Vorwort

Im November 1992 beschloß der Senat der Max-Planck-Gesellschaft die Gründung eines Max-Planck-Instituts für Physik komplexer Systeme in den neuen Bundesländern. Aufgrund des günstigen wissenschaftlichen Umfelds und der insgesamt guten Verkehrsanbindung wurde Dresden als Standort ausgewählt. Das Institut nahm im Juli 1993 mit Prof. Dr. Peter Fulde als Gründungsdirektor seine Arbeit zunächst in Stuttgart auf, da anfangs in Dresden entsprechende Räumlichkeiten nicht zur Verfügung standen. Im Januar 1994 begann die Arbeit in Dresden, wofür die TU Dresden dankenswerter Weise ein Provisorium in der Bayreuther Straße in unmittelbarer Nähe zur Universität zur Verfügung gestellt hatte. Die Institutseinweihung erfolgte am 2. Mai 1994 durch den Präsidenten der Max-Planck-Gesellschaft, Prof. Dr. H. Zacher. Der eingeladene Architektenwettbewerb für das neue Institutsgebäude war vom Architekturbüro Brenner und Partner mit J. Wittfoht gewonnen worden, so dass mit den Bauarbeiten im September 1995 begonnen werden konnte. Nach knapp zweijähriger Bauzeit wurde im Juli 1997 das neue Gebäude zusammen mit drei Gästehäusern dem Institut übergeben. Im Jahr 1998 erfolgte die Berufung von Prof. Dr. J.- M. Rost zum Direktor am Institut. Inzwischen haben zahlreiche Gäste aus dem In- und Ausland das Institut besucht.

Dresden, im März 2000

Preface

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 location in the new federal states (neue Bundesländer). Dresden was chosen because of an adequate scientific surroundings and reasonable traffic connections.

The institute started its activities in July 1993 in Stuttgart with Prof. Dr. Peter Fulde as its Founding Director (there was still a lack of proper office space in Dresden). The work in Dresden started in January 1994 at a temporary site generously offered by the Technische Universität Dresden. The location - Bayreuther Straße - was very close to the university campus. The official inauguration ceremony took place on May 2nd, 1994 under the presidency of Prof. Dr. H. Zacher.

The competition for the design of the new institute building was won by J. Wittfoht from the architectural firm Brenner und Partner. The construction work started in September 1995. After a construction period of two years the new building and the three guest houses were handed over to the institute in July 1997.

Prof. Dr. Jan-Michael Rost was appointed as a Director of the institute in 1998. In the mean time we have had a large number of guests from Germany and abroad who visited the institute.

Dresden, March 2000

Institutsstruktur

Die Struktur des Instituts weicht stark von derjenigen der meisten Max-Planck-Institute ab und ist am ehesten mit der des Max-Planck-Instituts für Mathematik in Bonn zu vergleichen. Die Grundidee ist, mit Hilfe eines großen Gästeprogramms den wissenschaftlichen Nachwuchs zu fördern und gleichzeitig zur Entwicklung der theoretischen Physik auf dem breiten Gebiet der komplexen Systeme beizutragen. Mit Hilfe eines umfangreichen Programms von Workshops und Seminaren, deren typische Dauer einige Wochen beträgt, soll der Nachwuchs der Universitäten mit neuen Entwicklungen auf dem Gebiet der komplexen Systeme früher als bisher bekannt gemacht werden. Dabei besteht die Hoffnung, dass diese Neuentwicklungen aufgegriffen werden und dass auf diese Weise zu deren Weiterentwicklung beigetragen wird. Für das Gästeprogramm ist Dr. S. Flach verantwortlich. Das Institut hat 17 Wissenschaftlerstellen, die sich auf insgesamt drei Abteilungen verteilen werden. Die Zahl der Wissenschaftler mit einem permanenten Vertrag beträgt gegenwärtig 4 unter Einschluß der Abteilungsleiter. Von den vorgesehenen drei Abteilungen existieren bisher zwei, nämlich die Abteilungen:

- **Elektronische Korrelationen in Molekülen und Festkörpern (Prof. Dr. P. Fulde)**
- **Endliche Systeme (Prof. Dr. J.- M. Rost)**

Die dritte Abteilung befindet sich noch im Stadium der Planung. Neben den Abteilungen tragen zum wissenschaftliche Programm insbesondere die Gastwissenschaftlern bei, von denen zu jedem Zeitpunkt zwischen 60 bis 70 am Institut beschäftigt sind. Die Aufenthaltsdauer von Gästen am Institut ist auf maximal zwei Jahre beschränkt.
Um die Institutsarbeit wissenschaftlich auf eine breitere Basis zu stellen und auch um das Gästeprogramm mehr zu strukturieren, hat das Institut frühzeitig mit Unterstützung des Präsidenten der MPG eine Reihe von Nachwuchs- und Arbeitsgruppen gegründet. Nachwuchsgruppen sind auf 5 Jahre eingerichtet. Ihr Programm ist von dem der Abteilungen sehr verschieden. Bei Beginn der Arbeiten darf der Leiter solch einer Gruppe höchstens 35 Jahre alt sein. Das Programm der Arbeitsgruppen steht dagegen im unmittelbaren Zusammenhang mit der Arbeit der Abteilungen, bzw. der Leiter der Gruppe ist einer Altersbeschränkung nicht unterworfen. Jede der Gruppen setzt sich zusammen aus dem Leiter, einem Mitarbeiter, 1 bis 2 Doktoranden und einem Gast. In Wahrheit sind die Gruppen jedoch größer, da sich gewöhnlich Gäste aus dem Gästeprogramm diesen anschließen.

Gegenwärtig gibt es folgende Nachwuchsgruppen:

- **Quantenchaos und Mesoskopische Systeme (Dr. K. Richter)**
- **Musterbildungen in Reaktions- und Diffusionsprozessen (Dr. M. Bär)**

sowie Arbeitsgruppen:

- **Nichtlineare Zeitreihenanalyse**
  (Dr. H. Kantz)
- **Nichtlineare Dynamik in Quantensystemen**
  (Dr. A. Buchleitner)
- **Quantenchemie**
  (Dr. U. Birkenheuer).

Die Gruppe Quantenchemie wird gegenwärtig neu aufgebaut, da deren früherer Leiter Dr. M. Dolg einen Ruf an die Universität Bonn erhielt. Es sei an dieser Stelle explizit betont, dass das Institut große Anstrengungen unternimmt, nicht in verschiedene Abteilungen und Gruppen zu zerfallen. Obwohl eine innere Institutsstruktur als notwendig angesehen wird, so wird der Kommunikation und Zusammenarbeit zwischen den Wissenschaftlern, unabhängig von ihrer formellen Gruppenzugehörigkeit, großes Gewicht beigemessen.

Structure of the institute

The structure of the institute is quite different from the majority of Max Planck institutes and can be best compared to the one of the Max Planck Institute for Mathematics in Bonn. The basic idea is to provide an optimal environment for young members of the scientific community and to contribute to the progress of theoretical physics in the broad field of complex systems with the help of a large scale Guest Program. Workshops and seminars with typical duration of several weeks each introduce in new topics and developments in the field of complex systems, faster and more efficient than before, to the scientific offsprings. The intention is that these new topics will be picked up and carried on, contributing to their further development. Dr. S. Flach is responsible for the Guest Program. The institute has 17 scientific staff positions for three departments. There are currently 4 scientists under permanent contract (including the directors). Of the three planned divisions two are already working, namely:

- **Electronic correlations in molecules and solids**
  (Prof. Dr. P. Fulde)
- **Finite systems**
  (Prof. Dr. J.-M. Rost)

The third division is in the stage of planning. The scientific work of the divisions is complemented by the scientific program of the guest scientists. Their number ranges from 60 to 70 at any time. The period of stay of a guest scientist is limited to a maximum of two years.

In order to put the scientific work of the institute on broad basis and in order to structure the Guest Program, the institute has founded several Junior Research Groups and Research Groups with the support of the president of the MPG. Both types of groups are set up for a period of 5 years each. The program of the Groups differs substantially from the research topics of the divisions. The head of a Junior Research Group should be not older than 35 years at the beginning of the groupś work. The research program of the Research Groups is related to the one of the corresponding division, and there are no restrictions concerning the age of the head of the group. Each group consists of a head, one staff member, a few PhD students and one guest. In reality the group size can be considerably larger, because visitors from the Guest Program may join.

Currently there exist the following Junior Research Groups:

- **Quantum Chaos and Mesoscopic Systems**
  (Dr. K. Richter)
- **Pattern Formation in Reaction-Diffusion Processes**
  (Dr. M. Bär)

and the Research Groups

- **Nonlinear Time Series Analysis**
  (Dr. H. Kantz)

- **Nonlinear dynamics in quantum systems**
  (Dr. A. Buchleitner)

- **Quantum Chemistry**
  (Dr. U. Birkenheuer)

The Quantum Chemistry group is currently in the process of reinstallation, since its former head Dr. M. Dolg accepted an offer from the Universität Bonn. It should be stressed explicitely here that the institute's policy is directed against a desintegration into different noninteracting divisions and groups. Although a certain internal structure is necessary, very important ingredients to conduct high-quality research are communication and collaboration between scientists, regardless of their formal group affiliation.

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Wissenschaftliche Tätigkeit am Max-Planck-Institut für Physik komplexer Systeme

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

Eine Beschreibung elektronischer Korrelationen erfordert Methoden die über die Einelektronnäherung oder die Hartree-Fock-Näherung hinausgehen. Falls die entsprechende Vielteilchenwellenfunktion untersucht werden soll, entfällt der Dichtefunktionalzugang. An seiner Stelle werden quantenchemische Methoden benötigt. Letztere müssen entsprechend verändert werden, um auf Festkörper, also unendliche räumlich periodische Systeme, anwendbar zu sein [1]. Bislang haben wir die Grundzustandswellenfunktion und -energie mit hoher Genauigkeit für eine Reihe von Festkörpern berechnet. In Zukunft werden wir uns entsprechenden Berechnungen von Energiebändern zuwenden. Dies verlangt eine enge Zusammenarbeit mit der Quantenchemiegruppe. Wir haben stark korrelierte Elektronensysteme mit vereinfachten Modellen beschrieben. Dieser Zugang diente z.B. der Untersuchung von Phänomenen wie der Ordnung von elektronischen Ladungen. Als Teilnehmer am Sonderforschungsbereich an der TU Dresden untersuchen wir das Zusammenspiel zwischen Supraleitung und Magnetismus (siehe Beitrag "Theoretical Model for the Superconducting and Magnetically Ordered Borocarbides", Seite 87). Kürzlich begannen wir mit Arbeiten zu Gläsern bei sehr tiefen Temperaturen (1-10 mK). In diesem Bereich werden starke Einflüsse von Magnetfeldern beobachtet, die wir phenomenologisch erklären konnten (siehe Beitrag "Mesoscopic quantum effects in cold glasses", Seite 85). Wir haben Quanteneffekte auf mesoskopischen Skalen identifiziert. Hier werden in Zukunft detailliertere Untersuchungen durchgeführt.

Andere untersuchte Themen sind z.B. Systeme mit großen Spins, nichtlineare Gitter, Breather etc.

[1] P. Fulde, Electron Correlations in Molecules and Solids
(3-rd ed. Springer Heidelberg, 1995)

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

Nichtlineare dynamische Systeme zeigen eine Vielfalt von komplexem Verhalten, wobei sogenanntes deterministisches Chaos einer der faszinierensten Aspekte ist.

Wir widmen einen großen Teil unserer wissenschaftlichen Arbeit ausgewählten, offenen Problemen im Verständnis von Nichtlinearität, wie beispielsweise der Wechselwirkung von Chaos und Rauschen, dem Übergang von deterministischem Chaos zu Zufall (siehe dazu den Beitrag "From a coupled map lattice to the Ising model", Seite 41), hochdimensionalem Chaos und der Dynamik von Systemen mit zeitverzögerter Rückkopplung.

Wenn eine im Laborexperiment oder in Feldmessungen gewonnene Zeitreihe komplexes, aperiodisches Zeitverhalten zeigt, so kann man spekulieren, ob dieses konkrete Signal durch ein relativ einfaches, deterministisches chaotisches System modelliert werden kann. Dieser inverse Ansatz wird seit dem Anfang der 80er Jahre verfolgt. Heutzutage besteht kaum Zweifel, dass die allermeisten interessanten Signale unserer Umwelt nicht niedrig-dimensional chaotischer Natur sind. Deshalb wird an Verallgemeinerungen gearbeitet, die Methoden der nichtlinearen Zeitreihenanalyse für größere Systemklassen anwendbar zu machen. Besondere Erfolge der letzen 2 Jahre wurden bei der Behandlung von Nichtstationarität und räumlich ausgedehnten Systemen erzielt (siehe Beitrag "Local estimates for entropy densities in coupled map lattices, Seite 45), wobei am Beispiel der Rauschunterdrückung für Sprache (siehe Beitrag "Denoising human speech signals using chaos-like features", Seite 35) die Möglichkeiten erkennbar sind.

Hand in Hand mit der Methodenentwicklung geht deren Anwendung in einer Vielzahl von Projekten, die teilweise in Zusammenarbeit mit experimentellen Gruppen, mit Industriepartnern oder mit Drittmitteln durchgeführt werden.

Auch in Zukunft werden die beiden Hauptrichtungen, nämlich Verbesserung des Verständnisses kompexen dynamischen Verhaltens und seiner Ursachen (in Zukunft stärker in Richtung auf statistische Physik) und die Methodenentwicklung und Methodenvergleiche in der Zeitreihenanalyse, weiterverfolgt. Wichtige neue Fragestellungen werden dabei sein:

(A) Statistische Aussagen über dynamische Systeme bei unscharfen Parametern.
(B) Dynamische Systeme mit vielen Freiheitsgraden.
(C) Zeitreihenanalyse für nichtlineare stochastische Prozesse.
(D) Meta-Dynamik im Parameterraum und ihre Rekonstruktion.
(E) Analyse von zeitlich veränderlichen Mustern.

Arbeitsgruppe: Quantenchemie
(Leiter: Dr. M. Dolg (bis 30. 9. 1999))

Die Arbeitsgruppe 'Quantenchemie' beschäftigte sich in den Jahren 1998 und 1999 mit der quantitativen *ab initio* Berechnung der Eigenschaften von Atomen, Molekülen, Clustern, Polymeren und Festkörpern. Die möglichst genaue Einbeziehung der wichtigsten Beiträge der Relativistik und der Elektronenkorrelation sowie die Interpretation der Bindungsverhältnisse standen hierbei im Mittelpunkt der Arbeiten.

Ein Schwerpunkt der Arbeiten war die Erweiterung der für Atome und Moleküle sehr erfolgreichen quantenchemischen *ab initio* Methoden auf unendliche Systeme, d.h. Polymere und Festkörper. Mit den ersten *full-CI*-Rechnungen an dem Modellsystem einer LiH-Kette und am dreidimensionalen LiH-Festkörper wurde dieses Ziel für Grundzustände nichtleitender Systeme erreicht. Coupled Cluster Rechnungen mit Einfach- und Doppelanregungen (CCSD) an komplizierteren Systemen sowie die Berücksichtigung von relativistischen Beiträgen einschließlich der Spin-Bahn-Wechselwirkung sind in Vorbereitung. Korrelationskorrekturen zu Bandstrukturen konnten von 2. Ordnung Störungstheorie (MP2) für Polymere auf dem Niveau durchgeführt werden.

Ein weiteres Arbeitsgebiet war die *ab initio* Berechnung der Struktur, Stabilität sowie anderer größenabhängiger Eigenschaften wie Ionisierungspotentialen und Elektronenaffinitäten von Clustern der Gruppen 2 und 12 sowie von Yb. Hierbei wurde, u.a. mit Hilfe von Ladungsfluktuationen und der Elektronenlokalisierungsfunktion, der Übergang von der Van der Waals Wechselwirkung in kleinen Systemen zur kovalenten Bindung in mittelgroßen Systemen studiert. Ein neues Hybridmodell für die Cluster von Quecksilber erlaubte dabei sehr genaue Untersuchungen von Systemen bis zu 55 Atomen. Neben relativistischen Pseudopotentialen, Rumpfpolarisationspotentialen und quantenchemischen Standardkorrelationsverfahren kam hier auch die Quanten-Monte-Carlo-Methode zum Einsatz.

Zahlreiche Untersuchungen beschäftigten sich mit Verbindungen der Lanthanoiden und Actinoiden, z.B. den Sandwichkomplexen mit Benzol und Cyclooctatetraen. Hierbei wurde neben in der Gruppe entwickelten relativistischen Pseudopotentialen und quantenchemischen Standardkorrelationsverfahren auch eigene auf dem *Dirac-Coulomb*-Hamiltonoperator sowie der *Zeroth-Order Regular Approximation* beruhende Dichtefunktionalprogramme eingesetzt.

Arbeitsgruppe: Quantenchemie
(Leiter: Dr. U. Birkenheuer (ab 1.3.2000))

Erklärtes Ziel der neuen Arbeitsgruppe 'Quantenchemie' ist die Berechnung korrelierter elektronischer Zustände (Grundzustand wie auch angeregte Zustände: Valenzbandlöcher, Leitungsbandelektronen) in periodischen Systemen auf der Basis quantenchemischer POST-SCF-Verfahren. Dieser wellenfunktionsbasierte Ansatz wird bewusst als Alternative zu den in der Festkörperphysik weit verbreiteten Dichtefunktionalmethoden angesehen. Er erlaubt es, detailliert und in kontrollierter Weise Ein-

blick in die Korrelationseffekte ausgedehnter Systeme zu erhalten wie er mit Dichtefunktionaltheorie nie zu errreichen ist.

Die vielversprechenden Vorarbeiten der Arbeitsgruppe in diese Richtung aufgreifend, sollen die entwickelte Methodik (Inkrementmethode) und das vorhandene Programmpaket (Wannier-Programm) so ausgebaut werden, dass damit korrelierte $N + 1$ und $N - 1$-Teilchenzustände in Festkörpern und Polymeren (Bänder) berechnet und so schlußendlich die Anregungspektren dieser Systeme bestimmt werden können.

Zu diesem Zweck muß das Wannier-Programm um die Möglichkeit des Einbezugs von Basisfunktionen zu höheren Drehimpulsen erweitert werden. Zur Reduktion des zu erwartenden hohen Rechenaufwandes ist eine Optimierung des Integralpakets durch Ausnutzung von Symmetrie und effizienter Integralabschätzungen vorgesehen. Einen weiteren wichtigen Fortschritt in der Bewältigung der Orthogonalitätsschwänze der Wannier-Funktionen verspricht der Übergang zu nicht-orthogonalen Orbitalgruppen in der Inkrementmethode. Ferner müssen die zu verwendenden CI-Programme (MOLPRO und/oder Turbomol) um die Möglichkeit des Einbezugs der Kristallumgebungseffekte (Coulombfeld, Austauschbeiträge und Lokalisierungspotentiale) erweitert werden. Absprachen in diese Richtung sind im Gange. Desweiteren soll evaluiert werden, in welchem Umfang auch eine Lokalisierung der virtuellen Orbitale für die Behandlung von Leitungsbandelelektronen bzw. Valenzbandlöchern notwendig wird; ggf. müssen geeignete Lokalisierungsverfahren erarbeitet bzw. getestet werden.

Klassische *ab initio* und DF-Rechnungen an periodischen und endlichen Systemen sollen, wie in der Vergangenheit auch, das Arbeitsgebiet abrunden.

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

Unser Name "Endliche Systeme" bringt das Interesse für solche Vorgänge zum Ausdruck, die typischerweise und im Gegensatz zur Festkörperphysik mit endlich vielen Freiheitsgraden zu tun haben. Dies beinhaltet die Anregung und Fragmentation von Atomen, Molekülen und Clustern. Ein Schwerpunkt der derzeitigen Arbeit liegt auf der Wechselwirkung dieser Systeme mit intensivem Laserlicht (siehe Beitrag "Irregular orbits generate higher harmonics", Seite 66). Unsere theoretischen Mittel der Beschreibung reichen von traditionell quantenchemischen Methoden über neuartige semiklassische Zugänge (siehe Beitrag "Threshold detachment by tunneling", Seite 63) bis hin zu klassischen Konzepten nichtlinearer Dynamik, wobei chaotische Phänomene eine wichtige Rolle spielen. Unter anderem ihnen widmet sich eine eigene Arbeitsgruppe "Nichtlineare Dynamik in Quantensystemen" unter der Leitung von Dr. Andreas Buchleitner.
Ein wesentliches Merkmal unserer Arbeit ist die Nähe zum Experiment. Dank innovativer Laser- und Detektortechnologie ist es möglich, Theorie und Experiment einem fruchtbaren, direkten und kritischen Vergleich auszusetzen [1]. Einen Schwerpunkt der Kooperation mit dem Experiment wird in Zukunft die Suche nach sinnvollen Fragestellungen bilden, die die extreme Datenfülle heutiger Experimente sinnvoll interpretieren und kanalisieren können. Wir hoffen hierbei paradigmatisch Wege zu einem erfolgversprechenden Umgang mit komplexen Systemen aufzuzeigen.
Zukünftige Forschungsarbeiten zielen besonders auf:

(A) die Wechselwirkung atomarer/molekularer Systeme mit intensiven Feldern, mit dem Schwerpunkt dynamische Korrelationseffekte,

(B) die Dynamik von Fragmentation und Anregung in atomaren und metallischen Clustern,

(C) die Suche nach globalen und dennoch sensitiven Größen zur Charakterisierung von Systemen mit endlich vielen Freiheitsgraden,

(D) Methodenentwicklung:

  (D1) genaue semiklassische Methoden zum Verständnis und zur Interpretation dynamischen Verhaltens (besonders relevant für (A)),

  (D2) Formulierung und Implementierung einer gemischten quanten-klassischen Beschreibung für eine explizite dynamische Beschreibung von 10-100 Teilchen (relevant für (B))

[1] The Theory of Two-Electron Atoms: "From the Ground State to Complete Fragmentation" G. Tanner, K. Richter and J.-M. Rost; Rev. Mod. Phys., in press (2000)

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

"Nichtlineare Dynamik in Quantensystemen" bezeichnet das Anliegen, Konzepte der nichtlinearen Dynamik in berechenbaren und experimentell zugänglichen Quantensystemen zu verwirklichen. Hinsichtlich der experimentellen Umsetzung zielen wir dabei vorwiegend auf einfache atomare Systeme, die in modernen quantenoptischen Experimenten präzise kontrollierbar sind. Im Rahmen einer Doktorarbeit über magnetische Billiards (K. Hornberger) ergibt sich jedoch auch ein gewisser Überlapp mit Nanostrukturen.

Einen wesentlichen Schwerpunkt unserer Arbeit bildet die möglichst näherungsfreie (vulgo: *"ab initio"*) quantenmechanische Beschreibung niedrigdimensionaler atomarer Systeme unter dem Einfluß elektromagnetischer Strahlung. Nachdem die numerische Simulation der klassischen und Quantendynamik des Wasserstoffatoms unter periodischem Antrieb inzwischen vollständig beherrscht ist, gilt unser Augenmerk derzeit insbesondere der Quantendynamik von Alkali-Rydbergatomen (siehe Beitrag "Residual symmetries in the spectrum of periodically driven alkali Rydberg states", Seite 69) und des Dreikörper-Coulombproblems (zusammen mit P. Schlagheck, Orsay) in einem oszillierenden Feld. Die typische Dimension des quantenmechanischen Eigenwertproblems erforderte die Entwicklung eines vollständig parallelisierten numerischen Diagonalisierungscodes (in Zusammenarbeit mit D. Delande, Paris, und K. Taylor, Belfast), der im Rahmen einer Doktorarbeit (A. Krug) derzeit für die erste präzise theoretische Behandlung des Ionisationsverhaltens von Alkali-Rydberatomen in Mikrowellenfeldern eingesetzt wird. Mit Hilfe der massiv parallelen Architektur der CRAY T3E des Rechenzentrums Garching der MPG sind wir erstmals in der Lage, Laborexperimente mit den exakten experimentellen Parametern (Rydbergquantenzahlen im Bereich 50 bis 80) numerisch nachzuvollziehen.

Neben der exakten numerischen Behandlung rangiert gleichrangig die physikalische Interpretation der gewonnenen (großen) Datensätze im Kontext von klassisch-quantenmechanischer Korrespondenz und klassisch chaotischer und/oder komplexer Dynamik. Aktueller Schwerpunkt ist hier eine Analogie des atomaren Ionisationsprozesses mit elektronischem Transport durch ungeordnete Festkörper. Das (in Zusammenarbeit mit I. Guarneri, Como, und J. Zakrzewski, Krakòw) eingeführte Konzept eines "atomaren Leitwerts" wird derzeit im Rahmen einer Diplomarbeit (S. Wimberger) hinsichtlich der Tragweite der Analogie Atom/Festkörper untersucht. Die grundlegende Fragestellung nach der Rolle quantenmechanischer Kohärenz bei der Propagation unter komplexer Dynamik motiviert ebenfalls eine im Rahmen einer binationalen Promotion (zusammen mit C. Miniatura, Nizza) betreute Doktorarbeit über kohärente Rückstreuung an kalten Atomen (C. Müller), d.h. an quantenmechanischen Streuern mit internen Freiheitsgraden.

Zweiter Schwerpunkt unserer Arbeit ist die Sensitivität kohärenter quantenmechanischer Entwicklung bezüglich der Kopplung an eine verrauschte Umgebung. Aktuelle Schwerpunkte sind der Einfluß von Rauschen auf den atomaren Anregungs- und Ionisationsprozeß (K. Hornberger), sowie die Nutzbarkeit rauschinduzierter Stabilisierungsphänomene (in Zusammenarbeit mit R. N. Mantegna, Palermo, und M. Kùs, Warschau) auf mikroskopischer Skala. Hier ist es uns unlängst gelungen (siehe Beitrag

"Stochastic resonance in the coherence of a quantum system", Seite 74), stochastische Resonanz in den *Kohärenzen* eines Zweiniveauatoms in kohärenter Wechselwirkung mit einer quantisierten Feldmode nachzuweisen. Die Arbeiten über stochastische Resonanz motivierten überdies ein neues Projekt (zusammen mit B. Kümmerer, Stuttgart) zur effizienten Präparation eines beliebigen Quantenzustandes (Doktorarbeit T. Wellens).

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

Unsere Gruppe hat ihre Arbeit im November 1995 aufgenommen. Die momentane Grösse der Gruppe von ca. 10 Mitgliedern wurde zuerst Anfang 1998 erreicht. Hauptforschungsgebiet ist Dynamik in ausgedehnten Nichtgleichgewichtssystemen. Dabei gliedern sich unsere Aktivitäten in drei Hauptgebiete.

Bildung komplexer räumlicher Strukturen: Spontane Strukturbildung wird in vielen physikalischen, chemischen und biologischen Systemen beobachtet. Wir beschäftigen uns besonders mit der Modellierung chemischer Reaktionen in Lösung und auf katalytischen Oberflächen sowie mit biologischer Musterbildung. Übergänge zwischen einfachen Mustern (Fronten, Pulse, periodische Muster, Spiralen) und komplexen Strukturen (Pulspaare, driftende Musterdomänen, raumzeitliches Phasen- und Defektchaos) werden durch numerische Simulationen von Reaktions-Diffusions-Systemen sowie mit Hilfe numerischer Stabilitäts- und Bifurkationsanalyse erforscht. Ein Hauptergebnis ist hierbei, daß Übergänge zu raumzeitlich chaotischen Mustern in der Regel durch Bifurkationen oder Instabilitäten einfacher, ,,kohärenter" Strukturen verursacht werden (siehe Beitrag "Complex Pattern Formation in Two Dimensions", Seite 20). Weitere Aspekte schließen die Untersuchung der Rolle von Anisotropie, Heterogenetitäten und raumzeitlichen ,,Treibens" in strukturbildenden Systemen ein. In Zukunft wollen wir uns der Erforschung dreidimensionaler Strukturen (,,Scrollwaves") sowie der engeren Zusammenarbeit mit Experimentatoren auf dem Gebiet der musterbildenden chemischen Reaktionen widmen.

Biophysik und Theoretische Biologie: Hier werden hauptsächlich Modelle aus Physiologie (intrazelluläre Kalziumdynamik) und Morphogenese (Aggregation und Schwarmbildung) untersucht. Ein Schwerpunkt ist die Aufklärung der Beziehung zwischen deterministischen Modellen (Differentialgleichungen) und stochastischen Beschreibungen (siehe Beitrag "Stochastic Spreading of Intracellular Ca^{2+} Release", Seite 25). Weitere neue Projekte in diesem Gebiet beschäftigen sich mit der Modellierung von Autoimmunkrankheiten, Aspekten aus der Immunologie sowie mit Modellen zur Polymerisierung von Aktin in der Fortbewegung von Bakterien und schließlich der Aggregation von Myxobakterien.

Statistische Mechanik des Nichtgleichgewichtes: In diesem Gebiet wird über Nichtgleichgewichtsphasenübergänge, Wachstumsmodelle, granulare Materie und stochastische Geometrie gearbeitet. Allgemein ergänzen diese Studien den deterministischen Ansatz im ersten Teil und sind auch relevant für musterbildende Systeme. Einige Ergebnisse sind in dem Bericht (siehe Beitrag "Order out of Disorder", Seite 29). Neue Projekte beschäftigen sich mit der Modellierung des Wachstums von Nanostrukturen bei der Metallisierung von Biotemplaten sowie mit der Beschreibung von Quasikristalloberflächen.

Nachwuchsgruppe: Quantenchaos und mesoskopische Systeme
(Leiter: Dr. K. Richter)

Mesokopische 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 mesokopischer Systeme beruht darauf, daß sie sowohl Quantenkohärenzeffekte (auf Mikrometerskala) als auch klassisch chaotische Dynamik aufwiesen. 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.

Die gegenwärtige Forschung in unserer Gruppe umfaßt drei Hauptrichtungen:

1. Die Untersuchung spektraler Statistik in komplexen Quantensystemen (siehe Beitrag "Signatures of Classical Chaos in Spectral and Transport Properties of Mesoscopic Quantum Systems", Seite 58). Hierzu gehören insbesondere die grundlegende Frage nach dem Zusammenhang zwischen semiklassischen Näherungen für spektrale Korrelationsfuntionen und Vorhersagen der Zufallsmatrixtheorie, sowie das Problem der "Vereinheitlichung" von Theorien für ungeordnete und chaotische Quantensysteme.

2. Die Anwendung der oben genannten Konzepte zur Erklärung von Eigenschaften elektronischer Mikrostrukturen wie beispielsweise Quantenpunkte (siehe Beitrag "Coulomb Blockade in Chaotic Quantum Dots: Interplay Between Interactions and Geometry", Seite 54) oder künstliche Übergitter. Unsere Arbeiten auf diesem Gebiet umfassen: Quantentransport (statische Leitfähigkeit als auch Transport in starken zeitabhängigen Feldern); optische, magnetische und thermodynamische Größen; Eigenschaften von Halbleiter- Supraleiter-Hybridstrukturen; nichtlineare Nanomechanik. Innerhalb dieser Schwerpunkte gibt es Zusammenarbeiten mit verschiedenen experimentellen Gruppen.

