can be heard

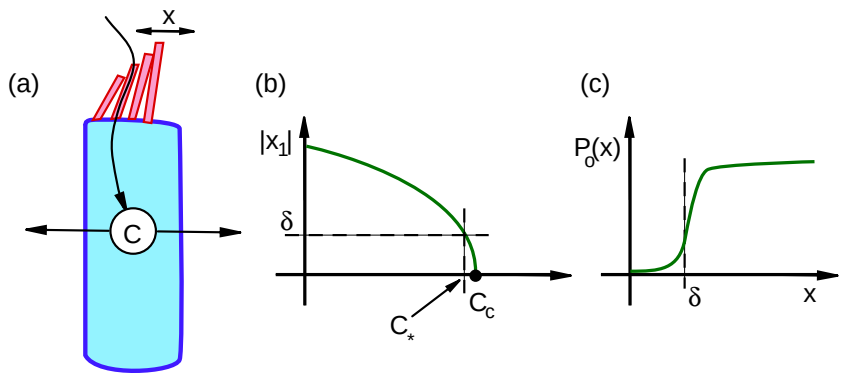

Figure 2: Simple self-tuning mechanism (schematic). (a) Regulation of the control parameter C associated with the concentration of ions such as Ca^{++} which enter the hair cell via transduction channels. A permanent outflux drives the system towards the oscillating side of the bifurcation, influx of ion via transduction channels provides a stabilizing feedback. (b) Fourier amplitude $|x_1|$ of spontaneous oscillations as a function of the control parameter near the bifurcation point C_c. Self-tuning brings the system to an operating point C_*. (c) Opening probability $P_o(x)$ of ion channels as a function of the deflection amplitude x. A signal is generated for deflections larger than δ.

if two pure frequencies f_1 and f_2 are played. Nonlinearities of the Hopf bifurcation can account for many of the observed two-tone interferences which are crucial for the analysis of complex sounds [11].

While the general principle of self-tuned critical oscillators seems to be at work in the ears of all vertebrates, the physical nature of the oscillators remains mysterious. In mammals (and humans) it is thought that so-called outer hair cells are the active elements involved. However, no direct evidence for their capability to oscillate exists so far. In non-mammalian vertebrates, which lack outer hair cells, oscillatory behaviors of hair bundles are studied that have been discovered recently [12, 13, 14]. They are candidates for the oscillators involved in hearing and might also be important in mammals. However, the physics behind the generation of oscillations and the details of the self-tuning mechanism remain to be uncovered.

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1.19 Understanding Complex Chemical Patterns

Lutz Brusch, Camilo Rodrigues Neto, Ulrich Storb and Markus Bär

Introduction. - Advances in experimental techniques (reactor design, imaging) have enabled chemists to record the spatiotemporal dynamics of reactions under sustained nonequilibrium conditions in 2D and to visualize even concentration patterns in 3D. These progresses enable the study of complex patterns, e. g. the transition to spatiotemporal chaos or modulated structures. Propagating and rotating waves of chemical concentration are frequently observed in the Belousov-Zhabotinsky medium. This autocatalytic chemical reaction possesses an intrinsic oscillatory dynamics. The underlying mechanisms of two dynamical instabilities of spiral waves (2D) and scroll waves (3D) are presented. For a wide range of parameters, *i.e.* quantitatively different compositions of the reactants, periodic waves are continuously emitted from self-organising sources in 2D (spirals) and 3D (scroll waves). Recently, saturated modulations of spirals (superspirals) and their breakup have been observed [1]. Fig. 1 (a),(d) shows experimental observations of a spiral and a superspiral, respectively. We show that the superspirals and their breakup can be explained by variants of the Doppler effect in nonlinear waves. Experimental work on the instability of a scroll wave, *i.e.* a stack of spiral waves in a three-dimensional reactor, upon an imposed parameter gradient is clarified by numerical simulations of the corresponding continuous model [2]. We find an instability of the scroll wave to lateral distortions that cause scroll breakup at the lateral boundaries.

Nonlinear Doppler effect and superspirals.- We analyse the novel superspiral structures in the framework of the complex Ginzburg-Landau equation (CGLE), a universal description of extended oscillatory media near the onset of oscillations [3]

$$\partial_t A = A - (1 - ic_3)|A|^2 A + (1 + ic_1)\Delta A \ , \tag{1}$$

where c_1 and c_3 are real and the field $A = A(x, y, t)$ has complex values describing amplitude and phase of oscillating chemical concentrations. Uniform spirals are reproduced with a stationary wave source in the center (Fig. 1 (b),(c)) where the oscillation amplitude $|A|$ has to vanish due to the rotational symmetry. In order to trigger the oscillatory instability of this source we added a weak and localized heterogeneity in the center of the domain. Now the source propagates on a circle around the heterogeneity and a superspiral results in the emitted wave field (Fig. 1 (e),(f)). These modulations saturate and regularly propagate outward but with different velocity than the underlying spiral arms.

For linear waves, the Doppler effect caused by a moving source alters the frequency of the emitted wave proportional to the velocity of the source. For nonlinear waves, we find that the amplitude of the modulation is not constant but typically exponentially damped away from the source. If the emitted wave are convectively unstable in an

infinite domain, saturated modulations or exponential growth of modulations are alternative possible scenarios. Autonomously rotating ("meandering") spiral cores have been observed experimentally. Previous theoretical work, based on linear analysis, has suggested that initial modulations will either decay or amplify due to nonlinearities, *i.e.* recover or destroy the uniform spiral, while transported away from the spiral center [4]. On the other hand, saturated traveling modulations of underlying waves are known to be critical to the survival of phase chaos, *i.e.* a mild form of spatio-temporal chaos in extended oscillatory media [5, 6]. In order to clarify this controversy and to illuminate the underlying mechanisms we investigate the radial dynamics of nonlinear waves emitted from a moving source. Projecting the possible circular movement of the source onto the radial direction yields a sinusoidal oscillation.

Within one-dimensional simulations of the CGLE (1) we now introduce a "source" boundary condition, *i.e.* $A = 0$ for $x < x_S$ that emits periodic waves with selected wavenumber q. The position of the source $x_S = \rho \cos 2\pi t/\tau$ depends on the radius ρ and the period τ of the rotation. Fig. 2 shows the numerical results at fixed parameters and provides evidence for an finite interval of periods τ with saturated modulations traveling as an envelope on top of the underlying wave field. We identify the saturated modulations of Fig. 2(b) as coherent structures, *i.e.*

$$A(x,t) = a(z)e^{i\phi(z)}e^{i(qx-\omega t)} \tag{2}$$

with unknown functions $a(z)$ and $\phi(z)$ of the comoving coordinate $z = x - vt$ and the wave number q and frequency ω of the underlying wave field. The CGLE possesses a one parameter family of plane waves ($a(z) = \sqrt{1-q^2}, \phi(z) = \phi_0, \omega = q^2(c_1 + c_3) - c_3$) parameterized by their uniform wave number $q(c_1, c_3)$ that is uniquely selected by

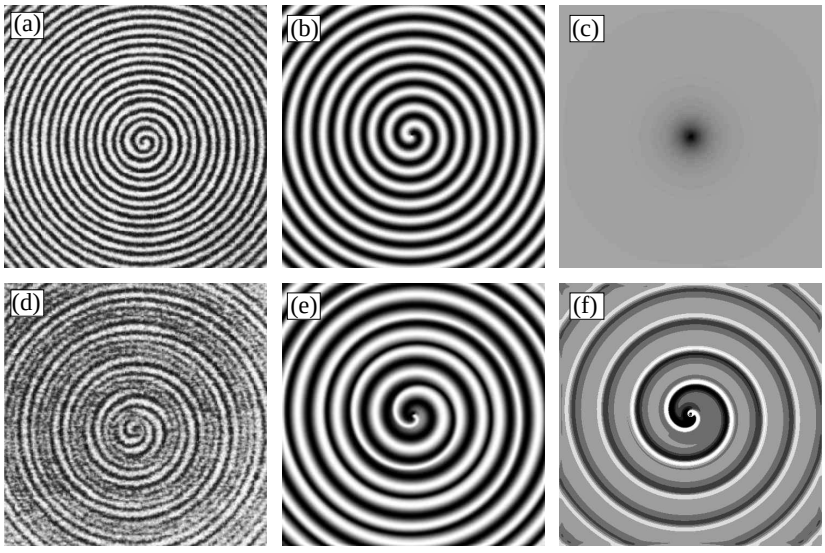

Figure 1: Uniform spirals (a-c) and superspirals (d-f) are observed in experiments (a,d) and numerical simulations (b,e) [1]. (c,f) represent the amplitude $|A|$ of local oscillations. Note the spiraling modulation in (f) that accompanies the modulation of the wave length in (e). (b,c,e,f) System with no-flux boundary conditions, (b,c) without and (e,f) with a localized heterogeneity in the center.

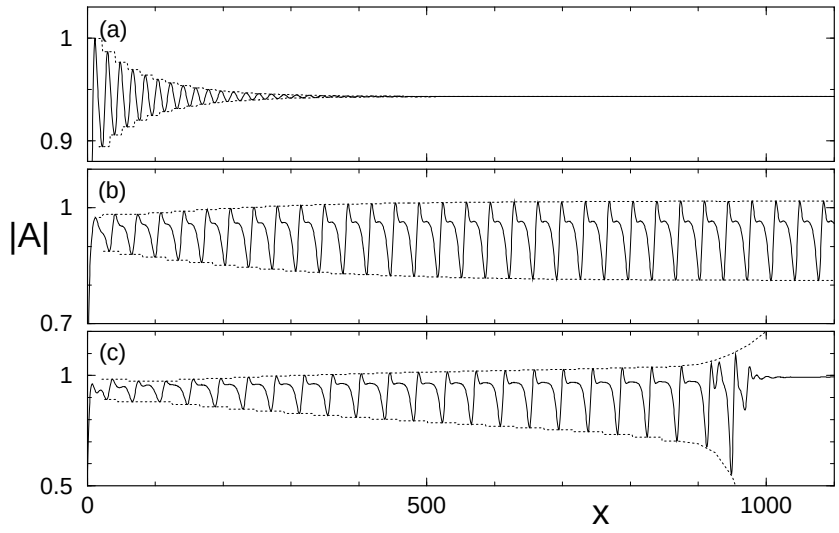

Figure 2: Snapshots of numerical simulations showing the amplitude profile $|A|$. The source at the left boundary oscillates with the period increasing from (a) $\tau = 8$, (b) $\tau = 13$ to (c) $\tau = 15$.

the source. Plane waves can experience a convective long wavelength instability, the Eckhaus instability (EI). After inserting the ansatz (2) into the CGLE (1) numerical bifurcation analysis may be employed to calculate the existence and stability properties of the saturated modulations [6]. We find a two-parameter family of solutions called modulated amplitude waves (MAWs) [5, 6]. MAWs may be parameterized by the average wave number $q(c_1, c_3)$ of the underlying wave field and the temporal period τ of the modulations that is determined by the moving source. MAWs cease to exist in saddle-node bifurcations (SN) if parameter values are changed accordingly. We calculated the threshold values $\tau_{EI}(q, c_1, c_3)$ and $\tau_{SN}(q, c_1, c_3)$. For a fast moving source, *i.e.* $\tau < \tau_{EI}(q, c_1, c_3)$, the modulations decay in radial direction since the uniform spiral is stable below the Eckhaus instability (Fig. 2(a)). For intermediate periods $\tau_{EI}(q, c_1, c_3) < \tau < \tau_{SN}(q, c_1, c_3)$ the modulations saturate in radial direction and form the superspiral (Fig. 2(b)). If the source moves very slow then $\tau > \tau_{SN}(q, c_1, c_3)$ and the modulations grow without bounds as they are advected away from the source no matter how small the radius ρ is (Fig. 2(c)). Adjacent wave fronts annihilate in a finite distance from the source ("superspiral breakup"). The distance from the source to the position of superspiral breakup decreases with further increasing period above $\tau_{SN}(q, c_1, c_3)$. Hence finite discs of superspirals are embedded in the surrounding phase of spatiotemporal chaos in agreement with experimental observations [1].

3D breakup of twisted scroll waves in a spatial gradient. - In collaboration with experimentalists (U. Storb, S. Müller) in the Biophysics Department of the University of Magdeburg we have studied the dynamics of scroll waves in a three-dimensional setup of the Belousov-Zhabotinsky reaction. A scroll wave is best viewed as a stack of rotating spirals, the line that connects center of rotation in the x-y plane is called filament and is initially parallel to the z-axis. If the rotation phase of the spirals seen in subsequents x-y projections varies, one speaks of a twisted scroll wave *resp.* a

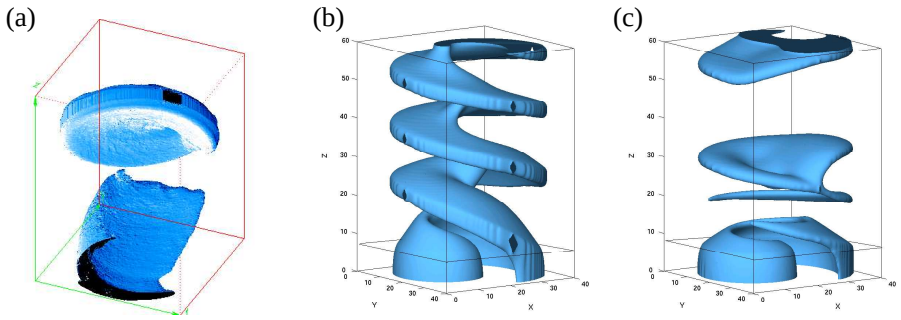

Figure 3: *(a) Experimental observation of filament breakup in the Belousov-Zhabotinsky reaction and simulations of (b) twisted scroll wave and (c) filament breakup in the Barkley model with a vertical gradient in excitability. Shown are surfaces of constant chemical concentrations.*

twisted filament. The experiments employ optical tomography to visualize the three-dimensional pattern dynamics. Under conditions of good excitability twisted scroll waves are observed, while for weak excitability breakup of a scroll wave at the bottom of the medium into planar waves at the top is found in the experiment (see Fig. 3a). We have reproduced that behavior in a simple two-variable model suggested by Barkley [7]

$$\begin{aligned} \partial_t u &= -\frac{1}{\epsilon} u(u-1)(u - \frac{v + b(z)}{a}) + \Delta u \\ \partial_t v &= u - v + \delta \Delta v \end{aligned} \tag{3}$$

where we imposed a vertical gradient in the excitability $b(z)$. This gradient is responsible for the spontaneous appearance of twist in the scroll wave. The twist compensates differences in the rotation frequency in different parts of the medium. It also leads to a bending in the filament of the scroll wave. If the bending amplitude becomes too large the filament may get attached to the system boundary and the scroll wave then ,,breaks" at this point and emits almost planar waves into the medium. A similar phenomena has been suggested as a mechanism for the formation of a fruiting body in colonies of the slime mold *Dictyostelium Discoideum* [8].

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1.20 Modelling Pattern Control on Templated Surfaces

Heiko Kühne, Lutz Brusch, Uwe Thiele and Markus Bär

Introduction. - Spontaneous pattern formation in chemical and biological systems typically occurs on a length scale between 1 μm and 1 cm. In material science, researchers try to exploit processes of self assembly to produce structures on the submicron scale (,,nanostructures"). Two questions arise: (a) Can the principles that have been found to operate in pattern formation on macroscopic scales be transferred to the nanoscale ? (b) Is there a way to influence and control pattern forming processes to obtain a desired structure on the nanoscale? We have modelled two experimentally relevant systems, the growth of metallic nanoclusters on biotemplates and the dewetting of thin fluid films on structured surfaces, with different approaches. In the first example, we use Monte-Carlo simulations of particles that adsorb and diffuse on a periodically structured biotemplate, a bacterial S-layer [1], where nanoscale clusters are observed experimentally under appropriate conditions (Fig. 1). Thin fluid films are subject to long range polar and apolar forces, therefore we use a continuum model derived from the Navier-Stokes equation and study the stability of striped film morphology on a striped substrate.

Metallisation of two-dimensional biotemplates. - Solid-on-solid models are often used for the investigation of surface growth phenomena. The adsorbates in the physical system are represented by columns of particles placed on a lattice. Particles are randomly deposited on the lattice and the top particle of each column may hop to neighbouring sites due to thermal activation. The hopping rates $\nu = \nu_0 e^{-\frac{E_A}{k_B T}}$ are chosen of Arrhenius type. The activation energy $E_A = E_0 + nE_N + sE_S$ consists of three essential terms, E_0 the ground activation energy represents the bonds of a particle to the underlying material and E_N stems from the binding to particles in the same layer. E_A is completed by the Ehrlich-Schwoebel barrier E_S which punishes jumps over edges. The heterogeneity of the substrate is implemented by varying E_0 in space. E_0^A is the ground activation energy on sites where particles prefer to stay - so called affinity centres, E_0^S represents all the other sites on the template and E_0^F is the corresponding term for metal atoms binding to other metal atoms (multilayer adsorption). The discrete model allows a mapping of the real unit cell structure to the model unit cell (Fig. 2).

For a given substrate, *i.e.* fixed ground activation energies, the choice of total deposited mass and of the rate by which the deposition takes place are crucial for the shape of the film at a given time. Morphology transitions from complete wetting to a film which maps the underlying structure perfectly are shown in Fig. 3. The weaker the binding

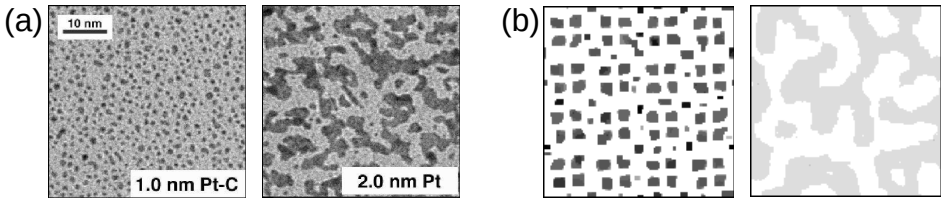

Figure 1: *Experimental observations (a) (TEM micrographs [1]) and simulation results (b) showing the formation of clusters on heterogeneous substrats for low deposition rates (left panel) and labyrinth like dewetting structures (coarsening) in case of homogeneous substrates or for fast diffusive adsorbat (right panel). Dark regiones mark the adsorbate.*

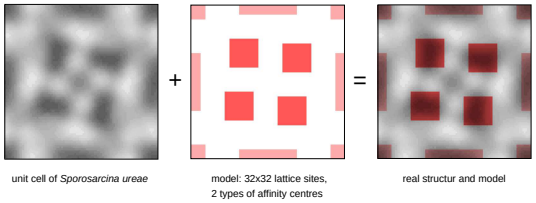

Figure 2: *Unit cell of Sporosarcina ureae calculated from TEM images of negatively stained native S layer [1] and adapted unit cell of the model with two types of affinity centres of different strength. The right picture combines both. Dark regions are pores of the S layer, the lattice constant has been determined as 13.2 nm.*

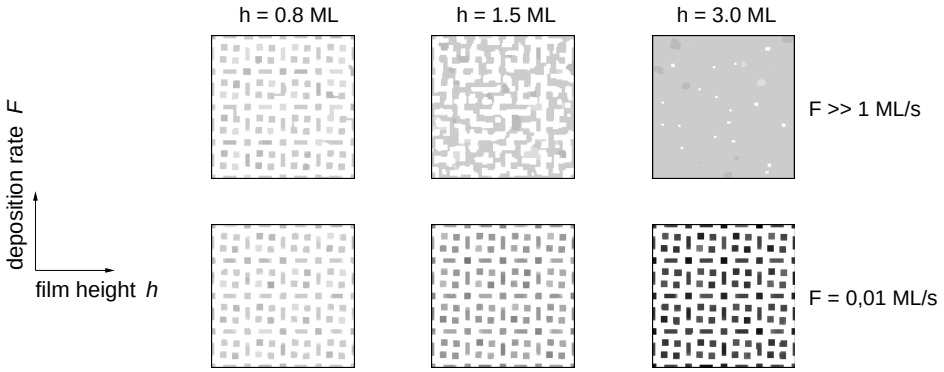

Figure 3: *Morphologies after $t = 1000s$ depending on the mean film height and the deposition rate. The system size amounts to 4x4 unit cells. Parameters are $E_S = 0.44eV, E_{A1} = E_{A2} = 0.6eV, E_F = 0.6eV, E_N = 0.1eV, E_S = 0.0eV$.*

to the affinity centres is the lower the rates of deposition and the smaller the total deposited mass have to be chosen to enable templating. For affinity centres of different strength within the unit cell a greater variety of patterns results. The proportion of clusters growing on the stronger affinity sites compared to those growing on weaker sites not only depends on the relative strength of the affinity sites but also on the deposition rate. These observations suggest the deposition rate as well as the deposited mass as important parameters easily adjustable in the experiments.

Thin film dewetting on structured substrates. - Here we study a model for a thin liquid film dewetting from a chemically heterogeneous substrate (template). Experimental work suggests a transition from the typical coarsening dynamics during dewetting on a homogeneous substrate to pinning, *i.e.* the identical imaging of the template structure, for strong heterogeneity [3]. These observations have been supported by numerical simulations but the underlying mechanisms remain unclear [4].

The evolution equation for the film thickness profile $h(x, y, t)$ is derived by combining the Stokes equation in long wave approximation with diffuse interface theory [5]:

$$\partial_t h = -\nabla\{(h - \ln a)^3 \nabla[\Delta h - \partial_h f(x, y, h)]\} \ . \tag{1}$$

Dimensionless quantities incorporating hydrodynamical parameters are chosen as in Ref. [6]. $a > 0$ describes the wetting properties and is set to 0.1 [5, 6]. The free energy

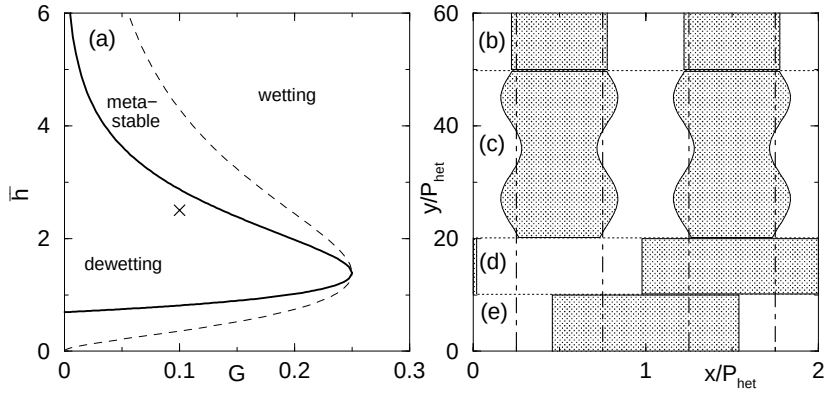

Figure 4: *(a) Phase diagram for thin films on a homogeneous substrate (after [6]). The cross marks the parameter values for which we present results in detail. (b) Schematic display of the template (dot-dashed line), the periodic film profile with the same spatial period (solid line). Shaded areas show where $h > \bar{h}$. (c) Initial stage of the transversal instability and (d),(e) final stages of variants of the longitudinal coarsening instability.*

$f(x, y, h) = \kappa(x)\, e^{-h}(e^{-h} - 2) + \frac{1}{2}Gh^2$ contains the ratio G of gravitation to mean molecular interactions and the spatially varying strength of the molecular interactions $\kappa(x)$. In the absence of heterogeneity, the model possesses two control parameters, the ratio G and the average film thickness $\bar{h}$ that represents conservation of mass. A phase diagram in G and $\bar{h}$ indicating the investigated region of spinodal dewetting is shown in Fig. 4(a). We choose $G = 0.1$ and $\bar{h} = 2.5$ for the following analysis.

We now introduce a heterogeneous substrate with a smooth change in the wettability that is modelled by a spatial sinusoidal modulation of the strength of the molecular interactions

$$\kappa(x) = 1 + \epsilon \cos(2\pi x/P_{het}) \; . \tag{2}$$

The amplitude ϵ and periodicity P_{het} of the template control the dewetting process. For a large range of ϵ and P_{het} we compute all stationary and spatially periodic solutions of Eq. (1) with period P by continuation techniques. Numerical stability analysis and calculation of the energy

$$E = \frac{1}{L_y P} \int_0^{L_y} \int_0^{P} \left[\frac{1}{2}(\nabla h)^2 + f(x, y, h) \right] dxdy \tag{3}$$

reveal stable solutions of lowest energy for each ϵ, P_{het}. On a homogeneous substrate dewetting occurs above the spinodal scale, *i.e.* $P > P_c \approx 33$. Our analysis predicts that the subsequent coarsening prevails for low values of $\epsilon * P_{het}/P_c$ while pinning is obtained for large values. If the heterogeneity has a larger spatial period than the critical dewetting mode, already weak heterogeneities are sufficient for pinning. At intermediate values we encounter a surprisingly large region of coexistence between coarsening dynamics and pinning. The respective transitions are accurately obtained by our method and presented in Fig. 5, the morphological phase diagram [7]. Templating can be best controlled by choosing the initial mass of fluid which yields the smallest P_c, *i.e.* the film thickness where the derivative $-\partial_{hh} f(x, y, h)|_{\bar{h}}$ is maximal.