3. Die Erforschung photonischer Mikrosysteme. Wir untersuchen die Dualität von klassisch chaotischer Strahldynamik und wellenoptischer Ausbreitung von Licht in kleinen deformierbaren Resonatoren. Diese Kavitäten, die man als photonische Billards auffassen kann, weisen interessante Abstrahlcharakteristiken auf (siehe Beitrag "The mode structure of microcrystal and microdroplet lasers", Seite 50) und sind daher als Resonatoren für neuartige Mikrolaser von großem Interesse.

Die zukünftigen Forschungsschwerpunkte der Gruppe orientieren sich zum einen an den oben genannten Richtungen auf dem Gebiet *mesoskopischer* Systeme; zum anderen beabsichtigen wir, unsere Aktivitäten auf der Physik von *Nanostrukturen*, wie beispielsweise ultrakleine Leiter und Netzwerke (bio)molekularer künstlicher Drähte zu verstärken. Dabei wollen wir mesoskopische Konzepte auf elektronischen Transport auf Nanoskala verallgemeinern. In Bezug auf die Physik molekularer Strukturen ist eine Zusammenarbeit mit der Nachwuchsgruppe Musterbildung (M. Bär) vereinbart.

Scientific Work at the Max Planck Institute for the Physics of Complex Systems

Division: Electronic Correlations in Molecules and Solids
(Prof. Dr. P. Fulde)

A treatment of electron correlations requires going beyond the independent-electron or Hartree-Fock approximation. If one wants to study the corresponding many-body wavefunction one cannot use a density-functional approach but instead must resort to quantum chemical techniques. The latter have to be modified properly, in order to be applicable to solids, i.e., infinite periodic systems [1]. In the past we have calculated with high accuracy the ground-state wavefunction and energy for a number of solids. In the future our aim will be directed towards similar calculations of energy bands. This requires a strong interaction with the Quantum Chemistry group. We have also been treating strongly correlated electron systems by simplified model Hamiltonians. With their help phenomena like electronic charge ordering have been investigated. As part of our participation in a Sonderforschungsbereich at the TU Dresden we also study the interplay of superconductivity and magnetism (see contribution "Theoretical Model for the Superconducting and Magnetically Ordered Borocarbides", page 87). Recently we have started work on glasses at ultralow temperatures (1-10 mK). In that regime strong magnetic field effects were observed which we could explain phenomenologically (see contribution "Mesoscopic quantum effects in cold glasses", page 85). Quantum effects on a mesoscopic scale were identified. They will be studied in much more detail in the future.
Other topics investigated include systems with large spins, nonlinear lattices, breathers etc.

[1] P. Fulde Electron Correlations in Molecules and Solids
(3-rd ed. Springer Heidelberg, 1995)

Group: Nonlinear Time Series Analysis
(Dr. 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 interaction between chaos and noise, the transition from chaos to noise, chaos with many degrees of freedom, and dynamics of systems with time delayed feedback (see contribution "From a coupled map lattice to the Ising model", page 41).

When a time series derived from an experiment or from field measurents shows complex, aperiodic oscillations, on can speculate how far a rather simple but chaotic determinsitic source is causing it. This inverse approach has been studied since the early eighties, but it is meanwhile evident that most phenomena of interest are not low-dimensional determinstic 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 and the analysis of spatially extended systems.

In addition to the develoment 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 parties funding. One example is noise redution of human voice (see contribution "Denoising human speech signals using chaos-like features", page 35).

Also future work will be split into the main two directions, namely improving the fundamantal understanding of complex dynamical behaviour (slightly more in the direction of statistical physics) and designing and applying time series methods for complex signals. Relevant issues include:

(A) Statistics of dynamical systems in the sense of fuzzy parameters.
(B) Dynamical systems with many degrees of freedom.
(C) Time series analysis for data from nonlinear stochastic processes.
(D) Meta-dynamics in the parameter space of dynamical systems.
(E) Analysis of temporally evolving spatial patterns.

Group : Quantum Chemistry
(Dr. M. Dolg (until 9/30/1999))

During the years 1998 and 1999 the 'Quantum Chemistry' research group worked on quantitative *ab initio* electronic structure calculations for properties of atoms, molecules, clusters, polymers and solids. Besides chemical bonding especially the contributions of relativity and electron correlation were investigated and interpreted.

A major area of research was the extension of the successful methods of molecular quantum chemistry to infinite systems, i.e., polymers and solids. *Full-CI* calculations of the model system LiH chain as well as the threedimensional LiH solid were completed and demonstrate the feasibility and usefulness of this approach for the ground states of nonconducting systems. Coupled Cluster calculations with single and pair excitations for more complicated systems as well as the incorporation of relativistic effects including spin-orbit coupling are underway. Correlation corrections to band structures were presented for polymers at the *MP2* level.

Another area of research was the *ab initio* investigation of structures, stabilities and other size-dependent properties as ionization potentials and electron affinities of clusters of the groups 2 and 12 as well as Yb. Charge fluctuations and the electron localization function were also applied to study the transition from Van der Waals interaction in small systems to covalent bonding in medium-sized systems. A new hybrid model for Hg clusters allowed the accurate investigation of systems with up to 55 atoms. Besides relativistic pseudopotentials, core polarization potentials and standard quantum chemical correlation methods the quantum Monte Carlo technique was also applied.

Many investigations dealt with compounds of lanthanides and actinides, e.g., sandwich complexes with benzene or cyclooctatetraene. Besides the pseudopotentials developed in the group and standard quantum chemical correlation treatments also own *Dirac-Coulomb*- and *Zeroth-order Regular Approximation*-based density functional programs were applied in these studies.

Group : Quantum Chemistry
(Dr. U. Birkenheuer (since 3/1/2000))

The declared target of the new 'Quantum Chemistry' group is the calculation of correlated electronic states (ground state as well as excited states: valence band holes and conduction band electrons) in periodic systems by means of quantum chemical POST-SCF methods. This wave function based approach is intentionally seen as an alternative to the density functional methods widely used in solid states physics. It allows a detailed and controlled insight into correlation effects in extended systems as can never be achieved with density functional theory.

Taking up the promising techniques already established in this field by the 'Quantum Chemistry' group the methods developed (increment method) and the existing program packages (Wannier program) should be extended in such a way that correlated $N + 1$ and $N - 1$ particle states of solids and polymeres (bands) can be evaluated which ultimatively leads to the excitation spectra of these systems.

To this end the possibility to include basis function with higher angular momentum has to be introduced to the Wannier program. To reduce the expected high computational effort an optimization of the integral package is planned which takes advantage of symmetry and effective integral estimates. Further progress in coping the orthogonality tails of the Wannier functions is believed to result from switching to non-orthogonal orbital groups in the increment method. In addition, the CI programs to be used (MOLPRO and/or Turbomol) have to be extended to allow the incorporation of the crystalline environmental effects (Coulomb field, exchange contributions, and localization potentials). Corresponding agreements are on the way. Moreover, it should be evaluated to with extent also a localization of the virtual orbitals will be necessary for the treatment of conduction band electrons or valence band holes; as the case may be, appropriate localization methods have to be developed and/or tested.

As in the past, classical *ab initio* and DF calculations on periodic and finite systems should round off the research activities.

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

We started to work at the institute in May 1999. Our name *Finite Systems* is meant to highlight our scientific interest in processes which typically involve a finite number of degrees of freedom.

This includes the excitation and fragmentation of atoms, molecules and clusters. A present focus of activity is the interaction of such systems with intense laser radiation (see contribution "Irregular orbits generate higher harmonics", page 66). Our theoretical tools range from traditional quantum methods over novel semiclassical approaches (see contribution "Threshold detachment by tunneling", page 63) to classical concepts of nonlinear dynamics. Thereby, chaotic phenomena play an important role. They are studied, among other things, by Dr. Andreas Buchleitner's group.

The characteristic hallmark of our work is a close contact with the experiment. Thanks to innovative laser and detector technology we have a fruitful, direct and critical comparison between experiment and theory [1].

A state-of-the-art experiment produces a tremendous amount of data. Hence, future research will be devoted to the development of new concepts to canalize and interpret this data. Thereby, we hope to demonstrate paradigmatically ways how to deal with complex systems. In particular, research in the near future will focus on:

(A) Interaction of atomic/molecular systems with intense fields, with an emphasis on dynamical correlation effects.

(B) Fragmentation and excitation dynamics in atomic and metal clusters.

(C) Search for global yet sensitive quantities to characterize systems of a finite number of degrees of freedom.

(D) Development of methods:

  (D.1) Semiclassical tools of high precision to understand and interpret dynamical behavior (relevant in particular for (A)).

  (D.2) Formulation and implementation of a mixed quantum-classical description for an explicit dynamical description of 10-100 particles (relevant for (B)).

[1] The Theory of Two-Electron Atoms: "From the Ground State to Complete Fragmentation" G. Tanner, K. Richter and J.-M. Rost; Rev. Mod. Phys., in press (2000)

Group : Nichtlineare Dynamik in Quantensystemen
(Dr. A. Buchleitner)

"Nonlinear Dynamics in Quantum Systems" designs the quest for the realization of basic concepts of nonlinear dynamics in experimentally and computationally accessible quantum systems. The experimental perspective largely aims at simple atomic systems which are precisely controllable in modern quantum optics experiments. A PhD thesis on magnetic billiards (K. Hornberger) additionally implies some overlap with nanostructures.

An important part of our work is devoted to the ideally approximation-free ("ab initio"), quantum mechanical description of low dimensional atomic systems exposed to electromagnetic radiation. Since the numerical modeling of the classical and quantum dynamics of periodically driven atomic hydrogen is nowadays essentially accomplished, we presently focus on the quantum dynamics of alkali Rydberg states (see contribution "Residual symmetries in the spectrum of periodically driven alkali Rydberg states", page 69) and of the three body Coulomb problem (together with P. Schlagheck, Orsay) in an oscillating field. The typical dimension of the quantum eigenvalue problem motivated the development of a completely parallelized version of the numerical diagonalization routine (in collaboration with D. Delande, Paris, and K. Taylor, Belfast). Within the framework of a PhD thesis (A. Krug) , this code is presently implemented for the first precise theoretical treatment of the ionization process of alkali Rydberg states subjected to microwave fields. The massively parallel architecture of the CRAY T3E of the computation center of the MPG at Garching allows for the first time for an exact numerical test of laboratory experiments, under precisely equal conditions (Rydberg quantum numbers in the range 50 to 80). Besides the exact numerical treatment, the physical interpretation of the (large) numerical data sets in the context of quantum-classical correspondence and classically chaotic and/or complex dynamics is of equal importance. A present key issue is an analogy between the atomic ionization process and electronic transport through disordered solid state samples. The recently introduced (together with I. Guarneri, Como, and J. Zakrzewski, Krakòw) concept of an "atomic conductance" is presently subject of a diploma thesis (S. Wimberger) exploring the range of validity of the implied analogy atom/solid state. The fundamental problem of the rôle of quantum coherence in quantum propagation under complex dynamics additionally defines the central motivation of a binationally supervised (together with C. Miniatura, Nice) PhD thesis on coherent backscattering of light from cold atoms (C. Müller), i.e. from quantum scatterers with internal degrees of freedom. A second topic of our work is the sensitivity of coherent quantum evolution with respect to the coupling to a noisy environment. At present, key issues are the influence of noise on the atomic excitation and ionization process (K. Hornberger), and the implementation of noise induced stabilization phenomena (in collaboration with R. N. Mantegna, Palermo, and M. Kùs, Warsaw) on a microscopic scale. Here, we recently succeeded (see contribution "Stochastic resonance in the coherence of a quantum system", page 74) to demonstrate stochastic resonance in the *coherence* of a two level atom in coherent interaction with a quantized radiation mode. Our work on stochastic resonance furthermore initiated a new project (together with B. Kümmerer, Stuttgart) on the efficient preparation of arbitrary quantum states (PhD thesis T. Wellens).

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

Our research group started its activities in November 1995 and has grown to its present size around January 1998. We deal with various aspects of nonequilibrium dynamics in extended systems. The main fields are:

Complex Pattern Formation: Pattern formation occurs in a wide variety of physical, chemical and biological systems. Our work concentrates on the modeling of chemical reaction in solution and on catalytic surfaces as well as on pattern forming biological systems. Transitions between simple patterns (fronts, pulses, periodic patterns, spirals) and complex patterns (bound pairs of pulses, drifting pattern domains, spatiotemporal phase and defect chaos) are investigated by numerical simulations of reaction-diffusion models and numerical bifurcation and stability analysis in 1D and 2D. A central result here is that transitions to spatiotemporal chaos are caused by instabilities and bifurcations of simple "coherent structures" (see contribution "Complex Pattern Formation in Two Dimension", page 20). Other aspects include the influence of anisotropy, heterogeneities and spatiotemporal forcing. Future projects include studies of patterns in in 3D (scroll waves) as well as collaborations with experimentalists studying chemical reactions.

Biophysics and Theoretical Biology: Here, mostly models from physiology (intracellular calcium dynamics) and morphogenesis (aggregation and swarming) have been considered. Emphasis here has been put on the relation between continuous deterministic models (differential equations) and stochastic models as e.g. in "Stochastic Spreading of Intracellular Ca^{2+} Release" (page 25), describing a stochastic model for intracellular calcium waves. Ongoing projects in this area include modeling of autoimmune diseases, aspects of immunology as well as a simple models for actin polymerization in bacterial propulsion and the aggregation of myxobacteria.

Nonequilibrium Statistical Mechanics: This subfield covers studies in nonequilibrium phase transitions, growth models, granular media and stochastic geometry. This supplements the deterministic approach inspired by nonlinear dynamics and is relevant to many pattern forming systems. Representative examples are described in the contribution "Order out of Disorder" (page 29). In addition growth models for nanostructure fabrication (metallization of microtubuli and bacterial S-layers) and surfaces of quasicrystals are under way.

Junior Research Group: Quantum Chaos and Mesoscopic Systems
(Dr. K. Richter)

Mesoscopic physics refers to systems in between the micro and 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.

Present research in our group comprises three main directions:

1. Spectral statistics of complex quantum systems (see contribution "Signatures of Classical Chaos in Spectral and Transport Properties of Mesoscopic Quantum Systems", page 58). In particular, the open link between semiclassical approaches and random matrix theory for spectral correlation functions and the question of "unifying" theories of disordered and chaotic quantum systems.

2. The application of the above concepts to describe properties of *electronic* microstructures such as quantum dots (see contribution "Coulomb Blockade in Chaotic Quantum Dots: Interplay Between Interactions and Geometry", page 54) or superlattices. In this respect we are interested in quantum transport (both for dc- and strong time dependent fields), optical, magnetic and thermodynamic quantities, properties of semiconductor-superconductor junctions, and nonlinear nanomechanics. Direct collaborations exist with several experimental groups.

3. The investigation of *photonic* microdevices. We study the duality of classically chaotic ray dynamics and wave-optical propagation of light in small resonant cavities. These cavities which act as photonic billiards exhibit interesting radiation characteristics (see contribution "The mode structure of microcrystal and microdroplet lasers", page 50) and serve as resonators for novel microlasers.

Future research of the group will focus, on the one hand, on mesoscopic phenomena along the lines described above and, on the other hand, on nanoscale devices, such as arrays of small conductors and networks of (bio)molecular wires. In this respect, a collaboration with the group on Pattern Formation (M. Bär) is envisaged. We are planning, and have already started, to extend concepts developed in mesoscopics for a better understanding of charge transport through nanosystems.

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Complex Pattern Formation in Two Dimensions

Markus Bär, Martin Falcke, Michal Or-Guil and Uwe Thiele

Chemical and biological reaction-diffusion systems often exhibit extended periodic patterns like rotating spiral waves or stripes and hexagons. Here, we give two examples of more complex patterns, localized spiral waves and stratified spatiotemporal chaos, and elaborate on the mechanisms involved. Occurence of localized spirals in a model for intracellular calcium waves is caused by a gap in the dispersion relation for planar waves. Stratified spatiotemporal chaos is generic in anisotropic, bistable media and can be rationalized from the orientation-dependent dynamics of interfaces connecting the two stable states.

Introduction. - Pattern forming processes are typically modelled by coupled, nonlinear partial differential equations that are usually not solvable in closed form and thus are investigated often by direct numerical integrations. This approach allows to reproduce the spatiotemporal dynamics for given parameters, initial values and boundary conditions, but often fails to give insight into the formation mechanism of complex patterns. Alternative approaches are the construction of approximate solutions by use of perturbation theory or the use of (numerical) bifurcation and stability analysis of traveling waves or periodic patterns. Here, we present one example for each of these strategies and show that they are essential in the understanding of complex pattern dynamics in two dimensions. In the first part, the appearance of localized spirals in a realistic three variable model for intracellular calcium dynamics is related to the existence of a gap in the dispersion relation for planar waves computed in a numerical bifurcation analysis. If the selected wavelength of the spirals falls into that gap, localized spirals are found. In the second part, a novel dynamic pattern, stratified spatiotemporal chaos in anisotropic bistable media is traced back to the angle-dependent dynamics of interfaces connecting the two stable states.

Dispersion gap and localized spirals in a model for intracellular calcium waves. - The system under consideration is a model for intracellular Ca^{2+} dynamics and waves. Ca^{2+} waves consist of a traveling range of increased Ca^{2+} concentration in the cytosol. The cytosol is the medium surrounded by the cell membrane, in which the cell organelles are embedded. Intracellular calcium waves were first observed in medaka eggs and later on in Xenopus oocytes [1].

The local dynamics inside these cells is nonlinear release and uptake of Ca^{2+} from intracellular stores like the endoplasmatic reticulum (ER) and the mitochondria. The model studied here extends previous approaches by incorporating mitochondrial calcium storage. Simulation results [2] compare favorably to experiments [3] with energized mitochondria. The relevant control parameter is the rate of mitochondrial Ca^{2+} uptake, $V_{max}^{(1)}$. Increase of $V_{max}^{(1)}$ changes the local dynamics from excitable to bistable and eventually leads to the destruction of spiral patterns. Spirals can be stabilized by the introduction of pinning sites (see upper left frame in left panel of Fig. 1). However, for large enough $V_{max}^{(1)}$ and for a wide range of pinning site radii, we observe formation of localized spirals [4].

The emitted waves get fragmented and disappear far away from the spiral center (see Fig. 1, left panel, bottom).

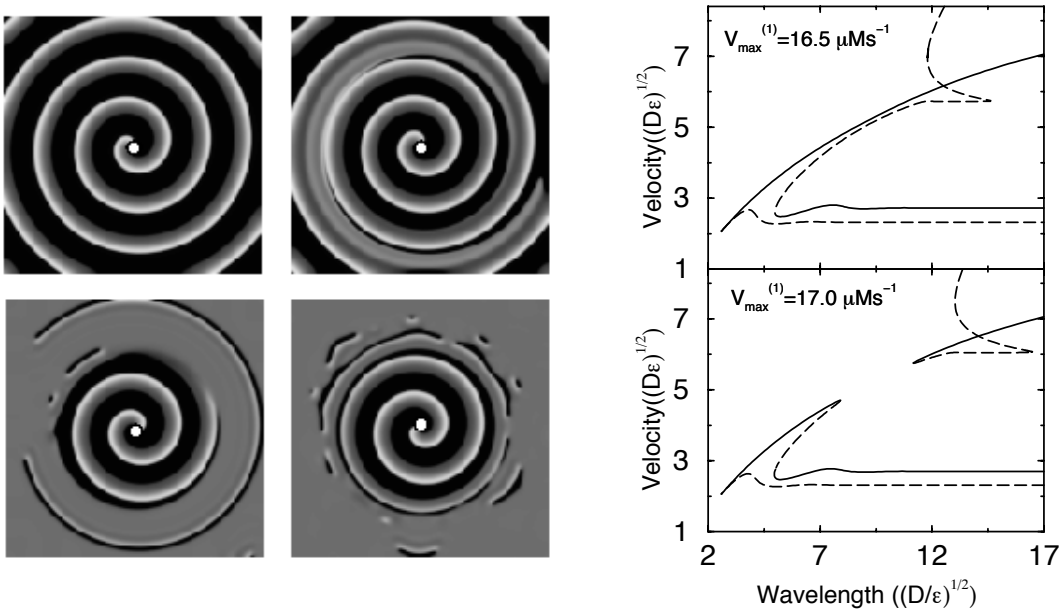

Figure 1: *Evolution of a localized pinned spiral formed by waves of increased cytosolic Ca^{2+} concentration in a numerical simulation left panel). Time increases from left to right and top to bottom in steps of 2 rotation periods. Bright areas indicate high Ca^{2+}. The system is in the bistable regime. The spiral is pinned by a non-excitable patch in the core (marked with a white dot). The size of the patch controls the period. Dispersion curves showing velocity and wavelength of wavetrain solutions for $V_{max}^{(1)}$=16.5 μ Ms^{-1} and $V_{max}^{(1)}$=17.0 μ Ms^{-1} (right panel). Dashed lines indicate unstable solutions, full lines stable ones.*

Performing in parallel a numerical bifurcation analysis for planar wavetrains, we find that our model is distinguished by the existence of four branches (two stable, two unstable) of wavetrains in the dispersion curve. In contrast, standard reaction-diffusion models posess only two branches of wavetrains (one stable, one unstable) [5]. At a critical value $V_{max}^{(1)}$, two of the four branches collide and a velocity gap - or a corresponding period gap - opens up (see Fig. 1, right panel). A systematic comparison to the simulations with localized spirals shows that these structures if the selected rotation period lies in the gap of the dispersion curve [4].

Stratified spatiotemporal chaos in anisotropic bistable reaction-diffusion media. - Anisotropy plays an important role in pattern formation processes in liquid crystals, on catalytic surface reactions and in biological media like cardiac tissue. Many qualitative features of pattern formation in reaction-diffusion systems are well described by the FitzHugh-Nagumo (FHN) model. Here we study its anisotropic variant

$$\begin{aligned} \frac{\partial u}{\partial t} &= \epsilon^{-1}(u - u^3 - v) + \delta^{-1}\nabla^2 u + \frac{\partial}{\partial y}[d\delta^{-1}\frac{\partial u}{\partial y}]\,, \\ \frac{\partial v}{\partial t} &= u - a_1 v - a_0 + \nabla^2 v\,, \end{aligned} \tag{1}$$

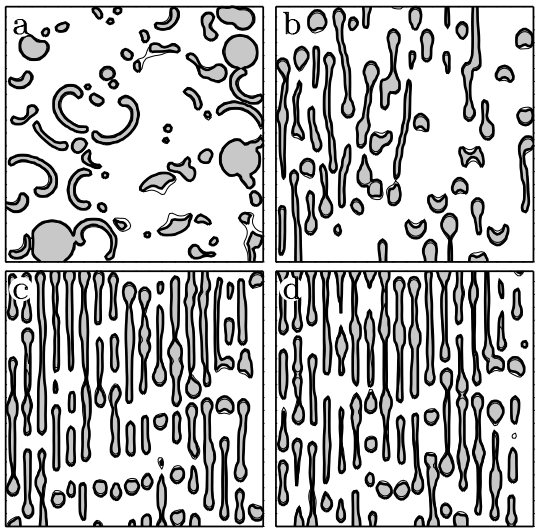

Figure 2: *Development of stratified chaos in Eq. (1) from initial spiral-defect chaos.*

The parameters a_1 and a_0 are chosen so that Eqns. (1) represent a bistable medium with two stationary and uniform stable states, an "up" state, (u_+, v_+), and a "down" state, (u_-, v_-). Front solutions connect the two states. Pattern formation in these equations can be analyzed by considering the number of front solutions. This number changes, when a single stable front that exists for values of $\eta := \sqrt{\epsilon\delta} > \eta_c$ is replaced by a pair of stable counter-propagating fronts and an additional unstable front for $\eta \leq \eta_c$. The corresponding saddle-node bifurcation is referred to as a front bifurcation. The anisotropy of the medium is expressed in the parameter d. Fixing all parameters except δ, the following sequence of patterns is observed: at small δ, stable traveling fronts, pulses and rotating spirals are encountered. For slightly larger δ irregular dynamic patterns known as spiral-defect chaos appear. Upon further increase of δ, we find an interesting behavior that has no counterpart in isotropic media, stratified spatiotemporal chaos (see Fig. 2). The most striking feature of stratified chaos is the existence of long range correlation in the x-direction, while the y-direction shows the rapid decay of correlations typical for extended chaotic systems. The pattern consist of stripe fragments that alternate between stretching and shortening by pinching off of grey droplets.

To get further insight, we have derived a velocity-curvature relation for the anisotropic Eq. (1), in the limit $\lambda := \sqrt{\epsilon/\delta} \ll 1$. The angle θ is taken between the tangent vector on the interface and the x axis. Since $\lambda \ll 1$ we distinguish between an inner region where $\partial u/\partial r \sim \mathcal{O}(\lambda^{-1})$ and $\partial v/\partial r \sim \mathcal{O}(1)$, and outer regions where both $\partial u/\partial r$ and $\partial v/\partial r$ are of order unity. Combining the equations for the inner and outer region and demanding continuity of the derivative $\partial v/\partial r$ at the interface gives an implicit relation between the angle dependent normal velocity of the front and its curvature

$$C_n + \frac{1+d}{\delta I(\theta)^2}\kappa = \frac{3I(\theta)(C_n+\kappa)}{\eta\sqrt{2}q^2\sqrt{(C_n+\kappa)^2+4q^2}} + \frac{3I(\theta)a_0}{\eta\sqrt{2}q^2}\,, \tag{2}$$

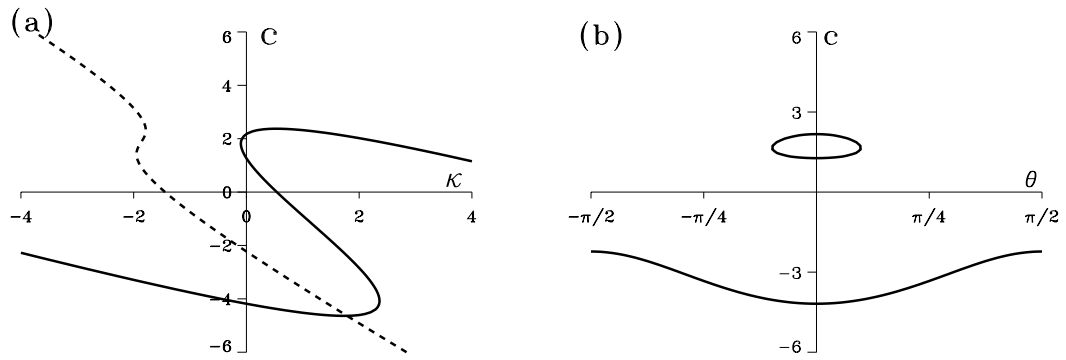

Figure 3: *Two views of the relation of Eqn. (2) corresponding to the parameters of the simulation in Fig. 2. (a) The velocity-curvature relation for fronts in the x direction ($\theta = \pi/2$, dashed curve) and y direction ($\theta = 0$, solid curve). (b) The velocity of planar ($\kappa = 0$) fronts at different angles. At $\theta = 0$ there is a pair of stable fronts and at $\theta = \pm\pi/2$ only a single front exists.*

where $q^2 = a_1 + 1/2$ and $I(\theta) = \sqrt{1 + dcos\theta}$. In Fig. 3a we have plotted the curvature-velocity relation for fronts in the x and y direction with the parameters of the simulation in Fig. 2. While the y direction is close to the front bifurcation, the x direction is far inside single-front regime. In the x direction the single front is moving with negative velocity towards the up state (displayed grey in Fig. 2). In the y direction, a fast moving front with positive velocity usually causes a stretching of the pattern along the y axis. Additional insight is obtained from the angle-velocity relation for planar fronts (Fig. 3b). One clearly sees the regions of single and multiple fronts along the angular orientation.

Both curves together explain in part the formation of stripes from fronts moving into the x-direction and the dynamic motion in the y-direction seen in Fig. 2. An additional element in the dynamics is the interaction of interfaces. The slow fronts in the x-direction form stable stripes, while the somewhat faster fronts with orientation in between x and y direction annihilate upon collision. The latter process leads to the pinch-off of grey droplets at the ends of stripe fragments and is necessary to sustain the chaotic dynamics.

Conclusion. - We have shown two examples where complex patterns in two dimensions can be rationalized from analyzing simple properties of the respective medium like the dispersion curve for planar periodic waves or the dynamics of moving interfaces. Another prominent example along these lines is the unraveling of two alternative mechanisms for spiral breakup in excitable media that has been explained by a careful analysis of the dispersion curves [7]. In general, the presented approach is feasible if the two-dimensional pattern dynamics can be reduced to its one-dimensional ingredients. This excludes some phenomena, *e. g.* the destruction of spirals starting in their core seen in [2]. Here a full understanding requires numerical bifurcation and stability analysis in two dimensions. That requires different numerical methods, in particular iterative schemes suitable to treat large-scale problems, and represents one of the challenges for the future.

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Stochastic Spreading of Intracellular Ca^{2+} Release

Martin Falcke

Calcium often acts as a second messenger in living cells so as to regulate multiple cellular functions. These functions include processes as diverse as muscle contraction and synaptic transmission. The Ca^{2+} signal initially employed in these processes consists of a transient increase in the intracellular concentration. This increase can arise from influx through the cell membrane or via Ca^{2+} release from internal stores. The release from internal stores like the endoplasmic reticulum is a nonlinear process, since calcium induces its own further release (Calcium Induced Calcium Release CICR). That allows for the formation of complex spatio-temporal signals in form of localized stochastic release events (puffs, sparks, [1, 2]) or - in large cells - waves of high Ca^{2+} concentration traveling across the cell [3].

Most relevant for our work, Parker et al. [2] showed for a single cell type, (the Xenopus oocyte), that there exists a continuum of wave phenomena. At low excitability, isolated puffs are observed. Abortive waves occur at higher excitability and a further increase of excitability leads to steadily propagating waves.

Ca^{2+} is released from the endoplasmic reticulum through channels spatially organized in clusters. There are a variety of channels showing CICR. Here, we will focus on the inositol 1,4,5-trisphosphate receptor channel IP_3R. This channel consists of four identical subunits. Each subunit has an activating binding site for IP_3, an activating site for Ca^{2+} and an inhibiting Ca^{2+} binding site. Experimental findings suggest that the channel is open if both Ca^{2+} and IP_3 are bound to the activating sites and at the same time Ca^{2+} is not bound to the inhibiting site, at at least three out of the four subunits. Binding of Ca^{2+} to the inhibiting site of one of these subunits closes the channel. It can reopen after dissociation of Ca^{2+} from the inhibiting sites. The bindings of Ca^{2+} to the activating and inhibiting sites are stochastic events rendering the opening and closing of the channel a stochastic process.

The observation of localized stochastic Ca^{2+} puffs and the rather small number of channels creating the localized event suggest that stochastic effects are relevant for Ca^{2+} wave propagation and need to be taken into account when waves are modeled mathematically. Indeed, abortive waves cannot be understood in terms of deterministic models, since in these models an excitation travels steadily if it travels at all.