Conclusion. - We have shown two examples for pattern control on templated surfaces. In the first example growth of nanoclusters is best realized with slow deposition rate

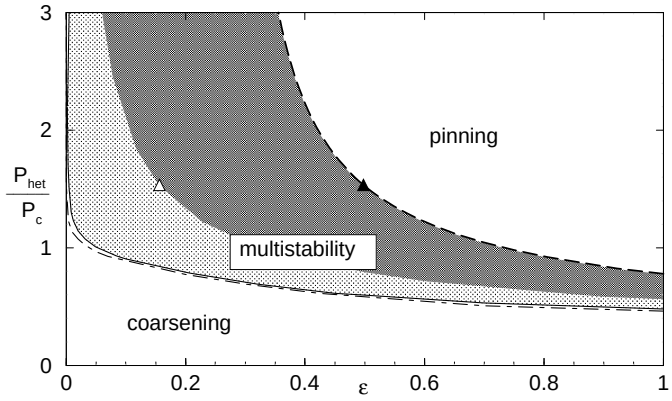

Figure 5: *Morphological phase diagram of templating on a heterogeneous substrate* (ϵ, P_{het}). *The shaded band separates parameters of pure coarsening from pure pinning. Inside the shaded band multistability is found with the desired pattern being the energetic minimum inside the dark shaded area.*

and small total deposit mass. In the second example we have studied the conditions for successful templating of thin films that are unstable to spinodal dewetting. The transition from the labyrinthine dewetting structure to the striped structure indicating successful template is first order and occurs with a large hysteresis.

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1.21 Myxobacterial Rippling: A Biological Migration-Collision Pattern

Uwe Börner, Andreas Deutsch, and Markus Bär

Myxobacteria exhibit a social life cycle with a variety of multicellular patterns. The rod-shaped cells glide along their long axis. Vegetative cells prey, grow and divide as individuals or in small swarms. Individual-based models of cohort migration have been reviewed in [1]. Under starvation conditions, bacteria start to act cooperatively, aggregate and finally build a multicellular structure, the fruiting body. Fruiting body formation is often preceded by a periodic pattern called *rippling* [2-4] (Fig. 1a). Bacteria organize into equally spaced ridges (dark regions) that are separated by regions with

low cell density (light regions). We examine the temporal dynamics of the density profile along a line perpendicular to the ripples (white line in Fig. 1a). The resulting space-time plot reveals a periodically oscillating standing wave pattern (Fig. 1b) with a wavelength of about 10-20 cell length and a temporal period of 10 *min*. Single cells move unidirectionally with the ripple waves in a typical back-and-forth manner [3].

Intercellular communication is essential to maintain a complex life cycle as the one exhibited by Myxobacteria. While other bacteria and ameobae (e.g. *Dictyostelium discoideum*) signal via diffusible chemicals (chemotaxis), myxobacterial rippling apparently depends on the membrane-bound protein C-factor; here signalling requires close end-to-end contact of cells [3]. Addition of C-factor (which can be extracted from rippling cells) increases the mean reversal frequency of cells [3]. Mutants that carry a mutation in the C-factor-encoding gene are unable to ripple and aggregate. Experiments with mixtures of C-signal-competent cells with such mutants exhibit an increased ripple wavelength [3]. Based on these findings Sager and Kaiser proposed the following mechanism for ripple formation: When two opposite moving cells collide head-on, they reverse their gliding direction due to exchange of C-factor [3]. In order to test this hypothesis we have designed a mathematical model.

Discrete model. - Our model for the formation of ripple patterns is based on the dynamics of individual cells. It is defined on a regular cubic lattice assuming discrete space and time coordinates, analogous to cellular automaton models. The spatial lattice constants are chosen in a way that bacterial cells (assumed as equally sized) cover exactly one node. Allowed cell positions are (i) directly on the substrate or (ii) on top of other cells. This reflects the experimental situation in which cells glide on the surface and are organized in heaps [2]. The total number of cells is constant (absence of replication and death). Once per time step all cells move to the neighboring node according to their orientation. Several exception scenarios ensure mobility of the densely

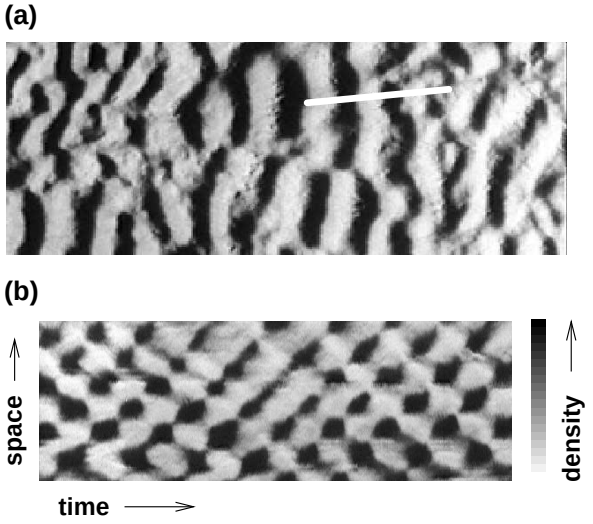

Figure 1: **(a)** *Ripples in aggregates of myxobacteria (snapshot from a movie by H. Reichenbach). The grayscale expresses the cell density. White bar: 300 μm.* **(b)** *Standing wave pattern in a space-time plot of the density along the white bar in (a) (parallel to the direction of wave propagation).*

packed cells. The basic interaction rule of the model is derived from the hypothesis described in the previous section. In the model, head-on-collision takes place if two counter-moving cells form a spatial arrangement in a way that their leading ends are close enough. A cell can be invoked in more than one collision event. Furthermore, we assume cells to be either sensitive or refractory. Refractory cells do not respond to C-factor, i.e. only sensitive cells reverse if invoked in collisions. After a cell has reversed it is temporarily refractory. The duration of this refractory phase is the most important ingredient for rippling [5].
We have also investigated the effect of introducing a second cell type representing C-factor deficient mutants. These mutants fail to encode the C-factor protein, thus they do not induce reversal of other cells in collisions. The mutant cell itself can receive C-signals and reverses after collisions with non-mutant cells. Reversal of mutants also results in temporary refractoriness; here we assume equal duration of this phase for mutants and non-mutants. There are no transitions between the mutant and the non-mutant cell type.

Mean-field approximation. - Apart from direct simulation one can perform a linear stability analysis on the following deterministic rate equations [5]:

$$\begin{aligned}
r_1(x,t+1) &= r_1(x-1,t) - F_r(x-1,t) + r_\tau(x-1,t) \\
r_2(x,t+1) &= F_l(x-1,t) \\
r_i(x,t+1) &= r_{i-1}(x-1,t), \\
l_1(x,t+1) &= l_1(x+1,t) - F_l(x+1,t) + l_\tau(x+1,t) \\
l_2(x,t+1) &= F_r(x+1,t) \\
l_i(x,t+1) &= l_{i-1}(x+1,t), \qquad i = 3 \ldots \tau.
\end{aligned} \tag{1}$$

l_i and r_i denote the average density of left- and right-moving sensitive ($i = 1$) and refractory ($i = 2 \ldots \tau$) cells. The *reversal* functions $F_r(x,t)$ and $F_l(x,t)$ estimate the collision probabilities.

Simulation results and discussion. - The refractory period turns out to be crucial for ripple formation. Regular patterns for refractory times $\tau \geq \tau_c \approx 4$ min can be observed. Two counter-propagating travelling waves of about equal amplitude form a standing wave, in agreement with the experimental observations. For refractory times $\tau < \tau_c$ we still observe pieces of waves without long-range correlations in space or time; for vanishing refractory time cells exhibit fluctuations near a homogeneous density state (Fig. 2a-f). Wavelength and wave period of the simulated ripples increase with τ [5]. The experimental values of wavelength and temporal period of the macroscopic rippling pattern (Fig. 1) are reproduced with a refractory time of ca. 4.5 *min*. The homogeneous solution of the rate equations (1) becomes linear unstable against an oscillatory instability for $\tau \geq 4$ min (Fig. 3a). The comparison of wavelength and period of the most unstable mode with the equivalent quantities extracted from Fourier analysis of the simulated data shows good agreement, in particular for $\tau < \tau_c$ (Figs. 3b,c).

The cell-based nature of the model enables us to investigate also the behavior of individual cells. They are found to move about a distance of half a wavelength before reversing [5], reproducing the back-and-forth movement of cells in the experiment. Pat-

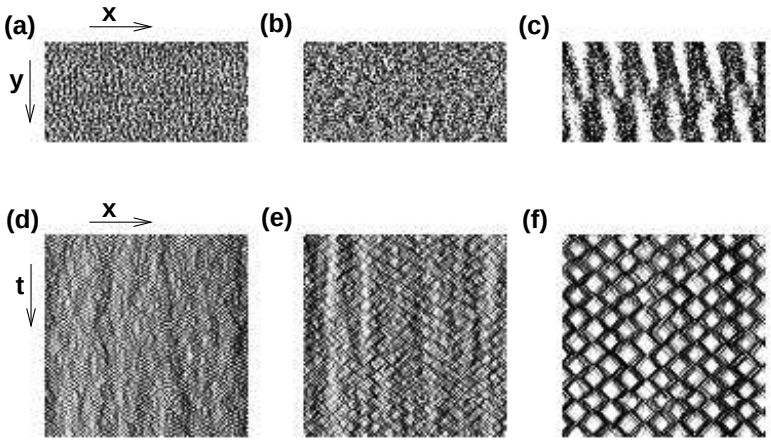

Figure 2: *Simulation snapshots for several refractory times (***(a)** $\tau = 1$ *min,***(b)** $\tau = 3$ *min,* **(c)** $\tau = 5$ *min). In* **(d-f)** *we show the corresponding space-time-plots. Please note the similarities of (c),(f) and Fig.1.*

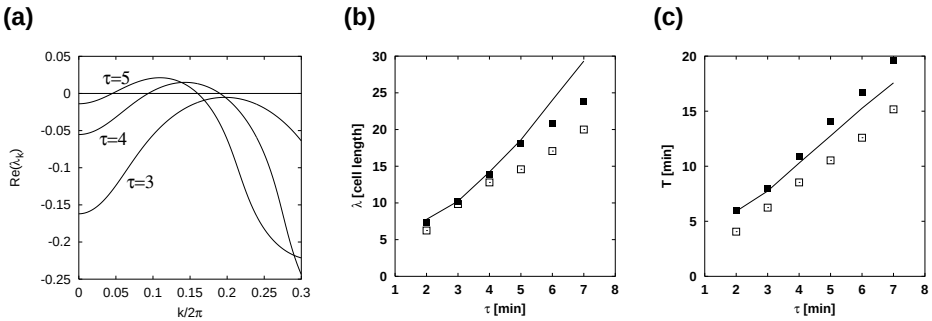

Figure 3: **(a)** *Numerically obtained real part of eigenvalues of the linearization of equation (1) with a suitably chosen reversal function [5] for sub- and supercritical values of* τ*. Only the branch with the rippling instability is shown. We compare wavelength* **(b)** *and period* **(c)** *of the ripple pattern found in simulations (squares) and in the mean-field equations (lines).*

terns produced in mutant-diluted systems (model extension I) are shown in Fig. 4. For a fairly large fraction (40%) of C-signal-defective mutants (Fig. 4a,d) the pattern is still recognizable and regular with long correlation lengths in space and time. Upon further increase of mutants the patterns are no longer visible from a snapshot (Figs. 4 b,c), though the space-time diagrams still show some periodicity and wave propagation (Figs.4 e,f). In the simulations the wavelength of the ripples does not show any clear tendency to change with the mutant fraction; this does not agree with the reported experiments [3].

Conclusions. - We presented a simple individual-based model for ripple formation including the interplay between cell migration and orientation-dependent interaction rather than a reaction-diffusion mechanism. The spatio-temporal synchronization is due to a refractory phase after reversal during which further cell reversal is prohibited. As our results show, collision-induced cell reversal as proposed by Sager and Kaiser is an appropriate mechanism for ripple formation only if it is supplemented by a refractory period. Wavelength and period of the pattern are determined by the duration of this period. The emergence of the pattern sensitively depends on the precision of this internal clock.

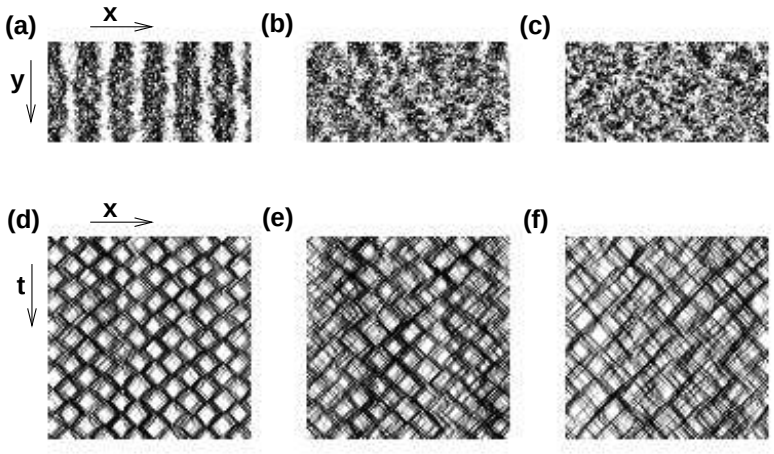

Figure 4: *Simulation snapshots for several fractions of C-factor-deficient mutants (***(a)** *40% mutants,* **(b)** *60%,* **(c)** *80%) and corresponding space-time-plots in* **(d-f)**.

Myxobacterial rippling provides a first example of pattern formation mediated by migration and direct cell-cell interaction. Related theoretical approaches use continuous models and assume a cooperative effect in the reversal of cells [7] or a combination of refractoriness and cooperativity [8]. Further analysis of these models as well as additional experiments are needed to clarify the details of the rippling mechanism. Similar processes may also be involved in myxobacterial fruiting body formation as well as selforganization processes in other multicellular systems.

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1.22 Correlations between periodic orbits and their rôle in spectral statistics

Martin Sieber and Klaus Richter

Complex quantum systems such as mesoscopic electronic devices, highly excited atoms and molecules, or optical microcavities, to name a few, have in common that they show

clear features of quantum coherence while simultaneously requiring statistical and nonlinear dynamics approaches. Such quantum systems with disorder or with a chaotic classical counterpart share the remarkable property that energy levels, eigenfunctions, transition amplitudes, or transport quantities exhibit universal features: They are independent of the details of the individual system and depend only on its symmetries. Energy level diagrams of these systems usually exhibit a variety of seemingly unstructured levels of high density. Then it is often irrelevant to study properties of individual quantum states but rather to consider statistical spectral features, such as fluctuations in the distributions of energy levels.

It was originally conjectured by Bohigas, Giannoni, and Schmit [1], and is by now numerically well established, that spectral correlations of classically chaotic quantum systems, in the semiclassical limit $\hbar \to 0$, agree with correlations between eigenvalues of random matrices. While such a connection with RMT has been proven for disordered systems using field theoretical methods [2], it remains an outstanding problem in the field of clean (disorder-free) quantum systems with a chaotic classical limit, often referred to as quantum chaos.

Semiclassical theory, being based on the Gutzwiller trace formula [3] represents one prominent approach towards an understanding of spectral statistics. It provides the most direct link between spectral quantities of the quantum Hamiltonian and properties of the chaotic dynamics of the corresponding classical system. A central quantity to characterize spectral statistics is the spectral two-point correlation function, $R(\eta)$, involving a product of two densities of states with energy separation η. A semiclassical approach to $R(\eta)$ is based on approximating the densities of states by the trace formula, which expresses them by sums over contributions from classical periodic trajectories. Hence a computation of $R(\eta)$ involves the evaluation of a double sum over classical trajectories.

Along this line, semiclassical theory has been applied [4] to better understand the observed universality in quantum energy spectra. It was shown [4] that by including only pairs of orbits with themselves or their time-reversed partner, the so-called *diagonal approximation*, the energy level correlator agrees with random matrix theory only in the limit of long-range correlations. To access the important spectral regime beyond these asymptotic results, the aim of this project, requires the direct calculation of so-called *off-diagonal* contributions from pairs of different classical paths, and necessitates further insight into classical correlations between trajectories.

In quantum chaos one main interest in recent years has been to further investigate the conjectured universality in the statistical distribution of energy levels [5]. To this end it proves convenient to consider the spectral form factor that is defined as the Fourier transform of the spectral two-point correlator $R(\eta)$,

$$K(\tau) = \int_{-\infty}^{\infty} \frac{\mathrm{d}\eta}{\bar{d}(E)} \left\langle d_{\mathrm{osc}}\left(E+\eta/2\right) d_{\mathrm{osc}}\left(E-\eta/2\right)\right\rangle_E e^{2\pi i \eta \tau \bar{d}(E)} \,. \tag{1}$$

Here, $d_{\mathrm{osc}}(E)$ denotes the oscillatory part of the density of states ($d(E) = \sum_n \delta(E - E_n) = \bar{d}(E) + d_{\mathrm{osc}}(E)$). In Eq. (1), the time is measured in units of the so-called Heisenberg time t_{H}, the inverse of the mean level spacing, i.e. $\tau = T/t_{\mathrm{H}} = T/(2\pi\hbar\bar{d}(E))$. The form factor is evaluated by averaging over an energy interval, $\langle \ldots \rangle_E$, that is small

in comparison to E but contains a large number of levels. An expansion of the random matrix prediction of the form factor for small τ gives $K^{\mathrm{GOE}}(\tau) = 2\tau - 2\tau^2 + \ldots$.

Semiclassical theory of spectral statistics has been developed in order to find an explanation for the observed agreement of numerical and experimental results with random matrix statistics. Its aim is to attribute this universal property of the quantum system to generic properties of trajectories of the corresponding classical system. For the spectral form factor the semiclassical approximation is obtained by expressing the density of states in terms of classical periodic orbits through Gutzwiller's trace formula [3], by inserting it into Eq. (1), and by evaluating the Fourier transform in leading order of $\hbar$. This leads to a double sum over periodic orbits. Each sum contains an infinite number of classical periodic orbits which exponentially increases with orbit length. Hence the double sum contains a huge number of pair terms. Most of the pairs consist of periodic orbits with classical actions that are uncorrelated. The sum over these orbits behaves like a sum over random complex numbers and their contributions cancel each other when summed over. We expect that the non-vanishing contributions come from a relatively small number of pairs of orbits to be indentified which are correlated. The strongest correlation occurs between orbits which have identical actions. In Berry's diagonal approximation only those pairs of orbits are considered which are identical or related by time inversion. In this way he obtained the leading term of the GOE form factor for small values of τ: $K(\tau) \approx 2\tau$ [4].

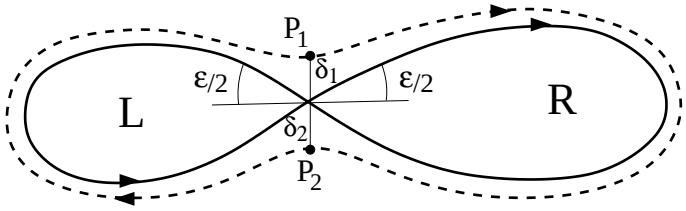

Figure 1: *An example of a self-intersecting classical periodic orbit with small opening angle ε, and its neighbouring periodic orbit (dashed line) (from Ref. [6]).*

To go beyond the diagonal approximation requires the evaluation of pairs of different orbits which are not related by any symmetry. In the following we sketch our derivation of the next term in the expansion of the form factor, namely the term $-2\tau^2$. It is obtained (in two-dimensional systems) from a class of pairs of self-intersecting periodic orbits with small opening angles and periodic orbits in their close vicinity as depicted in Fig. 1. The two orbits follow one loop in the same direction and the other loop in the opposite direction. In Ref. [6] it has been shown that such pairs of orbits indeed exist for small crossing angles $\varepsilon \ll \pi$.

In the following we will focus on a particular class of systems with uniformly hyperbolic dynamics, where all orbits possess the same Liapunov exponent λ and for which the calculations are simpler. We calculated the action difference between both orbits, entering into the form factor, and find [6] $\Delta S(\epsilon) \approx p^2\epsilon^2/(2m\lambda)$. Obviously, the action- and thereby phase-difference is vanishingly small for $\varepsilon \to 0$ and hence these orbit pairs are candidates for non-vanishing off-diagonal contributions to the form factor.

In order to proceed we have to evaluate the number of self-intersections of periodic orbits (since an orbit pair is associated with each self-intersection) and the distribution of the crossing angles. As a result of a longer computation [6] one finds for a trajectory with time T that the average number of self-intersections with an opening angle in an interval $\mathrm{d}\varepsilon$ around ε ($0 \leq \varepsilon \leq \pi$) is given by

$$P(\varepsilon, T)\,\mathrm{d}\varepsilon \sim \frac{v^2}{2\pi A} T^2 \sin\varepsilon \left[1 + \frac{4}{\lambda T}\log(c\varepsilon)\right]\,\mathrm{d}\varepsilon \tag{2}$$

for $T \to \infty$. Here, $P(\varepsilon, T)$ is the density of crossings of opening angle ε for trajectories of time T, A is the area, and c is a system dependent constant, $c \sim \pi$. The leading-order term for long times, $\sim T^2$, results from an ergodicity assumption. However, the evaluation of the form factor showed that the contribution from the T^2-term vanishes. Instead, the logarithmic term turned out to be of key relevance: It arises from the fact that the crossing density is reduced with respect to the ergodic result ($\log(c\varepsilon) < 0$ for small ε) owing to the hyperbolic character of the nonlinear dynamics [8].

We used this classical information to evaluate the contribution of the pairs of double-loop orbits to the spectral form factor. We did this by summing over all intersections of angle ε that occur in periodic orbits, and then integrate over ε. Altogether we finally obtained [6]:

$$K_{\mathrm{off}}^{(2)}(\tau) = -2\tau^2\,. \tag{3}$$

This result, which entirely stems from the $\log\varepsilon$ contribution in the integral, coincides precisely with the RMT prediction! We also confirmed numerically for the example of chaotic motion on a Riemannian surface that the analytical expression (2), and thereby Eq. (3), holds [6].

To conclude, we have shown that in chaotic systems a class of off-diagonal pairs of periodic orbits exists which evidently exhibit action correlations. This result is the first clear indication on the origin of off-diagonal contributions to the spectral form factor of complex quantum systems. Our findings suggest to draw the following conclusions: (i) It is possible to systematically evaluate off-diagonal contributions to the spectral form factor by the semiclassical method. (ii) The τ^2 term of the spectral RMT form factor is related to self-intersecting orbits in Fig. 1.

The problem to compute off-diagonal contributions to the spectral form factor is closely related to corresponding problems which involve energy averages over products of advanced and retarded Green functions. The method described opens up a variety of possible further applications. One prominent example is mesoscopic quantum transport. For clean chaotic systems, a semiclassical theory which adequately and quantitatively describes weak localization has been lacking for more than a decade [7]. Recently, based on the same technique as presented here, we obtained the correct weak-localization correction to the conductance in chaotic mesoscopic systems [8].

A systematic computation of higher-order contributions to the spectral form factor from multi-loop periodic-orbit configurations in chaotic systems remains as a challenging future program.

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1.23 Molecular-scale electronics

Gianaurelio Cuniberti

Introduction. - The incessant development of single molecule techniques is forcing a paradigm shift in the many neighboring branches of nano-science. This process does not exclude the modelling and design of electronic devices. Novel fabrication methods that create metallic contacts to a small number of conjugated organic molecules allow the study of the basic transport mechanism of these systems and will provide direction for the potential development of molecular-scale electronic systems [1]. The concept is now realized for individual components, but the economic fabrication of complete circuits at the molecular level remains challenging because of the difficulty of connecting molecules to one another. A possible solution to this problem is 'mono-molecular bridge' electronics, in which a single molecule will integrate the elementary functions and interconnections required for computation [2]. Indeed, the primary problems facing molecular electronics designing are measuring and predicting electron transport. That is due to the fact that molecular electronics is strongly dependent on the quality and nature of the contacts [3]. Nevertheless, the contact problem can be turned into a challenge. Even with the intrinsic barrier that the contacts represent, contacts can be strategically used to favor the design of specific devices [4]. However, this requires a more detail account of the atomic structure of the interface. Green functions and density functional theories (DFT) [5, 6] are the optimal instruments to characterize transport through single molecules clamped between two metallic contacts. This report provides, after a short section on the theoretical tools for investigating molecular scale transport, examples of several devices where the focus is given to the (I.) bridged molecule, to (II.) the role of the leads and to (III. and IV.) structures where both the molecule and the leads should be accounted at the same level due to the importance of the contacts.

Charge transport in molecular systems. - In dealing with molecular electron transport, a formulation that includes interference effects due to phase coherence as well as geometrical effects is needed. It was originally developed by Landauer [7] for a two-terminal geometry. The essential idea of the Landauer formulation is to relate the

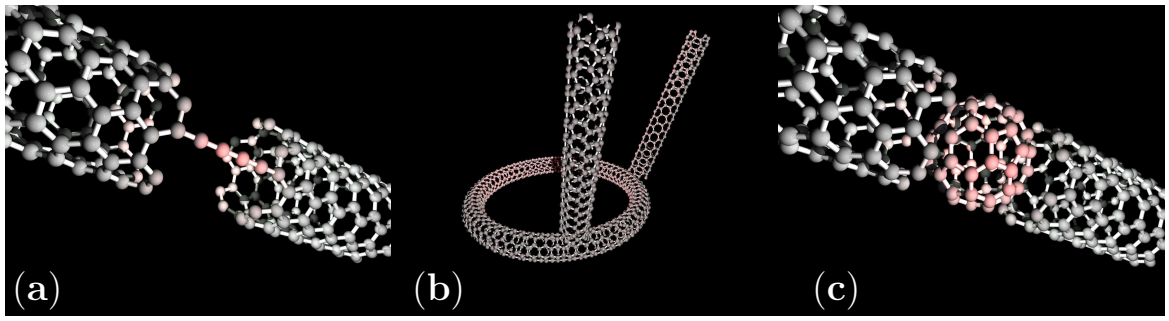

Figure 1: Examples of two terminal molecular electronic devices where carbon nanotubes leads clamp a molecular wire (a), a carbon nanotube ring (b), and a C_{60} molecule (c).

conductance to an elastic scattering problem and, ultimately, to transmission probabilities. The simplest way to derive this relationship is to separate the system at hand in three parts: a 'molecular' region connected to two ballistic leads, which are connected to electronic reservoirs at the chemical potentials $\mu_{\rm L}, \mu_{\rm R}$. It is assumed that electrons entering the reservoirs do completely lose their phase coherence. In equilibrium $\mu_{\rm L} = \mu_{\rm R}$, but if an infinitesimal voltage $eV = \mu_{\rm L} - \mu_{\rm R}$ is applied a non-equilibrium situation is induced and a current will flow. The scattering region is characterized by the energy-dependent transmission coefficient $T(E)$. In the zero-temperature, linear response ($eV \to 0$) regime it is found that the proportionality law between the conductance, g, and the transmission, $g = g_{\rm K} T(E_{\rm F})$, holds, where $g_{\rm K} = 2e^2/h$ is the von Klitzing conductance quantum and $E_{\rm F}$ is the Fermi energy of the whole system in equilibrium. In molecular transport, in the case of strong coupling, it is the electronic structure of the molecule influenced by the leads that determines the transmission properties which in turn play the decisive role for electron transport. For a general scattering region where inelastic effects are included, one can use non-equilibrium Green functions to derive an expression for the conductance which reduces to the one for the elastic case. An advantage of this derivation is that an explicit connection to the Green function of the scattering region dressed by the presence of the leads is established. The latter are introduced as self-energy corrections into the bare 'molecular' Green function. The result for the transmission probability is then given in terms of a trace over states in the scattering region of Green function and self-energy operators [6].

For system in which the issue of the contact between the leads and the molecules plays an important role, it becomes unavoidable to include some atoms belonging to the leads to the scattering region (already clean surface electrodes are usually energetically unstable, so that upon structural relaxation the surface topology may be modified and this will introduce additional scattering). From the point of view of electronic structure calculations, we have developed a scheme to cope with such situations. It enables to calculate *first-principles parametrized tight-binding* (TB) Hamiltonian matrix elements (at the DFT level). The TB-DFT scheme relies on a representation of the electronic eigenstates of the system within a non-orthogonal localized basis set, usually taken as a valence basis. The many-body Hamiltonian is then approximately represented by a two-center tight-binding Hamiltonian. The matrix elements, however, are calculated numerically, avoiding the introduction of empirical parameters as in conventional TB approaches.

I. Bridge molecules. (with L. Craco in collaboration with C. Dekker (TU-Delft), and D. Porath (Hebrew Univ. Jerusalem)) **-** As a first example of molecular de-

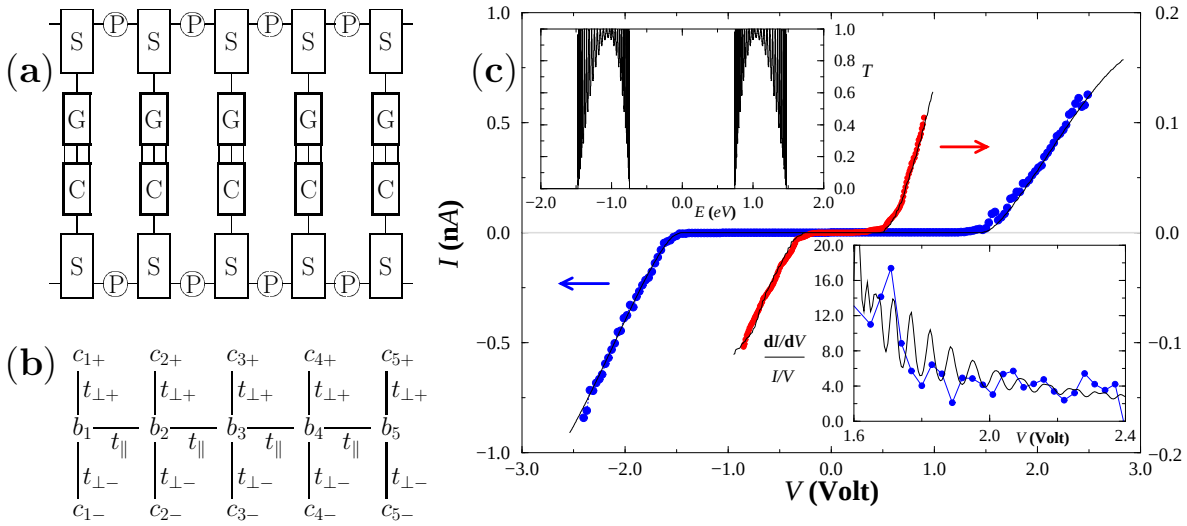

Figure 2: Schematic view (a) of a fragment of poly(G)-poly(C) DNA molecule; each GC base-pair is attached to sugar and phosphate groups forming the molecule backbone. In (b), the diagram of the lattice adopted in building our model, with the π stack connected to the isolated states denoted as $\pm$-edges. In (c), the low temperature I-V characteristics of two typical measurements at 18 K (blue circles) and at 3.6 K (red circles) are shown. Solid lines show the theory curves following the experimental data. The insets show the transmission calculated after the blue data (upper) and the normalized differential conductance (lower). The parameters used are 30 base pairs with $t_{\parallel} = 0.37$ eV and $t_{\perp\pm} = 0.74$ eV for the blue measurement, and $t_{\parallel} = 0.15$ eV and $t_{\perp\pm} = 0.24$ eV for the red one.

vice, we concentrate on a case in which it is not the structure of the lead electrodes to be relevant but the one of the molecule itself. Recently Porath *et al.* [8] have reported nonlinear transport measurements on 10.4 nm long polyguanine-polycytosine DNA, corresponding to 30 consecutive GC base-pairs, attached to bulky platinum leads (GC-device). The measured current-voltage (I-V) characteristics show typical semiconducting features at low temperature (under 10 K) with a gap of the order of 1 V. Furthermore, the poly(G)-poly(C) DNA molecule has typical electronic features of a periodic chain, as the first DFT calculations have indicated. This may support the idea that, differently from natural λ-DNA (complex sequence), where the sequence variability or the attachment to the surface could lead to electron localization over very few base-pairs, in short suspended GC-devices band-like conduction might be the relevant transport mechanism. Motivated by such considerations, we have introduced [9] a minimal model for charge transport through GC-devices and show that the semiconducting behavior of the observed low temperature I-V curves can be explained by the hybridization of the G-G π stack with the transversal backbone reservoirs. The result for the current obtained within a a tight-binding model for the hole injection into the GC-devices is presented in Figure 2. The I-V curves are in very good agreement with the experimental ones and have been obtained by generalizing the Landauer treatment to the nonlinear regime.

II. Carbon nanotubes as mesoscopic leads. (with G. Fagas, M. Porto, K. Richter, and J. Yi) **-** As second issue, we have focussed our attention on the role of the leads. Leads might give relevant contributions to the transmission when their lateral dimension is of the order of the contacted molecule. This is the case for carbon nanotubes (CNTs) conductors which have been in the focus of intense experimental and theoretical activity as another promising direction for building blocks of molecular-scale circuits. CNTs exhibit a wealth of properties depending on their diameter, on the orientation of graphene roll up, and on their topology, namely whether they consist of a single cylindrical surface (single-wall) or many surfaces (multi-wall). Among the different configurations in which CNTs have been employed, we would like to stress here two experiments which we have been considering. Figure 1.a shows a configuration resembling the experiment in Ref. [10] in which CNTs have been used as wiring elements connected by molecular wires. Given this particular configuration, we have shown that adopting CNT leads is strongly affecting the profile of the conductance [11]. Figure 1.b is the simplified version of the setup experimentally characterized in Ref. [12]. Two CNTs have been appended to two scanning tunneling microscope (STM) tips and have been put in contact with a CNT ring. We could show that both the rectification in the I-V characteristics and the peculiar STM images can be described by properly considering both the structure and the topology of the system [13].

III. Towards a first principle description. (with G. Fagas, and K. Richter in collaboration with R. Gutiérrez, F. Grossmann, and R. Schmidt (TU-Dresden)) **-** At this point we are left with the issue of characterizing the electronic

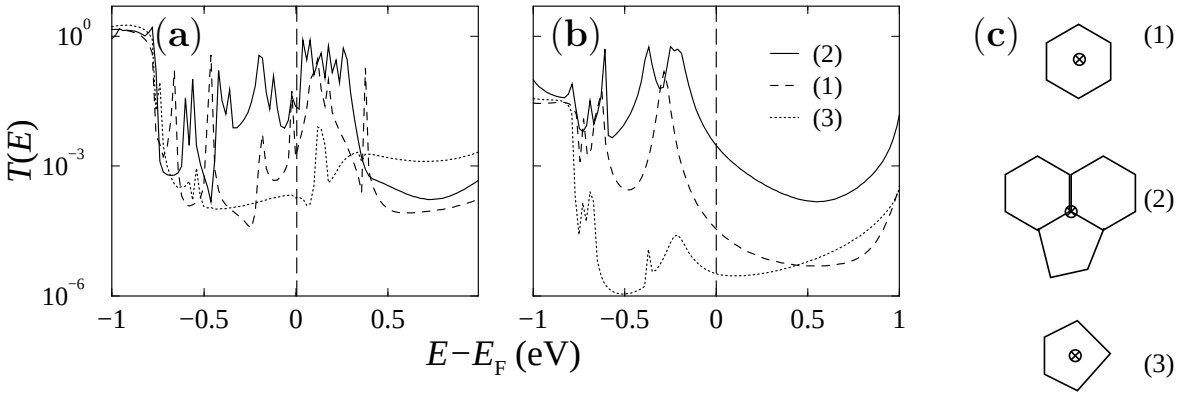

Figure 3: Transmission results for both unrelaxed (a) and relaxed (b) configurations. The tube-tube distance is fixed at 0.93 nm. Numbers classify three different molecular orientations of the C_{60} as depicted in (c); the nanotube symmetry axis is depicted by a cross inside a circle.

structure of the molecule as well as of the leads. We do this by discussing a single C_{60} molecule bridging two single metallic (5,5) armchair nanotubes (as in Figure 1.c) [14]. In this pure carbon system, charge transfer effects are negligible. The Fermi level of the whole system will therefore lie within the highest occupied - lowest unoccupied molecular orbital (HOMO-LUMO) gap of the isolated C_{60}. Therefore, the electronic transport will be mainly mediated by the overlap of the tails of the molecular reso-

nances within the HOMO-LUMO gap of C_{60}. The key problem we addressed was how severely orientational effects do influence the electronic transport. To this end several possible orientations of the C_{60} (depicted by the polygon(s) facing the tube symmetry axis in Fig. 3.c) have been considered for a fixed distance between the molecule and the tubes. For the sake of comparison, structurally unrelaxed and relaxed molecular junctions were considered. The basic results are displayed in Fig. 3, for both relaxed and unrelaxed structures. Surprisingly, at fixed distance, just an atomic scale rotation of the highly symmetric C_{60} molecule induces a large variation of the transmission at the Fermi energy by several orders of magnitude. As can be seen in Fig. 3.a, neglecting relaxation decisively influences the transmission properties of the molecular junction. This shows up as a different and less smooth behaviour of the transmission. The qualitative difference is related to the presence of dangling bond states on the CNT surfaces. Such states usually lie within a gap (a similar situation as that found, e.g., in semiconductor surfaces), in this case the HOMO-LUMO gap of the isolated molecule. They lead to the oscillatory behaviour in the transmission for unrelaxed junctions. Upon relaxation these states are partly saturated or they rehybridize, moving away from the middle of the gap. This rather sensitive dependence on the orientation could possibly be exploited in an electronic switching device on the nanoscale, as manipulation of fullerenes by using STM or atomic force microscope tips is becoming a standard technique in the field.

IV. The rôle of electronic correlations. (in collaboration with M. Thorwart, M. Grifoni, H. W. Ch. Postma, and C. Dekker (TU-Delft)) **-** In CNTs, quasi-

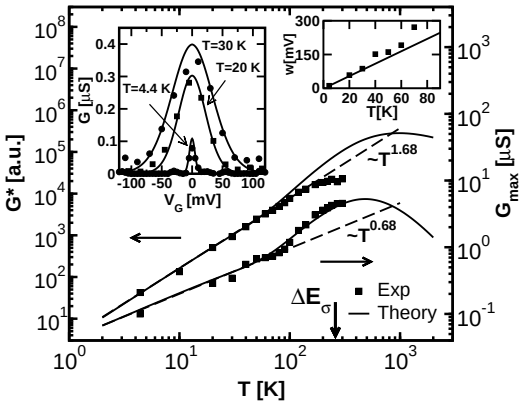

Figure 4: Conductance maximum $G_{\max}$ and integrated conductance G^* as a function of temperature. Solid line: theoretical prediction with the Luttinger interaction strength $g_\rho = 0.23$. Insets: Conductance peaks versus gate voltage (left), and peak width versus temperature (right).

onedimensionality and electronic correlations are expected to be reflected in a typical non-Fermi behavior. The rôle of electronic correlations of metallic single-walled CNTs can be accounted, at low-energy, via the Luttinger liquid theory [15]. Within this scheme, we have investigated correlated electronic transport in single-walled CNTs with two intramolecular tunneling barriers [16]. We suggest that below a characteristic temperature the long range nature of the Coulomb interaction becomes crucial to determine the temperature dependence of the maximum $G_{\max}$ of the conductance peak. Correlated sequential tunneling dominates transport yielding the power-law

$G_{\max} \propto T^{\alpha_{\mathrm{end-end}}-1}$, typical for tunneling between the ends of two Luttinger liquids. Our predictions are in agreement with recent measurements.

Acknowledgment. - S. Leoni is gratefully acknowledged for the ray-tracing of the devices in Figure 1.

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1.24 Aharonov-Bohm ring as a spin switch

Martina Hentschel, Diego Frustaglia, and Klaus Richter

Currently, the field of spintronics, where both the spin of the electron and its charge are manipulated, receives growing interest [1, 2, 3]. This is strongly motivated by the variety of potential applications of spin-based information processing. Considerable experimental efforts have been undertaken to, e.g., inject spin-polarized electrons into semiconductor devices. Recent successes [4] raise hope that the theoretically predicted spin-switch effect [5] that we will describe in the following will prove to be useful in the future.

The model system we consider is a ballistic ring built, e.g., from a two-dimensional electron gas of a semiconductor heterostructure, coupled to leads. It is subject to an

inhomogeneous magnetic field **B**, see Fig. 1. We study the spin-dependent magnetoconductance through the ring that is directly related to the transmission of electrons within the Landauer formalism. The magnetic flux through the ring gives rise to the well-known Aharonov-Bohm oscillations in the magnetoconductance that we expect to be changed by the existence of geometric phases in (sufficiently strong) inhomogeneous magnetic fields.

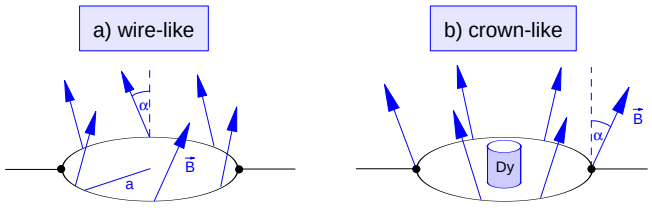

Figure 1: *Magnetic field texture for a) a wire-like and b) a crown-like magnetic field. The angle α is defined as the angle of the magnetic field with respect to the z-axis; here we mainly consider the case of in-plane fields, $\alpha = 90^0$. In experiments, a wire-like magnetic field can be created by means of a central current lead, while a crown-like field can be obtained by placing a (Dysprosium) micromagnet into the center of the ring.*

We consider electrons entering the ring with Fermi energy E_F. They are subject to the Zeeman interaction upon traversing the ring; spin-orbit coupling is neglected. The ratio between the spin (Larmor) frequency $\omega_L \propto |\mathbf{B}|$ and the orbital kinetic frequency $\omega \propto E_F$ defines the degree of adiabaticity that is higher in stronger magnetic fields.

We describe the system employing two different techniques. On one hand, we use a recursive Green function technique in a tight-binding formalism to model numerically a two-dimensional (2d) ring that can have several open transverse channels. On the other hand, we assume the ring to be one-dimensional (1d), allowing for an analytical description of the system for all magnetic field strengths [6]. A transfer-matrix approach [7], extended to spin-dependent transport, is used to model the transport through the ring, whereas the coupling between ring and leads is governed by a coupling parameter ϵ in the S-matrix.

The situation where the magnetic field lies in the plane of the ring turns out to be especially interesting, independent of the texture (tangential, radial, or combination) of **B**. Here we found a novel spin-flip effect that is illustrated in Fig. 2 in terms of (Fermi) energy-averaged transmissions. It exists both in 2d rings [left panels (a)-(c)] and 1d rings [(d)-(f)] where it can be rigorously proven [8].

We assume a tangent magnetic field of moderate strength in the ring plane [Fig. 2(b,e)], and electrons entering the ring with spin in field direction (up-polarized electrons, $\uparrow$). We study spin-dependent transmission through the ring as a function of an additional Aharonov-Bohm control flux ϕ. For $\phi = 0$, only electrons that keep their spatial spin direction are transported, $\langle T \rangle = \langle T_{\uparrow\uparrow} \rangle$. There are no electrons detected that have changed their spatial spin direction (and hence would still be aligned with the magnetic field), $\langle T_{\downarrow\uparrow} \rangle = 0$. This result holds irrespective of the field strength or adiabaticity. However, in the non-adiabatic limit, Fig. 2(a,d), the transmission is dominated by

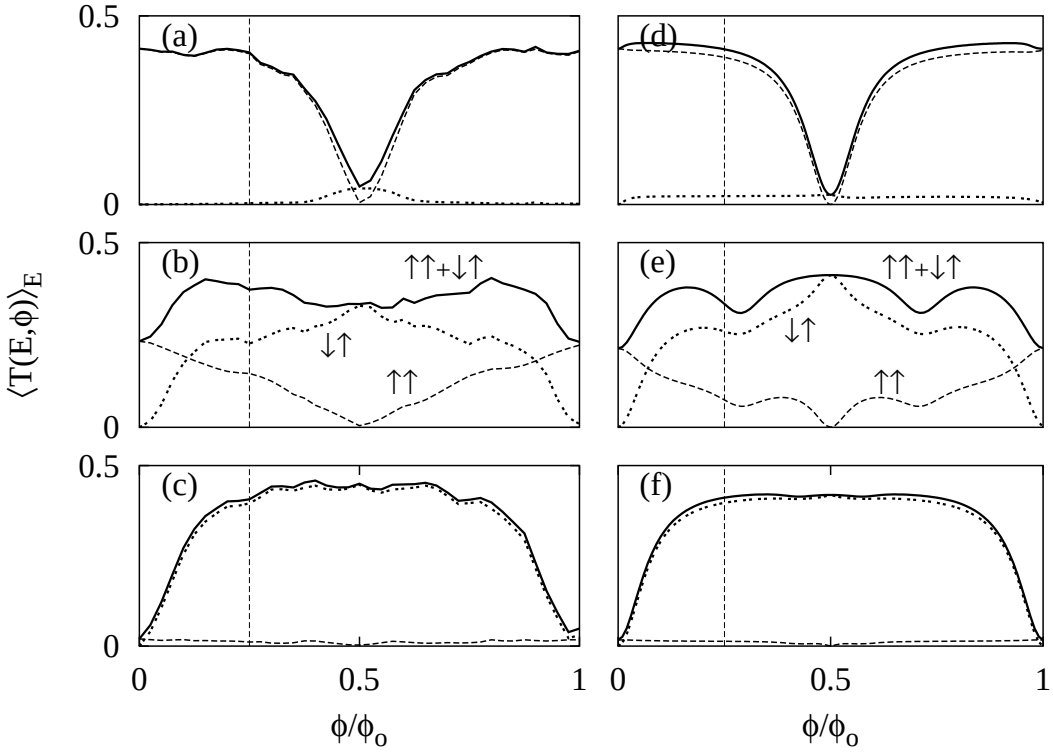

Figure 2: *Averaged transmission for up-polarized incoming spins through a quasi-1d ring as function of a (small) magnetic control flux ϕ measured in units of the flux quantum, $\phi_0 = hc/e$. We compare numerical results for 2d rings with one open transverse channel [left panels (a)-(c)] with analytical calculations for a strictly 1d ring [(d)-(f), $\epsilon = 0.3$] and find close similarity. The strength of the non-uniform in-plane magnetic field (and hence the degree of adiabaticity) increases from top to bottom: (a) weak, (b) moderate, (c) strong. The overall transmission $\langle T \rangle$ (solid line) is split into its components $\langle T_{\uparrow\uparrow} \rangle$ (dashed) and $\langle T_{\downarrow\uparrow} \rangle$ (dotted). Note the change in the polarization upon tuning the flux and the spin-switching mechanism at $\phi = \phi_0/2$. Equivalent results are obtained for down-polarized incoming electrons (not shown here).*

the $\langle T_{\uparrow\uparrow} \rangle$-component anyway, whereas the presence of the Berry phase in the adiabatic regime, Fig. 2(c,f), causes the total transmission to vanish for purely in-plane magnetic field.

Let us now turn on an Aharonow-Bohm flux of half a flux quantum, $\phi = \phi_0/2$. Then one finds only electrons that *switch* their spin (in space) to contribute to the conductance, $\langle T \rangle = \langle T_{\downarrow\uparrow} \rangle$ and $\langle T_{\uparrow\uparrow} \rangle = 0$, see Fig. 2 – this is exactly the opposite transmission behaviour of the $\phi = 0$ situation, and indeed constitutes a spin-switch effect. For other control fluxes $\phi \neq \phi_0/2$, both components, $\langle T_{\uparrow\uparrow} \rangle$ and $\langle T_{\downarrow\uparrow} \rangle$, contribute to the total transmission of incident up-polarized electrons (vertical dashed line in Fig. 2). We find a ϕ_0-periodicity of the behaviour, provided the control flux does not destroy the "in-plane field" condition.

For weak magnetic fields, Fig. 2(a,d), there exists an Aharonov-Bohm transmission minimum at $\phi = \phi_0/2$, whereas there is a transmission maximum for strong fields, Fig. 2(c,f) – the shift of the extrema by $\phi_0/2$ is a direct result of the presence of a Berry phase (causing a geometric flux equivalent to $\phi_0/2$) in the adiabatic regime. The

transmission in the adiabatic situation is dominated by electrons where the spin follows the magnetic field, $\langle T \rangle \approx \langle T_{\downarrow\uparrow} \rangle$. Hence, the spin-switch effect is masked both in the adiabatic and non-adiabatic situation.

We summarize this *spin-flip effect* as follows [5]: For ballistic microstructures subject to in-plane magnetic fields that are symmetric with respect to the lead axis we have demonstrated how an additional small Aharonov-Bohm flux ϕ can be used to control spin flips of incident polarized electrons, i.e., how to tune the polarization of the transmitted electrons, provided there is only one open channel in the leads. We point out that this effect, which arises from a subtle interference mechanism of the spatial and spin wavefunctions, holds for all degrees of adiabaticity though it is most striking in the intermediate regime, Fig. 2(b,e). In combination with a spin detector such a spin-flip device may be used to control spin polarized currents, similar to the spin field-effect transistor proposed in [1].

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1.25 Delay times of localized waves

Henning Schomerus

Interference of multiply scattered waves is a fundamental mechanism for phenomena in a variety of systems, ranging from electronic microdevices at low temperatures over electromagnetic wave guides and resonators to media which support classical waves, such as the elastic waves in the earth crust which originate from an earthquake or in an explorative underground detonation. Another field of application is in medicine, as in the examination of organs by ultrasound. Wave localization is maybe the most striking phenomenon which arises from multiple scattering. Localization can be understood as the systematic enhancement of the backscattered wave amplitude by constructive interference. In a wave guide geometry, it results in the exponential attenuation of the transmitted intensity

$$I(L) \propto \exp(-2L/\xi) \tag{1}$$

for lengths L of the wave guide greater than the localization length ξ, even in the absence of absorption. Localization was first investigated in mesoscopic systems [1]. Recently the undertaking of its realization and observation for microwaves [2, 3] and

optical waves [4, 5, 6] has attracted a lot of interest. One motivation is the prospect of achieving the feedback for a laser not by conventional mirrors but by multiple scattering, especially because wave localization provides a very efficient spatial confinement. However, the wave intensity I itself is not a good indicator of wave localization, because the same attenuation (1) can also arise from absorption.