We present a stochastic model for the IP_3R system. It is based on the DeYoung-Keizer-model [6, 7] for the kinetics of the IP_3 receptor channel. Furthermore, we introduce a new, general approach to the mathematical modeling of this class of experimental processes. In the paradigm used to date, the channels are perceived as an array of stochastic elements coupled by the Ca^{2+} concentration field c(r,t) (r and t denote the spatial and time coordinate resp.). The state of the complete system is determined by the states of all channel subunits at the current time and c(r,t). The Ca^{2+} concentration affects the transition probabilities between different states for the individual subunits and thereby couples channels by diffusion. The dynamics of Ca^{2+} concentration is determined by a diffusion equation with spatially discrete source terms corresponding to the clusters. It is reasonable to assume that the concentration profile evolves on a time scale much faster than that of the channel dynamics and in fact merely exhibits relaxation dynamics to an asymptotic state, as long as the channel configuration

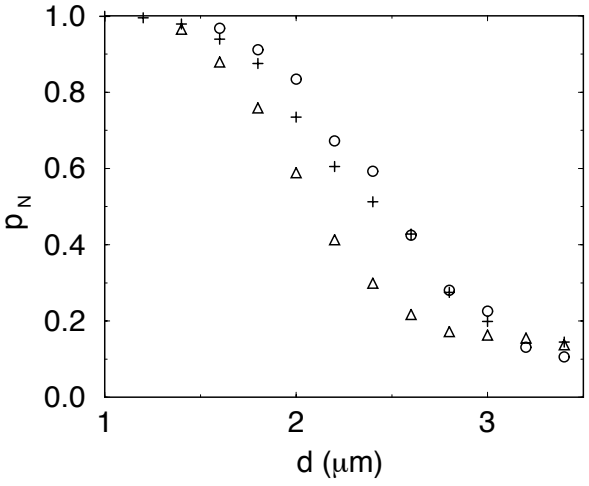

Figure 1: *The probability p_N that an active cluster activates a neighboring cluster in dependence on the cluster spacing d for the different models. The flux density ((single channel flux)/d) was kept constant. The line styles are: complete model (without adiabatic approximation) ∘, reduced model (with adiabatic approximation) +, reduced model with linearized transition rates △.*

remains unchanged. Then, one can ignore this transient period and use instead the time independent transition rates, which can be derived from the asymptotic state of the concentration profile for the actual configuration of channel states. That asymptotic Ca^{2+} profile $c(R_j, \{N_o\})$ depends on the cluster positions R_j and their numbers of open channels $\{N_o\}$. The adiabatic approximation reduces the complete model to a Markov process in the channel configuration space alone. Rather than study this complex Markov process, we make an additional approximation. The most important contributors to the calcium concentration at cluster j are the nearby open channels. We will therefore replace the dependence of $c(R_j, \{N_o\})$ on the overall set of open channels by a dependence on the number of open channels at a small number of nearby sites. Furthermore, we will approximate the full dependence of the calcium concentration on the channel variables as a sum of terms that depend separately on the number of open channels at each site [4].

The first issue we address concerns the transition from localized to propagating disturbances. Propagation can be characterized by the probability p_N that an active cluster activates a neighboring cluster. It can be obtained from the probability S(i) that an initial excitation travels at least up to the ith cluster: $S(i) \sim {p_N}^i$. p_N increases smoothly from 0 to 1 as we increase the coupling between clusters, increase the lifetime of the activated state of a cluster or increase the number of channels per cluster. Fig.1 compares simulation results with and without the adiabatic approximation for the Ca^{2+} diffusion equation. The results agree very well and clearly indicate that the Ca^{2+} dynamics can be eliminated adiabatically. A reduced model with linearized transition rates shows the same qualitative behavior (see Fig.1).

Our model reproduces the experimental finding of a continuum of wave phenomena, as shown in Fig.2a. The transition can be explained by the kinetics of the IP_3 receptor channel. An increase in $[IP_3]$ raises the IP_3 binding probability and hence the fraction of the open state of the channel. Additionally, inhibition decreases with increasing $[IP_3]$.

Simulations of this system also lead to a new type of spatio-temporal pattern that is characterized by backfiring, i.e. propagating pulses lead to the creation of counterpropagating pulses (in one dimension) or of new signaling centers (in higher dimension) in their wake. A typical picture in two dimensions is shown in Fig. 2b. One interesting new possibility concerns the formation of a spatio-temporally disordered calcium concentration pattern, as shown in Fig. 2c. This simulation shows that there is no

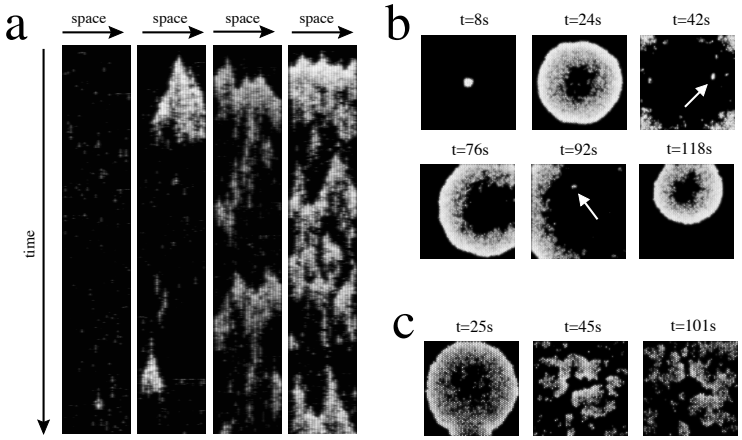

Figure 2: *a: Spontaneous wave patterns in one spatial dimension for different [IP_3] from left to right: 0.25 μM, 0.3 μM, 0.4 μM and 0.5 μM. Bright gray levesl indicate high Ca^{2+} concentration. Spontaneous, isolated sparks occur for I=0.25 μM. At I=0.3 μM, abortive waves appear. The waves at I=0.4 μM and I=0.5 μM no longer die out but instead disappear at the boundary or by collision. The time interval shown is 625s and the spatial extension is 600 μm. b: Backfiring in two spatial dimensions. An expanding ring emerges from an initial puff. It leaves behind small excited patches. Some of them (white arrows) set off another wave. c: Turbulent backfiring in two spatial dimensions. The initial wave leaves behind a turbulent state with wave fragments traveling in an irregular manner. The system size is 96μm x 96μm.*

need for heterogeneities to generate continuing wave patterns which are not spirals. In fact, once a single channel opens spontaneously, the wave activity can sustain itself via backfiring.

The pulses emitted during backfiring are initiated by active channels in the refractory tail of the original pulse. There are in principle two ways in which channels can be activated there; it is possible that they were originally activated by the first pulse and have not as yet become inhibited. Alternatively they may have already undergone the complete activation-inhibition-deinhibition cycle and hence can be re-opened. We always found the latter scenario to be the case for sample clusters in our simulations. The Ca^{2+} level in the refractory area is less than in the excited region but higher than the base level. This provides an increased opening-probability as compared to the medium in front of the pulse. If a group of re-opened channels stays open long enough for sufficient decay of the inhibition around it, it can set off another wave.

We found backfiring at intermediate channel numbers for parameters where the system would be bistable in the deterministic limit. With the channel number per cluster N_K and the flux strength of a single channel J the deterministic limit is $N_K \to \infty$ with JN_K=constant. The wave solutions in the bistable deterministic limit are fronts. However, as we showed before [8], to be in the bistable regime in the deterministic limit is not a necessary condition for backfiring to occur. Rather, backfiring occurs for parameters in the vicinity of a bifurcation separating the excitable from the bistable regime. For N_K smaller than the values for which backfiring occurs, abortive waves or steadily propagating pulses without backfiring were found. Reopening, obviously, is too unlikely to occur for small N_K.

Our stochastic model shows pulses for parameters where the system would be in the bistable regime in the deterministic limit; i.e. biological cells might be in the bistable regime, even when pulses are observed. That supports theoretical and experimental findings for bistability in Xenopus oocytes with energized mitochondria [5].

The occurence of pulses in the bistable regime and backfiring are effects of stochasticity for numbers of channels per cluster at the upper limit estimated from experiments. That suggess, that pattern formation in biological cells is typically in a regime where stochastic effects are relevant. Since spatially extended stochastic systems may exhibit oscillations for parameters with an excitable determinstic limit [9], our results open up the possibility that this is the case for Ca^{2+} oscillations in living cells as well. That is the subject of current research.

We have shown, that the Ca^{2+} dynamics can be eliminated adiabatically. That means that the original system can be reduced to an array of stochastic, coupled elements the behavior of which is determined by 6 independent parameters only. Hence, we derived a simple model allowing a thoroughly investigation of pattern formation in noisy systems. In that context, we plan to address a precise description of the conditions for backfiring and pulses in the regime with bistable deterministic limit next.

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Order out of Disorder

Ivan Dornic, Haye Hinrichsen, Dieter Joseph and Gudrun Schliecker

Understanding the mechanisms and the physical properties giving rise to the emergence of ordered structures or statistical regularities is a common feature of the subjects described in this section. The three topics we have chosen to present pertain to this line of thought. They concern the modelization of the growth of quasicrystals, the equilibrium properties of two-dimensionnal random cellular structures, and the kinetics of phase-ordering with or without surface tension.

Introduction

In the last two decades the physics community has become more and more interested in the investigation of disorder. In most cases, order and disorder were seen as counterparts competing in the game of life. Lately, it was recognized that this picture is over-simplified.

In this contribution we present examples, where order can be found *in* or can even emerge *out of* apparently disordered structures. In the first section, we model the growth of entropically stabilized non-periodic crystals (quasicrystals). In the second part, the disorder is increased and we describe how random cellular structures give rise to statistical regularities. The third section presents an overview how competing phases can order with or without surface tensions in between them.

Modelization of the growth of quasicrystals

Crystal structures and their lattices are *the synonym* for order in solid state physics. Therefore, a paradigma change was necessary after the discovery of quasicrystals in 1984 [1] which could not be periodic but were apparently as ordered as crystals. Instead of lattices quasiperiodic tilings are necessary for the description of the basic features like symmetry or degree of order [2]. These tilings can appear in an ideal, total ordered fashion or in a randomized way in which the buildings blocks (tiles) cover space face-to-face randomly. In the latter version the structure has new degrees of freedom because a topological entropy can be used to stabilize it. The question how these structures can grow and why they are prefered by nature in certain composition ranges is still unsolved. While the ideal tilings cannot be grown with local rules, the random quasiperiodic tilings face a growing strain in the above mentioned new degrees of freedom (named phasons in analogy with phonons) [3]. The expected amount of phason strain is not reported in experiment. Therefore, the question arose, if one can reduce this strain in the growth process.

To this end our model for the growth of entropically stabilized quasicrystals was developed. The main feature of the model is a fluctuating surface. During growth the surface can go further or retreat and therefore, can repair unfortuned configurations.

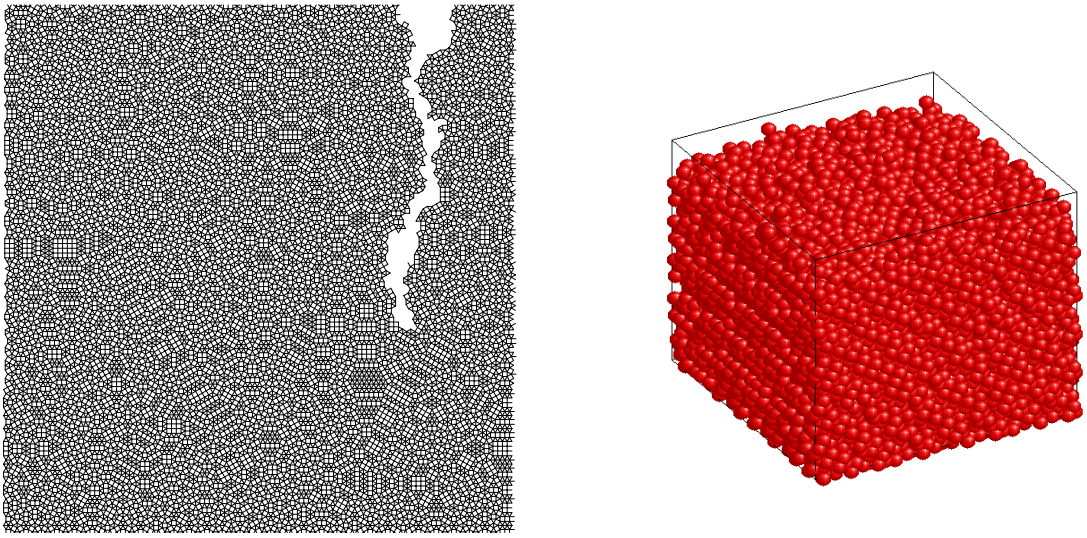

Figure 1: *Left: Detail of a 12-fold tiling consisting out of squares and equilateral triangles grown in vertical direction with a tear. Right: A 3D quasiperiodic tiling out of 6 different tetrahedra. Balls mark the vertices of the tiling*

The model consists of a bulk and a competing surface term. A chemical potential μ represents the energy one has to pay to attach a vertex to the tiling. The surface variable Ω is the part of the full-angle around the vertex subtended by complete tiles. The energy of the tiling is $H = \sum_i (\mu - \Omega_i)$ where the sum goes over all vertices of the tiling. Using this equation as a penalty function we performed Monte-Carlo simulations in 2D and 3D with various tilings [4, 5, 6]. Vertices were attached to or removed from the surface under the constrains that the directions of the bonds were consistant with the symmetry of the tiling and that a minimal distance between neighboring vertices is always respected.

We found that the additional phason strain during growth cannot be avoided but can be made as small as necessary. For a fixed length scale the phason strain goes to zero in the limit of vanishing growth velocity. This means that for a certain length scale the grown sample is indistinguishable from an equilibrium ensemble member. On the other hand we could show that the local phason strain is responsible for the nucleation of dislocations. As a biproduct the model was able to measure the equilibrium entropy of the tiling during the (non-equilibrium) growth process [4].

In this way, our model is an example how order (e.g. 12-fold symmetry, sharp diffraction peaks) can emerge out of certain kind of randomness. What happens if one relaxes the contrains on the tiles shows the next section.

Equilibrium properties of two-dimensional random cellular structures

In most natural structures, disorder and randomness are the rule rather than exception. Especially, random cellular structures can be observed in a huge variety of natural systems. In the past decade, the investigation and characterisation of their stationary-

state properties has become a subject of growing interest. Structurally, they are simply random tessellations of space by cells (cf. Fig. 2). In two dimensions, the cells are polygons with six numbers of sides in average, since always three cells meet at one vertex.

The work presented here addresses to the surprising statistical regularities concerning the topological properties [7] of planar random cellular structures. In particular, one observes quasi-universal laws not only for the distributions of the cells' shapes [8], but also for the correlations between neighbouring cells [9, 10]. The most promising theoretical approaches to this generally observed behaviour are based on a thermodynamic description of the system, partially established in [7, 11].

Starting point of the statistical-mechanics approach developped in [12] is the formulation of an effective interaction between the cells, i.e. a model Hamiltonian. In the spirit of a description of general properties (rather than of the physical and/or biological details of a given real system), the construction of the Hamiltonian is led by common empirical observations. They suggest a non-interacting part disfavoring cells with few and many sides, and a two-body term describing the interaction of the topological charges of two neighbouring cells:

$$H \;=\; \gamma \sum_{i=1}^{N} (k_i - 6)^2 + \frac{u}{2} \sum_{\langle i,j \rangle} (k_i - 6)\ (k_j - 6)$$

with $\gamma, u \geq 0$. The cells are labeled with $i, j = 1 \ldots N$, their numbers of sides are k_i, k_j. From this Hamiltonian, the topological one- and two-point functions can be obtained following essentially the methods of liquid state theory [13]. In agreement with common empirical observations and previous theoretical results [8, 7], a Gaussian cell shape distribution is obtained for the non-interacting system. In particular, a generalised "temperature" appears, acting as the relevant parameter governing the width of this distribution. The two-point correlations are approximated by the first nontrivial term in their systematic virial expansion, *i.e.* the Boltzmann factor [13]. This approximation is known to give reliable results in a situation, where many-particle effects are negligible.

Based on these results, the experimentally measured total number of sides of th eneighbours of a k-sided cell, $km(k)$ can be easily calculated. The results for weak interaction strength u are in convincing agreement with the semi-empirical Aboav-Weaire law [9], stating that $km(k) = (6 - a)k + 6a + \mu_2$. Whereas μ_2, the variance of the cell-shape distribution, is easily interpreted as a measure of randomness, the role of the Aboav-Weaire parameter a remained unexplained in previous theoretical investigations - especially its quasi-universal dependence on μ_2 empirically observed in [10] (see Fig. 2). Within our theoretical treatment, the slope was determined for three different values u/γ. The resulting curves represented in Fig. 2 are parametrized by the temperature: a 'cooling' of the system results in a decrease of μ_2 and a strong

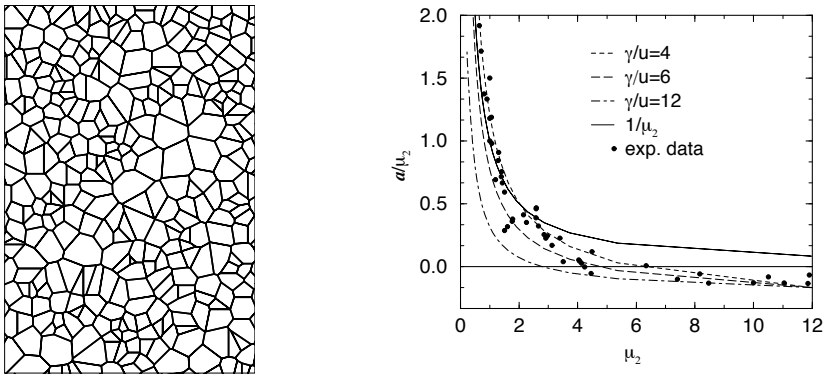

Figure 2: *Left: Part of a planar random cellular structure. Right: Results for the Aboav-parameter a: a/μ_2 is plotted versus μ_2 for different values of γ/u. The circles represent data from natural and model structures [10].*

increase of a/μ_2. In particular, the empirically observed behaviour is well reproduced by the curves which depend only weakly on the strength of the interaction parameter u. The fact that also small values of u/γ yield the empirically observed behaviour of a/μ_2 indicates that the Boltzmann approximation of the pair correlation function renders indeed a realistic description of the cell-shape correlations.
To conclude, the statistical-mechanics approach developped in [12] shows how a generalized temperature acts as the relevant parameter, governing the degree of disorder and correlations in random cellular structures.

Geometrical properties of domain walls

When an Ising model is suddenly quenched from a high-temperature, disordered point, deep into the phase coexistence region, the development of long-range order in the broken symmetry phase gives rise to a network of growing domains of each of the possible equilibrium states.

Such coarsening phenomena are of interest in many physical situations: spinodal decomposition, phase separation in metallurgy, soap froths, to quote a few. The driving force acting in all of these phase-ordering processes is surface tension, which entails that domain walls separating each phases move with a velocity proportional to their mean curvature. Since the latter is also of the order of the typical size of a domain, one immediately obtains the celebrated growth law $L(t) \sim t^{1/2}$. This result defines a broad universality class, which is characteristic of all the systems undergoing a dynamics which does not conserve locally the scalar order parameter.
However, the situation in the realm of non-equilibrium systems is richer, and phase-ordering can proceed through other mechanisms, since notions such as equilibrium phases and surface tension are not necesarily defined anymore when the dynamical rules do not obey detailed balance.
A known example of such an instance is provided by the so-called two-dimensional Voter model, which does display coarsening, but with several unusual features: conser-

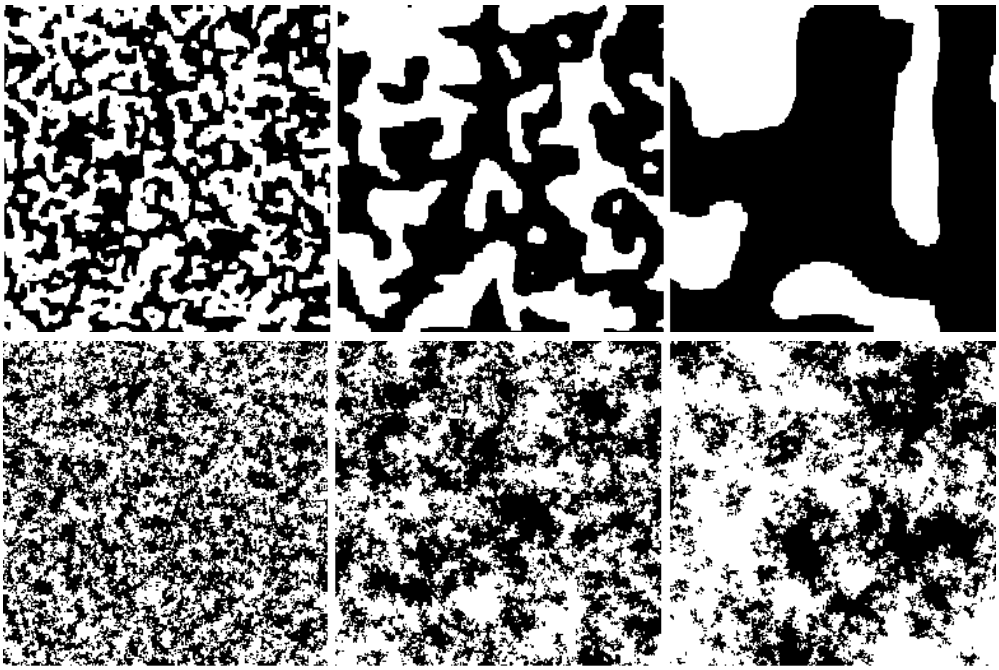

Figure 3: *Top: Coarsening in the 2D Ising model: competing equilibrium domains grow as* $L(t) \sim t^{1/2}$ *due to surface tension. Bottom: Domains in the voter model (no surface tension).*

vation of any initial magnetization, existence of all length scales up to $L(t) \sim t^{1/2}$ in the distribution of clusters, density of interfaces decaying as $\ln^{-1} t$ and not as $L^{-1}(t)$. The Voter model has therefore been perceived as a rather marginal system up to now. By introducing a variety of models with similar features, we have recently shown that this system was in fact defining a broad universality class of coarsening systems without surface tension, of which we have given two prescriptions to determine it in these non-equilibrium situations [14]. Unlike the original Voter case, the models we introduce do not exhibit either an explicit Z_2 symmetry or a decoupling of their hierarchy of correlation functions. Two prominent examples of non-equilibrium universality classes are represented by directed percolation (the paradigm of a dynamical transition from an active phase to an absorbing state), and by the Kardar-Parisi-Zhang equation (the simplest non-linear equation for kinetic roughening). By showing that the Voter model is in fact encompassing many models with similar phase-ordering properties, more order in the zoo of out-of-equilibrium systems has been obtained.

Conclusion

To summarize, we have presented a few examples that show how order and disorder can interact. On the one hand, apparently disordered structures can be characterized by only a few parameters that represent the basic features and allow classifications. On the other hand, only a few geometric contraints are necessary to grow entropically stabilized non-periodic structures which show high-order properties like discrete point-symmetries and at least Bragg-like diffraction data.

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Denoising human speech signals using chaos-like features

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Noise reduction for human speech is of high technological relevance. Background noises of all kinds are inconvenient in tele-communication, deteriorate automatic speech recognition, and cause serious difficulties for the users of electronic hearing aids. A well established remedy is filtering of the signal in the frequency domain, in the simplest case by band-pass filters. Due to the aperiodic nature of voice signals, expressed by broad band power spectra, simple filters distort the signal more than they reduce noise, such that more refined methods are required. As a consequence of the high technical relevance of this field, very sophisticated combinations of filtering techniques using Fourier transforms, wavelet transforms and other methods are in use in the specialized field of speech processing. Examples of state-of-the-art results are [1, 2], and a modern spectral subtraction scheme which became a kind of standard was introduced in [3].

The success of denoising human speech signals using chaos-like features is possible by the identification and exploration of quasi-deterministic structure in the voice. Hereby, the reconstruction of an embedding space allows to efficiently cope with the problem of non-stationarity. The different phonemes are identified implicitly. As argued before and as it will be proven below, the dynamics inside the single phonemes is very close to low-dimensional deterministic. Nonlinear time series analysis comprises a set of techniques for the analysis, manipulation, and understanding of aperiodic signals relying on the hypothesis of deterministic chaos [4, 5]. The application of this raw concept yields already typical gains in the signal to noise ratio which are comparable to the most recent results published in the signal processing literature (e.g. [1, 2]). The results can be improved by post-processing the denoised signal with other filters which rely on properties different from those exploited by our method to distinguish between signal and noise (e.g. spectral properties).

To get an impression of how the method works, assume that one has to eliminate noise from music stored on an old-fashioned long playing record, induced by scratches on the black disc. The task becomes almost trivial if one has several samples of this LP. When playing them synchronously, the signal part of the different tracks is identical, whereas the noise part is independent. Already simple averaging will enhance the signal. In deterministic chaotic signals, this redundancy is stored in the past: Since determinism means that similar initial conditions will behave in a similar way (at least for short periods), one solely has to look for almost repetitions of the present signal in the past. Based on this idea, several approaches for noise reduction for deterministic chaotic data have been developed [6]. One of them [7] will be sketched in the following.

Let a dynamical system be given by the map $\mathbf{F} : \Gamma \to \Gamma$ in a state space $\Gamma \subset \mathbf{R}^d$. The equation of motion thus reads $\mathbf{x}_{n+1} = \mathbf{F}(\mathbf{x}_n)$. Not knowing $\mathbf{F}$, one can determine it in linear approximation from a long time series $\{\mathbf{x}_k\}$, $k = 1, \ldots, N$, by determining a set

of neighboring points $\mathcal{U}_n$ of $\mathbf{x}_n$ and minimizing

$$s_n^2 = \sum_{k:\mathbf{x}_k \in \mathcal{U}_n} \left(\mathbf{A}_n \mathbf{x}_k + \mathbf{b}_n - \mathbf{x}_{k+1}\right)^2, \tag{1}$$

the one-step prediction error, with respect to $\mathbf{A}_n$ and $\mathbf{b}_n$ [8, 9]. The implicit relation $\mathbf{A}_n\mathbf{x}_k + \mathbf{b}_n - \mathbf{x}_{k+1} = 0$ expresses that data are confined to a hyperplane in the extended phase space. When the signal $\mathbf{x}_k$ is superimposed by random noise, $\mathbf{y}_k = \mathbf{x}_k + \eta_k$, the set $\mathcal{U}_n$ will no longer be embedded in a manifold whose tangent space is the hyperplane defined by $\mathbf{A}_n$ and $\mathbf{b}_n$, but will form a cloud scattered around it. Reducing noise now means to project the noisy $\mathbf{y}_n$ onto this hyperplane. If not $\mathbf{x}_k$ but only a scalar observable s_k is measured, one can reconstruct a phase space by the Takens time delay embedding method [10, 11], combining successive elements of the time series $\{s_k\}$ to vectors in $\mathbf{R}^m$, $\mathbf{s}_n = (s_n, s_{n-\tau}, \ldots, s_{n-(m-1)\tau})$. Here, the embedding dimension m and the lag τ has to be chosen suitably.

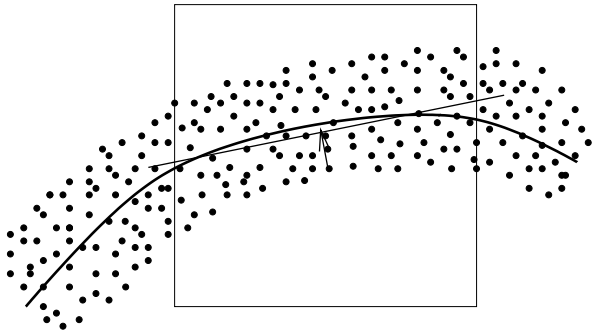

Figure 1: *Schematic representation of the noise reduction method.*

The noise reduction scheme outlined above is called *local projective noise reduction* as illustrated in Fig.1 and can be formalized by a minimization problem. The conceptual steps in the numerical algorithm are the following:

- For every delay vector $\mathbf{s}_n$, all neighbors in the delay embedding space are collected (i.e. $\mathcal{U}_n$ is formed).
- The covariance matrix $C_{ij} = \sum_{\mathcal{U}_n} (\hat{\mathbf{s}}_k)_i (\hat{\mathbf{s}}_k)_j$ is computed ($\hat{\mathbf{s}}_k$ means that the mean value (on $\mathcal{U}_n$) has been subtracted), and its singular values are determined.
- The vectors corresponding to the largest singular values are supposed to represent the directions spanning the hyperplane defined above by $\mathbf{A}_n$ and $\mathbf{b}_n$.
- To reduce noise, $\mathbf{s}_n$ is projected onto these dominant directions.

The method is iterated a few times for convergence. The choice of the parameters entering the algorithm (m, τ, diameter of $\mathcal{U}_n$, number of singular vectors to project on) is the crucial problem and has to respect the particular properties of the signal and of the noise.

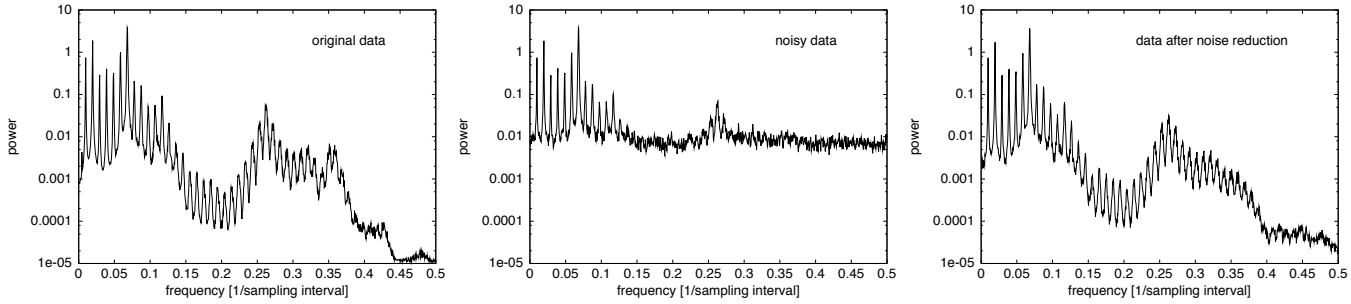

Figure 2: *The power spectrum of 3 seconds of the vowel "a": original recording, after adding noise numerically, and after nonlinear noise reduction. Most of the structure of the original spectrum below the noise level could be reconstructed.*

We use a recording lasting 3 seconds of the vowel "a" for a demonstration of the method for an aperiodic stationary signal. Is is contaminated numerically by 10 percent white noise, and afterwards filtered by the noise reduction algorithm. The power spectrum before adding noise, after adding noise, and after noise reduction is shown in Fig.2. Obviously, we were able to restore significant parts of the spectrum which are well below the noise level and thus invisible for any band-pass filter.

The voice signals studied in the following are taken from a language course on CD ROM with a sampling rate of 22.050 kHz, sampled with 12 bit. The data were converted to real numbers and numerically contaminated by different types and amplitudes of noise and subjected to the noise reduction algorithm. As a measure of performance, we use the gain in dB, given by

$$\text{gain} = 10 \log_{10} \frac{\sum (y_k - s_k)^2}{\sum (\hat{y}_k - s_k)^2}\,, \tag{2}$$

where s_k is the clean, y_k the noisy and $\hat{y}_k$ the signal after noise reduction. Additionally, we reconvert noisy and denoised signals into the `wav`-audio format and inspect the results accoustically.