Dynamical aspects of wave propagation in the presence of localization can be tested by probing the frequency dependence of the transmitted or reflected wave amplitude. When frequency is changed, the phase ϕ of the scattered wave changes in a systematic fashion: Without any scattering, the phase of the transmitted wave $\phi = \omega L/c$ allows to extract the travel time

$$\phi' = \mathrm{d}\phi/\mathrm{d}\omega = L/c \tag{2}$$

of the wave through the wave guide [7]. In a geometric-optics point of view, ϕ' can be interpreted as the travel time even when the wave is scattered many times, which is the case for diffusive wave propagation. However, this "classical" point of view can no longer be adopted if the non-perturbative effect of localization sets in. Recent experiments have succeeded in the direct measurement of the so-called single-mode delay time for specified incident and detected modes, both for microwaves [8] and optical waves [9]. (The attribute 'single-mode' means here that only one of the N propagating modes is excited, and only one mode is selected for detection, but does not imply any restriction of N itself.) These experimental efforts have promoted the single-mode delay times to quantities of interest in their own right. The measurements have been performed with wave guides shorter than the localization length, and their outcome [the probability distribution function $P(\phi')$] can be successfully described by diffusion theory [10].

Our theoretical investigations of the influence of localization on the delay times is based on the scattering formulation of wave transport and a single-parameter scaling equation, which describes how the statistical properties of the scattering matrix change when the length of the wave guide is increased incrementally. In the localized regime, a stationary limit is obtained for the properties of the reflected wave, while for the transmitted wave only a single dominant transport mode survives. Several indicators of localization can be derived from these observations, such as a strong correlation of the delay times of the different channels in transmission.

We have identified two particularly striking effects. The first phenomenon is a coherent backscattering effect which requires localization [11]: The typical delay times are reduced when the wave is detected in backscattering direction, by a factor $\approx \sqrt{2}$ [the precise value is $4096\sqrt{2}/(\pi 1371)$], see lower panel of Fig. 1. Without localization there is no dependence of $P(\phi')$ on the detection direction, see the top panel of Fig. 1. We confirmed these predictions by numerical simulations of wave propagation through a disordered wave guide.

The second phenomenon is seen in the transmitted wave. We predicted a very asymmetric distribution function $P(\phi')$ [12] (see Fig. 2), while diffusive propagation results in a distribution function which is totally symmetric around the median (same form as the distribution for reflection in the top panel of Fig. 1). This asymmetry indeed has been confirmed in the latest experiment [13] (as well as by our numerics). The functional form of the distribution function fits well with the theoretical predictions,

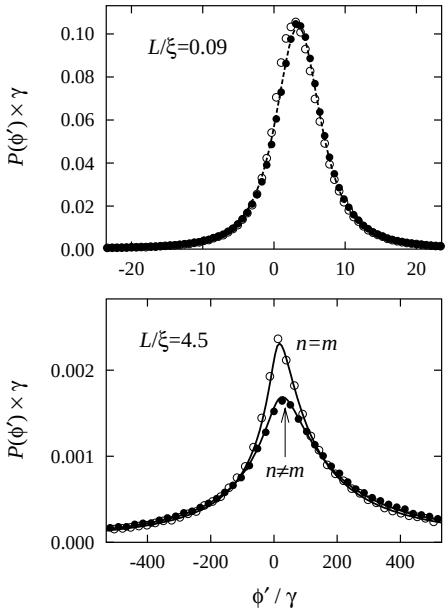

Figure 1: *Coherent backscattering effect in the distribution function of delay times. Top: diffusive regime. Bottom: localized regime.*

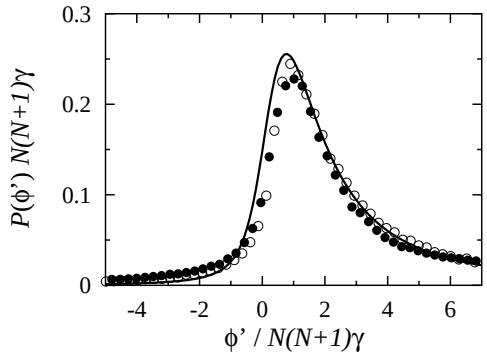

Figure 2: *Probability distribution function of the delay time in transmission, from theory and from numerical simulations.*

while a theory for the parameters is still missing for the experimental circumstances, in which the wave guide is not much longer than the localization length. Some understanding could be achieved by numerical simulations, which indicate that absorption must be very weak in the experiment (see Fig. 3).

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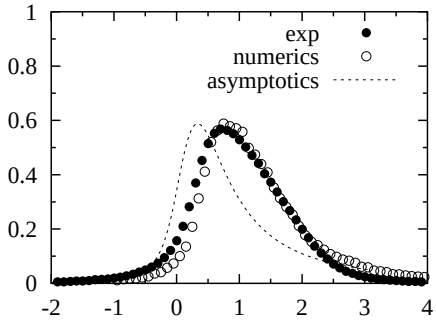

Figure 3: *Probability distribution function of the delay time in transmission, from experiment [13], numerical simulations, and the asymptotical prediction of the theory for a very long wave guide.*

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1.26 Hexagonal-shaped microcrystal lasers: Effects of corners and coupling

Jan Wiersig

A novel class of microlasers based on nanoporous molecular sieve host-guest systems has been fabricated recently [1, 2]. Organic dye guest molecules were inserted into the channel pores of a zeolitic microcrystal host. The aluminophosphate-crystals grow with natural hexagonal-shaped boundaries; see Fig. 1a. In terms of pump energy needed to reach lasing threshold these microlasers are comparable to semiconductor based vertical-cavity surface-emitting lasers (VCSELs). This makes them a promising candidate for future applications as e.g. optical communication devices. In collaboration with experimental physicists of the Technical University of Darmstadt and chemists of the University of Bremen (Volkswagen Foundation Project "Molekularsieblaser-Konglomerate im Infraroten") we study these microlasers in more detail. In particular, we try to improve their properties by coupling them to each other and/or to passive high-quality microresonators. Our theoretical approach is illustrated in the sequence of Figs. 1a-c. The real microlasers (Fig. 1a) are modelled by two-dimensional passive dielectric resonators using both numerical simulations of the full wave equations (Fig. 1b) and a semiclassical ray model (Fig. 1c). The resonant modes of dielectric cavities can be calculated analytically by means of separation of variables only for special geometries, like the circular cavity. In general, numerical methods are needed. Frequently used is the wave-matching method [3, 4] which is suitable for sufficiently slight deformations of an isolated circular cavity. To treat coupled cavities with sharp corners, we have invented a variant of the boundary element method (BEM) [5].

Figure 1b shows a TM polarized resonant mode of an isolated hexagonal cavity with low refractive index calculated with the BEM. The light is concentrated along the boundary (whispering-gallery mode) and escapes predominantly at the corners. The emission directionality is highly anisotropic, a desired property in optical applications.

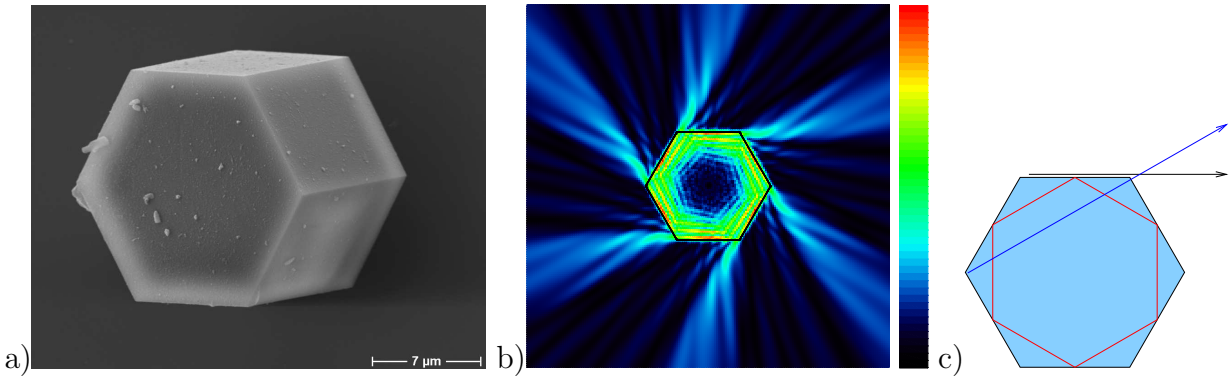

Figure 1: *(a) Hexagonal microcrystal laser, diameter is* $4 \ldots 50\mu m$ *and wavelength is* $600 \ldots 800nm$*. (b) False-colour representation of the near-field intensity pattern of a long-lived resonant mode calculated numerically from the full wave equations. Intensity is higher for redder colours, and vanishes in the dark regions. (c) Ray model. Red polygon marks a member of the family of whispering-gallery rays, other members are obtained by shifting the ray along the boundary. Arrows indicate emission due to boundary waves (black) and pseudointegrable dynamics (blue).*

These results are in agreement with the experiments and with earlier numerical results on *rounded* hexagons obtained from the wave-matching method [2]. However, we have observed that the modes in the hexagon with *sharp corners* and those in rounded hexagons differ substantially with respect to their lifetime and the exact emission direction. Apart from this unexpected sensitivity to rounding we found another interesting result: if the wavelength is fixed then the Q-factor (a measure of the quality of the mode) is approximately proportional to the diameter squared. Based on this finding we predict that the lasing threshold can be reduced considerably by increasing the size of the resonator.

The semiclassical (short-wavelength) approximation is applied in the field of quantum chaos to relate quantum (wave) dynamics to their underlying classical (ray) dynamics. Most research efforts have been focused on closed resonators, so-called billiards. Rational polygonal billiards (all angles between sides are rationally related to π) like the hexagon have, in general, peculiar properties due to the presence of corners, e.g. the classical dynamics is neither chaotic nor integrable but instead *pseudointegrable* [6, 7], classical Fourier spectra have multifractal properties [8], the quantum spectrum obeys critical statistics [9], and the quantum-classical correspondence is exotic [10]. Many concepts of quantum chaos have been carried over to *open* resonators, e.g. scars [11, 12]. However, semiclassical approximations have been introduced only in the case of smooth boundaries [3, 4].

In collaboration with J. U. Nöckel from the University of Oregon we develop a semiclassical ray model for hexagonal-shaped cavities which later might be extended to any rational polygon. According to geometric optics, a family of periodic rays (whispering-gallery rays) with identical lengths is confined within the hexagonal resonator by total internal reflection at the facets; see Fig. 1c. Responsible for emission of light are wave effects. We have identified three different wave effects, all of which are related to the corners. The most obvious one is *diffraction at corners*. The next one is propagation of *boundary waves* and their separation from the boundary at the corners as illustrated in Fig. 1c. The third effect is that waves smear out classical phase-space structures. To

take this into account one has to choose a small distribution of rays localized around the whispering-gallery rays as initial conditions rather than taking the whispering-gallery rays itself. As a consequence of the *pseudointegrable dynamics* the initial rays diverge slowly from the periodic rays until they fully separate from them at a corner leading directly to refractive escape as depicted in Fig. 1c. Our preliminary semiclassical model includes the boundary-wave and the pseudointegrable mechanism, whereas corner diffraction is ignored. The model allows for *analytic* evaluation of many quantities of interest, including the frequency spacing, the lifetimes, and the Q-factors. Moreover, it explains the sensitivity to rounding of the corners. In the future, we will include corner diffraction which seems to be important for the far-field pattern.

In Fig. 2a we see an example of two coupled hexagonal-shaped resonators. Careful comparison with the isolated hexagon demonstrates that the emission directionality has improved, whereas the Q-factor has remained unchanged. Figure 2b shows a hexagonal-shaped resonator coupled to a circular high-quality resonator. It turns out that the Q-factor of the mode in the composite system has been enhanced by a factor of 2.5 if compared to the corresponding mode in the isolated hexagon. In the experiments, silica spheres will be used rather than circular cylinders. Nevertheless, we believe that the 2D calculations will give deep insights, not only relevant for the experiments but also for the theory of dielectric resonators in general.

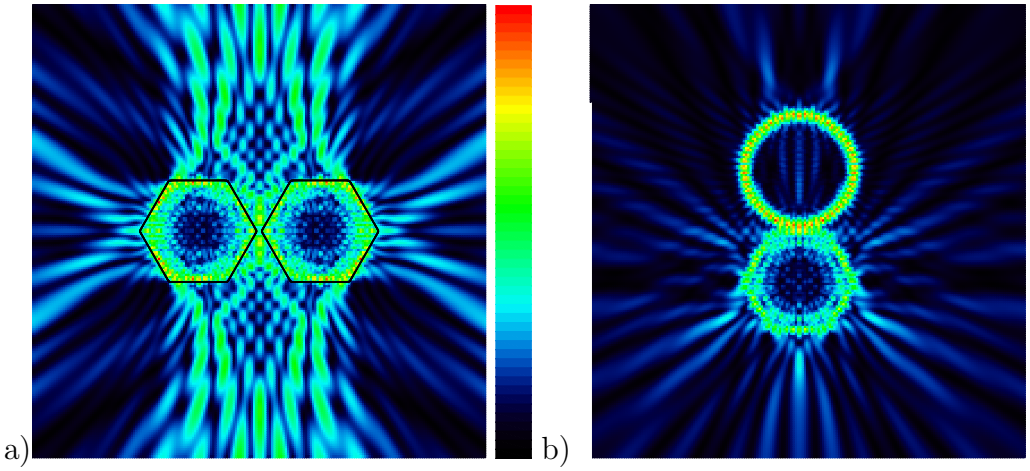

Figure 2: *Near-field intensity pattern of coupled microresonators calculated numerically from the full wave equations.*

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2 PhD Program

The training of PhD students is one of the central educative tasks of the mpi**pks**. 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**.

The success of this strategy becomes obvious from the growth of the number of PhD students at mpi**pks**. In 1996 we had a total of 20 PhD students at mpi**pks**, including 4 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 numbers grew continuously to 44 PhD students, including 13 from abroad, during the year 2001. The number of successful final PhD exams grew from 3 during the year 1996 to 7 during 2002.

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, a significant part is 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.

3 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 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 1996 the mpi**pks** hosted 35 guest scientists with contracts for at least three months. This number increased to 113 scientists during the year 2002. At the same time we enjoyed a significant increase in the number of senior scientists who use 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.

The guest scientists are typically in close collaboration with the research groups at mpi**pks**. Otherwise they conduct more independent research, which leads to synergetic effects. During the past six years we enjoyed several temporary collaborations at the institute on topics like *selforganized criticality, mathematical biology* and *Bose-Einstein condensation,* to name a few. 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. 151).

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. Rainer Klages* on *Statistical Dynamics of Nonequilibrium Systems*, and *Dr. Joachim Brand* on *Physics of Bose-Einstein Condensates*. Two PKS fellows have already left the institute: *Dr. Jaroslav Fabian* (*Spintronics*, see report on p. 143) accepted a professorship at Linz University, and *Dr. Heike Emmerich* (*Dynamics of Phase Boundaries Far From Equilibrium*) took a C2 position at the University Dortmund.

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 2000, 2001 and 2002 fellows were *Dr. Dominique Delande*, *Prof. Richard Prange* and *Prof. Alfredo Miguel Ozorio de Almeida* (see report on p. 145).

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 research collaborations of the research groups at mpipks with other institutes. Their number grew from 30 during the year 1996 to approximately 70 during the year 2002.

The Visitors Program also supported temporary synergetic research activities such as the *Initiative Biology* (p. 147), the *Mathematical Biology Group* (p. 149) and the *Formation of Correlations and Superconductivity working group* (p. 150).

3.1 PKS-Fellowship

Report by *Dr. Jaroslav Fabian:* Spintronics

Spintronics is a newly developing branch of electronics where spin, in addition to charge, determines the outcome of electronic devices. Traditional spintronic applications use metals as the media where the nonequilibrium spin is created, transported, and detected. The metal-based devices (the so called GMR–giant magnetoresistive devices) are already used in industry for magnetic read heads in personal computers.

Semiconductors are as of yet still waiting for their opportunity to enter the arena. The only reason for that is that an electronic generation of spin (spin injection) in a semiconductor like GaAs or Si has turned out to be extremely difficult. Recently, however, it was possible to achieve a significant spin injection into a semiconductor, when a ferromagnetic electrode was made of a magnetic semiconductor (and not metal, like Fe, used in metal-based spintronics). This is a great news, since semiconductor spintronics will potentially offer greater functionality than metal spintronics (we have a far greater control of electronics processes in semiconductors than in metals, mostly because we can vary the number of mobile carriers in semiconductors by doping), and the integration with the traditional semiconductor electronics should be easier (although of semiconductors, it is Si and not GaAs which is the most promising candidate–due to its band structure–for spintronics).

Once the spin injection is demonstrated, the question arises of what to do with the injected spin. While in Dresden, and in collaboration with my coworkers in the University of Maryland in College Park, Professor Sankar Das Sarma and Dr. Igor Zutic, I have pursued the study of spin transport in inhomogeneous semiconductors, in particular a p-n junction, in order to see to what extent the (nonequilibrium) spin properties of mobile carriers influence the electronic outcome (like the I-V curve) of the sample. We have designed two systems: the spin-polarized p-n junction, and the magnetic p-n junction. We have conducted a realistic device modelling of the two systems (after introducing the diffusion-recombination-relaxation equations for charge and spin transport in semiconductors).

A spin-polarized p-n junction is a p-n junction in which nonequilibrium spin is introduced into one (or both) regions (p and n). This can be done either optically (optical orientation) or electronically (spin injection). The first question we asked was: can the spin be transported (under an external bias) through the space-charge region separating the p and n regions? Our answer is yes. But more than that is happening: the spin gets amplified when crossing the region from a minority region into the majority one (say, if the electron spin in introduced in the p-region, and then it is transported

into the n-region, where electrons form the majority). This is the first manifestation of spin amplification. The phenomenon of spin amplification is also unique to semiconductors, as the space-charge region (and the built-in field) does not exist in metals due to the very effective charge screening. Other phenomena that we have demonstrated are the increase of an effective spin diffusion range in the p-n junction, the possibility of generating spin current in a spin-polarized solar cell, and an all-electronic control of spin (spin capacitance effect).

Next we considered what would happen if one side of the p-n junction would be doped with magnetic impurities (like Mn in GaAs) and placed into an external magnetic field. The magnetic impurities induce a large g-factor to mobile carriers (electrons and holes), so that the magnetic field induces a relatively large splitting between spin up and down levels. This has great ramifications. First, a similar question asked in the case of the spin-polarized p-n junction, of whether there is a spin injection through the space-charge region (from the magnetic into the nonmagnetic part) has a negative answer at reasonably low bias. Only at large bias, when the spin is out-of-equilibrium even in the magnetic region, the spin injection can take place. A very interesting effect of potential technological relevance occurs when a nonequilibrium spin is introduced into the nonmagnetic region. A huge giant-magnetoresistance results (that is, the current at a fixed bias diminishes when the magnetic field is switched from the direction parallel to the introduced spin to antiparallel). A curious effect, which also follows from our analytic formulation of the problem, is what we call the spin-voltaic effect. A current flows (or a voltage develops in a closed circuit) even if there is no bias. In analogy with solar cells, it is enough to maintain a steady nonequilibrium spin at the space-charge region to generate a charge flow. The flow changes sign when the magnetic field direction is reversed (the spin valve effect).

Finally, I have developed a theory for transient electron transport (ballistic and diffusive) in an inhomogeneous magnetic field, demonstrating a possibility of electron spin separation (a Stern-Gerlach-like effect) with conduction electrons.

Atomic vibrations in glasses

Atomic vibrations in glasses differ significantly from those in periodic crystals. Strong topological disorder inhibits both ballistic and diffusive (random-walk-like) propagation of the majority vibrational eigenstates. There are four distinct modes of vibrations in glasses, all different in spatial properties, thus in energy and momentum transfer. These modes are propagons (diffusive, random-walk-like modes), resonances (propagons trapped at topological defects), diffusons (modes above the Ioffe Regel limit, where the concept of mean free path makes no sense, diffusing intrinsically like a free quantum-mechanical particle), and the highest frequency modes are locons (localized, Anderson-like modes). The majority modes are diffusons, which determine thermodynamic and kinetic properties of (dielectric) glasses.

There is an outstanding question of how to meaningfully describe the difference between diffusons and propagons, in the sense of what physical characteristics beyond transport distinguishes between these two modes. During my stay in Dresden I was investigating spectral properties of diffusons and propagons from the perspective of random matrix theory. I found that diffusons differ from propagons at large spectral scales, measured, for example, by the Σ_2 statistics, which is the variance of the number

of energy (frequency) levels in a fixed interval. For propagons Σ_2 grows as a power law 3/2 with the interval size, as predicted by Altshuler and Shklovskii some time ago (but this prediction has never been verified before). For diffusons the power is quadratic. The reason for that remains unknown, as diffusons are not perturbative states like propagons, so no analytical treatment at present is possible to derive Σ_2 for these states.

Articles written at mpipks

- S. Das Sarma, J. Fabian, X. D. Hu, and I. Zutic, *Spin electronics and spin computation*, Solid State Commun. **119**, 207 (2001).
- I. Zutic, J. Fabian, and S. Das Sarma, *Spin injection through the depletion layer: A theory of spin-polarized p-n junctions and solar cells*, Phys. Rev. B **64**, 121201 (R) (2001).
- I. Zutic, J. Fabian, and S. Das Sarma, *A proposal for a spin-polarized solar battery*, Appl. Phys. Lett. **79**, 1558 (2001).
- I. Zutic, J. Fabian, and S. Das Sarma, *Theory of spin-polarized transport in inhomogeneous magnetic semiconductors*, Phys. Rev. Lett. **88**, 066603 2002).
- J. Fabian and S. Das Sarma, *Spin transport in inhomogeneous magnetic fields: a proposal for Stern-Gerlach-like experiments with conduction electrons*, Phys. Rev. B **66**, 024436 (2002).
- J. Fabian, *Spectral fluctuation of the atomic vibrations in glasses: Random matrix theory and beyond*, LANL preprint cond-mat/0104464.

3.2 Gutzwiller-Fellowship

Report by *Prof. Alfredo M. Ozorio de Almeida*

The Gutzwiller fellowship for 2002 was taken at a full stretch of twelve months, roughly coinciding with the European academic year, from the 19th August 2001. This was particularly convenient for interfacing European climate with the warm Brazilian winter.

Far from being a low academic season, both the beginning and the closure of my visit were the occasion for delivering sets of lectures. Indeed, my arrival coincided with the Wilhelm and Else Heraeus Summer School: *Dynamics of Complex Systems: Classical and Quantum Aspects* in Lutherstadt Wittenberg, 13-25/8/2001, where I delivered three lectures on Quantum Mechanics in Phase Space. My concluding activities in Dresden were the pair of lectures delivered at the mpipks Seminar *Microscopic Chaos and Transport in Many Particle Systems* and an invited talk at the homonymous workshop, in August 2002. The title was the same, but the subject matter evolved remarkably, as will be discussed at the end of this report.

Actually, the above was the third program at the mpipks in which I assumed an active role during my scientific visit. I also gave a talk at the *Q-Random* workshop, 27/1-1/2/2002 and at the workshop *Quantum Dynamical Concepts: From Diatomics to Biomolecules* in April, 2002. The latter was in combination with the formal mpipks Colloqium for the Gutzwiller Fellowship. In this, I presented a personal view of the Gutzwiller Trace Formula and its relation to the contemporary use of 'Semiclassics',

which was well received, since many people working in the wide range of subjects within the scope of the mpi**pks** do not have a clear appreciation of Gutzwiller's contributions. I also participated in a meeting at Ringberg, a very beautiful castle in Bavaria, organized by *Prof. Rost's* group in the mpi**pks** in collaboration with Prof. Rempe's group at the Quantum Optics Institute in Garching, 3-7/12/2001, at which I also gave a talk.

This was followed up by a visit to Garching in May, 2002 in combination with a visit to Prof. Frank Steiner's group in the University of Ulm. Previously, I also visited Prof. Klaus Richter at the University of Regensburg. Further afield, this Gutzwiller year was also the occasion of a ten days visit to Prof. Bohigas' group at the University of Paris-Orsay and a week's visit to the group of Prof. Berry and Prof. Keating at the University of Bristol. For both of these I counted on partial financial support from the mpi**pks**. In the latter case, my trip was chosen to coincide with my return to Europe after the second of two fortnightly visits to Brazil. These allowed me to provide continuing support for my group at CBPF-Rio. It should be noted that the previously agreed partition of my stay in Dresden into a period of six months, sandwiched between two periods of approximately three months, optimized the use of promotional flights with minimum financial bonus to the Max Planck Society.