The crucial aspect for the application of the nonlinear noise reduction algorithm is the choice of the correct embedding parameters and the dimension of the linear subspace onto which we project in order to capture the structure we want to preserve. The surprising issue of this paper is that structure in embedding space does in fact exist in human voice signals. Human voice forms an aperiodic and highly non-stationary signal. In Fig.6 we show the trace of the italian words "buon giorno". It is composed of sub-units, called phonemes, where the signal is almost periodic albeit unharmonic, so that it is reasonable to assume a limit cycle behavior on these episodes. The shape of the wave form changes smoothly and slowly inside a phoneme, but drastically from one phoneme to another (Fig. 3), which can be considered as different types of dynamics.

Careful investigation of time- and lengthscales, including the use of recurrence plots [12, 13] (Fig. 4), shows that the sound wave characterizing a single phoneme (duration between 50 and 150ms) has a characteristic profile on about 5-10ms. A kind

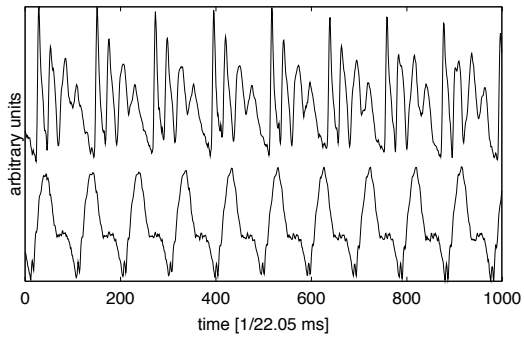

Figure 3: *Zoom into the time series representing two different phonemes (same scale, arbitrary offset).*

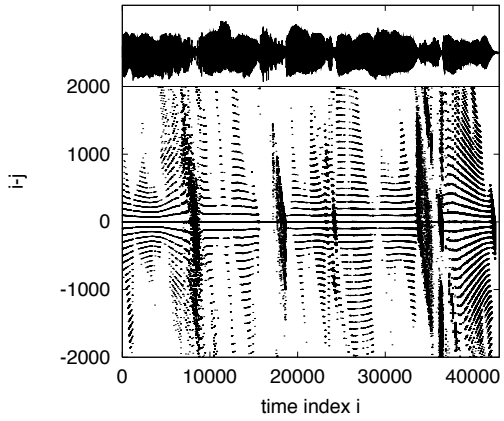

Figure 4: *Main panel: Section of a recurrence plot: In the plane of indices i, j a dot is printed, whenever the delay vectors fulfill $|\mathbf{s}_i - \mathbf{s}_j| < \epsilon$. Upper panel: The speech signal underlying the recurrence plot.*

of phase angle on this highly nontrivial oscillation will then identify the instantaneous amplitude. Thus our time delay embedding space should allow to identify the actual phoneme and the phase inside the phoneme. Both is achieved by 20 to 30-dimensional delay-vectors with a time lag of 3 to 5, covering a time interval of about 8ms. In this reconstructed state space neighbors represent very similar wave forms and carry thus the redundancy needed to reconstruct the original signal. The neighborhood sizes for the local linear reconstruction of the dynamical constraints are chosen to guarantee about 5-20 neighboring states. Although this number is undesirably small, it cannot easily be increased. A single phoneme does not offer more than $\approx$20 almost repetitions of a given wave. Searching for neighbors in other words (presumably in identical phonemes) introduces large numerical effort, requires longer sentences and, most importantly, does not improve the situation much, since changed amplitudes and dilatation or compression of identical phonemes in different words destroy the similarity. Thus all results presented here were gained from intra-phoneme neighbors. Fig.4 is a section of a recurrence plot proving these claims.

The high dimension of the embedding space helps to identify neighbors also for rather high noise levels: Usually, neighborhoods merge if all data are contaminated by large amounts of noise. Here, due to the fact that the signal is rather sparsely filling the 20 to 30-dimensional space, this is not a problem, and we find reasonable results (Fig.5). For noise levels bigger than 150% the computation of the singular values of the covariance matrix gives unreliable results and the filtering is performed via an averaging between the identified neighbors rather than a projection into the approximated sub-manifold. However, this may be seen as a degenerate projection onto a zero dimensional space and is fully contained in the general algorithm.

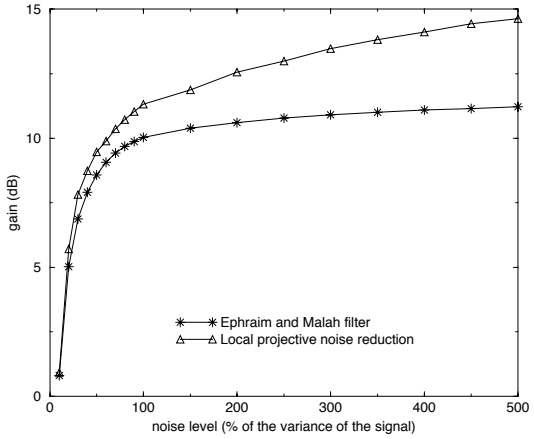

Figure 5: *The gain of the noise reduction scheme as a function of the noise level. The Ephraim-Malah adaptive filter [3] was used as a benchmark.*

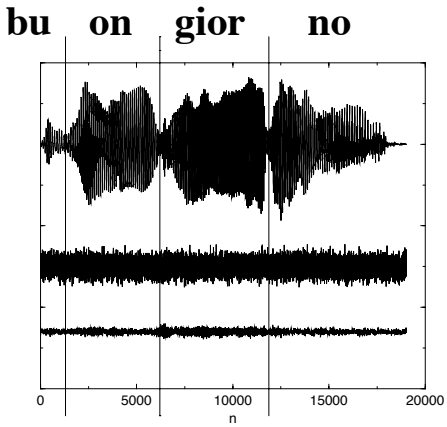

Figure 6: *The clean signal of "buon giorno", noise added to the signal, and the remaining noise after noise reduction (same scale, different offsets). The amplitude of the remaining noise varies systematically, i.e. the success of the noise reduction depends partly on the signal.*

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From a coupled map lattice to a kinetic Ising model

Frank Schmüser, Wolfram Just and Holger Kantz

Since the middle of the seventies the investigation of deterministic chaos has become one of the prominent fields in science, especially in physics. A lot of knowledge has been gained since that time, in particular for few degree of freedom systems, and a whole machinery of tools has been developed for the diagnostics of chaotic motion. We just mention Lyapunov exponents and fractal dimensions as the most popular quantities. Parallel to these developments the question has been raised to which extent the number of degrees of freedom enters the business. Unfortunately, much less progress has been achieved in this direction. Only few results are available and most of them are bound to the investigation of model systems. Within that context coupled map lattices (CMLs) have been introduced at the end of the eighties as a widely studied model class [1]. In these systems local chaotic units which are modelled by simple maps are placed on a lattice and are coupled to each other. For large lattices the dynamics of a CML becomes high dimensional chaotic. In comparison to non–linear partial differential equations, which can often model a system in a more realistic fashion, principal aspects of "spatio–temporal chaos" can be investigated more easily in coupled map lattices.

There is just one class of many degree of freedom systems which is fairly well understood, namely statistical mechanics at and near thermal equilibrium. Unfortunately, the systems studied in the field of space time chaos are often far from equilibrium so that the tools of equilibrium statistical mechanics may fail. Nevertheless, the reduction to relevant degrees of freedom, sometimes called coarse graining, may be equally successful in both areas. By elimination of irrelevant degrees of freedom one maps the microscopic deterministic equation of motion to a stochastic model where the noise captures the irrelevant information. In this way coupled map lattices can be related to spin systems with stochastic dynamics.

CMLs can also undergo phase transitions, if one changes a parameter. The just mentioned statistical methods become especially relevant in the study of these cooperative phenomena in CMLs. The CML that we have studied is motivated by the model of Miller and Huse [3], a prominent example for a CML with a phase transition. In the Miller Huse model antisymmetric chaotic maps are placed on a two–dimensional lattice and nearest neighbor lattice sites are coupled. For a sufficiently strong coupling a spontaneous magnetization develops in the corresponding spin system. This continuous phase transition resembles phenomenologically the one in the two dimensional Ising model. In [2] critical exponents were determined numerically and compared to the Ising case, but the results were inconclusive. In particular, their values depend on whether the CML is updated synchronously or asynchronously. One can summarise that the phase transition of the Miller Huse model is still far from being understood, in particular since no quantitative description of the spin dynamics could be derived.

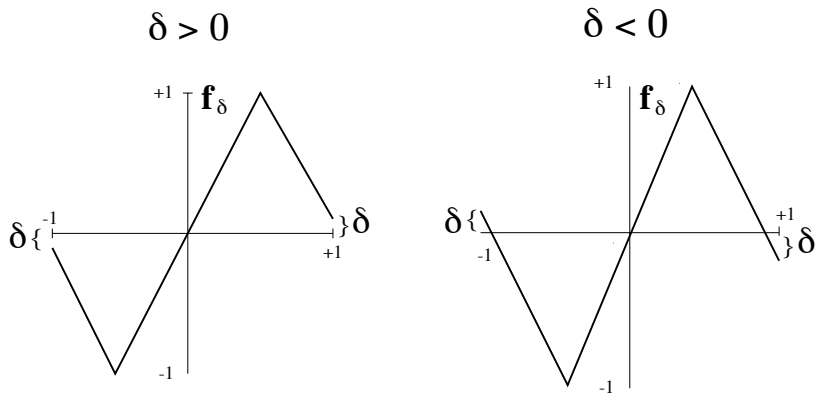

Figure 1: *The deformed antisymmetric tent map f_δ.*

In order to reach some progress in this direction we have investigated a slightly different model system with analytical methods [4, 5]. As a first step we also confined ourselves to a one dimensional lattice, i. e. a chain, with N sites. A deformed antisymmetric tent map f_δ (cf. fig. 1) operates on each lattice site and causes a locally chaotic dynamics. Nearest neighbours interact, so the full dynamics of the CML is given by

$$x_i^{t+1} := (1-\epsilon)\, f_\delta(x_i^t) + \frac{\epsilon}{2}\left(f_\delta(x_{i-1}^t) + f_\delta(x_{i+1}^t)\right) \quad . \tag{1}$$

Here t is the (discrete) time variable, and i labels the lattice sites. As can seen in fig. 1, the single site map f_δ undergoes a symmetry breaking bifurcation at $\delta = 0$ where two coexisting attractors merge into one. The CML depends on two parameters, the coupling strength ϵ and the deformation parameter δ.

An analytical treatment of the CML (1) is possible in the perturbative regime (ϵ, $|\delta| \ll 1$). The unperturbed case with $\epsilon = \delta = 0$ is easily solvable. On each lattice site the map $f_{\delta=0}$ possesses two coexisting attractors, the intervals $[-1, 0]$ and $[0, 1]$. Therefore the whole system has 2^N attractors, each one being an N dimensional cube. In the perturbative regime ϵ, $|\delta| \ll 1$ transitions between these cubes are induced. However, in this regime an orbit stays for many iterations within one cube, before it enters another one. This separation of time scales makes it possible to describe the dynamics of the CML in terms of transitions between cubes. Besides, in perturbation theory the attractors of the CML are given as unions of these cubes, if one neglects sets of volume $O(\epsilon, \delta)$.

Because of the local coupling in the CML (cf. eq. (1)) and the smallness of the coupling constant ϵ only the neighbouring coordinates play a role for a transition between two cubes. Hence the local dynamics of the CML can be reduced to three degrees of freedom. This reduction and the use of symmetries of the CML leads to three types of transitions between cubes in leading order perturbation theory. A transition of a certain type is possible only, if the deformation δ is smaller than a certain bound $\delta_{crit.} = -c\,\epsilon$ where c is a specific constant for this transition type. These constants c can be determined analytically by employing geometric constructions in the reduced

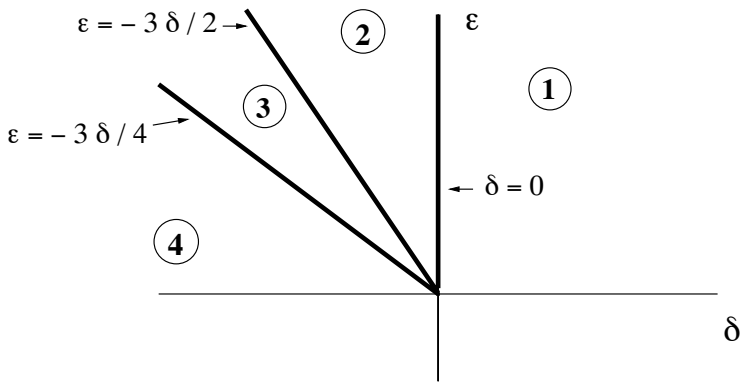

Figure 2: *Diagrammatic view of the bifurcation diagram for the CML studied here. Four parameter regions can be made out in the perturbative regime. Gray–shading indicates the type of coupling in the corresponding kinetic Ising model, antiferromagnetic (light) resp. ferromagnetic (dark).*

phase space. These critical values for the transitions determine the global bifurcations of the CML which take place in the perturbative regime. In the ϵ, δ parameter plane one can identify four regions with different ergodic behaviour (cf. fig. 2). Number and size of the coexisting attractors differ strongly in the various regions.

In region 1 and 2 where at most one transition type is allowed there are many coexisting attractors (the number of attractors grows exponentially with the system size). More interesting is the dynamics in regions 3 and 4, as will become clear after we have introduced a coarse graining of the CML. For this perspective on the CML two spin states for each lattice sites are introduced:

$$s_i(t) := \begin{cases} +1\,, & \text{if} \quad x_i^t \in [0,\,+1] \\ -1\,, & \text{if} \quad x_i^t \in [-1,\,0] \end{cases}$$

In this way an N dimensional cube can be identified with a spin chain of length N. Transitions between cubes correspond to stochastic spin flips at the coarse grained level. The stochastic dynamics of spin flips is a Markov process, because an orbit of the CML stays for a long time within a cube and the memory of a preceding transition resp. spin flip gets lost. Therefore the spin dynamics which is induced by the CML can be described by a master equation. In particular, for stationary solutions of the master equation detailed balance holds. One can show that the CML corresponds, in region 3 and 4, to a kinetic Ising model. There are three types of spin flips:

$$\begin{aligned} &\text{Type (a): e. g.} \quad \ldots\uparrow\uparrow\uparrow\ldots \rightarrow \ldots\uparrow\downarrow\uparrow\ldots. \\ &\text{Type (b): e. g.} \quad \ldots\uparrow\uparrow\downarrow\ldots \rightarrow \ldots\uparrow\downarrow\downarrow\ldots. \\ &\text{Type (c): e. g.} \quad \ldots\uparrow\downarrow\uparrow\ldots \rightarrow \ldots\uparrow\uparrow\uparrow\ldots. \end{aligned}$$

In region 4, where all three spin flip types are allowed, the stationary solution of the master equation can be interpreted as canonical distribution of the one dimensional

Ising Hamiltonian. The temperature T and the sign of the coupling J in the Hamiltonian are determined by

$$\frac{J}{T} = \frac{1}{4} \log\left(\frac{w_c(\epsilon,\delta)}{w_a(\epsilon,\delta)}\right) .$$

Here w_a and w_c are the rates for the spin flip type (a) resp. (c). The temperature thus depends on ϵ and δ. There is ferromagnetic and antiferromagnetic coupling in region 4 of the CML, but antiferromagnetic is predominant (cf. fig. 2).

In region 4 two spin flip types are allowed which describe the diffusion and annihilation in pairs of antiferromagnetic defects in the spin chain. Hence the spin dynamics relaxes to the ground state of the antiferromagnetic Ising model. The temperature of the spin dynamics is vanishing and is a dynamical critical phenomenon where diffusion sets the relaxation time scale. This correspondence to a critical spin dynamics explains the quadratic increase of the transient time with the lattice size for the CML. Overall, the transient dynamics of the CML can be identified with a critical non–equilibrium process of statistical physics.

To conclude: we have constructed a coupled map lattice in analogy to the Miller Huse model. Within our perturbative approach it has been possible to obtain the bifurcation diagram of this coupled map lattice analytically. Besides, we have successfully linked the dynamics of a coupled map lattice to properties of a kinetic Ising model on analytical grounds. The comparison with numerical simulations shows that the leading order of perturbation theory is a good description for parameter values $\epsilon, |\delta| < 5 \cdot 10^{-2}$. For further studies the adaption of the method to coupled maps on a two dimensional lattice seems desirable, since here also finite temperature phase transitions are possible. This would constitute a further step in the understanding of phase transitions in coupled map lattices as exemplified by the Miller Huse model.

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Local estimates for entropy densities in coupled map lattices

Eckehard Olbrich, Rainer Hegger and Holger Kantz

Many natural phenomena involving a huge number of degrees of freedom emerge from spatially extended systems (SESs), with translationally invariant equations of motion and spatial coupling. Thus an understanding of these kinds of systems is vital for the understanding of nature. Natural SESs are typically continuous in time and space and thus described by partial differential equations (PDEs). Nevertheless, a PDE can be approximated by a coupled map lattice (CML), i.e. a model discrete in time and space. CMLs were used as paradigmatic models to study general properties of spatio-temporal chaotic systems. A fundamental question concerning SESs is whether it is possible to extract characteristic quantities from local measurements. This problem is still unsolved in the realm of time series analysis. There were a considerable number of attempts, especially for the dimension density. [1] Nevertheless, the outcome was far from being satisfactory. Common to all these works is to use either time delay or purely spatial embedding for reconstructing the dynamical states or the invariant measure. The general problem is that local measurements can only reconstruct finite dimensional subspaces, though the whole phase space is infinite dimensional, in principle. Therefore, these subsystems are never fully deterministic, since they are coupled to the unobserved part of the phase space and are thus open systems.

However, in systems with local, e.g. nearest neighbour, interactions, the equations of motion include only a few local variables. Regarding only these variables the "local" future is governed by deterministic laws, while the whole dynamics in the measured subspace remains "stochastically" driven. The main idea we want to present is that the local deterministic structure can be exploited to estimate a dynamical entropy which will turn out to be a good approximation for the entropy density of the whole (mainly unobserved) system.

We will study a CML given by

$$x_i(n+1) = (1-\sigma) f(x_i(n)) + \sigma x_{i+1}(n) \;, \tag{1}$$

where i represents the position in space and n the time. σ is the spatial coupling constant. Although we study only the case of unidirectional coupling, the method can be generalised to the case of diffusive coupling easiely.

It is commonly observed that the dynamics of these CMLs is extensively chaotic in suitable parameter regions. Extensive means that the attractor dimension and the Kolmogorv-Sinai(KS)-entropy are proportional to the system size, here the number N of lattice sites. Thus it is possible to define dimension and entropy densities as intensive quantities.

In previous attempts to calculate entropy and dimension densities from observed time series either pure spatial or pure temporal embeddings were used. Since the dynamics for all these embeddings is non-autonomous with respect to equation (1), the corresponding projections of the invariant measure of the CML contain stochastic components so that the entropy diverges [2]. Seeing that we will use a novel embedding procedure ("pyramid embedding") which does not increase the dimension of the reconstructed measure when the dimension of the involved subspace is increased. This will enable us to compute the finite entropy related to the deterministic part of the dynamics in the subspace.

Consider a partitioning of a subspace $\Gamma_{\vec{s}}$ spanned by the components of a state vector $\vec{s}$ with a rectangular grid of mesh size ϵ. Via the invariant measure we can assign a probability p_i to every cell and define the entropy $H(\vec{s},\epsilon) = -\sum_i p_i \ln p_i$. For sufficient small ϵ its ϵ-dependence is given by $H(\vec{s},\epsilon) \propto -D \ln \epsilon$, where D is the information dimension of the projection of the invariant measure into the subspace spanned by $\vec{s}$. Let us choose a second subspace $\Gamma_{\vec{t}}$ spanned by the components of another state vector $\vec{t}$ satisfying

$$\vec{t} = \vec{F}(\vec{s}) \;, \tag{2}$$

which implies that the constraint $\vec{F}$ is determined by equation (1). $H(\vec{t},\vec{s},\epsilon)$ denotes the entropy of the joint probability p_{ij} for the system being in cell i of $\Gamma_{\vec{s}}$ and in cell j of $\Gamma_{\vec{t}}$. The projection of the invariant measure in the enlarged state space has the identical information dimension D due to the constraints (2). Therefore the conditional entropy $h(\vec{t}\,|\vec{s},\epsilon) = H(\vec{t},\vec{s},\epsilon) - H(\vec{s},\epsilon)$ will become independent of ϵ for sufficient small ϵ.

In the following we will use a abbreviated symbolic representation for the states appearing as arguments in the entropies. The pure spatial state of l neighbouring sites will be denoted by $(x_1(n), x_2(n), \ldots, x_{l-1}(n), x_l(n)) \rightarrow \underbrace{\square\square\square}_{l}$. Note that we can omit the time and space indices because of the stationarity and translation invariance.

The simplest way to choose state vectors $\vec{s}$ and $\vec{t}$ fulfilling the constraint (2) is $\vec{s} = (x_i(n), x_{i+1}(n))$ and $\vec{t} = (x_i(n+1))$. Using the symbolic writing we get

$$H(\vec{s},\epsilon) =: H\,(\square\square) \quad \text{and} \quad H(\vec{t},\vec{s},\epsilon) =: H\,(\blacksquare\square) \;.$$

In the symbolic notation of conditional entropies $h(\vec{t}|\vec{s})$ we will hatch $\vec{t}$:

$$h(\vec{t}\,|\vec{s},\epsilon) = H(\vec{t},\vec{s},\epsilon) - H(\vec{s},\epsilon) =: h\,(\blacksquare\square) \;.$$

The KS-entropy of a dynamical system is defined as the conditional entropy of the state of the system knowing the full past. Because the KS-entropy is proportional to the system size N in our case, we can introduce the entropy density η which is the

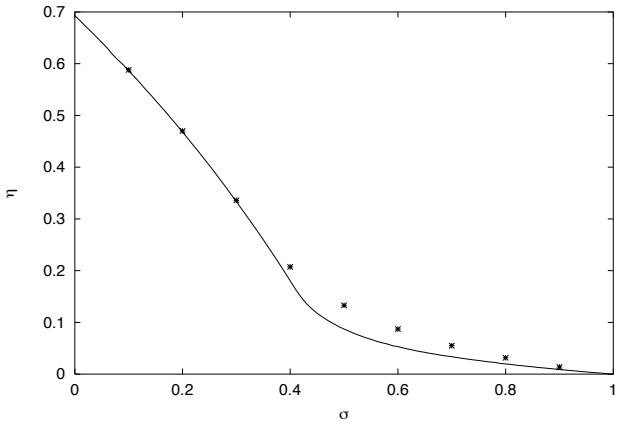

Figure 1: *Estimates of $h_p(1,1)$ (stars) compared to the entropy density computed via the Pesin identity, η_λ.*

KS-entropy divided by N. The definition of the entropy density can be written as

$$\eta = \lim_{N\to\infty} \lim_{m\to\infty} \lim_{\epsilon\to 0} \frac{1}{N}\, h\left(\underbrace{\qquad\qquad}_{N} \right) , \tag{3}$$

where the entropies are calculated for a finite CML with N lattice sites. We rewrite the r.h.s. of (3) in such a way that only a single site remains as the conditioned part in the conditional entropies:

$$h\left(\underbrace{\qquad}_{N} \right) = h\left(\underbrace{\qquad}_{N} \right) + \ldots + h\left(\underbrace{\qquad}_{N} \right) . \tag{4}$$

For any $\vec{s_2}$, $h(\vec{t}\,|\vec{s_1}\,\vec{s_2})$ fulfills the inequality

$$h(\vec{t}\,|\vec{s_1}\,) \geq h(\vec{t}\,|\vec{s_1}\vec{s_2}) \tag{5}$$

It says that the uncertainty about the state $\vec{t}$ is the larger the less I know about the rest of the system. Formally this can be shown using Jensen's inequality. If we apply (5) to (4) we get

$$h\left(\underbrace{\qquad\qquad}_{N} \right) \leq N h\left(\qquad \right) =: h_p(m,1) . \tag{6}$$

The index p means "pyramid" and denotes the form of the spatio-temporal embedding. The first argument m gives the number of time steps used for prediction and the second argument denotes the number of lattice sites predicted.

Now we can formulate an upper bound for the entropy density:

$$\eta \leq \lim_{\epsilon\to 0} \frac{1}{n} h_p(m,n) . \tag{7}$$

Similar to the usual conditional entropies in low dimensional systems the entropies $h_p(m,n)$ become constant on sufficiently small length scales (see e.g. Fig. 2). Thus the

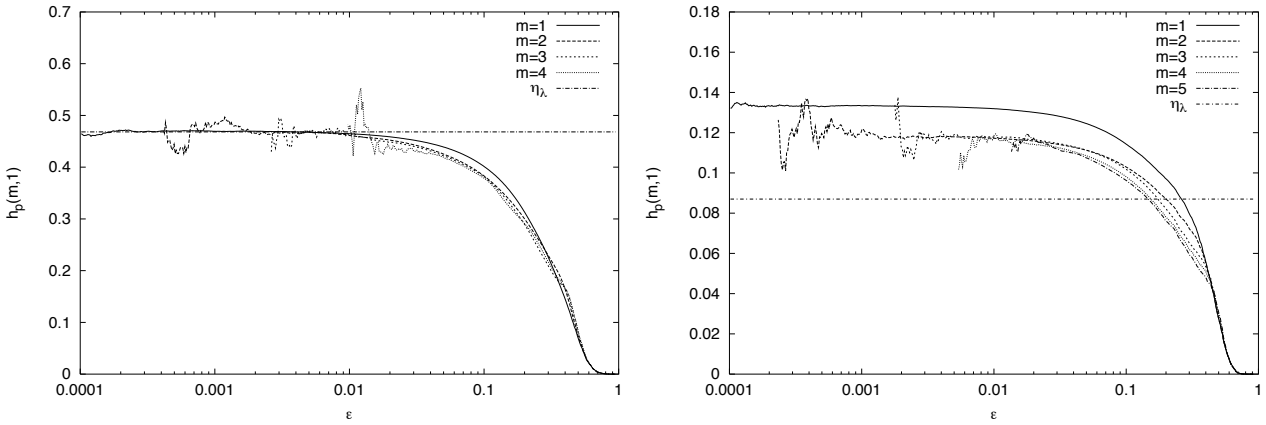

Figure 2: *Estimates of $h_p(m,1)$ for the unidirectional case, linear coupling with $\sigma = 0.2$ (left) and $\sigma = 0.5$ (right).*

entropies $h_p(m,n)$ provide an upper bound for the entropy density already on finite length scales ϵ.

While the results in the former section were derived for the usual Shannon entropy, for numerical investigations the entropies based on the correlation sum are much more convenient. They provide better statistics and require less computational effort. The correlation sum is defined as

$$C(\epsilon) = \frac{1}{N(N-1)} \sum_{i \neq j} \Theta(\epsilon - |\vec{s}_i - \vec{s}_j|) \; . \tag{8}$$

The quantity $H(\vec{s}, \epsilon) = -\ln C(\epsilon)$ can be regarded as a generalized entropy, the so called correlation entropy [3]. Although inequality (5) does no longer hold rigorously in this case, we can interpret the results provided by the correlation sum as approximate estimates of the entropy density as it was done with the usual correlation entropies as approximate estimates for the KS-entropies of low dimensional systems.

Fig. shows the estimates of $h_p(1,1)$ as a function of the coupling σ estimated by using the correlation sum (stars). They are compared to the results for the entropy density calculated by the Pesin identity (solid line) via the Lyapunov exponents $\eta_\lambda = 1/N \sum_i \lambda_i$ with $\lambda_i > 0$. The scaling with respect to ϵ can be seen in Fig. 2 with $\sigma = 0.2$ and $\sigma = 0.5$. In the example with $\sigma = 0.2$ the estimates of $h_p(m,1)$ are almost independent of m and turn out to be a good approximation of the entropy density, calculated by the Pesin-identity. This coincides with the observation in Fig. that the value of $h_p(1,1)$ is very close to the value calculated via the Lyapunov exponents for $\sigma \leq 0.3$. For larger coupling effects of correlations become visible. In Fig. 2 one sees that $h_p(2,1)$ is a remarkably better estimate than $h_p(1,1)$. Further increasing m gives no better results. The remaining difference between $h_p(m,1)$ and the Pesin value might be due to the spatial correlations in the system.

In summary, the method presented above [4] allows to estimate an approximation of the entropy density in coupled map lattices with local couplings using only observables

of local subsystems based on a rigorous upper bound.

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The mode structure of microcrystal and microdroplet lasers

Jens U.Nöckel

The work horse of optics is the *ray picture* – i.e., the short-wavelength limit of Maxwell's wave equations. In the form of the paraxial approximation, it is also the backbone of conventional optical resonator theory. Without such approximations, one is forced to resort to numerical solutions of the full wave equations, which in general reduces resonator design to trial-and-error. An exception are those few systems for which exact solutions can be obtained due to their symmetric, *separable* geometry.

Short-wavelength (or quasiclassical) approximations appear to be as important for light as they certainly are for electrons, and hence it is somewhat surprising that classical concepts such as "diffusion" familiar from condensed matter physics have not played a significant role in optical resonator design until recently. That is so because the engineer often has the freedom to choose geometries for which either the ray picture is simple or the wave equation is separable (up to small perturbations).

This is a luxury that we do not usually have with optical systems that occur in nature – specifically *self-assembled* dielectric microresonators formed from materials as diverse as aerosol droplets or microcrystallites. We study these optical cavities since they exhibit properties that are desirable for artificially patterned micro-optical devices as well. Because of this, the ray picture with its explanatory and predictive power is again of value. However, ray and wave properties combine in new ways when diffraction and interference compete with (a) *ray chaos*, induced by unconventional resonator geometries, and (b) the *openness* of the system due to its coupling to the environment.

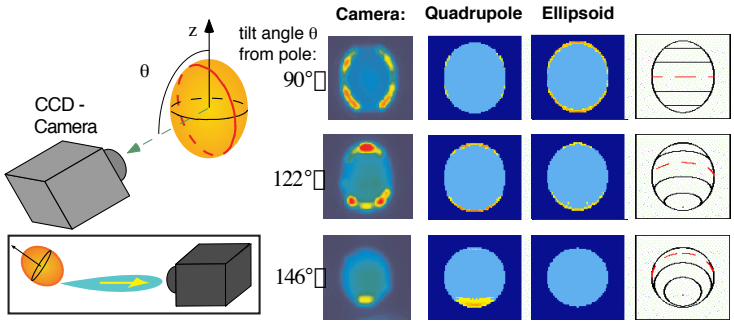

Figure 1: *Left: experimental setup, showing the tilted CCD camera and the droplet it images from different directions. Right: recorded CCD images at three tilt angles θ, compared to two ray simulations, differing only in the assumed droplet shape. Although a quadrupole and ellipsoid shape appear very similar to the eye, only the quadrupole agrees with experiment. The latitude circles as seen by the camera are shown in the rightmost column for orientation.*

Among the pioneering experiments in microcavity optics were spectroscopy and imaging of liquid **microdroplets** falling in air[2]. If they contain a suitable organic dye, excitation by a pump beam can cause these droplets to act as extremely efficient lasers. The feedback required for lasing is provided by long-lived modes whose emission properties are found to depend sensitively on the *shape* of the droplet. To understand these "morphology-dependent resonanaces", ray optics is an excellent framework: firstly, the droplets' diameter of $30-100\,\mu$m is much larger than optical wavelengths; furthermore, the mechanism by which the light is trapped in the droplets is *total internal reflection* at the interface to the outside air – a classical phenomenon in that it occurs almost indepently of wavelength.