As well as providing ample opportunity to discuss and interact with scientists passing through or working stably at the mpi**pks**, the generous terms of the Gutzwiller Fellowship allowed me to recommend the award of a postdoctoral fellowship for a collaborator during my stay. However, it proved more advantageous to bring more senior visitors for shorter periods, for which I am grateful to the flexibility of the mpi**pks**. Thus, Prof. Steven Tomsovic (Pullman - Washington, U.S.) worked with me from 10/2001 to 1/2002, as previously planned. Further on, the direction in which my research developed led me to request the visit of Prof. Marcos Saraceno (CNEA-Buenos Aires, Argentina) who then visited the mpi**pks** from 3/2002 to 5/2002. I am glad that promising work was also started with *Dr. Anatole Kenfack*, in collaboration with *Prof. Jan-Michael Rost* and *Dr. Tobias Schneider* and another project with *Dr. Gabriel G. Carlo*, also a postdoc at the mpi**pks**. The groups with which I had most scientific exchange were the ones headed by *Prof. Jan-Michael Rost*, by *Dr. Andreas Buchleitner* and by *Dr. Henning Schomerus*. In all respects, it is a pleasure to thank the hospitality of the above, as well as *Prof. Peter Fulde* and *Dr. Sergej Flach* of the Visitors Program. My stay and the solution of the problems that are a natural consequence of a year's transplanting were greatly helped by the patient and good natured assistance of *Gabriele Makolies, Katrin Lantsch, Claudia Pönisch* and *Mandy Stiegler*. The convivial working atmosphere that has been built up at the mpi**pks** is certainly an important asset for the future of this fairly new, but already very successful research institute and conference centre.

I close this report with a brief description of the content of my research in Dresden. I was able to take full advantage of the excellent working conditions, as well as the tranquility resulting from the distance from daily preoccupations in Brazil to really open out my research activities. Indeed, I have been working on semiclassical methods for over twenty years, in recognition of which I was awarded the Gutzwiller Fellowship. However, the main interest had originally been centred on the energy spectra of closed systems, i.e. the Gutzwiller Trace Formula. More recently the focus shifted to the phase space representation of individual states and their motion. But it was only in

this last year that I took up Prof. Saraceno's suggestion that these methods might be extendable to open systems. Thus, by the end of last year, I was able to show that the semiclassical evolution due to Lindblad operators that couple a subsystem to the outside environment can be combined with the internal Hamiltonian evolution. This work, referenced below, has now been submitted for publication after having circulated in the mpipks. During Prof. Saraceno's visit, we were able to adapt these semiclassical methods for the calculation of measures of decoherence, such as the growth of linear entropy, and we followed through computations for specific models. This work is well advanced and a preliminary report was the subject of my last talk in Dresden at the "Microscopic Chaos..." conference.

Parallel to this main advance, the work with Prof. Tomsovic (in collaboration with Prof. Caio H. Lewenkopf in Brazil) led to a critical assessment of formal resummation methods for periodic orbit contributions to the Gutzwiller Trace Formula in the case of integrable systems, for which exact comparisons can be made. This paper has also been submitted. The reference list below includes work which was concluded during the Gutzwiller Fellowship for 2002, for which I thank the mpipks and the Max Planck Society.

Articles completed and written at mpipks:

- *On the propagation of semiclassical Wigner functions*, P P de M Rios and AMOA, J. Phys. A **35** (2002) 2609-2617.
- *Homoclinic chaos in the dynamics of a general Bianchi type-IX model*, H P de Oliveira, AMOA, I Damião Soares and E V Tonini, Phys. Rev. D **65** (2002) 083511.
- *Hyperbolic scar patterns in phase space*, A M F Rivas and AMOA, Nonlinearity **15** (2002) 1-13.
- *On resumming periodic orbits in the spectra of integrable systems*, AMOA, C H Lewenkopf and S Tomsovic, quant-ph / 0207148 (submitted to J. Phys A)
- *Decoherence of semiclassical Wigner functions*, AMOA, quant-ph / 0208094 (submitted to J. Phys A).

Papers in preparation:

- *Quantum traces of Lyapunov stretching*, M Saraceno and AMOA (a summary of this, together with the previous paper, is also due to appear in a special number of Physica D dedicated to the conference on *Microscopic Chaos and Transport in Many-Particle Systems*)
- *Filtering of Wigner functions with chords*, AMOA, J M Rost and A Kenfack.

3.3 Initiative Biology

The *Initiative Biology* at mpipks was constituted in the late summer of 2000. The members made it their objective to point out the institute's engagement in the field of biophysics and theoretical biology, as well as improve communication between the researchers interested in biological problems who work in different groups and divisions. A major goal of the Initiative was to establish and intensify connections with experimentally working biophysicists, biologists and physicians.

It was expected that the methodical competence attained by the investigation of complex physical systems at the mpipks is applicable to modelling biological phenomena as well as evaluating experimental data. Particularly, the tools of non-linear dynamics used in the fields of mesoscopical physics, reaction-diffusion systems and time series analysis are to be mentioned, as well as methods of stochastical and statistical physics. The members of the Initiative at the mpipks pursued research projects on several biologically relevant subjects. Priorities are given to biological pattern formation and nanocluster growth on biotemplates (*Markus Bär*), electron transport in biomolecules and metallized DNA (*Gianaurelio Cuniberti, Klaus Richter*), interacting multicellular systems in morphogenesis and tumor growth (*Andreas Deutsch*), intracellular calcium dynamics (*Martin Falcke*), theoretical immunology (*Michal Or-Guil*) and population dynamics (*Nikolay Vitanov*).

Research highlights include the modelling of charge transport in molecular wires [1] and its application to DNA [2], the modelling of Ca^{2+} sparks, puffs and noisy waves in stochastic models for intracellular calcium dynamics [3], the modelling of the role of the mitochondria in intracellular calcium dynamics [4], the modelling of rippling patterns in aggregates of myxobacteria [5] as well as the modelling of swarming behavior of organisms by cellular automata [6]. Last but not least, first steps to model dynamical aspects of the immune system have been undertaken [7].

Common activities of the Initiative included one-day workshops with international participation on the current main topics (Focus Meetings) as well as conferences and lectures. The first *Focus Meeting on Biological Aggregation* (coordinators *A. Deutsch*, A. Stevens (Leipzig), and *M. Bär*) took place in October 2000. It was followed by meetings on *Immunology: T Cell Dynamics and Recognition* (coordinators *M. Or-Guil*, S. Bornholdt (Kiel)) in January 2001 and on *Electron Transport on the Molecular Scale* (coordinators *K. Richter* and *G. Cuniberti*) at the end of February. In March 2001, Focus Meetings on *Cytoskeleton* (Coordination *M. Falcke* and E. Frey (Harvard)) and *Protein Complexes* (*M. Falcke* and S. Diekmann (Jena)) did happen.

Already in October 2000 the mpipks had been host to an international conference on *Experimental and Theoretical Calcium Dynamics* (coordination *M. Falcke* with J. Lechleiter (San Antonio), J. Sneyd (Auckland) and D. Malchow (Konstanz)). In April 2001, Dr. Ursula Kummer (Bioinformatics, EML Heidelberg) presented a series of lectures on the basics of biochemistry, molecular biology and bioinformatics (invited by *M. Or-Guil*). Finally, an international conference on *Function and Regulation in Cellular Systems* with ca. 170 participants took place in June 2001, during which the Network MTBIO (*Modelling and Theory in Biosciences*, coordinator *A. Deutsch*) was presented to the scientific community. *A. Deutsch* and *M. Falcke* acted as coordinators together with J. Howard (MPICBG Dresden) and W. Zimmermann (Saarbrücken).

In parallel, *Dr. Frank Jülicher* (Paris) had been named director of mpipks and is leading the newly established department of *Biological Physics* since February, 2002. Research topics are force and motion generation in cells by motor proteins as well as the mechanical and dynamical properties of membranes, filaments and the cytoskeleton. The activities of the *Biological Physics* department on molecular motors and intracellular dynamics and the continuation of research on biological pattern formation in the research group on *Pattern Formation* (*Dr. M. Bär*) pick up some of the momentum generated by the *Initiative Biology* and ensure that mpipks will be a center of research

in biophysics and theoretical biology as well as a partner for experimentalists in the respective areas. Because of this, and the fact that most of its original members have left mpi**pks** for other positions, *Initiative Biology* was discontinued in May, 2002.

Selected Publications:

1. G. Fagas, G. Cuniberti, and K. Richter, *Conductance of a molecular wire attached to mesoscopic leads: contact effects*, *Acta Physica Polonica B* **32**, 437 (2001); *Molecular wire-nanotube interfacial effects on electron transport*, *Annals of the New York Academy of Sciences* **960**, 216 (2002); G. Cuniberti, F. Großmann, and R. Gutiérrez, *The role of contacts in molecular electronics*, in *Advances in Solid State Physics* **42**. ed. by B. Kramer, Springer, Berlin, 2002.
2. G. Cuniberti, L. Craco, D. Porath, and C. Dekker, *Backbone-induced semiconducting behavior in short DNA wires*, *Phys. Rev. B*, in press (2003).
3. M. Bär, M. Falcke, H. Levine and L. Tsimring, *Discrete stochastic modeling of calcium channel dynamics Phys. Rev. Lett.* **84**, 5664 (2000); M. Falcke, H. Levine and L. Tsimring, *Stochastic spreading of intracellular Ca^{2+} release*, *Phys. Rev. E* **62**, 2636 (2000).
4. M. Falcke, J. L. Hudson, P. Camacho, and J. Lechleiter, *Impact of Mitochondrial Ca^{2+} Cycling on Pattern Formation and Stability*, *Biophys. J.* **77**, 37 (1999); M. Falcke, M. Or-Guil and M. Bär, *Dispersion gap and localized spirals in a model for intracellular Ca^{2+} dynamics*, *Phys. Rev. Lett.* **84**, 5664 (2000).
5. U. Börner, A. Deutsch, H. Reichenbach and M. Bär, *Rippling patterns in aggregates of myxobacteria arise from cell-cell collisions*,Phys. Rev. Lett. **89** 078101 (2002).
6. A. Czirók, A. Deutsch and M. Wurzel, in *Polymer and cell dynamics*, W. Alt, M. Chaplain, M. Griebel, and J. Lenz (Eds.), Birkhäuser, Basel (2002).
7. M. Meyer-Hermann, A. Deutsch and M. Or-Guil, *Recycling probability and dynamical properties of germinal center reactions*, *J. Theor. Biol.* **210**, 265 (2001); G. Cuniberti and M. Or-Guil, *Coevolution of lymphocytes and mutating antigen in shape space*, in *Function and Regulation of Cellular Systems: Experiments and Models*, A. Deutsch, M. Falcke, J. Howard, W. Zimmermann (Eds.), Birkhäuser, Basel (2002).

3.4 Network MTBio: Modelling and Theory in the Biosciences

The Network MTBio (*Modelling and Theory in the Biosciences*) was founded at the mpi**pks** (founding workshop: 15.5.00). Foundation was preceded by a two-days workshop *Perspektiven der mathematischen und theoretischen Biologie* early in the same year (mpi**pks** 10.-11.3.00, organizers: W. Alt (Uni Bonn), *M. Bär* (mpi**pks**), *A. Deutsch* (mpi**pks**), A. Stevens (MPIMIS, Leipzig)) with approx. 70 participants. At this workshop various strategies were discussed how to further develop the interdisciplinary research field 'theoretical biology'. The participants agreed in launching an initiative for the foundation of a network *Modelling and Theory* instead of founding a usual 'society'. A network structure should be more adequate to represent the needs of the addressed highly interdisciplinary research field.

The Network MTBio is an initiative of researchers primarily from German universities and research institutes specialized in biophysics, bioinformatics and biomathematics. *Andreas Deutsch* (1999-2001 guest scientist at mpi**pks**) is in charge of the coordination of the competence- and communication network MTBio. The MTBio steering committee represents central modeling and theory competences and meets twice a year to discuss and to decide about network activities. MTBio membership is free and possible

at any time (registration at website www.mtbio.de). There are currently 370 members from all over the world (June 2002). MTBio members profit from a rich information data base (publications, workshops, open positions) and can distribute information themselves.

Focal point of the network is an internet platform that was possible with financial support from the Klaus Tschira foundation (Heidelberg) and the mpi**pks** (see www.mtbio.de). The main MTBio objective is to catalyze interdisciplinary communication and to initiate interdisciplinary research activities.

The network organizes workshops directed on biological key issues. The first international MTBio workshop *Function and regulation of cellular systems: Experiments and models* with approx. 180 participants took place in 2001 (25-30.6.01, mpi**pks**, scientific coordinators: *A. Deutsch*, *M. Falcke*, J. Howard (MPICBG), W. Zimmermann (University Saarbrücken)). Edited workshop proceedings will appear at Birkhäuser, Basel. The next international MTBio workshop will focus on developmental biology and evolution.

Further MTBio activities shall improve university education in the field *Modelling and Theory in the Biosciences*. Therefore, at the MTBio server information about ongoing university courses is collected and an initiative for a MTBio curriculum has been started.

3.5 International Working Group: Formation of Correlations and Superconductivity

(Ernst Helmut Brandt, Jan Koláček, Nai-Hang Kwong, Pavel Lipavský, Klaus Morawetz, Eugen Simánek)

As a consequence of a series of interdisciplinary workshops during the last years, an international working group *Formation of correlations and superconductivity* has been established between theoreticians and experimentalists from Prague (Czech Republic), Arizona (USA) and Dresden. Details can be found on the homepage http://www.mpipks-dresden.mpg.de/∼morawetz/work.html. The aim of this interdisciplinary working group is to contribute to the understanding of the relation between complexity and correlations with the help of the experiences from different fields. The key focus here is to describe the time-dependent formation of structures such as vortices in superconductors and clusters from a microscopic theory. The collaboration has published 16 papers (Phys. Rev. B, Ann. Phys.) and has organized 4 meetings and 2 workshops (mpi**pks**, WE-Heraeus) during the years 2001/2002.

3.6 Collaboration with Experimental Physics Groups

A number of joint collaborations with experimental physics groups in Germany, Europe and the US has been partially supported by mpi**pks**. The following list summarizes these collaborations for the period 1996-2002.

- *Surface reactions ($NO + CO$, $NO + H_2$, $O_2 + H_2$)* with R. Imbihl (Hannover) and M. Eiswirth (Berlin)

- *Intracellular Ca^{2+} waves* with J. Lechleiter (San Antonio)
- *Dynamics in neuronal output* with A. Selverston (San Diego)
- *Thin metallic films on biotemplates* with W. Pompe (Dresden)
- *Morphogenesis - myxobacterial aggregation* with H. Reichenbach (Göttingen)
- *3D patterns in the Belousov-Zhabotinsky reaction* with S. Müller (Magdeburg)
- *Patterns in the light-sensitive BZ reaction with heterogeneous forcing* with H. Engel (Berlin)
- *Measurements on quantum spin systems* with A. Loidl (Augsburg)
- *Interplay between magnetism and Kondo effect in metallic Ce compounds: Heavy fermions and non-fermi liquid effects* with G. Zwicknagl (Braunschweig)
- *Dielectric low-temperature properties of glasses* with P. Strehlow (Berlin)
- *Neutron scattering on solids* with T. Chatterji (Grenoble)
- *Highly correlated dynamics of two-electron atoms* with G. Kaindl (Berlin)
- *Laboratory for high magnetic fields* with F. Pobell (Rossendorf)
- *Measurement of Ericsson fluctuations in the electronic shell of the Helium atom* with H. Schmidt-Böcking (Frankfurt)

3.7 Conferences, Workshops and Symposia 2000-2002

1. *Vortices and Frustrations in 2D Magnet and Optical Systems*
   Workshop/Seminar: January 3 - 21, 2000 — 54 participants
   Scientific coordinators: A. Kosevich, F. G. Mertens

2. *Microscopic Structure and Dynamics of Vortices in Unconventional Superconductors and Superfluids*
   Workshop: February 28 - March 3, 2000 — 69 participants
   Scientific coordinators: R. P. Hübener, N. Schopohl and G. E. Volovik

3. *Perspektiven der Theoretischen und Mathematischen Biologie*
   Workshop: March 10 - 11, 2000 — 61 participants
   Scientific coordinators: W. Alt, M. Bär, A. Deutsch, A. Stevens

4. *Atomic Systems in Extreme Fieworkshopslds*
   Workshop/Seminar: March 13 - April 20, 2000 — 65 participants
   Scientific coordinators: C. Keitel, P. L. Knight, J.-M. Rost

5. *Satellite School "Journees des Actinides"*
   May 2 - 3, 2000 — 64 participants
   Scientific coordinators: P. M. Oppeneer, M. Richter

6. *TMR Meeting: Quantum Chemistry for the Excited State*
   May 5 - 9, 2000 — 31 participants
   Scientific coordinators: P. Fulde, S. Pleutin

7. *Biological Evolution and Statistical Physics*
   Workshop: May 10 - 14, 2000 — 69 participants
   Scientific coordinators: M. Lässig, A. Valleriani

8. *Gründungsworkshop Netzwerk Mathematische und Theoretische Biologie: Modellierung und Simulation in den Biowissenschaften*
   Workshop: May 15, 2000 — 15 participants
   Scientific coordinator: A. Deutsch

9. *Dynamics and Statistics of Complex Systems*
   Conference: May 18 - 19, 2000 — 97 participants
   Scientific coordinators: H. Kantz, T. Schreiber

10. *Quantum Dynamics in Terms of Phase-Space Distributions*
    Workshop: May 22 - 26, 2000 — 100 participants
    Scientific coordinators: T. Dittrich, H. J. Korsch, K. Richter

11. *Nonequilibrium Physics at Short Time Scales*
    Workshop/Seminar: May 29 - June 23, 2000 — 44 participants
    Scientific coordinators: K. Morawetz, P. G. Reinhard, E. Suraud

12. *Symposium on Entropy*
    Symposium: June 25 - 28, 2000 — 83 participants
    Scientific coordinators: A. Greven, G. Keller, G. Warnecke

13. *Statistical Mechanics of Space-Time Chaos*
    Workshop/Seminar: July 2- 28, 2000 — 77 participants
    Scientific coordinators: R. Livi, A. Politi

14. *Non-Perturbative Approach to Disordered Systems and Quantum Hall Effect*
    Workshop/Seminar: August 7 - 27, 2000 — 45 participants
    Scientific coordinators: V. I. Falko, A. Tsvelik

15. *Problems in Systems Neuroscience*
    Workshop/Seminar: August 28 - September 29, 2000 — 76 participants
    Scientific coordinators: J. L. van Hemmen, T. J. Sejnowski

16. *Collective Phenomena in the Low Temperature Physics of Glasses*
    Workshop: October 2 - 23, 2000 — 49 participants
    Scientific coordinators: C. Enss, S. Hunklinger, R. Kühn

17. *Experimental and Theoretical Calcium Dynamics*
    Workshop: October 24 - 27, 2000 — 59 participants
    Scientific coordinators: M. Falcke, J. D. Lechleiter, D. Malchow, J. Sneyd

18. *1st Focus Meeting: Biological Aggregation*
    October 30, 2000 — 15 participants
    Scientific coordinators: M. Bär, A. Deutsch, A. Stevens

19. *1. Dresdner Herbstseminar des Arbeitskreises Nichtlineare Physik*
    November 5 - 8, 2000 — 68 participants
    Scientific coordinators: H. Kantz, St. Müller, J. Parisi, W. Zimmermann

20. *2nd Meeting of the Network MTBio: Modelling and Theory in the Biosciences*
November 9, 2000 — 20 participants
Scientific coordinator: A. Deutsch

21. *LOCNET Network submeeting on Excitations in Josephson Junction Ladders*
November 20 - 21, 2000 — 54 participants
Scientific coordinator: S. Flach

22. *Workshop on GMR and TMR, RTN-Network Magnetoelectronics*
Workshop: November 30 - December 3, 2000 — 15 participants
Scientific coordinator: I. Mertig

23. *Dynamical Approaches in Atomic and Cluster Physics*
Workshop: December 4 - 9, 2000 — 60 participants
Scientific coordinators: P.-G. Reinhard, J.-M. Rost

24. *PhD Students' Day: Overview of Doctoral Theses*
December 14, 2000 — 50 participants
Scientific coordinators: A. Bernert, L. Brusch, E. Sinde

25. *1st Focus Meeting Immunology*
January 30, 2001 — 21 participants
Scientific coordinators: S. Bornholdt, M. Or-Guil

26. *Korrelationstage 2001*
Workshop: February 14 - 17, 2001 — 143 participants
Scientific coordinators: W. Brenig, K. W. Becker, A. Honecker

27. *Electron Transport on the Molecular Scale*
Symposium: February 23 - 24, 2001 — 62 participants
Scientific coordinators: G. Cuniberti, G. Fagas, K. Richter

28. *DFG Gutachterkolloquium zum Schwerpunktprogramm SPP 1116 Wechselwirkung in ultrakalten Atom- und Molekülgasen*
February 28 - March 02, 2001 — 52 participants
Scientific coordinator: M. Wilkens

29. *Statistical Mechanics of Information Processing in Cooperative Systems*
Seminar: March 5 - 23, 2001 — 41 participants
Scientific coordinators: M. Biehl, A. Engel, W. Kinzel

30. *Physics of Information and Synchronization in Stochastic Dynamics*
Workshop: April 1 - 4, 2001 — 74 participants
Scientific coordinators: P. Hänggi, J. Kurths, L. Schimansky-Geier

31. *Coherent Evolution in Noisy Environments*
Workshop/Seminar: April 2 - May 30, 2001 — 133 participants
Scientific coordinators: A. Buchleitner, R. Werner, A. Zeilinger

32. *Dynamics Days Europe 2001*
Workshop: June 5 - 8, 2001 — 280 participants
Scientific coordinators: H. Kantz, K. Richter, T. Schreiber

33. *1st International MTBio-Workshop on Function and Regulation of Cellular Systems: Experiments and Models*
Workshop: June 25 - 30, 2001 160 participants
Scientific coordinators: A. Deutsch, M. Falcke, J. Howard, W. Zimmermann

34. *Magnetic Correlations, Metal- Insulator Transitions and Superconductivity in Novel Materials*
Workshop/Seminar: July 16 - 27, 2001 157 participants
Scientific coordinators: W. Hanke, B. Keimer

35. *Nanostructures in Photovoltaics*
Workshop/Seminar: July 28 - August 4, 2001 84 participants
Scientific coordinators: R. Corkish, S. Kettemann, J. Nelson

36. *Nano-Physics and Bio-Electronics - A new Odyssey*
Workshop/Seminar: August 6 - August 31, 2001 81 participants
Scientific coordinators: T. Chakraborty, F. Peeters, U. Sivan

37. *Nonlinear Lattice Structure and Dynamics*
Workshop/Seminar: September 3 - 30, 2001 123 participants
Scientific coordinators: A. R. Bishop, S. Flach

38. *Control, Communication and Synchronization in Chaotic Dynamical Systems*
Workshop/Seminar: October 15 - November 23, 2001 60 participants
Scientific coordinators: S. Boccaletti, C. Grebogi, J. Kurths, Y.-C. Lai

39. *2. Herbstseminar des Arbeitskreises Nichtlineare Physik*
November 4 - 7, 2001 66 participants
Scientific coordinators: H. Kantz, B. Eckhardt, S. C. Müller, J. Parisi, W. Zimmermann

40. *Atomic Physics and X-ray Free Electron Laser Related Dynamics*
Workshop: December 12 - 15, 2001 52 participants
Scientific coordinator: J.-M. Rost

41. *PhD Students' Day: Overview of Doctoral Theses*
December 17, 2001 40 participants
Scientific coordinator: F. Mintert

42. *QRandom II*
Workshop: January 27 - February 1, 2002 56 participants
Scientific coordinators: A. Buchleitner, B. Kümmerer

43. *Computational Physics of Transport and Interface Dynamics*
Workshop/Seminar: February 18 - March 8, 2002 118 participants
Scientific coordinators: H. Emmerich, B. Nestler, M. Schreckenberg

44. *Models of Epitaxial Crystal Growth*
Seminar: March 4 - 22, 2002 35 participants
Scientific coordinators: M. Biehl, W. Kinzel, D. Vvedensky

45. *Quantum Dynamical Concepts: From Diatomics to Biomolecules*
Workshop/Seminar: April 2 - May 5, 2002 123 participants
Scientific coordinators: F. Grossmann, P. Jungwirth, R. Kosloff

46. *Topology in Condensed Matter Physics*
Workshop/Seminar: May 10 - July 31, 2002 99 participants
Scientific coordinators: M. Kleman, M. Monastyrsky, S. Novikov

47. *Quantum Dynamics in Atomic and Molecular Physics*
Workshop: June 13 - 14, 2002 47 participants
Scientific coordinator: J.-M. Rost

48. *Formation of Correlations, WE-Heraeus-Seminar in Bad Honnef*
Seminar: June 24 - 28, 2002 52 participants
Scientific coordinators: P. Lipavsky, K. Morawetz

49. *Microscopic Chaos and Transport in Many-Particle Systems*
Workshop/Seminar: August 5 - 25, 2002 83 participants
Scientific coordinators: R. Klages, R. Gaspard, H. v. Beijeren, J. R. Dorfman

50. *Chemical and Biological Activity in Flows*
Workshop/Seminar: August 26 - September 27, 2002 62 participants
Scientific coordinators: C. Grebogi, T. Tel, Z. Toroczkai

51. *Geometry and Mechanics of Structured Materials*
Workshop/Seminar: September 29 - October 25, 2002 53 participants
Scientific coordinators: R. Delannay, J. T. Jenkins, G. Schliecker

52. *Progress in Condensed Matter Theory*
Workshop: October 28 - November 1, 2002 82 participants
Scientific coordinators: K. Efetov, E. Khmelnitskii

53. *Electron Interference and Decoherence in Nanostructures*
Workshop: November 4 - 8, 2002 62 participants
Scientific coordinators: K.-H. Ahn, P. Mohanty, U. Weiss

54. *Electrons in Zero-Dimensional Conductors: Beyond the Single-Particle Picture*
Seminar: November 18 - 30, 2002 72 participants
Scientific coordinators: Y. Alhassid, Y. Gefen

55. *3. Herbstseminar des Arbeitskreises Nichtlineare Physik*
December 1 - 4, 2002 69 participants
Scientific coordinators: P. Hänggi, J. Peinke

56. *PhD Students' Day: Overview of Doctoral Theses*
December 5, 2002 50 participants
Scientific coordinator: F. Mintert

57. *Atomic Physics 2002*
December 9 - 13, 2002 59 participants
Scientific coordinators: A. Becker, J.-M. Rost

3.8 Workshop Participation and Dissemination of Results

3.8.1 Dissemination of Workshop Results

As the topics of Workshops and Seminars at mpi**pks** 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 mpi**pks** supports such efforts in various ways. The following list summarizes the relevant publications:

- Workshop:
  Localization in nonlinear lattices
  Physica D **119**, 1 - 238 (1998)
- Workshop:
  Novel physics in low-dimensional electron systems
  Physica E **1**, 21 - 320 (1997)
- Seminar and Workshop:
  Density matrix renormalization group and other recent advances in numerical renormalization group methods
  Peschel, I., X. Wang, M. Kaulke and K. Hallberg: *Density matrix renormalization.* Berlin, Springer 1999, 355 p.
- Seminar and Workshop:
  Dynamics of complex systems
  Physica E **9**, 327 - 624 (2001)
- Workshop No. 7:
  Biological evolution and statistical physics
  Lässig, M. and A. Valleriani: *Biological evolution and statistical physics.* Berlin, Springer 2002, 337 p.
- Seminar and Workshop No. 31:
  Coherent evolution in noisy environments
  Buchleitner, A. and K. Hornberger: *Coherent evolution in noisy environments.* Berlin, Springer 2002, 297 p.
- Workshop No. 33:
  1st international MTBio-workshop on function and regulation of cellular systems: experiments and models
  A. Deutsch et al., Basel: Birkhäuser (to be published)
- Seminar and Workshop No. 35:
  Nanostructures in photovoltaics
  Physica E **14**, 1 - 288 (2002)
- Seminar and Workshop No. 36:
  Nano-physics and bio-electronics - a new odyssey
  Chakraborty, T., F. Peeters and U. Sivan: *Nano-physics and bio-electronics: a new odyssey.* Amsterdam, Elsevier 2002, 354 p.