Whereas spherical droplets are separable systems, generic oval droplets are not. The latter exhibit highly anisotropic emission directionality, characteristic spectral line shifts and degradation of their resonance lifetimes[1]. In the ray dynamics, chaotic and non-chaotic ("regular") types of motion coexist. An important exception are oval cavities with the shape of a mathematical *ellipsoid*, for which no chaos exists. This raises the question if chaos can be relevant at all in oval droplets, because their shape could be approximated by an ellipsoid. Possible corrections could then be obtained by a perturbation approach.

The subtle distinction between an ellipsoid and the *quadrupolar* oval leads to qualitatively different predictions for the laser emission directionality in a geometric-optics simulation, cf. Fig. 1. Comparison with recent position - and angle - resolved imaging measurements unambiguously determines that the droplets are indeed quadrupoles, and *not* ellipsoids[3]. The emission directionality is thus a sensitive probe of the internal ray dynamics. Its structure is properly revealed only if one portrays the rays not in real space, but in a *phase space* spanned by the positions and orientations at which rays impinge on the surface. The lasing modes are found to be supported by rays that *diffuse in phase space* but are guided by stable structure which arises as a

non-perturbative consequence of the oval shape.

Because of their low refractive index, only a small portion of the phase space is available for long-lived modes in the droplets. The same holds for **zeolite microcrystals** which have recently been discovered as a novel class of composite laser media[4]. Encapsulated in the hexagonal nanopore matrix of the zeolite are dye molecules of the same type as in the droplet example, but the porous host material serves to impose order and stability on the fluorescent "guest" molecules. This leads to novel optical properties, among them polarized emission and lasing, in microcrystallites with hexagonal facets at less than $10\,\mu$m diameter, cf. Fig. 2 (a,b). The pump thresholds required for lasing can be as small as that of semiconductor based vertical-cavity surface-emitting lasers. The lasing modes exhibit a frequency spacing consistent with the optical paths shown in Fig. 2 (a). An infinite family of such periodic orbits with identical lengtsh exists, held in the cavity by internal reflection at the facets. Total internal reflection requires plane interfaces, which is well satisfied except at the corners. But the latter are in fact reached by a "degenerate" member of the periodic-orbit family in Fig. 2 (a).

As expected, experiment and numerical wave calculations, Fig. 2 (b) and (c), reveal that most oft the emission originates at the corners, whereas the internal intensity is distributed evenly over the whole periodic-orbit family of Fig. 2 (a). In contrast to the smooth droplets, the *directions* into which the light is radiated by these hexagonal crystals cannot be explained by geometric optics, because the radius of curvature at the corners is much shorter than the wavelength, leading to *corner diffraction*. In a simulation which approaches the limit of sharp corners starting from a shape with rounded corners via a continuous reduction of the radius of curvature ρ, one finds a crossover in the spectrum from level repulsion for $\rho \gg \lambda$ (=wavelength) to pronounced near-degeneracies which develop and stay practically unchanged as soon as $\rho < \lambda$. This qualitative change is indicative of a transition from quantum chaos to *pseudointegrability* (a nonseparable system without chaos); but it is not accompanied by a similar transition in the emission directionality: over

a large range of ρ above and below λ, the light emanates from the crystal approximately parallel to its facets. Intruigingly, that is in fact what the ray picture predicts for the case of rounded corners where it is again applicable.

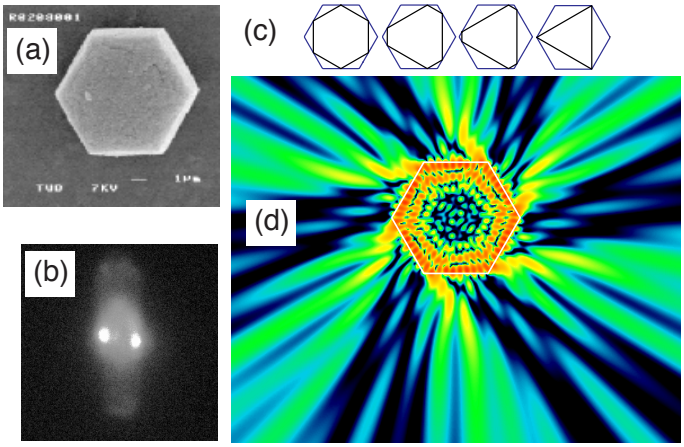

Figure 2: *Hexagonal dye-doped zeolite crystals: cross section (a) and laser emission (b). Periodic ray orbits in (c) are internally reflected, except for the rightmost one entering the corners. The cross-sectional field intensity (d) from numerical solution of the wave equation shows emission predominatly from the corners.*

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Coulomb Blockade in Chaotic Quantum Dots: Interplay Between Interactions and Geometry

Kang-Hun Ahn and Klaus Richter

The understanding of the interplay between many-body interactions and chaos has evolved to a prominent field in mesoscopic physics. This challenging issue brings together two seemingly disconnected fields, namely many-particle physics and quantum chaos. Classically chaotic independent-particle dynamics is found in mesoscopics for both, disordered systems due to scattering at impurities and *clean* quantum dots, where the shape of the confining potential can give rise to chaotic electron motion. While interaction effects in disordered systems have been intensively studied in the recent past, accounts on the inter-relation between many-body effects and chaotic dynamics in ballistic quantum dots are still rare (see, e.g., Refs. [1]). The latter systems can be modelled by quantum billiards that have served as prototypes to investigate quantum signatures of integrable and chaotic single-particle dynamics. Hence a generalization of these quantum chaos concepts to interacting particles in billiards appears natural.

Here we report on the influence of interactions and geometry on ground states of chaotic quantum dots[2]. Our work was partly motivated by new state-of-the-art measurements[3, 4] of charge transport through quantum dots with variable size and shape, which represent ideal tools to investigate experimentally interaction effects in confined chaotic systems. If such a dot with N electrons and ground state energy E_N is only weakly coupled to external leads a conductance peak is observed, upon tuning a gate voltage connected to the dot, whenever the chemical potential $\mu_N = E_N - E_{N-1}$ coincides with that of the leads. The spacing between neighboring peaks as function of gate voltage is proportional to the capacitive energy

$$\chi_N = E_{N+1} - 2E_N + E_{N-1} \; . \tag{1}$$

A number of recent experiments[3, 4] showed that fluctuations of χ_N resemble a Gaussian distribution, while the assumption of a constant interaction, which properly describes the mean conductance peak spacing, combined with random matrix theory (RMT) for the single particle fluctuations, predicts a Wigner-Dyson distribution. Moreover, the measured peak spacing fluctuations, $\delta\chi = (\langle\chi_N^2\rangle - \langle\chi_N\rangle^2)^{1/2}$, significantly vary between the different experiments and partly exceed the predicted fluctuations of the RMT model considerably.

We address the problem of interacting electrons in chaotic systems, in particular the responsible mechanisms for the large sample specific fluctuations observed, by modelling the quantum dots by a family of billiards which arise from a deformation of the unit disk[5]. They serve as appropriate tools to study systematically effects of electron interaction upon changing the billiard geometry. For the deformations to be considered

(see right insets in Fig. 1) the classical independent-particle dynamics is predominantly chaotic.

To include interactions we first calculated the single-particle eigenfunctions and -energies of a deformed billiard. We then used them to construct the Coulomb interaction matrix elements with $V(\mathbf{r}) = e^2/\epsilon r$ and the many-electron Hamiltonian.

We have studied both, ground state properties for many-electron quantum dots (up to ~ 40 spinless electrons) within a self-consistent Hartree-Fock (SCHF) approach[2, 6], and the spectral statistics and Fock space distributions of excited many-body states by diagonalizing the full hamiltonian of few interacting electrons[7]. Here we focus on our results on many-electron ground states relevant to Coulomb blockade physics. By comparing with our exact diagonalization results for few electrons we found that the SCHF results are very accurate, even for strong interactions.

The SCHF results for the capacitive energies χ_N, Eq. (1), do not show any visible dependence on N but rather on the dimensionless interaction strength R/a_B^*, where R is the system size and $a_B^* = \hbar^2\epsilon/m^*e^2$ the effective Bohr radius of the host material. (In terms of the quantity r_s we have $R/a_B^* = \sqrt{N} r_s$.) In the following we consider the variance of the capacitive energy fluctuations, $\delta\chi$, where the statistical average $\langle \ldots \rangle$ is performed over N, as in the experiments[3, 4].

The central result is summarized in Fig. 1. It shows $\delta\chi$ as a function of interaction strength for three different geometries depicted as insets close to the curves. For small size quantum dots (high density, $R/a_B^* \lesssim 12$) $\delta\chi$ is close to the RMT prediction, marked as the horizonal line, and in agreement with the RPA result of Ref. [9]. In terms of r_s, $\delta\chi$ retains the RMT value up to electron densities $r_s \approx 2$. Most interestingly, we find for larger R/a_B^* a cross-over to a regime where the capacitive energy fluctuations increase roughly linearly with increasing interaction strength. Such a clear-cut cross-over behavior has not been found in any tight-binding model for disordered systems [6, 8], indicating that it could be a property of confined ballistic systems.

Roughly, the cross-over to enhanced fluctuations $\delta\chi$ can be understood as follows: Electrons in states extending over the whole dot for small R/a_B^* move with increasing interaction to the edge due to the long-range Coulomb repulsion. This is illustrated in Fig. 2 which depicts the total charge densities for the case of eleven electrons and interaction strengths $R/a_B^* = 5$ and 15. Such ordered, charge density wave like structures as that in the right panel of Fig. 2 persist up to high electron numbers. We still found these states for $N = 40$, the highest N considered. When the states near the edge are fully occupied the corresponding mean field reduces the accessible space for the next electron above the Fermi level. Then the reduced effective size of the quantum dot gives rise to an enhanced level spacing which is accompanied by enhanced fluctuations, probed in Coulomb blockade experiments.

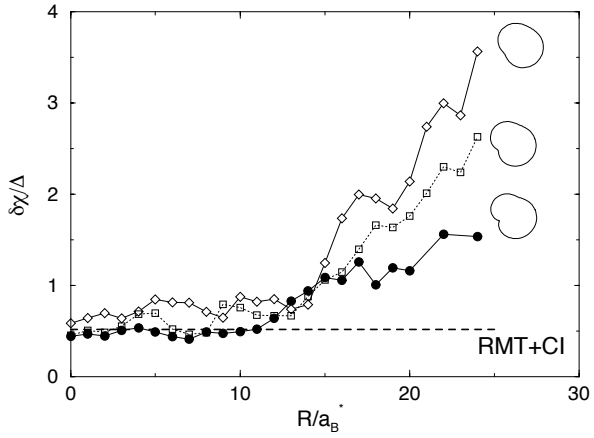

Figure 1: *Fluctuations of capacitive energies* $\delta\chi = (\langle\chi_N^2\rangle - \langle\chi_N\rangle^2)^{1/2}$ *in units of the mean level spacing* Δ *as a function of interaction strength for interacting electrons in three chaotic billiards of different shape shown on the right. For small* R/a_B^* *(or high electron densities)* $\delta\chi$ *agrees with predictions from the constant interaction model combined with random matrix theory (RMT+CI). However,* $\delta\chi$ *shows a clear cross-over near* $R/a_B^*=12$ *and increases with increasing* R/a_B^* *in the strong interaction regime.*

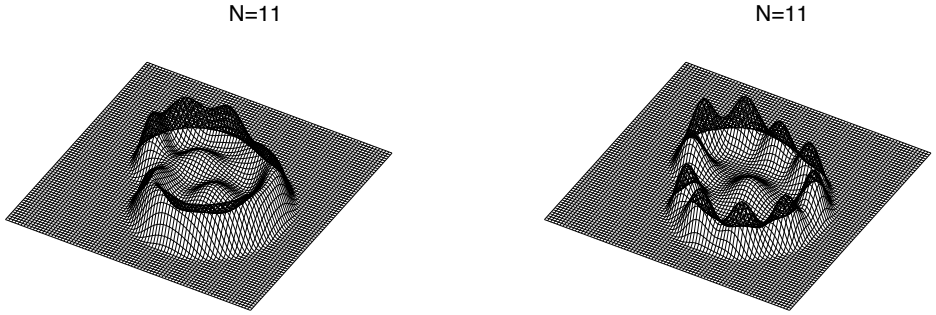

Figure 2: *Total charge densities of eleven interacting electrons for a chaotic dot (right bottom inset in Fig. 1). The left (right) panel shows charge reordering with increasing interaction strength,* $R/a_B^* = 5$ *(15).*

A systematic analysis of various geometries and particle numbers allowed us to extract the following common trends:

(i) An abrupt change in the mean-field potential for fixed N occurs when an electron from the inner region of the dot moves into a state close to the edge.

(ii) With growing system size (lower density) the electrons tend to be localized near the edge of the dot. *For* $R/a_B^* \gtrsim 12$ *the charges are reorganized in an ordered structure similar to a one-dimensional crystal or a charge density wave state.* Our results indicate that even for a chaotic geometry the SCHF single-particle states near the Fermi level in the strong interaction regime do no longer follow RMT owing to charge rearrangement. The reorganized charge states at the edge form a "crystal chain" but differ from a Wigner crystal where the electrons are localized in due to electron correlations. The charge rearrangement considered here results from the competition between the long-

range interaction and the confinement potential.

(iii) A strongly deformed quantum dot where part of the boundary is concave (insets in Fig. 1) renders the formation of edge states more difficult than the dot with a shape close to a disk. Thus the fluctuations $\delta\chi$ are the largest in the latter case and turn out to be system dependent, even if the non-interacting geometries all exhibit chaotic dynamics.

(iv) The shape dependence of the capacitive energy fluctuations found within our model, which does not include effects, e.g. from the dot surroundings, temperature, and spin, may be considered as one possible mechanism that leads to the different widths in the peak spacing distributions of the various experiments[3, 4].

Summarizing, we aim at a better understanding of quantum chaos for many-particle systems, in particular interaction effects in quantum confined chaotic systems. Our present results show that fluctuations in the ground state energies of quantum dots follow approximately a universal random matrix prediction for weak interactions, while there is a crossover to a regime where the fluctuations are strongly enhanced and scale roughly linear with interaction strength. This effect is non-universal depending on quantum dot shape and size. This enhancement is related to the rearrangement of charges into crystal-type states which appear in confined systems at much higher densities than the formation of the Wigner crystal in the two-dimensional bulk.

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Signatures of Classical Chaos in Spectral and Transport Properties of Mesoscopic Quantum Systems

Klaus Richter, Martin Sieber, and Oleg Yevtushenko

Disordered metallic systems and clean quantum systems with a chaotic classical limit behave in some aspects very similarly. In certain regimes, wavefunctions, energy levels or transition amplitudes have universal properties that do not depend on details of the system. They can be described by assuming that matrix elements of the Hamiltonian are randomly distributed. For disordered systems this connection with random matrix theory has been established by diagrammatic expansions and by non-perturbative field-theoretical methods[1]. The treatment of quantum systems with a chaotic classical limit requires different theoretical methods. In order to connect quantum properties to those of the underlying classical system one can apply semiclassical methods that describe for instance energy spectra, magnetic or transport properties in terms of classical trajectories. For example, it was possible to show in this way, by using mean properties of classical trajectories, that statistical distributions of energy levels agree for spectral long-range correlations with the random matrix result[2]. So far, it has not been possible to go beyond this limit of long-range correlations, since this would require information on correlations between classical trajectories which is presently not available. On the other hand, semiclassical methods have the advantage that they can be applied also to the non-universal regime in order to describe system-specific features.

One way to establish a connection between disordered systems and chaotic systems would be to add impurities to a clean system. We have followed this route in two complementary approaches which we summarize in the following:

(I) We examined whether a quantum point-like scatterer can have an influence on the statistical distribution of the energy levels of a chaotic system[3, 4].

(II) We studied the influence of "classical" scatterers on the quantum weak localization correction to the conductance. This quantity, which is based on two-particle Green functions, has much in common with correlations in the spectral density discussed in (I).

(I) *Spectral statistics of a chaotic system with a point scatterer* – The general expectation, based on the random matrix hypothesis, is that the energy level distribution of a clean chaotic system should not be changed with a point-like scatterer. This is supported by the observation that the semiclassical approximation for the density of states is not changed in leading order of $\hbar$. The influence of the scatterer is described semiclassically by a certain class of trajectories, so-called transient orbits that start from the scatterer and return to it. They contribute to the density of states in higher order of $\hbar$ than the leading order contribution from periodic orbits.

It was unexpected to find in [3] that the scatterer could nevertheless have an influence on spectral statistics. When spectral correlation functions are calculated by using mean properties of transient orbits, the so-called diagonal approximation, they show modifications which do not vanish in the semiclassical limit ($\hbar \to 0$). In order that this does not lead to deviations from random matrix statistics, these terms have to be cancelled by off-diagonal terms which contain information about correlations between different trajectories. As was remarked above, the calculation of correlations between trajectories is an outstanding, unsolved problem in general quantum systems. For the transient orbits that describe the influence of a scatterer, however, the off-diagonal terms could be calculated explicitly and systematically. This was done in [4], and it was shown that they indeed cancel the diagonal terms. This implies that the scatterer does not change the statistical distribution of energy levels.

Furthermore, these calculations also allowed for the semiclassical evaluation of parametric spectral statistics. Universality in chaotic systems is not only expected in the properties of single systems, but also in the way in which system properties vary when a parameter of the system is changed. Random matrix theory makes predictions about correlations between densities of states for different parameter values. By calculating the diagonal and off-diagonal terms in [4] it was shown that the parametric spectral statistics of a chaotic system with a point scatterer agree indeed, for small changes of the parameter, with those of random matrix theory. The parameter in these systems is the strength of the scatterer.

(II) *Weak localization effects in antidot systems* – Weak localization (WL), a decrease in the average conductivity with respect to the classical one, is one prominent quantum interference effect observable in a mesoscopic conductor. It was initially found in disordered samples and can be attributed to the constructive interference of diffusive time-reversed trajectories backscattered from (point-like) impurities [6].

WL in ballistic conductors has been studied mainly for small phase-coherent cavities where the elastic mean free paths exceed the relevant device dimensions considerably[7]. Hence backscattering arises from specular reflections at the boundaries and WL should carry features of the underlying classical, possibly chaotic, dynamics.

Ensembles of regularly or randomly placed disk-like classical scatterers in a clean two-dimensional system probably represent the closest ballistic counterpart to impurity scattering in a disordered system. Such a Lorentz gas (see Fig. 1) can be experimentally realized in a high-mobility two-dimensional electron gas patterned with so-called antidots, artificial potential pillars (upper right inset in Fig 2). In this case the usual WL theory for disordered systems is no longer valid: It is well suited to describe coherent backscattering from (point-like) impurities where the scattering is regarded as a *quantum* process [6]. This provides a "quantum splitting" of classical trajectories at impurities allowing the formation of pairs of time-reversed backscattered paths.

Moreover, the electron motion can be regarded as a delta-correlated, diffusive process. Antidots with a diameter a considerably larger than the Fermi-wavelength $\lambda_{\rm F}$ act as *classical* scatterers. Therefore, WL in antidot structures calls for a generalization of WL theory beyond the diffusion approximation in order to account for correlations in the ballistic classical dynamics. In this context semiclassical methods[7, 8] are again attractive, since they provide a close link between the classical dynamics and quantum effects. However, approaches, which exploit the genuine semiclassical limit $\hbar \to 0$ by using stationary-phase arguments, turn out to be too crude to correctly account for ballistic WL.

According to suggestions by Argaman[9] and Aleiner and Larkin [10] it is the exponential separation of initially close orbits in a chaotic system with classical scatterers like antidots, which provides a mechanism for a minimal wave packet of size $\lambda_{\rm F}$ to split into two parts which then follow time-reversed paths before they interfere constructively upon return (see Fig. 1). This approach goes beyond the standard semiclassical stationary-phase arguments introducing another relevant timescale for WL in a chaotic system: the Ehrenfest time for the spreading of the wave packet over a distance of the size a of the antidots, $t_E = \lambda^{-1} \ln (a/\lambda_F)$. Here λ is the mean Lyapunov exponent of the classical system. This approach accounts for correlations in the chaotic ballistic dynamics in the "Lyapunov region" for timescales up to the Ehrenfest-time t_E [10]. For times larger than t_E the classical mechanics is assumed to be uncorrelated and is treated as diffusive again. The result for ballistic WL then reads[10, 5] in the experimentally relevant regime

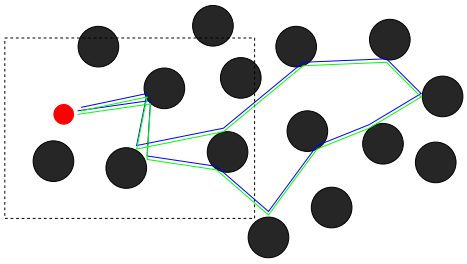
$$\Delta\sigma \simeq -(e^2/\pi h) \exp\{-t_E/\tau_\phi\} \ln(\tau_\phi/\tau)\,. \tag{1}$$

Here, τ_ϕ is the temperature-dependent phase relaxation time and τ is the transport time governing the classical (Drude) conductivity. The standard result for WL in disordered systems is recovered in the limit $t_E \to 0$.

We compare measurements of the temperature dependence of the WL correction $\Delta\sigma$ in antidot structures with theoretical results based on Eq.(1)[5]. The antidots act as classical scatterers since their diameter is significantly larger than the Fermi-wavelength. As shown in Fig. 2 the temperature dependence of $\Delta\sigma$ is well fitted by an exponential law

$$\Delta\sigma(T)|_{B=0} \sim \exp(-T/T_c) \tag{2}$$

for an unusually wide range of $1.2\text{K} \leq T \leq 44$ K with $T_c \simeq 14.5$K. This T-behavior can hardly be explained in the framework of WL in diffusive systems. In order to apply Eq. (1) we have computed the relevant quantities as follows: The Lyapunov exponent λ has been estimated within the simplified model of a 3-disk billiard[11] confirmed by numerical simulations for a disordered Lorentz gas[12]. The T-dependence enters into $\Delta\sigma$ through the overall dephasing rate $\tau_\phi^{-1} = \tau_{e-e}^{-1} + \tau_{e-ph}^{-1}$: It is dominated by *electron-electron* (e-e) interactions at low T ($T < 10$K), while *electron-phonon* (e-ph) scattering



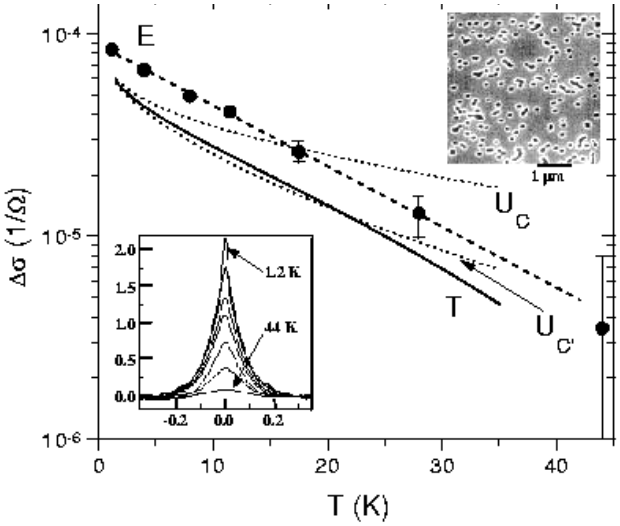


Figure 1: *(left) Sketch of a pair of paths which contribute to coherent backscattering in an antidot system. Orbits of a minimal wavepacket (small filled circle) separate on the scale of the Ehrenfest time by a distance of the order of the size of the classical disk scatterers.*

Figure 2: *(right) Temperature dependence of the weak localization correction $\Delta\sigma$ in an antidot system. Experimental data (filled dots and dashed line) are compared with our theoretical results (solid line T and dotted lines $U_C, U_{C'}$). The line T is the result of WL theory for ballistic systems, Eq. (1). The dotted curves, U_C and $U_{C'}$, show results of the usual WL theory, Eq. (1) with $t_E \to 0$, for diffusive systems for two different strengths of the electron-phonon interaction. Upper inset: Electron micrograph of a disordered antidot array with mean antidot distance 300 nm. Lower inset: Measured $\Delta\sigma$ in units of h/e^2 as a function of magnetic field (in Tesla) for temperatures between $T = 1.2K$ and 44 K.*

must be considered at higher temperatures (here $T > 10$K). We have estimated $\tau_\phi(T)$ using models of dephasing in dirty systems [13, 14] which yield $\tau_{e-e}(T) \simeq A/T$ (with $A \simeq 57$ ps / $T[K]$ for the present experiment) and $\tau_{e-ph}(T) = C/T^2$. Using the estimates for λ, t_E, and $\tau_\phi(T)$, Eq. (1) gives the solid line in Fig. 2.

Up to $T \simeq 15$K, the temperature dependence is predominantly given by e-e interaction and the slope of the theoretical curve, which shows considerable agreement with experiment, is rather insensitive to τ_{e-ph} and, consequently, to the constant C. By variation of C, which remains the only free parameter, we have adjusted the slope of the theoretical line to the experimental one at $T \geq 15K$. We have found a reasonably good agreement of the experimental and theoretical slopes over nearly the entire, wide temperature range.

In contrast, the usual theory for WL in diffusive systems (Eq. (1) with $t_E = 0$), which predicts a logarithmic T-dependence, cannot adequately describe the experiment. There exists no choice for C in τ_{e-ph} which would lead to a reasonable agreement with the experimental data over the whole temperature range (dotted curves U_C and $U_{C'}$ in Fig. 2; the C' chosen in $U_{C'}$ already leads to unrealistically small values of τ_ϕ).

Thus we find a manifestation of classical correlations in the chaotic electron motion of weak localization in antidot systems. This work indicates a way to extract the Ehrenfest time and the classical Lyapunov exponent from the measured quantum correction to the conductance.

The experimental part of the project was performed by G. Lütjering and D. Weiss.

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Threshold detachment by tunneling

Jan M. Rost

Given a negative ion which is approached by an electron at extremely low relative speed – is there a chance to detach the bound electron from the ion and if so, how does it happen?

First, this *does* happen and is realized experimentally in ion storage rings where the electrons are injected parallel to the ions with an absolute velocity close to the speed of light but with well controlled relative motion of some meV. Threshold detachment from the deuteron (D^-) and the oxygen (O^-) negative ions by electron impact [1, 2], and also from B^- [3] have been reported.

This process can be understood theoretically as tunneling of the outgoing electrons under the barrier created by their own mutual repulsion as sketched in Fig. 1 [4].

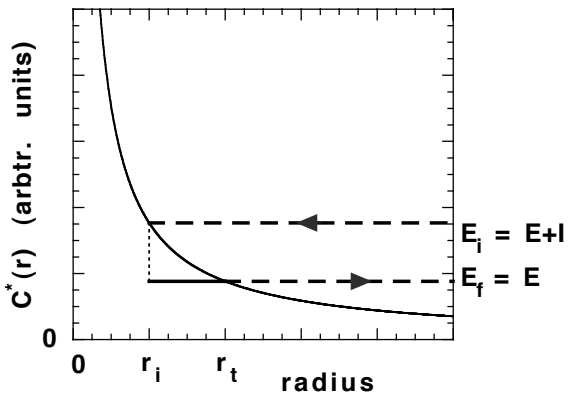

Figure 1: *Sketch of tunneling threshold dynamics on the fixed point manifold with potential $C(r)$ from Eq. (1). The classically allowed incoming and outgoing trajectory on the respective energies E_i and E_f is shown (dashed lines) as well as the tunneling part (solid thick line) which determines the threshold fragmentation probability.*

Quantitatively, the dominant energy variation of the cross section is determined by the corresponding Gamow factor, i.e.,

$$\sigma(E) = \sigma_B P(E) \equiv \sigma_B \exp(-2\Gamma(E)/\hbar) \tag{1}$$

where $i\Phi \equiv \Gamma = \int_{r_i}^{r_t} p dr$ is the tunneling action along a specific classical two-electron orbit and σ_B is a smooth background. The orbit corresponds to a classical fixed point in all degrees of freedom but the (hyper)radial one, $r = (r_1^2 + r_2^2)^{1/2}$, where the r_i are the electron-atom distances. More precisely, the two electrons leave the atom back to back (interelectronic angle $\theta^* = \pi$) and with the same speed ($r_1(t)/r_2(t) = \tan\alpha^*$). This scenario is the Wannier configuration known from the usual, classically allowed threshold ionization process which occurs, e.g., in electron impact ionization of atoms [5]. That only the fixed point orbit is relevant close to threshold is justified by the fact that all available energy (which approaches zero for $E \to 0$ and $r \to \infty$) must be put into the radial degree of freedom r in order to fragment the system. Hence, the system

evolves asymptotically in a frozen configuration where neither its geometrical shape ($\theta = \theta^*$), nor the relative interparticle distances $r_1/r_2 = \tan\alpha^*$ change. Moreover, due to the Coulomb scaling properties, any partial wave with angular momentum L reduces in scaled coordinates to an S-wave since the scaled angular momentum reads $\tilde{L} = L\sqrt{E}$ [6]. Therefore, only the S-wave has to be considered. Hence, the radial motion on the fixed point manifold is governed by the Hamiltonian (atomic units are used unless otherwise stated)

$$H = \frac{P_r^2}{2} + \frac{C(\alpha^*, \theta^*)}{r}\,, \tag{2}$$

where the effective charge $C = 2^{-1/2}$ results from the evaluation of the electron-electron repulsion $V = |\vec{r}_1 - \vec{r}_2|^{-1}$ at the fixed point.

For each energy $E = H$ we can calculate the tunneling action $\Gamma(E)$ entering from the imaginary momentum $p = (-P_r^2)^{1/2}$ of Eq. (1). The integration limits are the outer turning point r_t where the orbit becomes classically allowed, $p(r_t) = 0$, and a starting point r_i, see Fig. 1. In contrast to threshold fragmentation under attractive Coulomb forces tunneling threshold fragmentation depends on the initial configuration, at least as far as the value of r_i is concerned which will influence shape and magnitude of $P(E)$ in Eq. (1).

A realistic approximation for r_i is the classical turning point of the incoming electron, as it appears on the fixed point manifold whose dynamics is specified by Eq. (1). Hence, to determine this turning point of the *incoming* electron we put $P_r = 0$ in Eq. (1) at the incoming electron energy of $E_i = E + I$ to yield

$$r_i = C_*/(E + I). \tag{3}$$

The initial momentum of the *outgoing* electron pair $p(r_i) = \sqrt{2I}$ follows from the Hamiltonian Eq. (1) on the final energy surface $E_f = E$. The situation is sketched in Fig. 1. Evaluating the tunneling integral the threshold detachment probability $P(E)$ in Eq. (1) reads in dimensionless units explicitly

$$P(E) = \exp\left[-4C\alpha\sqrt{\frac{m_e c^2}{2E}}\left(\arctan\sqrt{\frac{I}{E}} - \frac{\sqrt{IE}}{I+E}\right)\right], \tag{4}$$

where $\alpha = 1/137$ is the fine structure constant, $m_e c^2 = 511\text{keV}$ is the rest mass of the electron, and $C = C_*$ is the repelling charge of the two electrons on the fixed point manifold in units of e, see Eq. (1). One can cast Eq. (4) into a more familiar form of atomic units by noting that $m_e c^2/\alpha^2 = e^2/a_0 = 27.2116\text{eV}$ is just the atomic energy unit. Clearly, the tunneling mechanism breaks the scaling invariance of $P(E)$ for different systems characterized by different ionization potentials I since $P(E)$ does not only depend on E/I but also on $m_0 c^2/E$. This is one of the major differences compared to Wannier's classical result for threshold ionization under attractive Coulomb forces [5].

Different threshold cross sections are shown in Fig. 2 corresponding to detachment from the ions B^-, D^-, and O^- respectively. The theoretical cross sections are obtained by fitting the experimental cross sections to Eq. (1) with

$$\sigma_B(E) = \sigma_0/(b_0 + E/I), \tag{5}$$

where σ_0, b_0 are fitting parameters and $P(E)$ is the analytical tunneling probability from Eq. (4). The $\sigma_B(E)$ obtained in this way are indeed smooth functions [4].

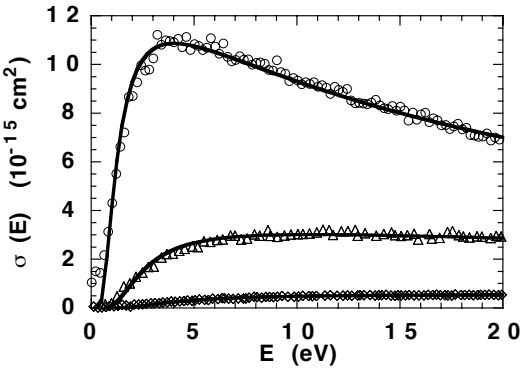

Figure 2: *Sketch of tunneling threshold dynamics on the fixed point manifold with potential $C(r)$ from Eq. (1). The classically allowed incoming and outgoing trajectory on the respective energies E_i and E_f is shown (dashed lines) as well as the tunneling part (solid thick line) which determines the threshold fragmentation probability.*

In summary, separating the rapidly changing detachment probability $P(E)$ from the background cross section $\sigma_B(E)$ we have shown that threshold fragmentation under asymptotic repulsive Coulomb forces can be treated on the same footing as the well established threshold ionization under attractive Coulomb forces. In contrast to the classical result for attractive forces, threshold detachment of negative ions by electrons can be interpreted to proceed via quantum mechanical tunneling of the outgoing electron pair. This implies a breaking of the scale invariance of $P(E)$ with respect to energy since $P(E)$ depends on $m_e c^2/E$ irrespectively of the target properties while $P_{CL}(E)$ under attractive Coulomb forces is scale invariant.

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Irregular orbits generate higher harmonics

Gerd van de Sand and Jan M. Rost

In the scattering terminology for time-independent problems we can distinguish at different energies direct and indirect (time-delayed) collision processes where the latter give rise to resonances. Belonging to different (in principle observable) energies these processes are not summed coherently.

In contrast the time-dependent Hamiltonian for an atom (binding potential $V(x)$) in a laser field

$$H = p^2/2 + V(x) + E_0 x \cos \omega t \tag{1}$$

mixes energies and therefore, direct and time-delayed indirect contributions can interfere. This gives rise to the enhanced quantum (Fig. 1a) and semiclassical (Fig. 1c) harmonic spectra compared to the classical one (Fig. 1b).

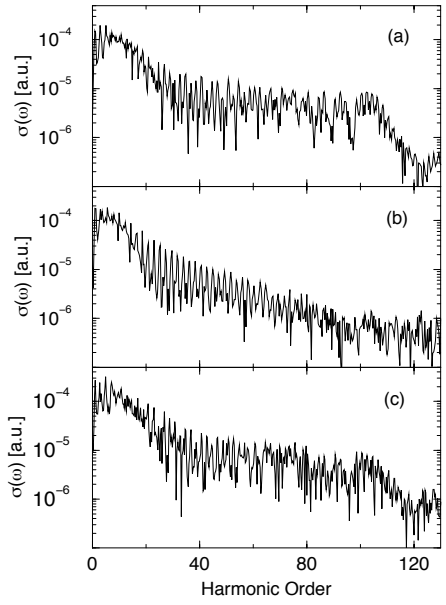

Figure 1: *Quantum (a), classical (b), and semiclassical (c) spectrum of higher harmonics according to Eq. (2).*

To proof that this enhancement, also known as plateau, is due to interference, one must carry out a full semiclassical calculation of high harmonic generation (HHG) which has not been done so far due to considerable technical difficulties. However, using a uniformized propagator following the ideas of Hermann and Kluk [1, 2] we have succeeded in obtaining a converged semiclassical spectrum of HHG. Moreover, we were able (i) to prove that HHG is a pure interference effect, and (ii) to identify the different types of trajectories which interfere with each other. We have probed HHG in the setting of laser assisted scattering [3], i.e., we start an electronic wavepacket under the influence of the laser field 70 a.u. away from the ion and observe the emitted radiation

$$\sigma(\omega) = \int d(t) e^{i\omega t} dt \tag{2}$$

where

$$d(t) = -\left\langle \Psi(t) \left| \frac{dV(x)}{dx} \right| \Psi(t) \right\rangle , \tag{3}$$

is the time-dependent dipole acceleration and $|\Psi(t)\rangle$ has evolved from a Gaussian $|\Psi(0)\rangle$ under the time-dependent Schrödinger equation with the Hamiltonian of Eq. (1). For the technical details we refer the reader to [4]. Typically 10^6 classical trajectories are necessary to converge the semiclassical expression for $d(t)$ from Eq. (3). Among the classical trajectories from which the semiclassical dipole acceleration Eq. (3) is constructed we can distinguish trajectories which suffer a time delay when passing the nucleus (i.e. $x \approx 0$) from the "mainstream" trajectories which are not slowed down. Furthermore, among the time-delayed trajectories we can identify two groups. Trajectories of the first group (dotted line in Fig. 2) get "stranded" on top of the barrier of the effective potential $V_{eff}(x) = V(x) - E_0 x$. The second group is formed by trajectories which become temporally "trapped", (solid line in Fig. 2). The trapped trajectories are chaotic in the sense of an extreme sensitivity to a change in initial conditions [4].

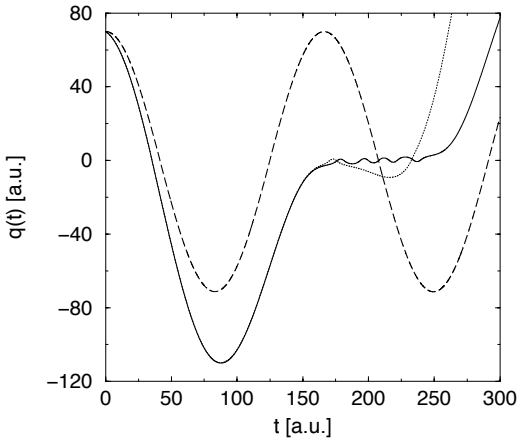

Figure 2: *Examples for direct (dashed line), stranded (dotted line) and trapped (solid line) trajectories, see text.*

Having identified the orbits, or equivalently, the initial conditions, which are responsible for the higher harmonics we can artificially construct a harmonic spectrum without those contributions to double check that they are really responsible for HHG. This has been done in the semiclassical spectrum of Fig. 3b where the time-delayed trajectories (about 3% of all initial conditions) have been discarded. Clearly, the plateau has disappeared and the spectrum is similar to the purely classical spectrum with trajectories for all initial conditions included (Fig. 1b). Discarding only the trapped trajectories (0.6%) smears out the cutoff and leaves a reduced plateau for lower harmonics (Fig. 3a). Hence, the quantitative semiclassical reproduction of the quantum HHG spectrum together with the absence of higher harmonics in the classical case (Fig. 1) *and* in the semiclassical case if irregular, time-delayed trajectories are discarded (Fig. 3) confirms our explanation of the origin of the higher harmonics.

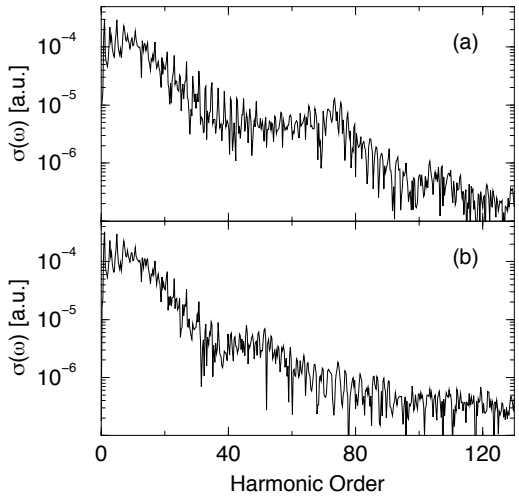

Figure 3: *Semiclassical HHG spectrum as in Fig. 1 but without trapped trajectories (a), and without time-delayed trajectories (b), see text.*

To summarize we have shown that higher harmonic generation can be interpreted as a semiclassical interference effect between regular and time-delayed trajectories of the electron. The time-delay is either due to a temporal trapping which generates chaotic dynamics or due to a stranding on top of the potential barrier. Along with this time delay goes a characteristic difference in action compared to the undelayed mainstream orbits. Remarkably, despite the chaotic dynamics of the trapped trajectories, one can obtain a converged semiclassical spectrum if a proper semiclassical propagator such as the Hermann-Kluk propagator is used which does not break down at the (abundantly occuring) caustics. The resulting semiclassical harmonic spectrum agrees well with the quantum spectrum.

We would like to thank O. Frank for the calculation of the quantum spectrum and C. H. Keitel for helpful discussions. Financial support from the DFG under the Gerhard Hess-Programm and the SFB 276 is gratefully acknowledged.

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Residual symmetries in the spectrum of periodically driven alkali Rydberg states

Andreas Krug and Andreas Buchleitner

The excitation and subsequent ionization of Rydberg states of atomic hydrogen by microwave fields is one of the most prominent examples of the manifestation of classically nonlinear dynamics in a realistic physical system [1]. Given a driving field frequency comparable to the classical Kepler frequency of the unperturbed Rydberg electron, the electron's classical trajectory goes chaotic for sufficiently large driving field amplitudes, finally leading to its ionization on a finite time scale [2]. As a matter of fact, already before the onset of classically chaotic motion, i.e. at not too large driving field amplitudes, individual quantum eigenstates of the atom in the field exhibit energies and ionization rates which are determined only by the orbital parameters of the classical trajectory they are associated with [3]. Those orbits which are the least stable under the external perturbation induce the largest ionization rates for their associated eigenstates. Consequently, in this near-integrable regime of classical dynamics, it is possible to classify the eigenstates of the atom in the field through quantum numbers associated with the orbital parameters of unperturbed Kepler ellipses, i.e. with the angular momentum and the Runge-Lenz vector [3].

A considerable part of experimental data has been accumulated in experiments on Rydberg states of alkali atoms rather than of atomic hydrogen [4]. A priori, a classical-quantum correspondence as briefly sketched above for atomic hydrogen cannot be established here, due to the absence of a well and uniquely defined classical Hamiltonian. In particular, the atomic core destroys the symmetry characteristic for the hydrogen atom and the Runge-Lenz vector is no more a constant of motion.

It is the purpose of the present project to develop a rigourous treatment which allows for the first time for a *direct* comparison of hydrogen and alkali ionization dynamics under *precisely the same* conditions, without adjustable parameters. First results of our numerical experiments directly address the above question of quantum-classical correspondence for periodically driven alkali atoms.

The nonrelativistic Floquet Hamiltonian [5] of a one-electron atom exposed to a linearly polarized microwave field of (constant) amplitude F and frequency ω, in the length gauge, employing the dipole approximation and atomic units, writes:

$$\mathcal{H}(t) = \frac{\mathbf{p}^2}{2} + V_{\rm atom}(r) + Fz\cos\omega t - i\partial_t,\ r > 0. \tag{1}$$

To find the eigenstates ("dressed states") of the atom in the field, we make the Ansatz:

$$|\Psi_\varepsilon\rangle = \sum_k \exp(-ik\omega t)|\Psi_\varepsilon^k\rangle = \sum_{k,\ell} \exp(-ik\omega t) Y_{\ell,m}(\theta,\phi)|\Psi_{\varepsilon,\ell}^k\rangle/r, \tag{2}$$

with $Y_{\ell,m}(\theta,\phi)$ the spherical harmonics. The additional quantum number k counts the number of photons that are exchanged between the atom and the field, and ε denotes the quasi-energy of the atom in the field. Due to the transfer of angular momentum associated with the absorption (emission) of a photon, the generalised parity $\Pi = (-1)^{k+\ell}$ is conserved.

As a unique one-particle potential $V_{\rm atom}(r)$ for alkali atoms is unknown, we use a variant [6] of R-matrix theory to describe the interaction of the outer electron with the atomic core. Due to the continuum coupling induced by the external field, all atomic bound states turn into resonances with finite ionization rates Γ_ε. Complex scaling [7] of the Hamiltonian allows to extract the latter, together with the energies ε of the atom in the field. Our method generalizes the approach outlined in [6] to periodically driven systems. Its basic ingredients are described in [8].

This theoretical apparatus is now applied to alkali atoms in a microwave field. Since we want to identify the core induced effects in the alkali problem as compared to the hydrogen spectrum, we use parameter values which have been employed in earlier work on microwave driven Rydberg states [3] of hydrogen. To keep the comparison as transparent as possible, we focus on a microwave frequency $\omega = 1.07171794 \times 10^{-4}$ a.u. which is nonresonant with the hydrogen level spacing in the vicinity of the atomic initial state with principal quantum number $n_0 = 23$. The field amplitude is fixed to $F = 1.072 \times 10^{-7}$ a.u., slightly below the onset of appreciable (chaos-induced [2]) ionization of atomic hydrogen [3]. This choice of parameters defines a near-integrable phase space structure for the classical dynamics of driven hydrogen, with an unambiguous signature in the associated quantum energies emerging from the $n_0 = 23$ manifold. The black dots in fig. 1 illustrate the situation: The driving field lifts the angular momentum degeneracy of the substates of the manifold, which reorganize according to their localization properties in classical phase space [3]. Those states with maximum angular momentum and spherical symmetry experience the strongest field induced ("ac-") shift in energy, whereas those with maximum radial component of the Runge-Lenz vector and "λ-symmetry" [3, 9] remain essentially unaffected by the external perturbation. Since the low angular momentum states are strongly mixed by the field (to build states with λ-symmetry [9]), a new (semiclassical) quantum number p [3] is used to label the n_0 substates of the manifold in the field. The associated eigenstates exhibit spherical symmetry for $p = 0 \ldots 9$, and λ-symmetry for $p = 10 \ldots 22$, respectively [3]. Note that low and high p-values correspond to negligible ionization rates of the atom in the field, due to the *classical* stability of the associated trajectories under external driving [3].

In the presence of a non-hydrogenic core, the Runge-Lenz vector is no more a conserved quantity and the λ-symmetry defining associated eigenstates of the field free atom [9] is destroyed. Therefore, no symmetry argument is available to predict a similar (semi-

classical) organization of the alkali energy levels under external driving, alike the one observed for atomic hydrogen [3]. Notwithstanding, our results for Li Rydberg states exposed to precisely the same external perturbation as for the hydrogen results clearly show that the symmetry properties of the driven Coulomb problem prevail even in the presence of the core. As evident from the open triangles in fig. 1 (a), the hydrogenic part of the Li manifold exhibits globally the same (semiclassical) structure as the hydrogen levels. For low values of p ($\simeq 0 \ldots 9$) this is not surprising as the associated classical trajectories (large angular momenta) do not probe the atomic core [3]. However, for large p-values ($\simeq 10 \ldots 20$), the classical solution of the Coulomb problem does impinge on the nucleus and will certainly suffer scattering off the nonhydrogenic core. Yet, in the presence of the field, this scattering obviously mixes states of λ type only and does not affect the overall separation of the spectrum in spherical and λ states, as a remnant of the classical phase space structure of the driven Coulomb dynamics. Neither does the presence of the core appreciably affect the ionization rates of the dressed states, as obvious from fig. 1 (b). Only at $p = 10$ is there a local enhancement of the width (by approx. one order of magnitude), due to the near resonant coupling of the state to the nonhydrogenic eigenstate originating from $|n = 41, \ell = 0\rangle$, via a six-photon transition (similarly, a very weak mutliphoton coupling slightly enhances the width of the $p = 12$ state). Closer inspection of fig. 1 (a) shows additional structure in the alkali spectrum, on top of the globally hydrogen-like structure: for large values of p (≥ 11), the alkali levels are shifted with respect to the hydrogenic energies. These shifts can be recovered by diagonalization of the hydrogen problem within the restricted subspace spanned by the hydrogenic levels of the alkali Rydberg manifold [10]. In other words, the shifted energies are the solutions of the eigenvalue equation

$$PH_{\rm hyd}P|\Phi^{k_0}\rangle = (E + k_0\omega)|\Phi^{k_0}\rangle, \tag{3}$$

where $H_{\rm hyd}$ is obtained from from (1) setting $V_{\rm atom}(r) = -1/r,\ r \in]0, \infty[$, and P the projector onto the hydrogenic subspace of the alkali manifold labeled by the principal quantum number n_0 and the photon number k_0. Such a procedure is legitimate as long as the states emerging from the nonhydrogenic part of the alkali manifold have vanishing overlap with the complete hydrogen manifold emanating from (n_0, k_0).

Solving (3) for E is tantamount to finding the roots of

$$\det(Q\frac{1}{H_{\rm hyd} - (E + k_0\omega)}Q) = 0, \tag{4}$$

with $Q = 1 - P$ the projector onto the orthogonal complement of the hydrogenic subspace for given (n_0, k_0). Without loss of generality we choose $k_0 = 0$ hereafter. Consequently, for one single non-vanishing quantum defect δ_{ℓ_0}, (4) becomes

$$\sum_{\varepsilon} \frac{|\langle n_0, \ell_0|\Psi_{\varepsilon}^{k_0=0}\rangle|^2}{\varepsilon - E} = 0, \tag{5}$$

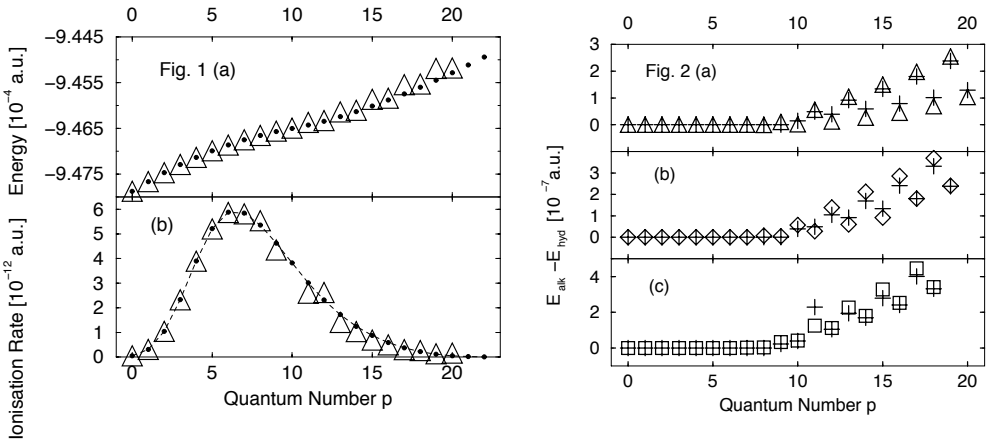

Figure 1: *Energies (a) and ionisation rates (b) of Rydberg states with principal quantum number $n_0 = 23$ of Li (triangles) and of atomic hydrogen (dots) exposed to a linearly polarized microwave field. The Li spectrum lacks two of the 23 substates of the manifold, due to the nonvanishing quantum defects of the $\ell = 0$ and $\ell = 1$ statesBoth spectra almost coincide (in energy and ionisation rate) even for larger values ($p \geq 10$) of the quantum number p, despite the fact that the localization properties of the associated eigenstates originate in the dynamical symmetry of the Coulomb potential [9] The latter, which is* destroyed *by the presence of a nonhydrogenic core in alkali atoms. The ionization rate of the $p = 10$ state of Li is locally enhanced with respect to the corresponding hydrogen eigenstate, due to a six-photon resonance with the $|n = 41, \ell = 0\rangle$ state.*

Figure 2: *Shifts $E_{\rm alk} - E_{\rm hyd}$ of the energies $E_{\rm alk}$ of Li (a, triangles), Na (b, diamonds), and Rb (c, squares) as compared to those, $E_{\rm hyd}$, of the $n_0 = 23$ manifold of atomic H in a linearly polarized microwave field, with the same parameters as in fig. 1. Due to the nonvanishing quantum defects [11], three (Na) respectively four (Rb) energy levels are missing in (b) and (c). The nonvanishing shifts for large $p \geq 9$ values can be accounted for by projecting out the low ℓ components, eq. (4). The agreement between this perturbative approach (crosses) and the exact quantum results (open symbols) is always better than the average level spacing of the hydrogen manifold (dots in fig. 1), except for the relatively large discrepancy at $p = 11$, in (c). The latter is due to a multiphoton resonance between the alkali eigenstate and a nonhydrogenic (low ℓ) state.*

where $|n_0, \ell_0\rangle$ spans the orthogonal complement of the hydrogenic subspace of the alkali atom within the $(n_0, k_0 = 0)$ manifold. Note that (4) has to be evaluated for different values of the generalized parity Π, and that we have to solve (5) separately for $\ell_0 = 0$ and $\ell_0 = 1$, in order to recover the level shifts observed for Li in fig. 1. The result of the projection method, compared to the exact numerical result, is shown in fig. 2 – the agreement is very good. Since the low p states essentially exhibit spherical symmetry with large angular momentum projection, their overlap with $|n_0, \ell_0 = 0(\ell_0 = 1)\rangle$ vanishes and their energies remain unshifted as compared to the hydrogen results.

The same scenario applies for the heavier alkali elements, as illustrated in figs. 2 (b) and (c). Here we plot the shifts of the exact energies of Na and Rb with respect to the hydrogen levels, as they emerge from the $n_0 = 23$ manifold, for precisely the same field parameters as used for the Li results. Since for these elements also the $\ell_1 = 2$ (Na) and the $\ell_1 = 3$ (Rb) states are separated from the hydrogenic manifold due to their

large quantum defects, the range of Q in (4) is two-dimensional. Again, the projection method gives very good agreement with the numerical result. In addition, we note that the larger the dimension of the range of Q, the smaller the values of p for which the alkali levels are shifted. This is a consequence of the dominance of small ℓ components in large p states and of large ℓ components in small p states, since the heavier the element the larger the ℓ values affected by non-negligible quantum defects.

In conclusion, the energy levels of alkali Rydberg states emerging from the hydrogenic n_0-manifold clearly reflect the phase space structure of the microwave driven Coulomb problem, despite the presence of a symmetry breaking atomic core. Also the ionization rates of the atoms reflect the underlying classical phase space structure, with the exception of local enhancements due to multiphoton resonances with nonhydrogenic sublevels of other manifolds.

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Stochastic resonance in the coherence of a quantum system

Thomas Wellens and Andreas Buchleitner

Recently it was shown, that stochastic resonance (SR) [1, 2, 3], the noise-induced enhancement of a weak periodic signal fed into a nonlinear detection device, can be used to control the quantum jumps of a quantum system between its metastable states [4, 5]. In the general terminology of SR, these states are associated with well separated values of the reaction coordinate monitored on output of the detection unit. SR manifests in the almost periodic switching of the reaction coordinate between these values, at the frequency of the weak signal fed into the device, for an optimal, *non-vanishing* noise level. In quantum systems, generic quantum transport effects (such as tunnelling [6] or quantum noise [5]) contribute to the transitions between the metastable states and compete with the (classical) thermal activation. The characteristic features that result from that competition have been discussed, e.g., in [2-6].

Yet, there is another, fundamental aspect of quantum SR which so far remained unaddressed: If we consider a closed quantum system living on a two-dimensional Hilbert space, the superposition principle provides us with a continuous family of equivalent basis sets to monitor its temporal evolution. On the other hand, the coupling of such a two-state system to an environment selects a preferred basis – the above-mentioned metastable states – which is most robust with respect to environment-induced decoherence [7]. Any generic quantum state will rapidly decohere into a mixture of these basis states, and this suggests that quantum SR – with a characteristic time scale comparable to the typical residence times in either of the metastable states – is only detectable in a reaction coordinate defined by an observable diagonal in the preferred basis [6]. As we shall demonstrate, this apparent dilemma can be circumvented by inducing the two-state system's metastability not via direct coupling to an environment but rather by its coherent interaction with a bistable quantum system which – in turn – is coupled to a thermal bath. Such a system is experimentally realized in the micromaser [8], where a sequence of two-level atoms coherently interacts with a single mode of the quantized radiation field (i.e. with a harmonic oscillator) sustained by a resonator with an extremely small though finite damping rate. We shall see that the bistability of the quantized radiation field can be monitored in different components of the atomic Bloch vector, what ultimately allows for the noise-induced amplification of a feeble signal inscribed in the coherence of the atomic two-state system, via the interaction with the bistable maser field.

At a given time, at most one atom is present in the micromaser cavity, and the radiation mode of frequency ω resonantly couples the upper and the lower atomic energy eigenstates $|u\rangle$ and $|d\rangle$, during a fixed interaction time $t_{\rm int}$. Consequently, the atomic Bloch vector performs a Rabi nutation eventually leading to the emission/absorption of

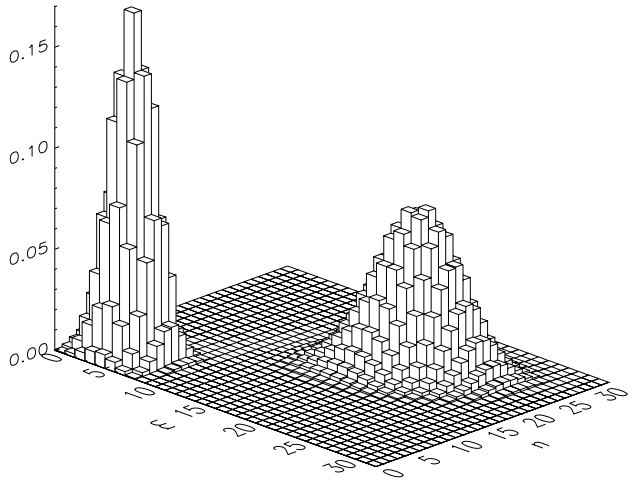

Figure 1: *Stationary state of the photon field density matrix* $\rho^{(\mathrm{ss})}_{n,m}$*, with two metastable states* $\rho^{(1)}$ *(left peak) and* $\rho^{(2)}$ *(right peak). Nonvanishing coherences between different photon numbers* n *and* m *only exist if both,* n *and* m *belong to either* $\rho^{(1)}$ *or* $\rho^{(2)}$*. Initial atomic superposition, Eq. (1):* $a = \sqrt{0.9}$*,* $b = -i\sqrt{0.1}$*, temperature* $T = 0.5$ K.

a photon in/from the cavity mode. In the most general scheme, each atom is prepared in a coherent superposition

$$|\psi\rangle = a|u\rangle + b|d\rangle, \tag{1}$$

with $|a|^2 + |b|^2 = 1$, before entering the resonator.

In addition to the interaction with the two-level atoms, the photon field is damped due to the nonvanishing coupling to the cavity walls at temperature T. Hence, for $t \to \infty$, the photon field density matrix will approach a stationary state $\rho^{(\mathrm{ss})}$, where photon losses due to the damping of the field are counterbalanced by photon gains due to the pumping with the atoms. In particular, for certain values of the experimental parameters, $\rho^{(\mathrm{ss})}_{n,n}$ displays two maxima as a function of the photon number n, corresponding to the *bistable operation mode* of the micromaser. An example is shown in Fig. 1.

The maser bistability illustrated in Fig. 1 reveals itself in a single realization of the dynamics, i.e. in a series of single atomic detection events as they are monitored in the experiment [9]. On exit from the resonator, the detection probability of an atom in a given final state ($|u\rangle$, $|d\rangle$, or a superposition of both) generically exhibits quantum jumps between two well separated equilibrium values at random times, as a signature of the corresponding jumps of the photon field between the two metastable states $\rho^{(1,2)}$ [9]. In terms of the atomic Bloch vector $\langle\vec{\sigma}\rangle$, $\langle\sigma_z\rangle = +1$ and $\langle\sigma_z\rangle = -1$ distinguish the atomic energy eigenstates $|u\rangle$ and $|d\rangle$, respectively, whereas $\langle\sigma_{x,y}\rangle$ probe *coherences* between the atomic energy eigenstates. The appropriate measurement scheme now allows for the detection of the metastability in $\langle\sigma_z\rangle$ or $\langle\sigma_y\rangle$,[1] as well as in

[1]With our choice of the phase angle of the initial atomic coherence ($ia^*b \in \mathbb{R}$, corresponding to $\langle\psi|\sigma_x|\psi\rangle = 0$), the metastability *cannot* be detected in the $x-$component of the atomic Bloch vector.

linear combinations thereof:

$$\sigma_\chi = \cos(\chi)\sigma_z + \sin(\chi)\sigma_y. \tag{2}$$

The expectation value $\langle\sigma_\chi\rangle$ defines our *reaction coordinate*.

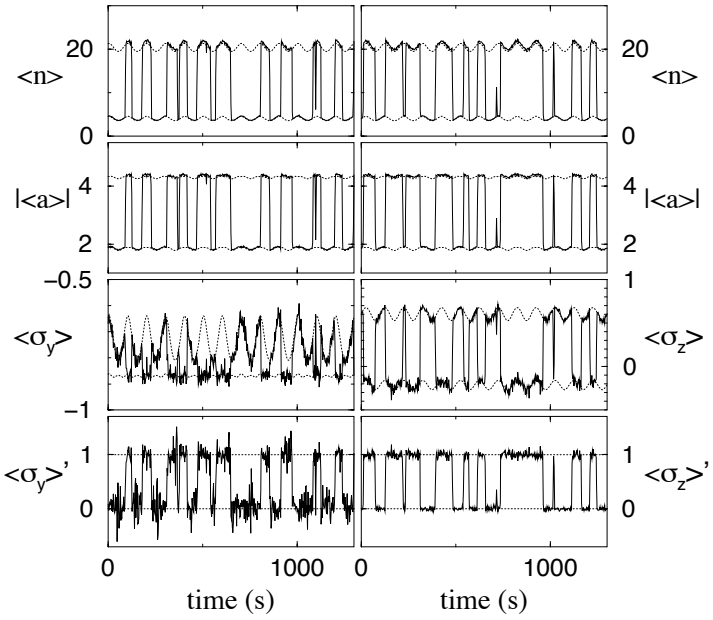

Figure 2: *A single realization of the maser dynamics at $T = 0.5$ K: Time evolution of (from top to bottom) (i) the mean photon number, (ii) the expectation value of the photon annihilation operator (proportional to the electric field amplitude [10]), (iii) the atomic Bloch vector on exit from the cavity, and (iv) the modified Bloch vector, obtained from (iii) by filtering out the intrastate modulation via Eq. (4). In the left (right) column, the $y-$ ($z-$) component of the atomic Bloch vector is measured. An average over small time intervals of length $\Delta t = 2.5$ s ($\simeq$ 40 cavity decay times γ^{-1}, ca. 1700 atomic detections) has been performed. The dotted lines indicate the expectation values corresponding to the metastable states $\rho^{(1)}$ ($\langle n\rangle^{(1)} \simeq 4$) and $\rho^{(2)}$ ($\langle n\rangle^{(2)} \simeq 21$) of the photon field.*

Because of the backaction of the measurement on the photon field [10], a variation of the measurement scheme also influences the transition rates between the metastable states $\langle\sigma_\chi\rangle^{(1,2)}$. However, our numerical tests indicate that this dependence is a relatively weak one: For the parameters of Fig. 1, the transition rates are approximately $1-5$ % slower when measuring in $z-$direction ($\chi = 0$) than in $y-$direction ($\chi = \pi/2$), with the difference getting smaller for higher temperatures.