- Seminar and Workshop No. 43:
  Computational physics of transport and interface dynamics
  H. Emmerich et al., Berlin: Springer (to be published)
- Seminar and Workshop No. 46:
  Topology in condensed matter physics
  M. Kleman et al., Berlin: Springer (to be published)
- Seminar and Workshop No. 49:
  Microscopic chaos and transport in many-particle systems
  Physica D (to be published)

3.8.2 Number of Workshops and their Participants

The total number of participants per workshop or seminar is shown in the following figures for the years 2000, 2001 and 2002. One can see that we have reached our full size of operation roughly since 1999. The large number of participants in 2001 (fig. 1) is due to the organization of the "Dynamics Days Europe" which took place in Dresden, organized by mpi**pks**. The figures 2-4 allow to differentiate between participant numbers from different countries or regions of affiliation - Germany, Europe including Israel, and others.

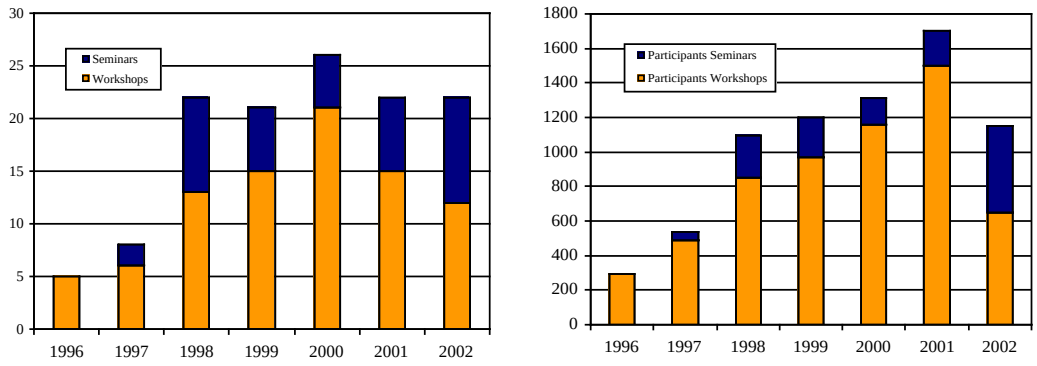

Figure 1: Development of the number of workshops/seminars and their participants.

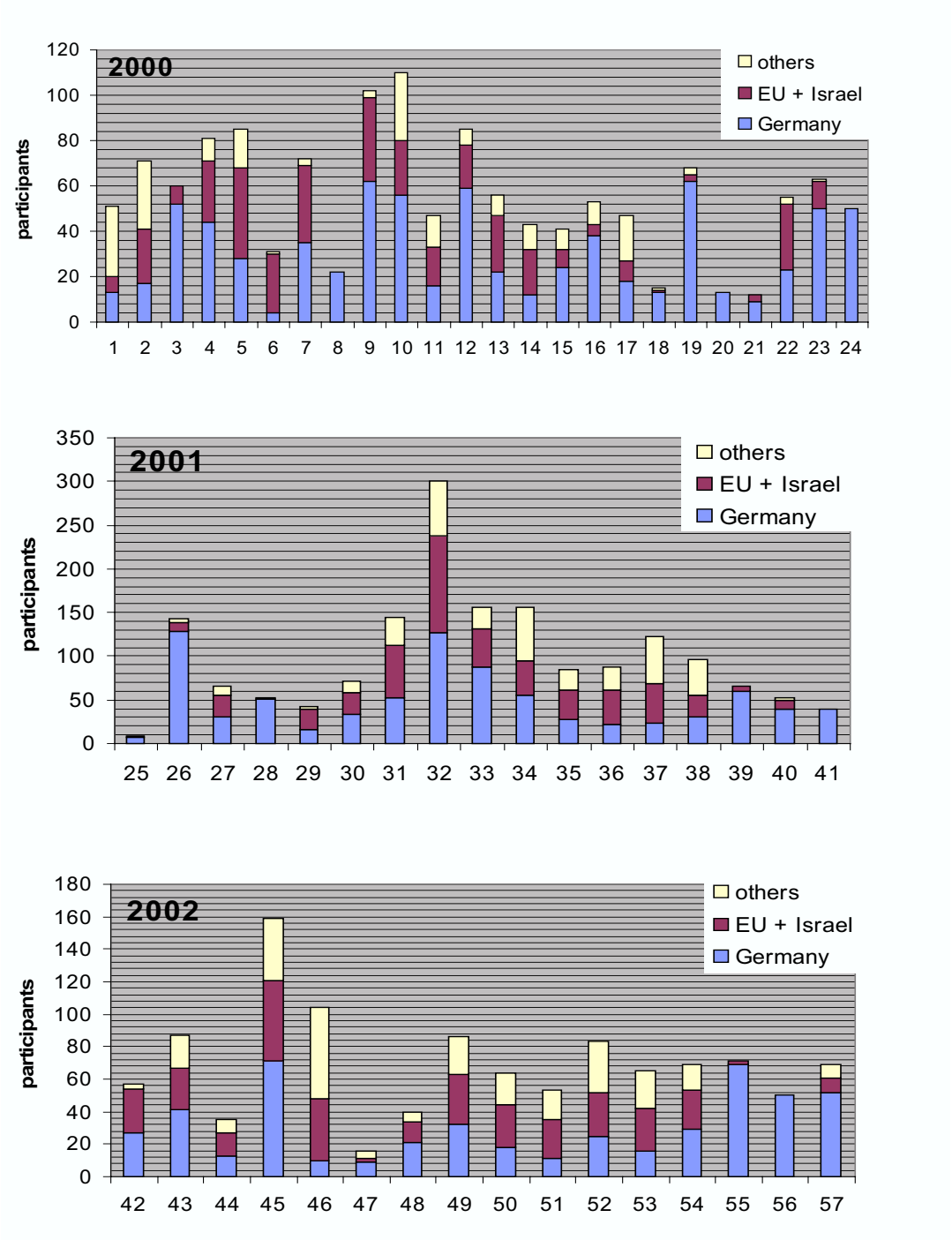

Figure 2: *Workshop/Seminar participants in the years 2000-2002. The numbers on the abscissa refer to the workshops listed on p. 151*

3.9 Workshop Reports

Biological Evolution and Statistical Physics

Workshop, scientific coordinators: Michael Lässig and Angelo Valleriani

In the era of genomic research, also the interaction of physics and biology has entered a new stage. This workshop has played a pivotal role in a new field that can be called the *physics of biological information*. Biological information is encoded, it reproduces and evolves. It is translated into structures and patterns over an enormous range of scales from single molecules to species networks coupled over entire continents. The statistical theory of biological information lives not only in three-dimensional space. It involves various abstract spaces in which this information is encoded and evolves, such as nucleotide sequences, gene networks, or topologies of the 'tree of life'.

This workshop has highlighted areas where the application of physics concepts and methods is likely to have an impact in the near future. The diversity of the invited speakers - biologists, physicists, and mathematicians - underscores the interdisciplinary character.

The conference address has been given by Manfred Eigen. The session topics and the invited speakers have been:

- **Genomics** (Terence Hwa, Dannie Durand, Hanspeter Herzel, David Krakauer)
- **RNA and Proteins** (Ralf Bundschuh, Peter Schuster, Richard Goldstein, David Rand)
- **Spatial and Modular Structures** (David Nelson, Nadav Shnerb, Peter Grassberger, Paulien Hogeweg, John McCaskill)
- **Phylogeny** (Ellen Baake, Nicolas Galtier, Mike Charleston, Mark Pagel, Mike Steel)
- **Population Genetics** (Peter Hammerstein, Ulf Dieckmann, Diethard Tautz)
- **Fitness and Selection** (Peter Stadler, Joachim Krug, Eric van Nimwegen, Werner Ebeling, Dietrich Stauffer)
- **Large Scale Evolution** (Paul Higgs, Ugo Bastolla, Douglas Erwin)

Participants' reactions to this workshop have been unanimously enthusiastic. The comments emphasized that it offered a genuine exchange of ideas and has attracted the attention of many young scientists and called for a timely follow-up workshop here. Some of the scientific contacts established have continued in the subsequent workshop at the Institute for Theoretical Physics in Santa Barbara and have resulted in collaborations. Conference proceedings have been published by Springer.

The organizers wish to express sincere thanks to the mpi**pks** for making this event possible and for the generous support.

Quantum Dynamics in Terms of Phase-Space Distributions

Workshop, scientific coordinators: T. Dittrich, H. J. Korsch, K. Richter

Our meeting was intended as a forum to present ongoing research on the dynamics of quantum phase-space distributions, to demonstrate their usefulness and versatility in applications, and to compare to and make contact with other approaches.

We were glad to reward the hospitality of the institute by offering the contribution of one of our most distinguished speakers, Eric Heller (Harvard), as a joint session with the mpi**pks**–TU-Dresden colloquium. Prof. Heller showed convincingly that the semiclassical propagation of Gaussians in phase space is a universal tool for the description of complex quantum dynamics. Similarly broad overviews, with emphasis on applications in quantum chemistry, were presented by Bill Miller (Berkeley) and Eli Pollak (Rehovot). Peter Hänggi (Augsburg) advertised the application of phase-space distributions to the analysis of localization in disordered solid-state systems; Wolfgang Schleich (Ulm) surveyed quantum-optics applications, featuring recent experiments. Questions of methodology and formalism were considered by Robert Littlejohn (Berkeley) and Alfredo M. Ozorio de Almeida (Rio de Janeiro); Steve Zelditch (Baltimore) made contact with closely related problems currently discussed in mathematics. Fritz Haake (Essen) and Shmuel Fishman (Haifa) had fresh results on Ruelle resonances, showing how phase-space concepts can provide new and otherwise inaccessible insight into quantum chaos. Uzy Smilansky (Rehovot) discussed action correlations among periodic orbits and thus built a bridge to developments around trace formulae. Talks by young, not yet established researchers (Frank Großmann and Martin Sieber (Dresden), Dmitry Jakobson (Chicago), Bilha Segev (Haifa), Gregor Tanner (Nottingham), Joshua Wilkie (Burnaby)) contributed appreciably to the high level of the meeting and the strong representation of ongoing research. A very special highlight was the lecture by Sir Michael Berry (Bristol), who filled the institute's seminar room up to the last seat with his lively demonstration that even in perception processes like seeing, phase-space distributions play an essential role. We have the impression that in this meeting a community formed that up to now had existed only virtually.

Concentrating on the scientific quality of the talks and posters, we tried to free participants from duties not directly related to the actual meeting. In particular, we decided to replace a printed proceedings volume by "virtual proceedings", in the form of links from the web site of the conference program to publications relevant for the respective contributions, provided by their authors. We are convinced that, in this way, an overview over recent literature around the subject of the meeting can be given, without any additional publishing.

Non-Perturbative Approach to Disordered Systems and Quantum Hall Effect

Workshop & Seminar, scientific coordinators: V. I. Falko, A. Tsvelik

This workshop aimed to designate ways for developing theoretical approaches that enable one to treat electron-electron interaction and disorder in phase-coherent electron systems on equal footing. Problems in focus of this meeting included theories of

quantum Hall effect liquids, quantum transport and quantum chaos in disordered systems, Kondo effect in quantum dots in the Coulomb blockade regime, and a mysterious metal-insulator transition discovered in high-mobility 2D electron gases.

The workshop has brought together more than 40 participants from Europe, USA and Israel: experts in the field of quantum disordered systems, exactly solvable one-dimensional models and conformal field theory, active researchers in Mesoscopics and theory of nanostructures, and junior scientists who decided to devote their career to this difficult area of condensed matter theory. The core of the workshop has been formed by the recognized authorities in this field whose works formed the foundations and the variety of modern field theory approaches in these areas: B. Altshuler (Princeton), C. Beenakker (Leiden), K. Efetov (Bochum), L. Glazman (Minneapolis), A. Ludwig (UCSB, USA), N. Reed (Yale), A. Tsvelik (Oxford), M. Zirnbauer (Köln). Groups from SUNY/Stony Brook, Technion/Haifa, Delft U, Lancaster U, Oxford U and Cambridge U which are currently active in mesoscopic physics research and in the studies of quantum Hall effect were represented by the younger generation of researchers: I. Aleiner, A. Kamenev, Yu. Nazarov, V. Falko, J. Chalker, and Dr. Simons, respectively.

More than a third of the workshop has been represented by junior researchers, for many this was the first meeting of this kind they attended. [...] Thanks to the splendid facilities provided by the mpi**pks**, we were able to balance the program of the meeting and to complement morning lectures by group discussions and small seminars where younger participants were actively involved. A working atmosphere created in the Institute was so stimulating that, during the three weeks of the event, a full solution has been achieved of an ambiguity of the problem of electron quantum diffusion in the presence of a random magnetic field in 2D systems.

In a short term, the success of this meeting can be judged upon several new collaborations started and already resulted in numerous publications. N. Reed, J. Chalker and A. Ludwig have initiated the collaboration on the spin-Hall effect. L. Glazman and I. Pustylnik have solved the mystery about the speeded electron-electron energy relaxation in metallic wires; I. Aleiner and V. Falko, and Yu. Nazarov and V Falko have published a series of papers on spin relaxation in quantum dots explaining strange observations by the Harvard group of C. Marcus; B. Altshuler, who is always the centre of attraction for the youth, has pushed forward theory of two-level systems in relation to the two-channel Kondo problem. B. Altshuler, A. Altland and J. Meyer and V. Falko with T. Jungwirth have started to work on, and later solved, the problem of parallel magnetoresistance in 2D semiconductor structures, now their review article is in preparation.

In the longer term, the investment has been made into merging together supersymmetric sigma-model techniques used in quantum chaos and replica sigma-models and shaping analytical skills of the next generation of researchers who are interested in the theory of mesoscopic strongly correlated systems.

Problems in Systems Neuroscience

Workshop & Seminar
Scientific coordinators: J. L. van Hemmen, T. J. Sejnowski

Systems Neuroscience is devoted to many-neuron systems performing information processing. The key question is: How does a system of interacting neurons perform this task? To gain some preliminary insight, it may be helpful to follow the stream of information as it passes through the brain.

Sensory systems such as eyes and ears collect data in space and time so that temporal coding is one of the central issues related to describing incoming information. In vertebrates neurons produce action potentials or spikes, voltage pulses of 1 ms duration that convey the information. During evolution quite intricate forms of spike dynamics have arisen but a full understanding is still absent. Hence modeling spike activity in systems of interacting neurons and the ensuing collective dynamics is one of the most important issues in the field.

Special feedforward configurations of neurons transmit incoming information to higher areas, assemblies of neurons. The collection of neurons that provide input to a specific neuron "higher-up" is called a receptive field. This notion plays a dominant role in the study of both the visual and the auditory system and directly leads to the question: How do receptive fields arise and what role do they play in information processing? Do they originate from genetic coding or from development during experience as an animal grows up?

The collection of receptive fields of many neurons occurring in an area is called a *map*. It is, so to speak, a neuronal representation of the outside world. Once again one can question its origin. Maps in subsequent areas give rise to intricate dynamics, the structure of which is to be clarified, and are tied together through feedback, which is also what attention is due to.

This seminar in the millennium year 2000 was inspired by the mathematician David Hilbert. At the International Mathematicians Congress in Paris in 1900 Hilbert presented 23 mathematical problems that have had an important role in the development of mathematics in the twentieth century.

Inspired by Hilbert's magnificent example, the focus of the present symposium was on *identifying key problems*. Now 23 speakers were invited to present a specific fundamental question in the context of systems neuroscience during the workshop (August 4–8). More specialized sessions on auditory and visual topics as well as attention were preceding and following the workshop.

It is fair to say that the seminar and, in particular, the workshop were a great success. Well-known scientists such as Jean Bullier, Catherine Carr, Amiram Grinvald, Andreas Herz, Michael Merzenich, Klaus Pawelzik, Henning Scheich, Murray Sherman, Mike Stryker, and Steve Zucker were participating. In addition, several upcoming postdocs were providing as speakers a dynamic foreland paving the way for critical discussions.

The organizers, L. van Hemmen & T. Sejnowski, are the editors of a book on "23 Problems in Systems Neuroscience", to appear with Oxford University Press. This book will have a broad visibility and is expected to reach a wide audience.

Physics of Information and Synchronization in Stochastic Dynamics

Workshop, scientific organizers: P. Hänggi, J. Kurths, L. Schimansky-Geier

The theme of the workshop was devoted to timely topics in statistical physics, nonlinear physics and biophysics. In particular, the focus was on prominent questions such as how noise can play a constructive role in nonlinear systems responsible for information processing and/or what is the role of noise for synchronization and how synchronization – if it exists at all – is modified in the presence of noise.

The goal of this workshop was to promote original ideas among practitioners and theoreticians of various scientific disciplines and to work out the common groundworks for the understanding of novel phenomena in these and related interdisciplinary fields. The main topics were:
(i) physics of information (ii) phase dynamics in stochastic systems, (iii) stochastic resonance in physics and biophysics, and (iv) synchronization in chaotic and noisy systems.

The characterization of the underlying physics then requires new measures of complexity. In this context the use of synchronization and information theoretic measures play an increasingly prominent role as was demonstrated theoretically with presentations by W. Ebeling (Berlin), P. Gaspard (Brussels), H. Kantz (Dresden), A. Longtin (Ottawa) and N. Stocks (Warwick) for such complex systems involving language, wheather, neuronal activity, etc. Most stimulating lectures by P. Callenbach (Augsburg), J. Freund (Berlin) and M. Rosenblum (Potsdam) have shown evidence for the powerful abilities of an effective phase description in noisy and chaotic processes. F. Moss and A. Neiman (both St. Louis) presented new interesting, experimental synchronization results for the sensory systems of the paddlefish and the crayfish where these theoretical measures of synchronization theory have been applied. B. Blasius (Potsdam) presented a challenging lecture on the issue of spatial phase synchronization in the ecological systems and the role of disorder therein.

Among other highlights of the workshop were the lectures devoted to the role of noise in the dynamics of ion channels by S. Bezrukov (Bethesda) and stochastic resonance phenomena in assemblies of ion channels by I. Goytschuk (Augsburg) and P. Jung (Athens). These contributions could establish the constructive role of internal noise for the control of the response of the channels with respect to external stimuli. In such ensembles the noise level can be controlled via the size of the system, thereby modifying the total number of participating channels. A similar theoretical reasoning for a physical model was proposed by A. Pikovsky (Potsdam) who termed the effect "System size resonance".

Still other fascinating presentations centered around noisy dynamical models that relate to specific technological applications. P. Reimann (Augsburg) has shown analytically how a giant increase of diffusion in periodic potentials can occur. Likewise, C. van den Broeck (Limburgs) inspected the role of fluctuations in ensembles of parametric oscillators. These theoretical results were complemented by experiments on coupled noisy oscillators in the contribution of V. Anishchenko (Saratov). M. Rubi (Barcelona) reported challenging results on the possibility of a noise reduction via the addition of

several multiplicative noise sources.

The interesting lectures together with the lively poster presentations at this workshop have given evidence to the broad interest in this scientific area and did underpin the vitality of the field of stochastic synchronization of nonlinear information processing dynamics. Several cooperations between groups working in this field (Augsburg-Katowice-Berlin-Barcelona-Potsdam-Saratov) were intensified during the workshop. These colaborations have already resulted in joint publications. Moreover, a bookshow covering the multifacetted aspects of stochastic physics and nonlinear dynamics, which was organized by Dr. Caron from Springer publishers, attracted widespread attention among all participants of all ages.

Coherent Evolution in Noisy Environments

Workshop & Seminar
Scientific coordinators: A. Buchleitner, R. Werner, A. Zeilinger

The key motivation for this International School/Seminar/Workshop was to bring together experts from quantum information, photonic band gap materials, and noise induced stabilization phenomena (such as Stochastic Resonance), sharing a common interest in decoherence. The event had a strongly interdisciplinary scope from mathematics to experimental physics. Special emphasis was directed towards the training of promising PhD students and young PostDocs, and this has been ensured by a series of advanced lectures on selected topics of the seminar program.

The structure of the entire program was subdivided in an International School, during the first seven weeks, and an International Workshop, during the last week. During the School, nine lectures (5×90 minutes each, from monday to friday, before lunch) on key topics of the program were presented by internationally reputable experts (H. Briegel, B.-G. Englert, G. Ingold, B. Kümmerer, P. Lambropoulos, M. Raizen, W. Strunz, H. Weinfurter, K. Wiesenfeld), and of high or even very high didactic quality. It was essential that lectures started from elementary foundations and proceeded to cutting edge problems along a steep learning curve. Applicants were only admitted for periods which fitted with the lecture schedule (i.e., partial attendance to various lectures was disencouraged). Two regular afternoon seminars were organized – to allow oral presentations of current research topics of the participants, or to deepen special aspects of the lectures. This combination of lectures and seminars provided a stable structure, which, in particular, stimulated discussions and common projects between the less and the more experienced participants (the latter including K. Dietz, P. Hänggi, T. Leggett, A. Schenzle, and U. Weiss) and the lecturers. The Workshop was conceived as a climax to the School, as well as an independent event. Besides a dense program of talks (by S. Haroche, G. Vidal, H. Maassen, T. Wellens, M. Arndt, G. Agarwal, Y. Imry, G. Gerber, H. Walther, G. Alber, L. Lugiato, D. Shepelyansky, H. Schomerus, G. Giacomelli, R. N. Mantegna, H. J. Carmichael, C. Köstler, S. Fishman, M. Grifoni, H. Lichte, J. P. Paz, D. Cohen, U. Becker, J. Zakrzewski, C. Miniatura, B. v. Tiggelen, C. Müller, E. Akkermans, A. Lagendijk, J. Schmiedmayer, S. Kilin, M. Keyl, L. Davidovich, M. Kus, H. Briegel, M. Wilkens, H. Schmidt-Böcking, V. Meyer, G. Leuchs, Y. Yamamoto) from the different areas mentioned above, two extensive poster sessions allowed the presentation of recent results of the participants. A public evening

lecture by A. Zeilinger (title: "Was Quanten alles können"), in the lobby of the mpi**pks**, attracted approx. 150 guests, followed by vivid discussions between lay(wo)men and workshop participants over snacks and drinks in the lobby of the institute. [...]

The School/Workshop stimulated numerous fruitful discussions, and allowed to establish contacts between so far rather disconnected research areas (which, in some cases, already led to common research projects). Due to the positive feedback to the School, the larger part of the lecturers agreed upon writing a textbook on the subjects treated during the school, much in the spirit of the Les Houches series. The book should appear in print by the end of 2002.