We can now inscribe a small periodic signal in the atomic coherence, by modulating the amplitudes of the initial coherent superposition (Eq. (1)):

$$\begin{aligned} a(t) &= [0.9 + 0.05\sin(\omega_s t)]^{1/2}, \\ b(t) &= -i[0.1 - 0.05\sin(\omega_s t)]^{1/2}. \end{aligned} \tag{3}$$

The modulation period $t_s = 2\pi/\omega_s = 100$ s $\gg \gamma^{-1} \gg$ t$_{\rm int}$ approximately equals the average residence times in the two metastable states, for $T \simeq 0.5$ K. Two examples

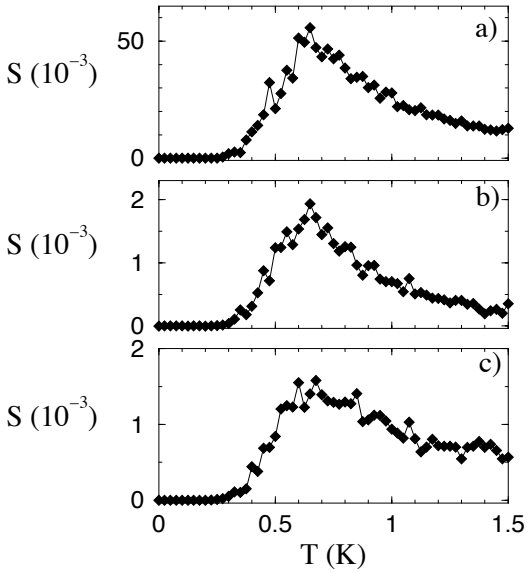

Figure 3: *Output signal power S of the $\chi-$component $\langle\sigma_\chi\rangle'$ of the modified atomic Bloch vector, Eqs. (7,9), vs. temperature T, for a) $\chi = 0$ (i.e. measuring σ_z), b) $\chi = 0.7 \times \pi/2$, and c) $\chi = \pi/2$ (i.e. measuring σ_y), in response to a weak periodic modulation of the atomic superposition, Eq. (3), at period $t_s = 100$ s. In all three cases, SR is observed: At an optimal temperature of $T \simeq 0.6$ K the output signal power exhibits a maximum. Each data point corresponds to approx. 25 million atomic detection events.*

of a single realization of the maser dynamics in presence of this modulation are shown in Fig. 2, for two different measurement schemes of the outgoing atoms (in $y-$ and in $z-$direction). The simulations were performed using a quantum trajectory method similar to the one described in [11]. Clearly, the quantum jumps of the photon field as well as the corresponding jumps of the atomic Bloch vector are visible in Fig. 2.

As obvious from Fig. 2, $|\langle\sigma_y\rangle^{(2)} - \langle\sigma_y\rangle^{(1)}|$ is comparable to the intrastate modulation of $\langle\sigma_y\rangle^{(1)}(t)$, i.e. the response of $\langle\sigma_y\rangle(t)$ to the small periodic signal (quantified by the output signal power S defined below) is dominated by the intrastate modulation which obscures the contribution from the jumps between the metastable states. We therefore subject $\langle\sigma_\chi\rangle$ to an affine transformation

$$\langle\sigma_\chi\rangle' = m(t)\langle\sigma_\chi\rangle + c(t), \tag{4}$$

in order to filter out the intrastate modulation. From $\langle\sigma_\chi\rangle'$ we now extract the output signal power S (defined as the area under the signal peak in the power spectrum of $\langle\sigma_\chi\rangle'(t)$, at the signal frequency ω_s [5]), which is shown in Fig. 3 as a function of the temperature T of the environment, for three different final state projections $\chi = 0$, $\chi = 0.7 \times \pi/2$, and $\chi = \pi/2$. Clearly, in all three cases S assumes a maximum at about $T = 0.6$ K, and noise-induced signal enhancement is observed. The cause of the similar temperature dependence of $S(T)$ in all three cases is the weak $\chi-$dependence of the transition rates between the metastable states.

We have seen that stochastic resonance can be achieved not only in the populations but also in the coherences of a two-state quantum system, a transmission "channel" which is classically inaccessible.

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Discrete breathers

S. Flach

The study of dynamical nontopological localization in nonlinear Hamiltonian lattices has experienced a considerable development during the past decade[1],[2],[3]. The discreteness of space - i.e. the usage of a spatial lattice - is crucial in order to provide structural stability for spatially localized excitations. Spatial discreteness is a very common situation for various applications from e.g. solid state physics.

To make things precise let us consider a d-dimensional hypercubic spatial lattice with discrete translational invariance. Each lattice site is labeled by a d-dimensional vector l with integer components. To each lattice site we associate one pair of canonically conjugated coordinates and momenta X_l, P_l which are real functions of time t. Let us then define some Hamiltonian H being a function of all coordinates and momenta and further require that H has the same symmetries as the lattice. The dynamical evolution of the considered system is given by the standard Hamiltonian equations of motion. Without loss of generality let us demand that H is a nonnegative function and that $H = 0$ for $X_l = P_l = 0$ (for all l). Call this state the classical ground state. Generalizations to other lattices and larger numbers of degrees of freedom per lattice site are straightforward.

When linearizing the equations of motion around $H = 0$ we obtain an eigenvalue problem. Due to translational invariance the eigenvectors will be spatially extended plane waves, and the eigenvalues Ω_q (frequencies) form a phonon spectrum, i.e. Ω_q is a function of the wave vector q. Due to the symmetry of the Hamiltonian Ω_q will be periodic in q. Moreover the phonon spectrum will be bounded, i.e. $|\Omega_q| \leq \Omega_{max}$. Depending on the presence or absence of Goldstone modes Ω_q might be gapless (zero belongs to the spectrum, spectrum is acoustic) or exhibit a gap ($|\Omega_q| \geq \Omega_{min}$, spectrum is optical). Increasing the number of degrees of freedom per lattice site induces several branches in Ω_q with possible gaps between them.

Let us search for spatially localized time periodic solutions of the full nonlinear equations of motion, i.e. $X_{|l|\to\infty} \to 0$ and $X_l(t) = X_l(t + T_b)$ (same for P). These solutions are coined discrete breathers. If a solution exists, we can expand it into a Fourier series in time, i.e. $X_l(t) = \sum_k A_{kl} \mathrm{e}^{\mathrm{i}k\omega_b t}$ ($\omega_b = 2\pi/T_b$). Spatial localization implies $A_{k,|l|\to\infty} \to 0$. Insert these series into the equations of motion. This results in a set of coupled algebraic equations for the Fourier amplitudes[3]. Consider the spatial tail of the solution where all Fourier amplitudes are small and should further decay to zero with growing distance from the excitation center. Since all amplitudes are small, we can linearize the equations. This procedure decouples interaction in k-space and we obtain for each k a linear equation for A_{kl} with interaction in l. This equation will contain $k\omega_b$. It will in fact be identical to the above discussed equation linearized around $H = 0$ and it will contain $k\omega_b$ instead of Ω_q[3]. If $k\omega_b = \Omega_q$ the corresponding

amplitude A_{kl} will not decay in space, instead it will oscillate. To obtain localization we arrive at the nonresonance condition $k\omega_b \neq \Omega_q$[3]. This condition has to be fulfilled for all integer k. For an optical spectrum Ω_q frequency ranges for ω_b exist which satisfy this condition. For acoustic spectra $k = 0$ poses a problem. We will discuss this case below in more detail.

The nonresonance condition is only a necessary condition for generic occurence of discrete breathers. More detailed analysis shows that breathers being periodic orbits bifurcate from band edge plane waves[4]. The condition for this bifurcation is an inequality involving parameters of expansion of H around $H = 0$[4].

Discrete breathers (periodic orbits) appear generically as one-parameter families of periodic orbits. The parameter of the family can be e.g. the frequency (or the energy, action etc). Note that we do not need any topological requirement on H (no energy barriers). Indeed breather families have limits where the breather delocalizes and its amplitude becomes zero.

With the help of the nonresonance condition we can exclude the generic existence of spatially localized solutions which are quasiperiodic in time. Indeed in the simplest case we would have to satisfy a nonresonance condition $k_1\omega_1 + k_2\omega_2 \neq \Omega_q$ for ω_1/ω_2 being irrational and all possible pairs of integers k_1, k_2. This is impossible[5].

To understand spatial decay properties of discrete breathers let us consider

$$H = \sum_l \left[\frac{1}{2} P_l^2 + V(X_l) + \sum_{l' \neq l} W_{l-l'}(X_l - X_{l'}) \right] \tag{1}$$

with $V(z), W_l(z)$ being nonnegative functions and $V(0) = W_l(0) = 0$. If $\partial^2 V/\partial z^2$ is nonzero for $z = 0$ then Ω_q is optical. In the opposite case the phonon spectrum is acoustic. If Ω_q is optical and Ω_q^2 an analytical function in q (this is realized for any finite range interaction $W_{l>l_c} = 0$ but also e.g. for $W_l(z)$ exponentially decaying in l) the interaction part of H is called short-ranged. To compute the spatial decay of a breather solution we use the above mentioned linearized equations for its Fourier amplitudes A_{kl}. With the help of Green's function method we find[6]

$$A_{kl} \sim \int_{1.\mathrm{BZ}} \frac{\cos(ql)}{(k\omega_b)^2 - \Omega_q^2} \mathrm{d}^d q \ . \tag{2}$$

Here the integration extends over the first Brillouin zone. Due to general properties of convergence of Fourier series[7] we conclude that for short-range interactions A_{kl} decay exponentially in l, where the exponents depend on k [5]. The exponent of A_{kl} tends to zero whenever $k\omega_b$ approaches an edge of Ω_q. Note that in such a limit the linearization of the algebraic equations in the tails of the breather ceases to be correct for a finite number of selected $k' \neq k$ and nonlinear corrections to (2) apply[8]. Still the spatial decay is exponential.

Consider a one-dimensional lattice with algebraically decaying interactions $W_l(z) \sim 1/l^s$ and $\partial^2 V/\partial z^2|_{z=0} \neq 0$. Since Ω_q^2 is nonanalytic in q for this case, (2) implies that for large distances l the spatial decay of a breather will be algebraic[6]: $A_{kl} \sim 1/l^s$. However for $s \to \infty$ the spatial decay becomes short-ranged (nearest neighbour interactions). To understand the crossover to exponential decay in this limit, consider (2) for the case when $k\omega_b$ is very close to the edge of Ω_q which is characterized by some wave vector q_c. Since the integrand nearly diverges near q_c we may use a stationary phase approximation and expand Ω_q^2 around q_c taking into account only the leading order term. For $s > 3$ the leading order dependence of Ω_q^2 on q will be proportional to $(q - q_c)^2$. The nonanalytic behaviour is then hidden in higher order terms in $(q - q_c)$ and does not contribute within the approximation[6]. Since we approximate Ω_q^2 by an analytical function, we will obtain exponential decay in space. However we know that the asymptotic dependence of A_{kl} on l will be algebraic. We thus conclude that in the mentioned case of $k\omega_b$ being close to the edge of Ω_q the spatial decay will be exponential for intermediate distances, but becomes algebraic for distances larger than some crossover distance l_c. High-precision numerical computations confirm this prediction[6]. The crossover distance can be estimated to be given by

$$\frac{\ln l_c}{l_c} \approx \frac{\nu}{s} \tag{3}$$

where ν is the exponent of the spatial decay obtained within the stationary phase approximation[6]. From result (3) it follows that for $s \to \infty$ $l_c \to \infty$. This is an expected result, since in this short-range interaction limit we recover exponential decay in the whole space. More surprising is that also the limit $\nu \to 0$ (i.e. $k\omega_b \to \Omega_{q_c}$) yields $l_c \to \infty$. Exponential decay is thus also obtained in the whole space whenever the (multiple of a) frequency of the breather solution comes close to the edge of Ω_q.

When Ω_q contains zero, i.e. when the linearized equations around $H = 0$ yield Goldstone modes, the dc component of a breather solution A_{kl} with $k = 0$ deserves special attention. All ac components ($k \neq 0$) can be analyzed similar to the case of an optical spectrum. If the Hamiltonian is invariant under the transformation $X_l \to -X_l$ then time-periodic solutions being invariant under this transformation will have $A_{kl} = 0$ for even k which includes $k = 0$. However if such a parity symmetry is broken, all Fourier components will become nonzero.

Assume that Ω_q^2 is analytical in q. Since the $k = 0$ component can not decay exponentially in space, at large distances from the breather the leading order part of the solution will be given by its slowly decaying dc part, the static lattice distortion. Its corresponding linearized equation will be similar to the equation for a strain in continuum mechanics, which is induced by some local deformation (the breather center) of the system[9]. The strain will decay algebraically in space. The constraint of finite energies leads to the requirement that the monopole contribution to the local deformation is zero for $d = 1, 2$. The resulting algebraic decay $A_{0l} \sim 1/|l|^{d-1}$ induced by a

dipole has been numerically confirmed for $d = 2$ [9].

A direct consequence of the spatial decay properties of discrete breathers is the possible appearance of nonzero energy thresholds. We remind that breathers show up as one-parameter families of time-periodic solutions in phase space. When sliding along such a family all parameters characterizing the breather will continuously change. Physically important is the presence or absence of an energy gap. First we observe that the only limit where the breather energy could vanish is the limit of zero amplitudes, i.e. the limit when ω_b approaches the edge of Ω_q. Let us estimate the far field energy part of a breather E_b

$$E_b \sim \int_1^\infty r^{d-1} F_d^2(\delta r) \mathrm{d}r \tag{4}$$

where the energy density is proportional to $A_{1r}^2 \sim F_d^2(\delta r)$. Since in the considered limit the spatial decay will be weakly exponential (no matter whether Ω_q^2 is analytical or not) the function $F_d(\delta r)$ is bounded by an exponential function with exponent δ. Assuming that the dispersion near the band edge in Ω_q is in leading order quadratic in $(q - q_c)$, we find $\delta \sim |\omega_b - \Omega_{q_c}|$. In the same limit, using perturbation theory for weakly nonlinear plane waves with amplitude A and frequency ω_b, we can estimate $|\omega_b - \Omega_{q_c}| \sim A^2$. Since the breather in the considered limit is a slightly distorted (localized) plane wave, we finally arrive at[10]

$$E_b \sim |\omega_b - \Omega_{q_c}|^{1-d/2} \quad . \tag{5}$$

This result implies that the breather energy can not assume arbitrary small values for $d \geq 2$. Consequently in such a case breathers have nonzero lower bounds on their energy (and similarly on their action). In some nongeneric cases nonzero energy gaps may occur even for one-dimensional systems[10]. Also nonanalytical dispersion Ω_q^2 may lower the critical lattice dimension[6].

Although discrete breathers are generic solutions for lattice Hamiltonians, they are not easily obtained in a closed analytic form. In the following we will present classes of functions H for which closed expressions can be obtained, though no special integrability requirement for H has to be fulfilled. What is needed in first place is separability of time and space. This can be obtained for homogeneous potential functions. Consider the one-dimensional lattice Hamiltonian

$$H = \sum_l \left[\frac{1}{2} P_l^2 + \frac{1}{2} (X_l - X_{l+1})^2 h(S_l) \right] \tag{6}$$

where $h(z)$ is some function and $S_l = \frac{X_l}{X_{l+1}} + \frac{X_{l+1}}{X_l}$. Making the ansatz $X_l(t) = u_l G(t)$ we find $\ddot{G} = -\kappa G$ and a set of nonlinear coupled algebraical equations for the amplitudes u_l which contains the separation parameter κ. These equations can be explicitely solved with e.g. $u_l = (-1)^l \mathrm{e}^{-\beta|l|}$. A necessary and sufficient condition is that the function $h(z)$ satisfies

$$h(-z_0) = -z_0(z_0 + 1) h'(-z_0) \tag{7}$$

for a positive value of $z_0 > 2$ (note that (7) is not a differential equation)[11]. The exponent β is defined by $z_0 = 2\cosh\beta$. The locality of condition (7) allows to generate whole classes of $h(z)$.

It is also possible to define Hamiltonian functions in higher lattice dimensions with explicit breather solutions. Let us briefly introduce these models. Define $\hat{L}X_l = \sum_{l',|l-l'|=1} X_{l'}$ and $S_l = \frac{\hat{L}X_l}{X_l}$. Then the Hamiltonian

$$H = \sum_l \left[\frac{1}{2} P_l^2 + \frac{1}{2} (\hat{L}X_l)^2 h(S_l) \right] \tag{8}$$

allows for explicit breather solutions[11] if the function $g(z) = \frac{1}{2} z^2 h(z)$ satisfies two local equalities at z_0 and z_1:

$$g(z_0) = g(z_1) \ , \ g'(z_0) = g'(z_1) \ . \tag{9}$$

Compactons have been discussed for PDEs by Rosenau[12]. The basic idea is to consider field equations which lack linear dispersion terms. On a lattice it is easy to implement an analogous idea. All we have to require is that $\partial H / \partial X_l$ vanishes for $X_l = 0$ and arbitrary values of all other variables. This is satisfied for

$$H = \sum_l \left[\frac{1}{2} P_l^2 + V(X_l) + F(X_l) \sum_{l' \neq l} W_{l-l'}(X_l - X_{l'}) \right] \tag{10}$$

with $F(0) = F'(0) = 0$ (simplest choice is $F(z) = z^2$). Indeed in such a case it is possible to excite a cluster (or several clusters) of lattice sites with nonzero displacements and momenta, but the dynamics will be restricted to the initially excited sites, leaving all unperturbed sites with $X = P = 0$ unchanged.

The discrete breather concept has been recently used for different experimental situations. Light injected into a narrow waveguide which is weakly coupled to parallel waveguides (characteristic diameter and distances of order of micrometers, nonlinear optical medium based on GaAs materials) disperses to the neighbouring channels for small field intensities, but localizes in the initially injected wave guide for large field intensities[13].

Bound phonon states (up to seven participating phonons) have been observed by overtone resonance Raman spectroscopy in PtCl mixed valence metal compounds[14]. Bound states are quantum versions of classical discrete breather solutions.

Spatially localized voltage drops in Nb-based Josephson junction ladders have been recently observed and characterized[15] (typical size of junction is a few micrometers). These states correspond to generalizations of discrete breathers to dissipative systems.

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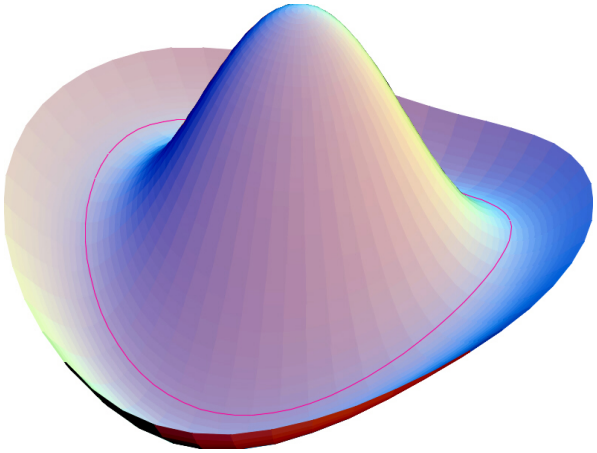
Mesoscopic quantum effects in cold glasses

S. Kettemann, P. Fulde, P. Strehlow

In 1998 Strehlow et al. made the remarkable observation that below 10 mK the multicomponent glass $BaO - Al_2O_3 - SiO_2$ responds sensitively to an applied magnetic field. The effect is seen in the change of the dielectric function $\delta\epsilon(H)$ with field which is 5 - 6 orders of magnitude larger than expected. Since spin effects can be excluded the origin of this behavior must be due to orbital effects. We have developed a theory which can explain some of the unexpected experimental observations (Phys. Rev. Lett. **83**, 4325 (1999)). Starting point is the tunnelling model familiar for glasses. Hereby one should realize that the tunnelling motion of an ion, i.e., O^{2-} or a group of ions is circular rather than linear



The tunneling path has the form of the rim of a Mexican hat.

because changing bond angles costs less energy than changing bond lengths. When a magnetic field is applied, a phase change takes place in the wave function for each ring according to Bohm-Aharonov. This phase change is periodic in the flux quantum ϕ_0, but huge fields of order 10^5 Tesla are required before that situation is reached. However, the tunnelling systems interact with each other via electric and elastic dipole interactions. A simple estimate shows that the dipole interaction between tunnelling systems which are 10^{-8} m apart (a typical distance) is of order 100 mK. Thus at low temperatures those systems are locked together and tunnel coherently. In analogy to interacting Fermion systems one may assume a one to one correspondence between the excitations of the coupled tunnelling systems and that of uncoupled ones but with renormalized parameters. The latter are here the effective charge q of the tunnelling particles and the maximum height of the potential barriers separating the two minima of a tunnelling system. With these assumptions the minimum tunnelling matrix element is magnetic field dependent, i.e., $t_{min}(\phi) = t^{(0)}_{min} cos(\pi\phi/\phi_0)$. One finds that the effective charge q is of order $q = 4 \cdot 10^5 |e|$ where $|e|$ is the electron charge. With this model prediction have been made as regards $\delta\epsilon(\phi)$ which have been verified subsequently by experiments.

Apparently the multicomponent glass is a system which at low temperatures is described by a wave function extending over a region of several microns. Therefore, it seems that glasses at ultra low temperatures are characterized by a wave function the range of which is between that of atoms (microscopic dimensions) and superconductors (macroscopic dimensions).

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Theoretical Model for the Superconducting and Magnetically Ordered Borocarbides

Alessandro Amici, P. Thalmeier, P. Fulde

The discovery of borocarbides in 1994 renewed the interest of the condensed matter community on a long debated issue: the mutual interaction between superconductivity and magnetic order. Borocarbides are a family of compounds with formula unit $R\mathrm{Ni_2B_2C}$, where R stands for Y, Lu or a rare-earth element. Several borocarbides undergo a transition into a superconducting state at temperatures between 3 K and 16 K. In addition most of the compounds containing magnetic rare-earth ions order magnetically in the same range of temperatures. The first challenge for the theory is the variety of the magnetic structures observed: incommensurate spin-density waves and helices, commensurate antiferromagnets, high field spin-flop structures, etc. However the outburst of experimental and theoretical activity on borocarbides during the past five years has been mainly motivated by the mutual interaction between superconductivity and magnetic order observed in these compounds.

After V. L. Ginzburg [1] in 1957 demonstrated the strong competition between ferromagnetism and superconductivity, the first who claimed the possibility of coexistence between superconductivity and long range magnetic order were W. Baltensperger and S. Strässler [2] in 1963. They examined the case of antiferromagnetic order and paired electrons in the magnetic Bloch-states resulting from the underlying exchange field. Even if the Hamiltonian lacks time-reversal symmetry, it is invariant under the composition of the two operations of time-reversal and translation by a lattice vector. This more general symmetry assures that no static pair-breaking is introduced by antiferromagnetic order and the overall effect of its presence is a small reduction of the effective interaction between phonons and electrons.

¿From the experimental point of view the problem of the coexistence were successfully approached only in 1977 when two families of superconducting and magnetically ordered materials were discovered. The materials $R\mathrm{Rh_4B_4}$ and $R\mathrm{Mo_6S_8}$, known respectively as rhodium borides and Chevrel phases, share the characteristics to be ternary, rare-earth, transition-metal compounds. The pioneering theoretical predictions by Ginzburg and by Baltensperger and Strässler were nicely confirmed by the experiments and the theories for ferromagnetic and antiferromagnetic superconductors were further developed in order to understand numerous interesting details.

After the discovery of borocarbides [3],[4] it was immediately realized that these compounds share several characteristics with the old magnetic superconductors with the addition of a wide variety of new magnetic structures that compete or coexist with superconductivity. Furthermore, the wide possibility of doping, both on the rare earth site and on the nickel site, and the rapid availability of large single crystals permitted to collect an amount of experimental data much larger and more detailed than the data

on the old magnetic superconductors. ¿From a theoretical point of view borocarbides are a strict test for the theories of antiferromagnetic superconductors due to the numerous parameters that can be fine tuned experimentally. Moreover, the presence of incommensurate magnetic structures coexisting or competing with superconductivity calls for a non-trivial generalisation of the known theories.

The main aim of the our work has been to provide a general framework for the treatment of superconductivity in the presence of arbitrary magnetic structures via the generalisation of the BCS theory to the paired magnetic Bloch-states. The formalism can be seen as a generalisation of the treatment of the antiferromagnetic superconductors by W. Baltensperger and S. Strässler. It naturally includes the case of the antiferromagnet, but can be exploited as well in the cases of transverse helical and collinear modulated order, which are the two cases of interest for the borocarbides. The focus has been kept on the complex phase diagram of $HoNi_2B_2C$ and related compounds, where the mutual influence between the two ordered states is amplified by the proximity of their transition temperatures, $T_c \simeq 8.5$ K and $T_m \simeq 6$ K.

The complex magnetic properties of these compounds have been addressed on the line of the magnetism of rare-earth intermetallics. We could reproduce a number of features of the low-temperature anisotropic metamagnetic phase diagram of $HoNi_2B_2C$ [5] using a model which includes the crystal-electric-field potential acting on the rare-earth ions and the Ruderman-Kittel-Kasuya-Yosida interaction among them [6]. The minimal theoretical treatment required to reach reasonable agreement with the experiments is relatively sophisticated and, even then, finer details call definitely for the inclusion of further physical ingredients (e.g., magnetoelastic coupling or more general terms in the RKKY interaction). On the other hand, the functional form of the RKKY interaction extracted from the low-temperature data, immediately gives us the key to interprete the incommensurate-to-commensurate lock-in transition observed at $T_N \simeq 5$ K. Overall the magnetic properties of borocarbides appear a challenging problem by themselves, even before considering their coupling with superconductivity.

The problem of the mutual interplay between superconductivity and a magnetically ordered state can be approached at different levels of complexity. In our work we attacked the first level, namely the mean-field solution of a system of band electrons interacting with the magnetically ordered structure via the exchange potential. We have derived the mean-field equations of magnetic superconductivity using a multi-bands formalism which may be applied to any possible commensurate magnetic structure, no matter how complicated. Even if the actual possibility to solve numerically these equations is limited to magnetic structures with small magnetic unit cells (realistically less than ten crystal unit cells), we found that some general characteristics of the magnetic phases may be used to qualitatively estimate the tendency for superconductivity to coexist with them [7]. Some of these qualitative features of the underlying magnetic structure, such as the presence of a ferromagnetic component or the possibility of nesting of

the Fermi surface at the magnetic **Q**-vector, were already known to strongly suppress superconductivity, and have been commonly used in the interpretation of the behaviour of borocarbides. Within our formulation we could identify at least one additional wide class of magnetic structures with a possibly-strong detrimental effect on superconductivity. They are those magnetic phases whithout ferromagnetic component which, nevertheless, split the spin-degeneracy of the energy bands on large parts of the Fermi surface. It is worth noting that the transversely-polarised spin-density-waves observed in a few borocarbides, belong just to this non-trivial class of magnetic structures.

In our opinion however, the more remarkable outcome of our work is not to have identified one more piece of evidence for the *competition* between magnetic order and superconductivity, rather than the opposite: we have found that magnetic structures not belonging to the above mentioned classes appear to affect superconductivity in essentially the same way an antiferromagnet does, hence allowing for the *coexistence*. In this case indeed the main effect on the superconducting properties is a slight weakening of the effective attractive interaction among conduction electrons in the magnetic Bloch-states. Even if most of these superconductivity-compatible magnetic phases are quite exotic, with the helices being the noteworthy exception, they are nevertheless interesting from the theoretical point of view because the whole category appears to be much wider than the previous approaches would suggest. In particular we have shown that the arguments based on the time-reversal-plus-translation symmetry, often used in the theory of the antiferromagnetic superconductors, may provide a sufficient condition for the coexistence, but not a necessary one.

One more feature appearing in such a general formulation of the theory has attracted our attention, and has revealed extremely valuable in the process of constructing an intuitive picture of the physics of magnetic superconductors. Cooper pairs formed by electrons in the Bloch states associated with any kind of magnetic ordered states *do not decay*, exactly as non-magnetic BCS pairs do not. Therefore, the detrimental effect on superconductivity is not produced by "pair-breaking", in any possible meaning of the term. It has to be kept firmly in mind that the effect on superconductivity of a magnetically ordered structure is completely different from the one of an isolated magnetic impurity.

Eventually, we set up a simplified model for the description of superconductivity in the class of Ho-related borocarbides. Specialising our superconducting theory to the helical structure we found the quantitative relation between the magnetic order parameter $\mu(T)$ and the effective attractive interaction parameter $\lambda(\mu(T))$, that in the magnetic superconductors take the place of the BCS parameter λ [8]. Such a relation holds for any commensurate value of the **Q**-vector associated with the helical order and has a well-defined, *calculable* limit in the case of incommensurate structures. Moreover, the relative reduction of the interaction parameter due to helical magnetism is estimated to be of the order of the 10% in the family of the Ho-related borocarbides. With

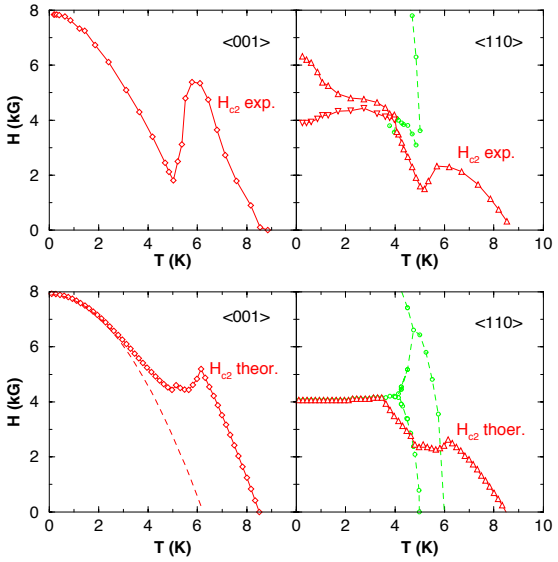

Figure 1: *(Upper row) Experimental $H_{c2}(T)$ curves along two high symmetry directions. (Lower row) Calculated $H_{c2}(T)$ curves and metamagnetic phase transitions (small circle). The upper critical field along $\langle 110 \rangle$ is strongly reduced by the anisotropic magnetic response of the magnetically ordered rare-earth moments.*

the assumption that the relevant magnetic phases in the complex phase diagram of $HoNi_2B_2C$ are the antiferromagnetic and the c-axis helical ones, we are able to calculate a model upper-critical-field phase diagram with excellent qualitative agreement with the experimental one [7] as shown in fig. 1. In spite of the fact that most of the works on the experimental $H_{c2}(T)$ curves interprete the fairly large depression as a hint of the destructive effect on superconductivity of the incommensurate phases, our calculation provide a completely different interpretation. Indeed, the dip in the theoretical curve results from a small but rapid decrease of the effective interaction parameter $\lambda(T)$ due to the onset and fast developing of the magnetic order parameter. The incommensurate-to-commensurate transition does not change significantly the influence of magnetic order on superconductivity, and the recovery of the upper critical field below $T_N \simeq 5$ K is actually related to the sudden saturation of the magnetic order parameter, rather than to the commensurate character of the low temperature phase. Further comparisons with the data from pure samples at high pressure and from slightly doped compounds show clear rational patterns which are easily explained within the same picture.