Nanostructures in Photovoltaics

Wokshop, scientific organizers: P. Corkish, S. Kettemann, J. Nelson

More than 80 participants from 20 countries came together to face the challenges of the next generation of photovoltaics in this interdisciplinary workshop. The opening on Sunday morning started with a survey of the current state of research and development of high efficiency solar cells, the physical limits of the efficiency of conventional single gap solar cells and of tandem solar cells, as compared to the one of innovative concepts like hot electron and multiband solar cells (M. Green, Sydney; P. Würfel, Karlsruhe). The advantages of multi quantum wells for the optimization of solar cell performance were outlined by K. Barnham (Imperial College, London) with recent experimental results.

The introductory lectures continued on Monday, with a review of the preparation and optical characterization of lateral heterostructures (D. Heitmann, Hamburg) and the theory of the optical properties of nanostructures (S. Koch, Marburg), as well as an introduction to the mesoscopic photovoltaic effect and the theory of weak localization (V. Falko, Lancaster). These lectures established the link to basic research and reminded the participants that the photovoltaic effect is, beyond its application in solar cells, a subject of present-day research efforts.

An introductory comparison between photovoltaics and photoelectrochemistry (M. Archer, Cambridge) was followed by a review of the current state of research in nanoporous dye sensitized solar cells (J. Nelson, Imperial College, London).

The limitations as well as the potential of nanostructuring of solar cells were critically discussed by H. Queisser (MPI für Festkörperforschung, Stuttgart), an expert and historical witness who contributed immensely to the understanding and development of photovoltaics, in a particularly clear and motivating way.

Having the common basis of these first two days of introductory lectures in photovoltaics, new solar cell concepts and the physics of nanostuctures, the following research presentations in talks and posters captured the great interest of all the participants.

The prospect on the 3rd generation of solar cells (M. Green, Sydney) and quantum dot solar cells (A. Nozik, National Renewable Energy Lab., Golden, Colorado), followed new results from basic research on nanostructures like the resonant tunneling spectroscopy of insulating quantum dots. (D. Vanmaekelbergh, Debye Institute, Utrecht),

and the theory of many-body effects in the photoluminescence of nanostructures (M. Raikh, Salt Lake City).

After a presentation of the newest developments in solar cell technology of tandem solar cells, using III-V- compounds, (M. Yamaguchi, Toyota, Nagoya), as well as the improvement of Si thin film solar cells by self-organized growth of Ge islands, (H. Presting, DaimlerChrysler AG, Ulm), there followed the plenary talk by S. Ganichev (Univ. Regensburg/Ioffe Inst. St. Petersburg). He gave a thrilling account of the very recently discovered conversion of the photon spin of circularly polarized light into a directed spin-polarized electrical current in quantum wells.

Further major progress was reported on the theory of multiband solar cells (A. Luque, Madrid; A. Brown, Sydney; S. Kettemann, Hamburg), the properties of multiquantum well solar cells (N. Ekins-Daukes, London; A. Freundlich, Houston; R. Morf, Zürich; N. Anderson, Amherst; C. Honsberg, Atlanta; A. Varonides, Scranton), the work on many open questions concerning the charge transfer and transport in dye sensitized, nanoporous semiconductor solar cells (M. Grätzel, Lausanne; T. Lian, Emory Univ., Atlanta; F. Willig, HMI Berlin; B. O'Reagan, Petten, Niederlande; A. Hinsch, Fraunhofer ISE, Freiburg; A. Kambili, Bath, GB; A.R. Kumarasinghe, UMIST, Manchester; S. Nakade, Nokia, Tokyo; K. Tennakone, Sri Lanka; A. Konno, Hamamatsu, Japan; U. Rau, Stuttgart; D. Vanmaekelbergh, Debye Institut, Utrecht), the preparation and characterization of nanostructured materials for photovoltaics (R. Caruso, MPIKG, Golm; R. Könenkamp, HMI Berlin; A. Rogach, Hamburg; F. Schauer, Brno; C. Wang, BUAA, Beijing), as well as on the rapid progress in organic solar cells (V. Dyakonov, Oldenburg; T. Markvart, Southampton; L. Schmidt-Mende, C. Ramsdale, Cavendish, Cambridge; S. Tuladhar, Ben Gurion Uni., Sede Boker).

The diversity of all these contributions showed impressively that photovoltaic research has produced promising novel concepts in recent years whose further development demands a better and deeper understanding of the physics of nanostructures. The success of this interdisciplinary workshop was to a large extent due to the contributions by young postdoc researchers and students to the poster sessions and research talks and their fruitful interactions with the leading scientists in the physics of nanostructures and in photovoltaics.

The results of this first workshop on nanostructures in photovoltaics will be published in a special issue of Physica E (Low Dimensional Structures) in May 2002.

We thank the Max-Planck-Institut für Physik Komplexer Systeme for all its support and Ms. Mandy Stiegler for managing the workshop office in a friendly and tireless manner. We also thank the Centre for Third Generation Photovoltaics, University of New South Wales, for providing a copy of the published proceedings to each participant.

Nano-Physics & Bio-Electronics – A new Odyssey

Seminar & Workshop
Scientific organizers:
T. Chakraborty, F. Peeters, U. Sivan

The major aim of the meeting was to bring together experts from various disciplines, such as physics, chemistry, biology, computer science, etc. in order to have a unique

meeting to assess the rapid developments in the field. In the first two weeks, many world-class experts reviewed the field of conventional nanoscale physics. Most notably, Prof. T. Ando presented an extensive review on carbon nanotubes, and Prof. B. Halperin discussed at length the properties of metal nanoparticles and quantum dots. In addition, there were several talks on the experimental and theoretical developments of the basic and applied aspects of quantum dots. Physical properties of quantum dots covered in these two weeks included Kondo effect, quantum computing, quantum cryptography, optoelectronic devices, optical spectroscopy and transport in quantum dots. There was also a one-day session on the quantum cascade lasers. Important speakers included D. Mowbray, M. Grundmann, A. Shields, J. Faist, and many others.

In the remaining two weeks of the meeting, the speakers described various aspects of DNA-related nanoscience and technology. Talks covered topics that included electronic properties of DNA, computations via DNA self-assembly, molecular electronics with single DNA, biology-based nano-electronics, molecular machines from DNA. Invited speakers for these topics included N. Seeman, C. Dekker, P. Kuekes, E. Winfree, H. Bouchiat, H. Lipson, and many others.

As stated above, our main aim was to organize an interdisciplinary meeting of experts on nano-scale science and technology, and, in particular, on the emerging field of bio-related nanotechnology. We believe that the meeting succeeded in that goal. There were several very lively informal discussions on the issues presented in the formal talks. Some of the invited speakers have written up extended version of their talks which will be published as a book by Elsevier in April, 2002.

Computational Physics of Transport and Interfacial Dynamics

Seminar & Workshop
Scientific organizers: H. Emmerich, B. Nestler M. Schreckenberg

The meeting has closely pursued the recent progress of research in computational physics and materials science, particularly in modelling both traffic flow phenomena and complex multi-scale solidification. These branches of science have become topics of considerable diversity linking disciplines as different as physics, mathematical and computational modelling, nonlinear dynamics, materials sciences, statistical mechanics and foundry technique. The international workshop brought together experts from different fields in order to (i) enhance the exchange of knowledge, to assess common interests and to provide closer cooperation between different communities of researchers, (ii) create a comprehensive and coherent image of the current research status and to formulate various possible perspectives for joint future activities. Special attention was devoted to the exchange of experiences concerning numerical tools and on the bridging of the scales as necessary in a variety of scientific and engineering applications. An interesting possibility along this line was the coupling of different computational approaches leading to hybrid simulations. To this end we explicitly addressed researchers working with different numerical schemes as diverse as cellular automata, coupled maps, finite difference and finite element algorithms for partial differential equations (e.g. phase-field computations). The following scientific topics were treated in the contributions:

- Fundamentals and modelling of microstructure formation: Free boundary prob-

lems, phase transitions, solidifiation, interfacial dynamics, Ginzburg-Landau equations, Cahn-Hilliard equations, phase-field modelling.

- Numerical simulations on different time and length scales: Fluid dynamic computations, adaptivity, finite element-discretizations, discrete modelling techniques such as molecular dynamics and Monte Carlo.
- Multi-scale problems in crystal growth, porous media, solidification and traffic flow.

The three-weeks seminar was attended by 87 participants from 22 different countries. In the first week the organizers Emmerich and Nestler gave a lecture-based course for younger researchers to introduce the topics of the subsequent two-weeks intensive workshop. Throughout all three weeks the scientific newcomers used the opportunity to present their research interests and results in either short talks, discussion rounds or poster sessions. In addition they had the chance to meet and discuss with experts from both fields: transport and interface dynamics. The second and third week of the workshop were scientifically supported by a large number of important researchers. Among them are Peter Berg (Canada), Kurt Binder (Germany), Massimo Conti (Italy), Wolfgang Dreyer (Germany), Charlie Elliott (UK), Martin Glicksman (USA), Peter Hänggi (Germany), Dieter Herlach (Germany), Serge P. Hoogendoorn (Netherlands), Alain Karma (USA), Stefan Luding (Netherlands), Kai Nagel (Switzerland), Michael Rappaz (Switzerland), Alfred Schmidt (Germany), Robert Sekerka (USA), Jürgen Sprekels (Germany), Stefan Turek (Germany), James A. Warren (USA), Adam A. Wheeler (UK).

Proceedings will be published by Springer.

Quantum dynamical concepts: From diatomics to biomolecules

Workshop & Seminar
Scientific organizers: F. Großmann, P. Jungwirth, R. Kossloff

Novel theoretical approaches to solve the time-dependent Schrödinger equation for systems with increasing complexity were in the topical focus of the whole event. In addition to the 32 theoretical talks, three experimental talks were held during the central workshop, revealing the challenges for theory. Key talks have been given by Eric J. Heller (Harvard) and William H. Miller (Berkeley) who were dealing with the fundamental aspects of approximate semiclassical theories and Benny Gerber (Jerusalem) who applied mixed classical/quantum approaches to time-dependent phenomena in large molecules and clusters. Another highlight was the experimental talk by Tobias Brixner (Würzburg) on controlling chemical reactions with taylored femtosecond laser pulses. Moreover novel density functional theory based methods for large systems, like water clusters, have been discussed by Dominik Marx (Bochum). Quantum aspects in the dynamics of biomolecules have e. g. been covered in the talks of Wolfgang Domcke (Munich) and Sharon Hammes-Schiffer (Penn State). In his well attended public evening lecture, Peter Hänggi (Augsburg), gave an introduction to molecular electronics, on the time-dependent quantum aspects of which he also focussed in his scientific contribution to the workshop. Younger participants have used the two poster sessions

and especially the 4 surrounding seminar weeks (which were held on a tutorial level) for intense discussion groups and contacts to the senior participants.

The last workshop talk by John Briggs (Freiburg) was critically investigating the role of time in quantum theory. It became clear that although the time-independent Schrödinger equation might be more fundamental, nevertheless, the time-dependent Schrödinger equation is an extremely valuable tool for understanding and predicting new interesting phenomena in the realm of physics and chemistry.

Microscopic Chaos and Transport in Many-Particle Systems

Seminar & Workshop
Scientific organizers: R. Klages, P. Gaspard, H. van Beijeren, J. R. Dorfman

This meeting concentrated on the connection between dynamical systems theory and statistical physics with a major emphasis on the description of nonequilibrium systems. A fundamental problem in this field is to analyze the fractal properties of nonequilibrium steady states as generated by microscopic chaos in the motion of atoms and molecules composing fluids. In particular, one tries to find relationships between characteristic quantities of chaos and transport properties and to assess their validity.

Some of the most central topics were

The Evans-Cohen-Gallavotti fluctuation theorem. The "founding father" D. Evans gave a very good review of the various versions of this important theorem; G. Gallavotti discussed some very interesting applications in hydrodynamics far from the microscopic realm for which the theorem was envisioned originally, and C. Maes derived a quite general version of the fluctuation theorem valid for Hamiltonian systems coupled stochastically to heat baths. Z. Kovács showed that the fluctuation theorem still holds in certain specific cases where not all mathematical conditions are satisfied.

Hydrodynamic modes, generalizations of hydrodynamic modes and other long wave length collective modes. P. Gaspard showed how hydrodynamic modes may be constructed for various systems ranging from simple toy models to many interacting particles. J. R. Dorfman and I. Claus lectured on the same topic and D. Wojcik and T. Prosen shed some light on the generalization of these concepts to quantum mechanical systems. The subject of how to generalize hydrodynamics and hydrodynamic modes to low-dimensional systems in which transport is anomalous was treated by P. Grassberger, T. Geisel, D. Isbister, Y. Klafter, G. Radons and S. Tasaki. H. Posch reported on collective very slowly growing modes in the Lyapunov spectrum of many particle systems. Theoretical treatments of this were reported by M. Mareschal, A. de Wijn and T. Taniguchi, but so far none of them is capable of completely explaining the eigenvalue spectrum observed in the simulations.

Thermostats. The physical status of mathematical thermostats such as the Nosé-Hoover and the Gaussian ones remained much disputed. R. Klages gave a good review of this subject and it also came up in the talks by D. Evans, D. Panja, G. Morriss, S. Hess, and W.G. Hoover as well as in many private discussions.

Introductory lectures were provided by O. de Almeida, P. Cvitanovic, C. Maes, D. Evans and P. Gaspard. Younger people could present their posters in form of 4-minute

talks during a special workshop session, and they competed for book awards for the three best posters. Newcomers with very interesting contributions were N. Davidson, who does experiments on atom-laser interactions, B. Li and D. Alonso, both working on non-dispersing but nonetheless diffusive billiards, and H. Larralde, who reported on billiards with rotating scatterers. The 86 conference participants were from 22 different countries, 18 of them were Ph.D. students, 22 postdocs, and 11 were active participants from the mpi**pks**.

This conference was very valuable as a platform for the exchange of ideas. It sharpened the contours of problems to be solved yet, of issues on which the opinions are still divided and of directions to follow in the future. The excellent setting and organization contributed much to its success, and the full program could be carried through despite the serious flooding that occurred in Dresden. The main scientific results of this conference will be published as proceedings in a special issue of *Physica D*.

Progress in Condensed Matter Theory

Workshop, scientific organizers: K. Evetov, E. Khmelnitskii

The conference was dedicated to the 70th birthday of Prof. Anatoly Larkin. His scientific interests extend over a very broad spectrum of directions of research in Condensed Matter Physics and this gave an opportunity to attract to the conference key players in diverse branches of Theoretical Physics. The following topics were discussed at the conference: 1. Superconductivity, magnetism and strongly correlated systems. 2. Disordered systems. 3. Mesoscopic and Nanoscience. 4. Spin glasses. 5. Quantum Hall Effect. Most of the participants were outstanding scientists from all over the world. The list of the participants includes P.W. Anderson (Princeton, USA), E. Abrahams (Rutgers, USA), B. Altshuler (Princeton, USA), V. Ambegaokar (Cornell, USA), C. Beenakker (Leiden, Netherlands), M. Fisher (Maryland, USA), H. Fukuyama (Tokyo, Japan), P. Fulde (Dresden, Germany), B. Kramer (Hamburg, Germany), T. M. Rice (Zurich, Switzerland), G. Schon (Karlsruhe, Germany), D. Thouless (Seattle, USA), C. Varma (Lucent, USA), P. Wölfle (Karlsruhe, Germany) and many other leading scientists. Newcomers could present themselves at two poster sessions and several of them made oral presentations. The conference was a big event. The key experts working in different branches of the Condensed Matter Physics could gather together and get information on what is going on not only in their fields of expertise but also in other branches of Condensed Matter Physics. The conference was invaluable for young people who had an opportunity to listen and talk to the top scientists in the world.

4 Externally Funded Research and Relations to Industry

4.1 DFG Projects

Individual Projects

- *Ballistischer Transport im Rahmen der Fredholm-Theorie*, Dr. Klaus Richter
- Kooperationsprojekt *Complex systems in condensed matter physics - strong correlation and disorder*, Prof. Peter Fulde

- *Experimentelle und theoretische Untersuchung von räumlich lokalisierten Anregungen in nichtlinearen Gittern*, Dr. Sergej Flach
- *Der Einfluss klassischer Mechanik auf physikalische Schwelleneffekte in der Quantenphysik*, Prof. Jan-Michael Rost
- *Der Einfluss viskoser und viskoseelastischer Eigenschaften auf die Stabilität von Ferrofluidschichten in statischen Magnetfeldern*, Dr. Adrian Lange

Schwerpunktprogramme

- *Quasikristalle: Struktur und physikalische Eigenschaften (SPP 1031)*, Dr. Dieter Joseph
- *Zeitreihenanalyse von Bifurkationen elasto-plastischen Typs auf der Grundlage von extrem kurzen Zeitreihen (SPP 1114)*, Prof. Holger Kantz
- *Wechselwirkung in ultrakalten Atom- und Molekülgasen (SPP 1116)*, Prof. Jan-Michael Rost, Dr. Thomas Pattard

Sonderforschungsbereiche and Forschergruppen

- *SFB 256 Nichtlineare partielle Differentialgleichungen*, Dr. Andreas Deutsch
- *SFB 276 Korrelierte Dynamik hochangeregter atomarer und molekularer Systeme*, Prof. Jan-Michael Rost
- *SFB 393 Numerische Simulationen auf massiv parallelen Rechnern*, Dr. Bernhard Mehlig
- *SFB 463 Seltenerd-Übergangsmetallverbindungen: Struktur, Magnetismus und Transport*, Prof. Peter Fulde
- *SFB 609 Modellierung von Erstarrungsvorgängen unter Magnetfeldeinfluss*, Prof. Holger Kantz
- Forschergruppe *Nanostrukturierte Funktionselemente in makroskopischen Systemen*, Dr. Markus Bär, Heiko Kühne

4.2 BMBF funding

- Mitgliedschaft im Kompetenzzentrum *"NanOp" für die Nanostrukturen in der Optoelektronik*, Dr. Klaus Richter
- *Modellierung mesoskopischer Dielektrika, insbesondere Scheiben- und Ringresonatoren mit hohem Brechungsindex*, im Rahmen des Schwerpunktes *Innovative Laser bei 1,3 und 1,5 Mikrometer*, Dr. Klaus Richter
- *Fehlerfrüherkennung durch Zeitreihenanalyse*, Prof. Holger Kantz
- BMBF-Förderung im Rahmen deutsch-kanadischer wissenschaftlich-technischer Zusammenarbeit; Sektor: Materials/Physical Technologies: *Application of semiclassical methods to complex systems relevant to nanotechnology*, Dr. Klaus Richter

- Projekt im Rahmen der Förderung regenerativer Energien:*Nichtlineare Methoden zur Last- und Energieangebotsprognose in lokalen Energiesystemen, insbesondere bei Windenergie und Photovoltaik*, Mario Ragwitz, Prof. Holger Kantz

4.3 EU funding

- TMR-Network *Quantum transport on the atomic scale*, Dr. Andreas Buchleitner
- INTAS-Network *Periodically Driven Zero-Dispersion Systems*, Dr. Klaus Richter
- COST P5 Initiative *Mesoscopic Electronics*, Dr. Klaus Richter
- CERION/ ESPRIT IV Participant of the *Canadian European Research Initiative on Nanostructures*, Dr. Klaus Richter
- TMR-Network *Quantum Chemistry of the Excited State*, Prof. Peter Fulde
- TMR-Network *Localization by nonlinearity and spatial discreteness, and energy transfer, in crystals, biomolecules and Josephson arrays*, Dr. Sergej Flach

4.4 Additional external funding

- VW-Stiftung: *Molekularsieblaser-Konglomerate im Infraroten*, Dr. Jan Wiersig
- VW-Stiftung, Zusammenarbeit mit Natur- und Ingenieurwissenschaftlern in Mittel- und Osteuropa: *Entanglement measures and the influence of noise*, Dr. Andreas Buchleitner, together with Dr. K. Życzkowski, Polish Academy of Sciences, Warsaw
- VW-Stiftung, *Faltenbildung als dynamische Instabilität bei der Blechumformung durch Drücken*, Prof. Holger Kantz
- VW-Stiftung, *Schleifbranderkennung durch Analyse von Schallemissionssignalen*, Prof. Holger Kantz
- DAAD (PROCOPE), *Spektrale Eigenschaften von Mehrelektronenatomen im elektromagnetischen Feld*, Dr. Andreas Buchleitner, together with Dr. D. Delande, Universite Pierre et Marie Curie, Paris
- GIF, *Self-organization phenomena in catalytic surface reactions: from nanoscale to microscale*, Dr. Markus Bär
- HLRB Grand Challenge Projekt: *Spectral Properties of Atomic Rydberg States in Intense Electromagnetic Fields*, Dr. Andreas Buchleitner
- Verbundprojekt im Rahmen des Programms *Technische Anwendungen von Erkenntnissen der Nichtlinearen Dynamik*, Dr. Eckehard Olbrich, Prof. Holger Kantz
- Klaus Tschira Stiftung, Unterstützung des Netzwerkes MTBio, *Dr. Andreas Deutsch*
- Robert Bosch Stiftung, *Winterschule für Sächsische Gymnasien*, Prof. Holger Kantz, Uta Gneisse

4.5 Stipends

- *Dr. Gianaurelio Cuniberti*, Schlössmann stipend
- *Dr. Gudrun Schliecker*, Schlössmann stipend
- *Prof. Guram Adamashvili*, DAAD reseach stipend
- *Elisangela Feretti Manfra*, DAAD PhD stipend
- *Dr. Anatole Kenfack*, AvH research stipend
- *Prof. Eric Heller*, AvH research award
- *Prof. Laxmi Chand Gupta*, AvH research award
- *Joseph Choi*, NSF funded PhD stipend

4.6 Cooperations with Industry

Prof. Holger Kantz: Assisted by Garching Innovation, we have been trying to set up cooperations with industrial companies in order to explore the applicability of nonlinear methods for wind speed predictions. The company Boreas in Dresden Hellerau supplied us with several data sets which enabled us to perform more precise statistical tests with our method. Negotiations about licensing of the patent have been performed with one major German manufacturer of wind converters, and currently a cooperation with a Spanish company is prepared.

A second field of industrial cooperation is the analysis of human speech. A local company in Dresden has started to explore the applicability of nonlinear noise reduction methods for the preprocessing of human speech signals for the purpose of automatic speech recognition.

4.7 Patents and Licences

- *Dr. Mario Ragwitz, Prof. Holger Kantz*
  Verfahren und Vorrichtung zur Steuerung von Windenergieanlagen, 2000
- *Dr. Klaus Richter, Dr. Martina Hentschel et al.*
  Nichtlinearer 2D-Laser mit zur Auskopplung integriertem Lichtventil, 2000
- *Dr. Tobias Letz*
  Verfahren zur Stabilisierung der Ausgangsleistung eines Festkörperlasers und Festkörperlasersystems, 2001
- *Prof. Holger Kantz*
  Verfahren und Vorrichtung zur Vorhersage von Strömungsparametern turbulenter Medien, 2002

5 Teaching and Education

5.1 Lectures at Universities

Sommersemester 00

Theoretische Quantenoptik - Dr. A. Buchleitner, LMU München

Theoretische Biophysik - Dr. M. Bär, TU Dresden

Stochastic processes - Prof. H. Kantz, Uni Wuppertal

Wintersemester 00/01

Hydrodynamics and turbulence - Prof. H. Kantz, Uni Wuppertal

Sommersemester 01

Nonlinear dynamics and chaos - Prof. H. Kantz, Uni Wuppertal

Theoretische Biophysik - Dr. M. Falcke, TU Chemnitz

Wintersemester 01/02

Theoretische Quantenoptik - Dr. A. Buchleitner, LMU München

Deterministic chaos and nonequilibrium statistical mechanics - Dr. R. Klages, TU Dresden

Physik am Samstag - Prof. J.-M. Rost, TU Dresden

Sommersemester 02

Strukturbildung in nichtliniearen Systemen - Dr. M. Bär, Universität Magdeburg (Lehrstuhlvertretung *Professur für nichtlineare Phänomene*)

Forschungsseminar Biophysik - Dr. M. Bär, Universität Magdeburg (Lehrstuhlvertretung *Professur für nichtlineare Phänomene*)

Ringvorlesung: Aspekte der Zeit - Dr. K. Morawetz, Prof. J.-M. Rost, Kathedralforum Dresden

Wintersemester 02/03

Stochastic processes and the Fokker-Planck Equation - Prof. H. Kantz, mpi**pks**

Ringvorlesung: Aspekte der Zeit - Dr. K. Morawetz, Prof. J.-M. Rost, Kathedralforum Dresden

5.2 Degrees

5.2.1. Habilitations

- *Schliecker, G.: Disorder of Shapes and Shape of Disorder,* Dresden 2000
- *Hetzel, R.: The Determinant Quantum Monte Carlo Method,* Dresden 2001
- *Bär, M.: Complex Patterns in Reaction-Diffusion Systems,* Dresden 2002

5.2.2. Dissertations

- *Abdurahaman, A.: Correlated ground state ab initio studies of polymers,* Dresden 2000
- *Amici, A.: Magnetic order and superconductivity in $HoNi_2B_2C$ and related borocarbide compounds,* Dresden 2000
- *Massoth, M.: Elektronische Korrelationen, Kristallfeldanregungen und magnetische Wechselwirkungen in Nd_2CuO_4,* Dresden 2000
- *Schautz, F.: Modellpotentiale in Quanten-Monte-Carlo-Methoden,* Dresden 2000
- *Sinde, E.: Nichtbeschattbarkeit durch Dimensionsvariabilität in dynamischen Systemen,* Wuppertal 2000
- *Brusch, L.: Complex Patterns in Extended Oscillatory Systems,* Dresden 2001
- *Frustaglia, D.: Spin-Dependent Transport in Mesoscopic Quantum Systems,* Dresden 2001
- *Hentschel, M.: Mesoscopic wave phenomena in electronic and optical ring structures,* Dresden 2001
- *Hornberger, K.: Spectral Properties of Magnetic Edge States,* München 2001
- *Krug, A.: Alkali Rydberg States in Electromagnetic Fields: Computational Physics Meets Experiment,* München 2001
- *Letz, T.:Theoretische Aspekte der Regelung eines frequenzverdoppelten Festkörperlasers und der Einfluss von Rauschen auf seine Dynamik,* Oldenburg 2001
- *Matassini, L.: Signal analysis and modelling of non-linear non-stationary phenomena,* Wuppertal 2001
- *Müller, C.: Schwache Lokalisierung von Licht in einem Gas kalter Atome: Kohärente Rückstreuung und interne Quantenstruktur,* München and Nice (France) 2001
- *Ragwitz, M.: Datengetriebene Modelle stochastischer dynamischer Systeme am Beispiel hydrodynamischer Turbulenzen.* Wuppertal 2001
- *Bernert, A.: Theorie der Phasenübergänge in NaV_2O_5,* Dresden 2002
- *Ferretti Manffra, E.: Properties of systems with time delayed feedback,* Wuppertal 2002

- *Kaiser, A.: Nichtlineare Methoden zur Quantifizierung von Abhängigkeiten und Kopplungen zwischen stochastischen Prozessen basierend auf Informationstheorie,* Wuppertal 2002
- *Nicola, E.: Interfaces between competing patterns in reaction-diffusion systems with nonlocal coupling,* Dresden 2002
- *Schneider, T.: Zur Photoionisation einfacher Atome - quantenmechanische und klassische Zugänge,* Dresden 2002
- *Siedschlag, C.: Mechanismen der Ionisation atomarer Systeme in intensiven Laserpulsen,* Dresden 2002
- *Wellens, T.: Entanglement and control of quantum states*
  München 2002

5.2.3. Diploma

- *Wimberger, S.: Der Leitwert von Atomen,* LMU München 2000
- *Marschinski, R.: Metodi non lineari per l'analisi di serie temporali e multivariate di dati,* Bologna 2001

5.3 Appointments and Awards

Appointments

- *Prof. Klaus Richter* accepted the offer for a C4 professorship at the University Regensburg.
- *Prof. Holger Kantz* accepted the offer for an adjunct professorship at the Physics Department of the University Wuppertal.
- *Dr. Martin Sieber* accepted the offer for a lecturer position at the University Bristol.
- *Prof. Martin Albrecht* accepted the offer for a Junior Professorship at the University Siegen.
- *Dr. Marco Ameduri* accepted the offer for a Senior Lecturer in Physics at the Weill Cornell Medical College in Qatar.
- *Prof. Jaroslav Fabian* accepted the offer for a professorship at the University Linz.

5.3.2 Awards

- *Schmüser, F.:* Otto-Hahn-Medaille 2000
- mpi**pks** (*U. Gneisse):* Max-Planck-Preis für Öffentliche Wissenschaft 2000
- *Müller, C.:* Wissenschaftspreis der Universität Würzburg 2001
- *Or-Guil, M.:* Nachwuchsgruppe der Volkswagenstiftung 2001
- *Brusch, L.:* Otto-Hahn-Medaille 2002

- *Cuniberti, G..:* Nachwuchsgruppe der Volkswagenstiftung 2002
- *Flach, S.:* Stephanos Pnevmatikos International Award 2002
- *Hornberger, K.:* Otto-Hahn-Medaille 2002

6 Public Relations

Open House Day

On November 16th, 2001 we opened the doors for everyone interested in visiting our institute. During talks, video shows and poster presentations the members of our institute conveyed the importance and fascination of their research to a broad audience. The resonance was very good, about 500 visitors participated in the event, which included:

- an Invited Lecture by Prof. Dr. Peter Fischer, Universität Konstanz
- Short lectures about the scientific work at the institute
- Physical experiments
- Physics Quiz with nice prizes for fast and sharp thinking

Journal *Kontakt*

mpi**pks** participates in the editorial board of the alumni journal *Kontakt* (with Technische Universität Dresden, Forschungszentrum Rossendorf e.V., Institut für Festkörper- und Werkstoffforschung Dresden, Institut für Polymerforschung Dresden e.V., Max-Planck-Institut für Chemische Physik fester Stoffe, Herz- und Kreislaufzentrum der TU Dresden). The journal appears every 3 months with regular news about mpi**pks**.

Wissenschaft im Rathaus • Science in the City Hall

The mpi**pks**, the Technische Universität Dresden and the city of Dresden have launched a series of public lectures (about 3 per year) called *Wissenschaft in Rathaus*. The following lectures were delivered during the period 2000-2002:

- 5 April 2000, Prof. Dr. Wieghardt - MPI für Strahlenchemie in Mülheim, *Spurenelemente - Ihre Wirkung in Mensch und Tier*, about 200 participants
- 13 September 2000, Prof. Dr. Jens G. Reich - Max-Delbrück-Centrum Berlin-Buch, *Gene und Klone: Das Menschenbild der neuen Biologie*, about 500 participants
- 9 November 2000, Prof. Rolf Emmermann - GeoforschungsZentrum Potsdam *Geotechnologien - Das neue Bild unserer alten Erde*, about 300 participants
- 14 March 2001, Prof. Otto Krätz - Universität Stuttgart, *Der Chemiker - Held oder Finsterling?*, about 300 participants

- 22 May 2001, Prof. Günter Blobel, (Nobelpreis 1999) - Rockefeller University, New York, *Wie eine Zelle sich organisiert*, about 700 participants
- 20 September 2001, Dr. Gerhard Thiele - Astronaut ESA, *Wie Raumfahrt das Bild der Erde verändert*, about 500 participants
- 28 March 2002, Prof. Dr. Christine Nüsslein-Volhard - MPI für Entwicklungsbiologie, Tübingen, *Von Genen und Embryonen*, about 350 participants
- 12 September 2002, Prof. Dr. Peter Hartmut Graßl - MPI für Meteorologie, Hamburg, *Der globale Klimawandel hat begonnen. Können wir ihn dämpfen?*, about 300 participants
- 14 November 2002, Prof. Dr. Peter Gruss - Präsident der MPG, *Stammzellen - Wohl oder Wehe?*, about 440 participants

mpipks school contact program

mpi**pks** conducts annual lectures for high school students to increase interest in natural sciences and mathematics among future potential students and to establish and strengthen contacts to the staff members of high schools, especially to physics teachers. Prof. Dr. Otto Krätz (Universität Stuttgart) gave a lecture on *Die Chemie auf den Jahrmärkten des 18. Jahrhunderts* to an audience of about 240 high school students on September 27th, 2000. Prof. Dr. Friedrich Kreißl (Technische Universität München) gave a lecture on *Feuer und Flamme, Schall und Rauch* to an audience of about 250 high school students on September 25th, 2001.

In addition mpi**pks** offers regular workshops on modern aspects of physics research for high school physics teachers:

- 13. April 2000, *Chaos und Quantenphänomene*
- 12. September 2000, *Einführung ins Chaos*
- 13. March 2001, *100 Jahre Quantenphysik*
- 11. September 2001, *Über die Entstehung von Mustern in der Natur*
- 28. February 2002, *Supraleitung*
- 4. September 2002, *Von Plastiktüten und Flachbildschirmen: Die Physik der elektrisch leitenden Kunststoffe*

On the 25th of April 2002 we had the first *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 difficulties when pursuing a scientific career. About 50 female students participated in this event.

mpi**pks** offers Praktika to interested high school students, with durations from 2 weeks to several months. At the moment there are six students enrolled.

In addition mpi**pks** offers lecturing at high schools on a permanent basis. High school staff teachers are informed about the current lecture topics offered and are encouraged to request for a specific lecture. About ten lectures are given annually.

Winter school for high school students

Among the different PR activities, we have particularly focussed on high school teachers and high school students. Together with the Fetscher Gymnasium (secondary school in Pirna), we have applied for and obtained funding from the Robert Bosch foundation within a program called "NatWorking". This program aims exactly at the establishment of links between academia and high schools. Our joint project consists in a series of three winter schools for high school students. For about 60 participants, we arrange an entertaining and educating mixture of scientific talks on a level accessible by interested students in the highest two years of a secondary school, of more interactively designed exercises, and of discussions on issues concerning the sciences as subjects of study and profession. The first three days' school in February 2002 was already very successful. Based on these experiences, the outline was slightly modified for the second school, which took place from Feb. 3-5, 2003. Since biological physics gained a stronger emphasis, we could make use of the excellent facilities of the Hygienemuseum (museum for hygienics), in particular of their experimental labs. It seems that this school was extremely well received from both students and accompanying teachers.

7 Budget of the Institute

Figures 1 and 2 show a breaking down of the budget for personnel and for research for the three years 2000, 2001, and 2002.

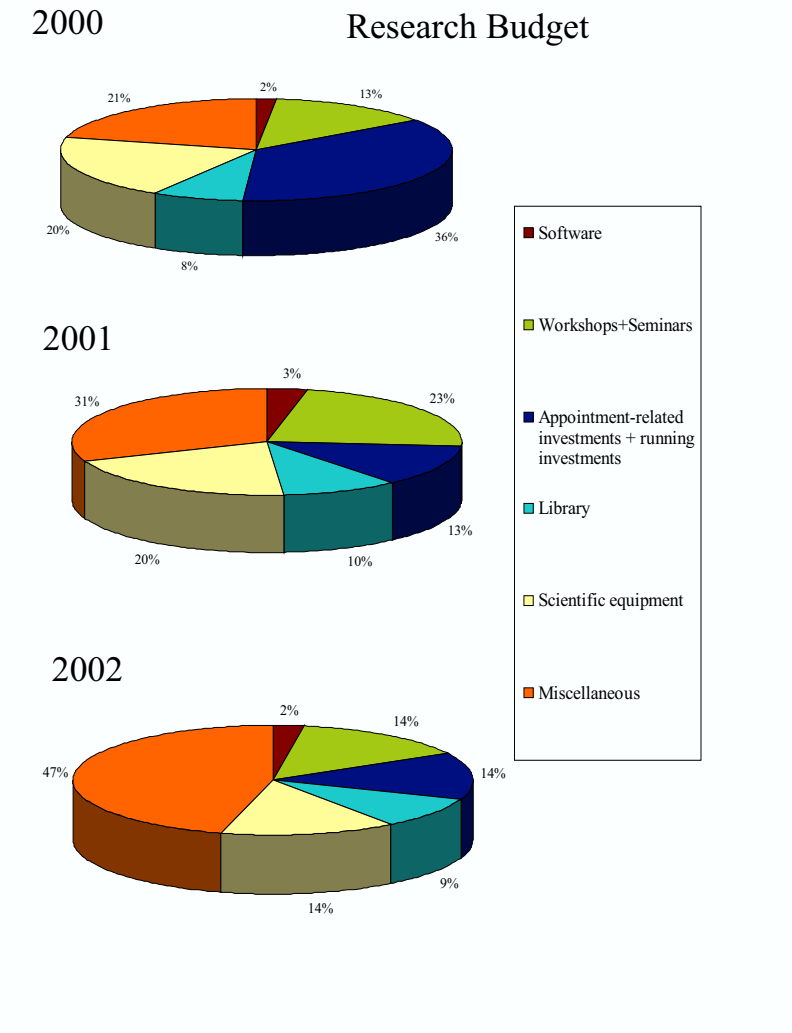

Figure 1: *Research budgets during the past three years*

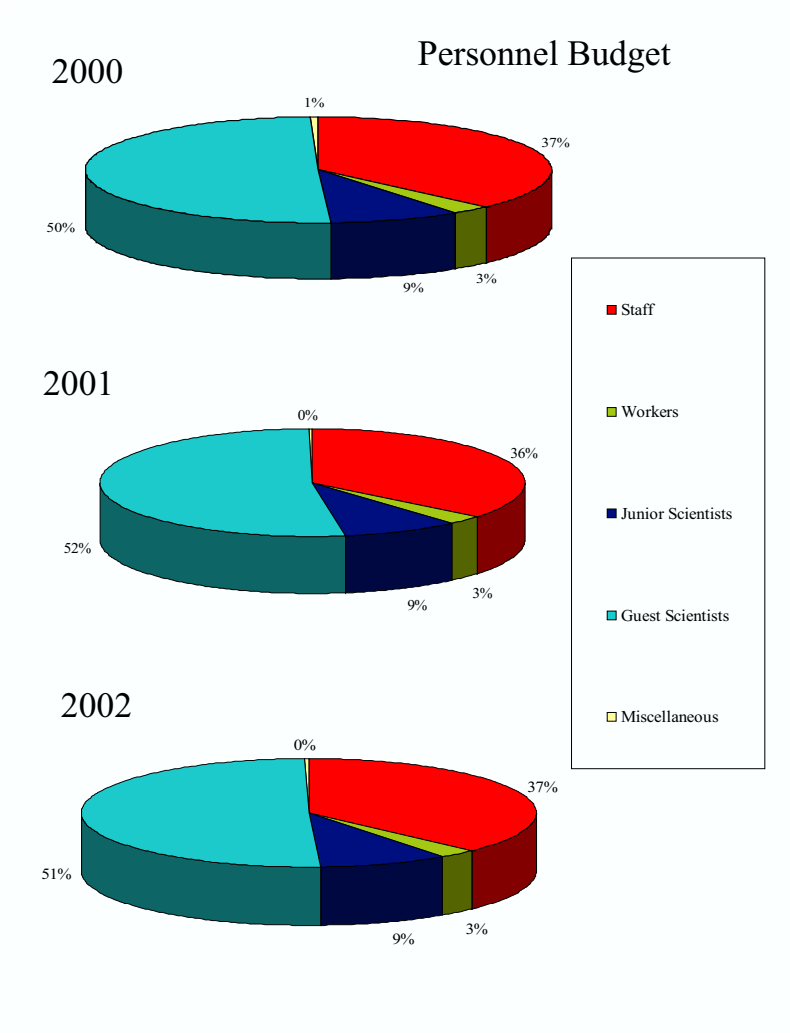

Figure 2: *Budgets for personnel*

8 Equipment und premises

8.1 Computer Facilities

The computer requirements in our institute are mainly characterised by a very high demand for computing power and relatively moderate requests for graphics. 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 160 computers with a total of 240 CPU's. The computers offer from one to four CPU's and a maximum of 32 Gigabytes of main memory and three Terabytes of local disk space. We use both ATM (LAN emulation) and Fast Ethernet as a local area network interconnect. In order to maximize the computational throughput in our computing cluster, we run a network queueing system which achieves an overall average utilization of more than 90 % of the available CPU time. 2002 was the first year to see an inhomogeneous unix cluster in our institute. This was caused by the fact that standard PC hardware has developed quickly and delivers CPU speeds near or beyond the performance of high-end servers and workstations at a fraction of the price. As a consequence we introduced a first cluster with 20 2-processor AMD servers running a Linux operating system. By the end of 2002 we even decided to give away our 16 processor server in favor of a Linux based PC cluster that will deliver several times the cpu performance of that server.
Besides the unix cluster there are about 20 PC's at our institute, running a Windows operating system, mainly for office applications. We also offer about 20 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 Terminal server 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 34 MBit/s which we share with our neighboring institute.

The computer department is run by three employees with their respective main tasks being unix and networks, web and windows and hardware. Smaller to medium programming tasks are done by our staff and a student who is working part-time in the computer department. Larger programming tasks have to be given to external companies.

Future

In the near future we are planning to introduce more Linux based PC's. This will allow us to probably double the available computing power in 2003 as expressed in the available MFlop rate. There are plans to introduce Linux on 64 Bit PC processors

(either from AMD or Intel) as they become available in 2003 which will allow for an addressable memory space of more than 2 GByte with relatively cheap hardware. By 2005 we will have to decide which way to go with our main servers. If Linux has become mature it will be tempting to leave the proprietary operating system - Tru64 Unix from HP (formerly Compaq, formerly Digital) right now - in order to become independent from hardware vendors and still have the option to run the same flavor of operating system on the entire 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 interconnecting 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. 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

8.2 Library

The library collection is primarily intended to support research within the institute but it can also be used by visitors from outside the institute. The library is permanently accessible for members of the institute including guests, and can be used by the public from Monday to Friday 8:00 am. to 4:30 pm.

Located on the ground floor and in the basement of the institute the library offers eight reading desks and a special corner with armchairs for discussion and studies of the several daily national and international newspapers as well as some magazines.

The journal volumes are arranged in the shelves in alphabetical order. The older volumes (before 1980) are stored in the basement. The most recent issues can be found in special boxes. The monographs are arranged in systematical order (Regensburger Systematik). Furthermore, a computer is available for searching the online catalogue. Via the homepage of the institute up-to-date electronical access to journals, databases and information of the services of the Max-Planck-Society are offered.

At the moment the library has about 2712 monographs (2000: 2287 ; 2001: 2511 ; 2002: 2712) and 78 journals (2000: 69 ; 2001: 78; 2002: 78).

Books or references, which are not available in the library can be ordered through inter-library lending (data from last years: 2000: 749; 2001: 909; 2002: 734)

The library management system Bibliotheca of the B.O.N.D.GmbH has now been used for four years. Users can borrow literature themselves with the automatic lending system of the Sensormatic GmbH, which was installed four years ago and has been working successfully.

There are two special photocopying machines available for books and journals only. A scanner is also part of the equipment.

The library committee discusses in quarterly meetings new developments.

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 offers three guest houses with different apartment types for up to 42 guests.

Guest House no. 1 comprises 20 single and 5 double rooms (with two separated bedrooms and a telephone. Some of them have 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 no. 2 offers ten apartments with kitchen for up to two persons and three large ones with two bedrooms, a living room, bathroom and kitchen for up to three persons (e.g. families). All apartments have TV connection ports and telephones, some of them have a balcony. In the basement of guest house no. 2 two washing machines and two tumble dryers are available. They are accessible from all three guest houses.

Guest House no. 3 allows to accommodate guests in four large apartments similar to the ones from guest house no. 2. They are situated on the second floor, the apartments on the first floor have been transformed into offices. Like in the other two guest houses, guest house no. 3 offers TV connection ports, telephones and partly 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 extra beds, cots and TV sets.

9 Committees

9.1 Scientific Advisory Board

According to the statutes of the Max Planck Society the mpipks 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:

Aharony, A. Professor Dr.	School of Physics & Astronomy Tel Aviv University, Tel Aviv 69978 Israel
Bensimon, D. Professor Dr.	Laboratoire de Physique Statistique Ecole Normale Superieure 24, rue Lhomond, 75231 Paris cedex 05 France
Efetov, K. Professor Dr.	Institut für Theoretische Physik III Ruhr-Universität Bochum Universitätsstraße 150, 44801 Bochum
Eschrig, H. Professor Dr.	Institut für Festkörper- und Werkstoffforschung Dresden e.V. Helmholtzstraße 20, 01069 Dresden
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
Lhuillier, C., J. C. Professor Dr.	Physique Théoretique des Liquides Université Pierre & Marie Curie 4, Place Jussieu, 75252 Paris Cedex 05 France

Peyerimhoff, S. D.
Professor Dr.
Lehrstuhl für Theoretische Chemie
Universität Bonn
Wegelerstraße 12, 53115 Bonn

Pietronero, L.
Professor Dr.
Dipartimento di Fisica
Universita degli Studi di Roma
La Sapienza
Piazzale Aldo Moro 2, 00185 Roma
Italy

Stark, J.
Professor Dr.
Department of Mathematics
University College London
Gower Street, WC1E 6BT, London
United Kingdom

Wegner, F.
Professor Dr.
Institut für Theortische Physik
Universität Heidelberg
Philosophenweg 19, 69120 Heidelberg

9.2 Board of Trustees

In accord with the statutes of the Max Planck Society the mpipks 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 mpipks 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 2006):

Birgel, D.	Chefredakteur Dresdner Neueste Nachrichten Hauptstrasse 21, 01097 Dresden
Eschelbacher, H. C. Dr.-Ing.	Ministerialdirigent im Bundesministerium für Bildung, Wissenschaft, Forschung u. Technologie Heinemannstraße 2, 53175 Bonn
Freiesleben, H. Professor Dr.	Fachrichtung Physik Technische Universität Dresden Zellescher Weg 16, 01062 Dresden
Harter, J. Dr.	Geschäftsführer Infineon Technologies Dresden GmbH & Co.OHG Königsbrücker Str. 180, 01099 Dresden
Junker, F. Dr.	Mitglied des Vorstandes König & Bauer AG Friedrich-List-Str. 47-49, 01445 Radebeul
Mehlhorn, A. Professor Dr.	Rektor der Technischen Universität Dresden Mommsenstraße 13, 01069 Dresden
Müller, H. Dr.	Mitglied des Vorstandes Dresdner Bank AG Jürgen-Ponto-Platz 1, 60329 Frankfurt/M
Rößler, M. Dr.	Sächsischer Staatsminister für Wissenschaft und Kunst Wigardstrasse 17, 01097 Dresden
Schmidt, J. Dr.	MdB a.D. Straße der Jugend 40, 09633 Halsbrücke

Tschira, K. Dr.	Geschäftsführender Gesellschafter Klaus Tschira Stiftung gGmbH Schloss Wolfsbrunnenweg 33, 69118 Heidelberg
Wagner, H. Dr.	Oberbürgermeister a.D. Wachauer Strasse 8, 01067 Dresden

10 Members of the MPI for the Physics of Complex Systems

(as of December 2002)

1. mpi**pks positions** — **38**

   1.1 Scientific personnel
   - Scientific members: 3
   - Research staff (including four junior research groups): 17

   1.2 Technical staff: 5

   1.3 Administration and infrastructure staff: 13

2. **Externally funded research staff** — **4**

3. **PhD students** — **27**

   3.1 German PhD students (MPG funding): 21

   3.2 Foreign PhD students (MPG funding): 3

   3.3 PhD students (external funding): 3

4. **Guest scientists** — **56**

   4.1 German guest scientists: 19

   4.2 Foreign guest scientists (MPG funding): 37

The research positions are generally limited in time. Only *Prof. H. Kantz*, head of the group "Time Series Analysis" is employed on a permanent C3 position. Furthermore, *Priv. Doz. Dr. S. Flach*, head of the Visitors and Workshop Program, is a permanent staff member of the scientific service with a BATIb position.

11 Publication list 2000-2002

11.1 Publications 2000

Abdurahman, A., A. Shukla and M. Dolg: Ab initio treatment of electron correlations in polymers: Lithium hydride chain and beryllium hydride polymer. Journal of Chemical Physics **112**, 4801 – 4805 (2000).

– Correlated ground-state ab initio calculations of polymethineimine. Chemical Physics **257**, 301 – 310 (2000).

Abel, M., L. Biferale, M. Cencini, M. Falcioni, D. Vergni and A. Vulpiani: Exit-times and [454]-entropy for dynamical systems, stochastic processes, and turbulence. Physica D **147**, 12 – 35 (2000).

Ahn, K.H. and P. Fulde: Parity effects in stacked nanoscopic quantum rings. Physical Review B **62**, R4813 – R4816 (2000).

Ahn, K.H. and K. Richter: Coulomb-blockade peak spacing fluctuations in chaotic quantum dots. Physica E **6**, 388 – 391 (2000).

Albrecht, M., P. Fulde and H. Stoll: An ab initio estimate of correlation effects on the band gap of covalent semiconductors: diamond and silicon. Chemical Physics Letters **319**, 355 – 362 (2000).

Alexeeva. N.V., I.V. Barashenkov and G.P. Tsironis: Impurity-induced stabilization of solitons in arrays of parametrically driven nonlinear oscillators. Physical Review Letters **84**, 3053 – 3056 (2000).

Amici, A. and P. Thalmeier: Theoretical model for superconductivity in magnetic borocarbides. Journal of Low Temperature Physics **117**, 1641 – 1645 (2000).

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Bär, M., M. Falcke, H. Levine and L.S. Tsimring: Discrete stochastic modeling of calcium channel dynamics. Physical Review Letters **84**, 5664 – 5667 (2000).

Bär, M., A. Hagberg, E. Meron and U. Thiele: Front propagation and pattern formation in anisotropic bistable media. Physical Review E **62**, 366 – 374 (2000).

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Bhattacharya, J. and P.P. Kanjilal: Revisiting the role of correlation coefficient to distinguish chaos from noise. European Physical Journal B **13**, 399 – 403 (2000).

Bhattacharya, J.P, P.P.Kanjilal and S.H. Nizamie: Decomposition of posterior alpha rhythm. IEEE Transactions on Biomedical Engineering **47**, 739 - 747 (2000).

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