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Ab Initio Quantum Chemistry for Atoms, Molecules and Clusters, Polymers and Solids

Michael Dolg

Introduction

The main area of research of the 'Quantum Chemistry' group at MPI-PKS were accurate *ab initio* electronic structure calculations for finite systems, i.e., atoms [1, 2], molecules [3, 4, 5, 6, 7, 8, 9, 10, 11] and clusters [12, 13, 14, 15, 16], as well as the extension of quantum chemical methods to infinite systems, i.e., polymers [17, 18, 19, 20] and solids [21, 22, 23, 24, 25]. Besides method development in the latter field, e.g., the coding of a Wannier-function-based Hartree-Fock program for polymers and solids [17, 21] and the evaluation of correlation corrections to ground state total energies within the incremental scheme based on self-consistently determined localized orbitals [20, 25], methodologic work has also been done on the field of energy-consistent relativistic *ab initio* pseudopotential (PP) schemes [11], relativistic Dirac-Coulomb-Hamiltonian-based and scalar-relativistic Zeroth-Order Regular Approximation (ZORA) Hamiltonian-based Kohn-Sham density functional theory (DFT) approaches [1, 2, 3, 8], quantum Monte Carlo (QMC) techniques [10] as well as various techniques to analyze chemical bonding, e.g., charge fluctuations evaluated for real-space and Hilbert-space partitionings of the system [10] as well as the electron localization function. The developed methods and programs were then applied, together with approaches and codes of other groups, to various systems of chemical or physical interest, e.g., the electronic structure of sandwich complexes of benzene [7, 8] and cyclooctatetraene [5, 6], the possible existence of tetravalent Hg compounds [9], the open question of the YbO ground state [3], the electronic structure of Gd diatomics with very high spin multiplicities [4], structures and energetics of group 2, 12 and Yb clusters [12, 13, 14, 15, 16] or structural and cohesive properties of polyethylene [17], polyamino- and polyiminoborane [18], polyacetylene [19] or solids as GdN [22]. In order to get quantitatively meaningful results, both relativistic effects and electron correlation effects were included systematically in all studies of heavy-element systems. Some other work aimed at deriving model Hamiltonian parameters for solid state physics impurity problems [26], interpreting electron correlation phenomena in small molecules [27] or developing suitable hybrid model (HM) approaches for the study of large metal clusters [14]. In addition, pure computational chemistry was applied to investigate the mechanisms of some organic reactions [28, 29].

Some of the most challenging systems for *ab initio* electronic structure calculations contain lanthanides and actinides [30]. Even for atoms and ions it is very difficult to account accurately for the very large relativistic and electron correlation effects, especially when processes are investigated in which the f occupation number changes. Relativistic PPs developed previously in the group together with large-scale wavefunction-based correlation treatments were calibrated against experimental data (Figs. 1 and 2) [1, 2, 11].

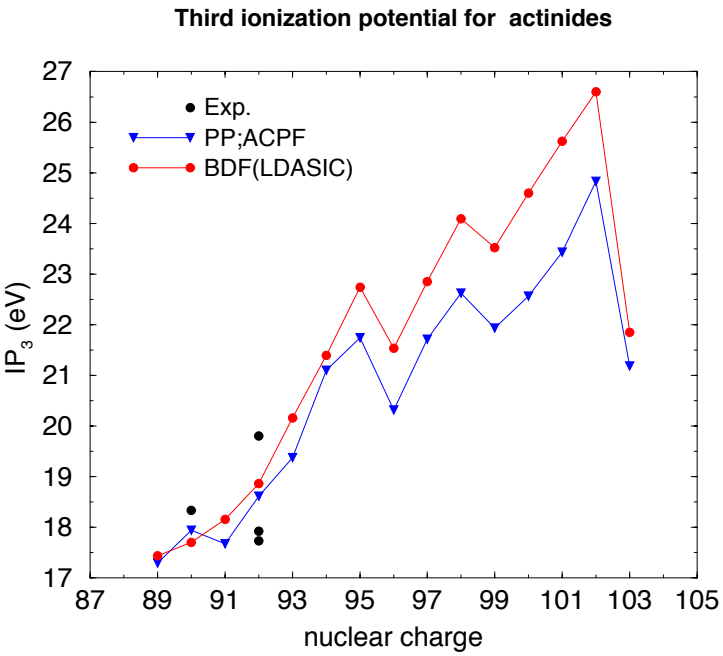


Fig. 1. *Third ionization potential of actinide atoms from relativistic pseudopotential (PP) averaged coupled--pair functional (ACPF) calculations corrected for spin--orbit coupling and all--electron density functional calculations including a self-interaction correction (BDF,LDASIC)[2].*

In addition a four-component gradient-corrected DFT code developed in the group (*Beijing Density Functional, BDF*; W. Liu, G. Hong, D. Dai, L. Li, M. Dolg, Theor. Chem. Acc. 96 (1997) 75) proved to yield very promising results both for atoms and f-element diatomics [3, 4]. Both approaches usually give essentially the same trends and their results can be used as a guide to further experimental studies. A computationally more efficient scalar-relativistic DFT code was also developed and tested in a study for the thermodynamic stability of the bis-η^6-benzene complexes of transition metals, lanthanides and actinides. The agreement with corresponding relativistic PPs large-scale coupled-cluster studies including single, double and perturbative triple excitation operators (CCSD(T)) is quite satisfactory. In particular, the thermodynamic stability of bis-η^6-benzene actinide complexes was predicted. It should be noted, however, that most experimental data for the stabilities is very uncertain or actually only estimated (Fig. 3) [7, 8].

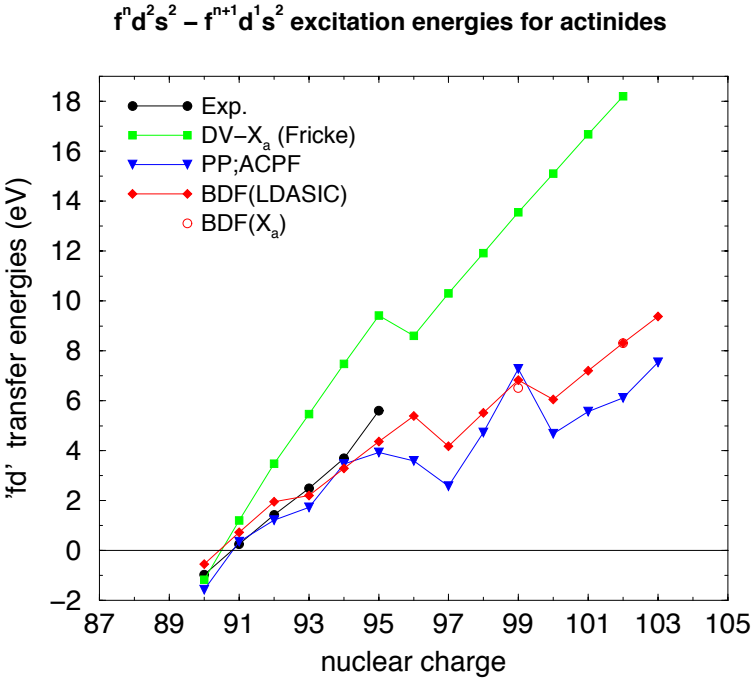


Fig. 2. *$f \rightarrow d$ excitation energies of actinide atoms from relativistic pseudopotential (PP) averaged coupled-pair functional (ACPF) calculations corrected for spin-orbit coupling and all-electron density functional calculations including a self-interaction correction (BDF,LDASIC)[2].*

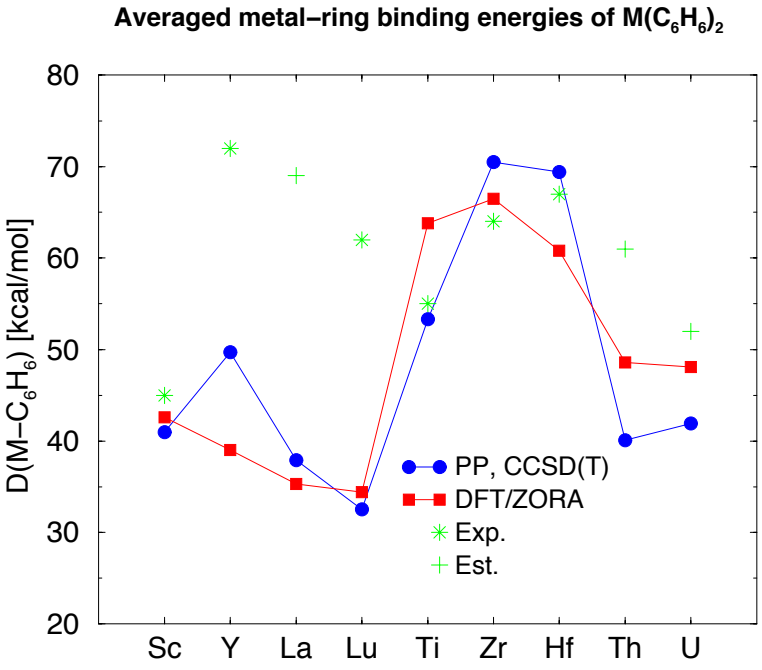


Fig. 3. *Averaged metal-ring binding energies of bis-η^6-benzene complexes from relativistic pseudopotential (PP) coupled-cluster calculations including singles, doubles and perturbative triples (CCSD(T)) and gradient-corrected density functional (DFT) calculations based on the scalar-relativistic Chang-Pélissier-Durand Hamiltonian (ZORA) [7, 8].*

Clusters

Using a previously developed analysis of complete active space multi-configuration Hartree-Fock self-consistent field (CASSCF) wavefunctions in a local orbital basis (M. Mödl, M. Dolg, P. Fulde, H. Stoll, J. Chem. Phys. 105 (1996) 2353) the covalent contributions to bonding in group 2 and 12 dimers have been analyzed in terms of the local

spin on one of the atoms and the charge fluctuations in an orbital group associated with one of the atoms (Fig. 4). He_2 and H_2 serve as limiting cases for pure Van der Waals interaction and a typical covalent single bond, respectively. It is seen, that both group 2 and 12 dimers as well as Yb_2 have noticeable covalent bonding contributions. A similar analysis, although in context of the interpretation and analysis of covalent chemical bonds in diatomic first-row main group molecules also appeared [27].

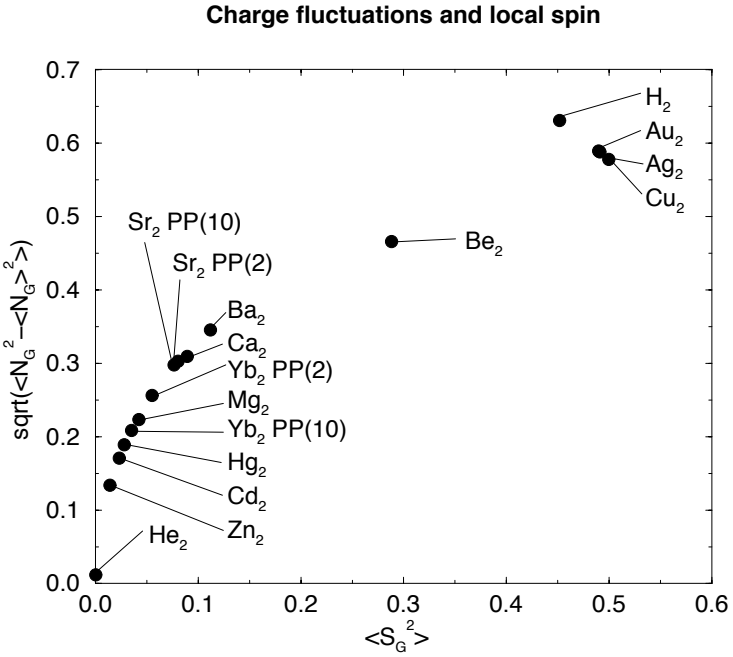


Fig. 4. *Local spin and charge fluctuations of various homonuclear diatomics from complete active space multiconfiguration Hartree-Fock self-consistent field calculations with a $ns-np$ active orbital space. G denotes a group of localized $ns-np$ orbitals on one of the atoms, N_G and S_G are the local occupation number and spin operators, respectively [16].*

Instead of a partitioning in Hilbert space built from localized orbitals orbitals of a CASSCF wavefunction, an alternative partitioning in real space was also investigated with QMC calculations [10]. For correlated calculations the results obtained with both approaches reveal the same trend (cf. H.-J. Flad, F. Schautz, Y. Wang, M. Dolg, MPI-PKS report 1995-1997, Fig. 3), however, the real space QMC approach is suitable for the study of larger clusters, where a too large active space would result. Another alternative is the use of the electron correlation function (ibid., Fig. 5) [13, 16].
DFT or model Hamiltonian approaches are inadequate for the study if size-dependent properties of clusters of groups 2, 12 and Yb. The transition from van der Waals interaction to covalent (and ultimately metallic) bonding must be described in an unbiased way, e.g., by wavefunction-based highly-correlated quantum chemical *ab initio* methods using a suitable relativistic Hamiltonian. Several PP CCSD(T) and QMC studies for small and medium-sized clusters have been performed during the reporting period [12, 13, 16].

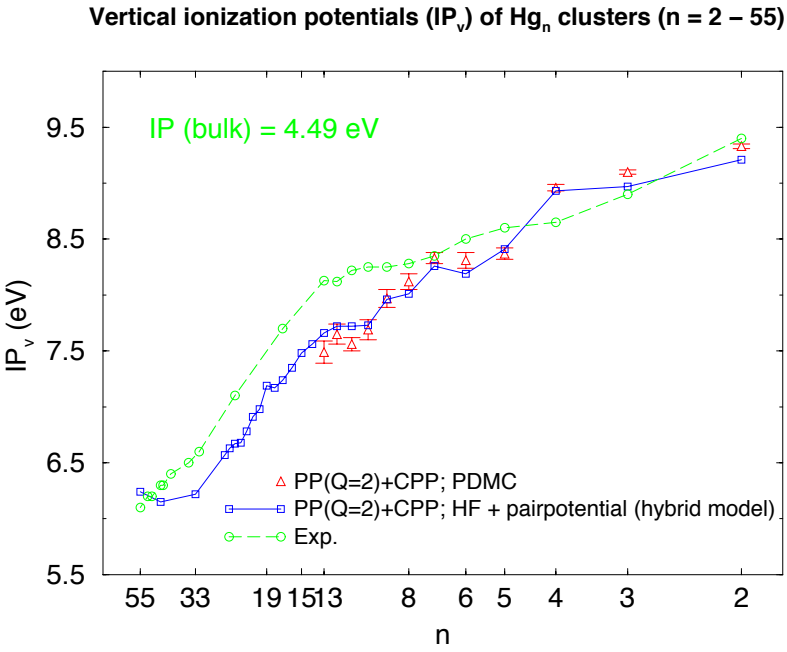


Fig. 5. *Ionization potentials of Hg clusters from two-valence-electron pseudopotential plus core-polarization calculations (PP(Q=2)+CPP) using a hybrid model (HM) for covalent and van der Waals interactions as well as pure diffusion quantum Monte Carlo results (PDMC) for the optimized structures [14].*

Large clusters of mecury became accessible within a HM approach, based on a relativistic energy-consistent two-valence-electron PP. Static and dynamic core-polarization effects, i.e., polarization at the HF level as well as core-valence correlation, were accounted for by a core-polarization potential (CPP), covalent bonding contributions at the valence-only HF level, and finally van der Waals-type correlation contributions by a pairwise additive potential of the form R^{-6} times a cut-off factor for small distances R. The correlation contributions were extracted from accurate small-core pseudopotential large-scale CCSD(T) calculations including also spin-orbit corrections for the Hg_2 dimer. The point-charge model for the core-core repulsion was corrected by a Born-Mayer-type pair-potential derived from frozen-core calculations for the $Hg^{2+}Hg^{2+}$ core system. The model was successfully tested against more rigorous calculations for clusters with up to 15 atoms and applied to clusters with up to 55 atoms. Additional recent advances will allow to go beyond this cluster size. The results are quite satisfactory, e.g., the calculated ionization potentials follow closely the trend of the experimental values (Fig. 5) and the calculated cohesive energy per atom is readily extrapolated towards the experimental limiting bulk value of 0.64 eV (Fig. 6). It should be noted that with the exception of the second ionization potential of atomic Hg used as a reference for adjusting the cut-off parameter in the CPP, no experimental information was used in the calculations. Future calculations will also account for dynamics on the Born-Oppenheimer surface.

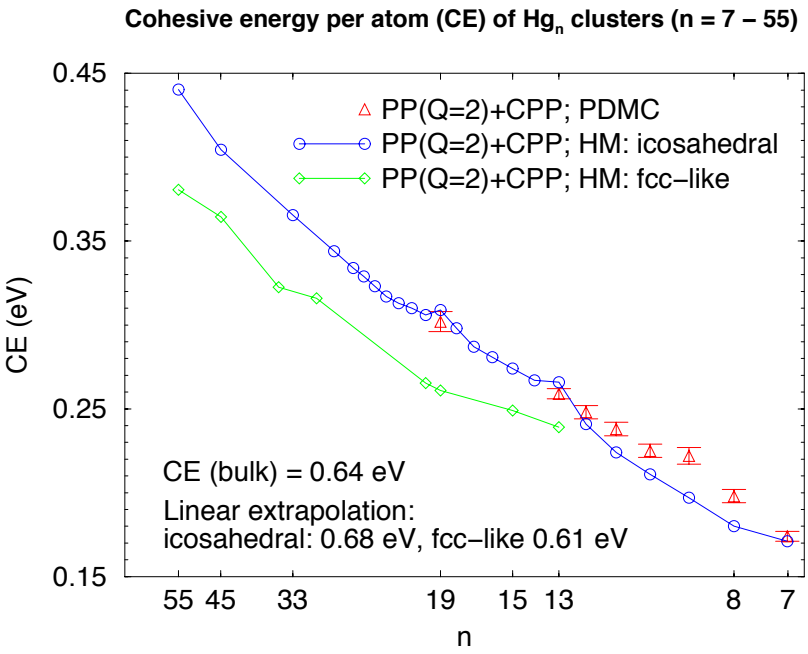
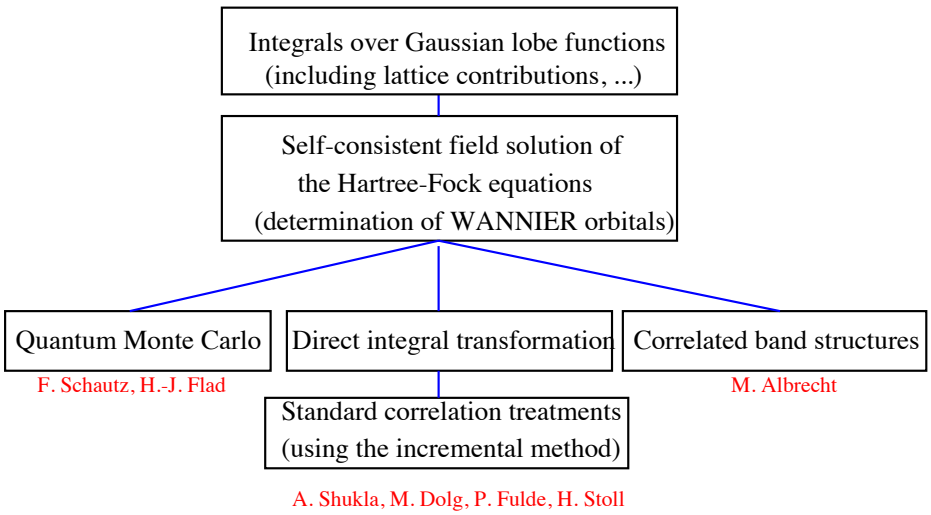


Fig. 6. *Cohesive energy per atom of Hg clusters from two-valence-electron pseudopotential plus core-polarization calculations (PP(Q=2)+CPP) using a hybrid model (HM) for covalent and van der Waals interactions as well as pure diffusion quantum Monte Carlo results (PDMC) for the optimized structures [14].*

Polymers and Solids

In collaboration with H. Stoll (Stuttgart) and P. Fulde (Dresden) the group developed a HF code (WANNIER) for infinite systems, which generates Wannier functions within the self-consistent field procedure (Fig. 7). These localized one-particle basis functions are then used, together with a suitable localized virtual orbital space, for subsequent correlated *ab initio* calculations of polymers and solids. The full-CI calculations on the model systems LiH chain [20] and the three-dimensional solid LiH [25] demonstrate the soundness of the approach. Further studies included, e.g., the polymers of polyaminoborane and polyiminoborane (Fig. 8), where also correlation corrections for the band structure were evaluated (Fig. 9).

Structure of the WANNIER polymer and solid code



possible future extensions: evaluation of properties, wavefunction analysis, treatment of impurities, treatment of surfaces, ...

Fig. 7. *Overview over the WANNIER polymer and solid program system.*

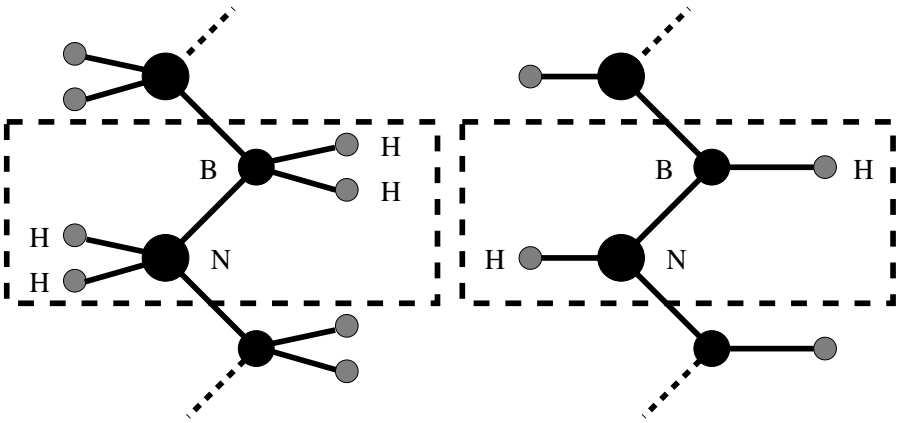


Fig. 8. *Unit cells of polyaminoborane and polyiminoborane [18].*

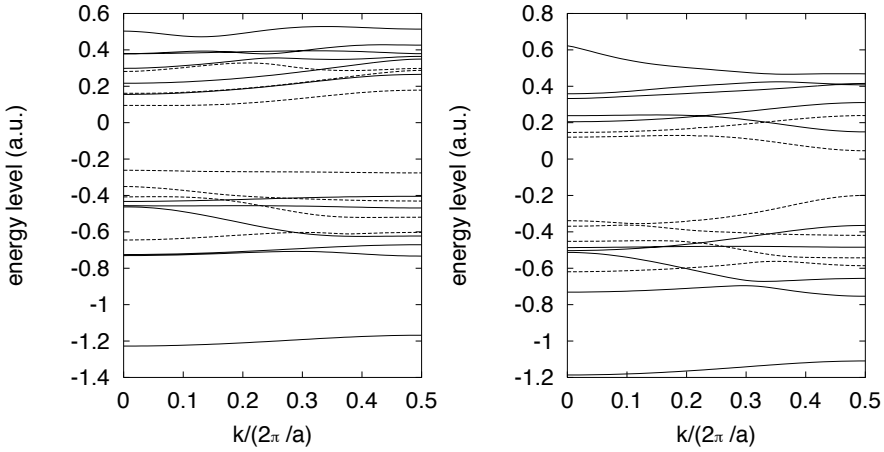


Fig. 9. *Band structures of polyaminoborane and polyiminoborane. The Hartree-Fock results are denoted by solid lines, the correlation-corrected Møller-Plesset-results by dashed lines. Only the valence orbitals of $(BNH_4)\infty$ and $(BNH_2)\infty$ were considered, resulting in a total of 10 and 12 bands, with 5 and 6 occupied bands, respectively. Correlation corrections are given only for the highest occupied and lowest unoccupied bands [18].*

Future extensions of the code, already partially being implemented, will include relativistic PP as well as CPP routines, a CCSD correlation treatment and the possibility to include spin-orbit effects. Although the program developed so far is definitely not a code for routine calculations of larger systems, it certainly demonstrates that quantum chemical methods are indeed applicable to infinite systems. The main advantage of such an approach is, in contrast to the commonly used 'dirty fast tricks' (DFT) and in particular to all kinds of model Hamiltonians, that systematic improvements of the applied approximations are possible. Long-term goals should be high-level correlation treatments, e.g., r_{12}-wavefunction-based CCSD(T) for infinite systems, however, this might take a decade and give work to a dozen of postdocs.

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Quantum Monte Carlo - Method and Applications

Friedemann Schautz and Heinz-Jürgen Flad

Within the Research Group "Quantum Chemistry" we were concerned with the development and application of Quantum Monte Carlo (QMC) methods. The focus of method development was on the use of model potentials (MP) within the QMC framework. On the side of applications we were especially interested in molecules and clusters containing heavier elements, which were treated by relativistic pseudopotentials, as well as in the calculation of properties.

Model Potentials in Quantum Monte Carlo calculations

Pseudopotentials became very useful in the context of QMC since they allow the elimination of core electrons which do not contribute to chemical bonding thus making calculations much more efficient and also include relativistic effects.

So called model potentials are an alternative to pseudopotentials. While pseudopotentials are obtained from a fitting procedure with respect to some reference data, model potentials can be produced by transforming a subset of single particle functions from a Self Consistent Field (SCF) calculation. If one does not aim at transferability between different systems this amounts to the Frozen Core approximation in Quantum Chemistry.

This Frozen Core approximation is useful in cases where orbital relaxations on SCF-level are to be taken into account and when one wants to replace arbitrary parts of the system. It is mandatory when quantum chemical methods are applied to infinite systems without introducing periodic boundary conditions (embedding)[10] .

Since QMC algorithms are local in the many electron configuration space but pseudopotentials as well as model potentials are nonlocal operators, their use in QMC requires an additional localization step using a trial wavefunction (for an overview see e.g. [11]). In the case of pseudopotentials this procedure is well understood and has been tested in many applications.

In comparison to pseudopotentials additional difficulties arise because of the fact that model potentials contain a projection operator preventing a collapse into the "frozen" part of the system. A localization procedure suitable for model potentials has been developed and implemented into our QMC-program. It has been tested in first applications to model systems [9].

Quantum Monte Carlo studies of correlation effects in molecules and clusters.

The stochastic solution of the Schrödinger equation within the framework of quantum Monte Carlo (QMC) methods provides an alternative to the algebraic approach. Especially short-range correlations corresponding to the behavior of the wavefunction near the electron cusp can be treated properly by means of r_{12} dependent correlation factors. The antisymmetry of the wavefunction enforces the only approximation based on the nodal structure of the trial wavefunction. In combination with relativistic pseudopotentials and polarization potentials QMC has been proven to be a useful tool even for systems containing heavy elements [1]. A comparison with other *ab initio* methods

reveals a remarkably good agreement with coupled cluster calculations. Besides the energy it is possible to calculate energy derivatives like dipole moments [2] and static dipole polarizabilities [3] using finite difference formulas as well as expectation values of local operators [2], including such cases like local charge fluctuations [3, 4] which are otherwise difficult to evaluate.

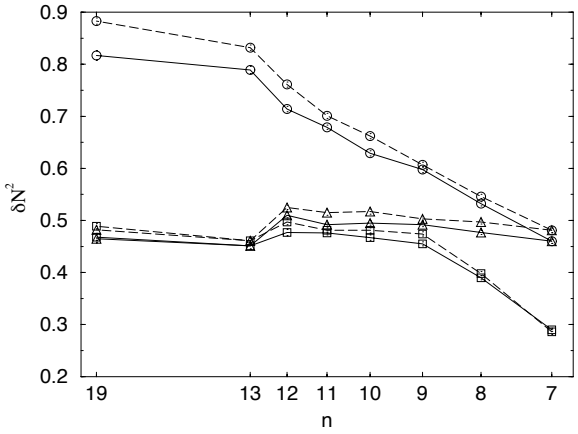

Figure 1: *Charge fluctuations for atomic domains* $\delta N^2 = \langle \hat{N}_A^2 \rangle - \langle \hat{N}_A \rangle^2$ *calculated with QMC methods. Solid (dashed) lines refer to correlated (uncorrelated) calculations. Three different types of atoms corresponding to the pentagonal bipyramidal subunit have been selected (central peak atom ◯, opposite peak atom △, ring atom □). The error bars in the QMC results are below* ± 0.007 *and therefore have not been plotted.*

One of the basic motivations for studying clusters is the question how bulk properties evolve with increasing cluster size. It is an important challenge for theory to relate the evolution of these properties to changes of the type of chemical bonding. An outstanding example are the clusters of divalent elements [6] which undergo a transition from van der Waals to covalent and finally metallic types of bonding with increasing cluster size. QMC methods can be used for these systems with almost invariable accuracy over a large range of cluster sizes and provide an accurate description of electron correlation. Properties measured in experiments like cohesive energies, ionization potentials and electron affinities are obtained with good accuracy and can be used for the calibration of more approximate methods [4, 6]. Although these properties provide some insight into the type of chemical bonding it would be desirable to study more local properties of the correlated wavefunctions. An example for such a property are atomic charge fluctuations which are intimately related to the type of bonding [7]. We have calculated these charge fluctuations with respect to atomic Wigner-Seitz cells but more realistic atomic domains based on Bader's description of atoms in molecules [8] using zero-flux surfaces of the density present no principal technical difficulty. Figure 1 shows the dependence of charge fluctuations on electron correlation in the case of mercury clusters ranging from Hg_7 to Hg_{19}.

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Konferenzen, Workshops und Symposien 1998-1999

Conferences, Workshops and Symposia 1998-1999

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International Workshop and Seminar on Disordered Dynamical Systems 107

International Symposium on Recent Trends in Modern Physics and Chemistry 108

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Report on

Nonlinear Time Series Analysis

February 11 - 21, 1998

Scientific directors: H. Kantz, D. Kaplan, T. Schreiber
61 participants

Motivation and goal
Nature supplies an overwhelming richness of dynamical, i.e. time dependent phenomena. Their understanding or prediction can be of value in many applications. Moreover, dynamical properties often shed light on underlying mechanisms. The experimental, but often also numerical observation of dynamics requires an analysis of time series data, i.e. data where the time ordering carries part of the information. Analysis methods derived from concepts of deterministic nonlinear dynamics and classical chaos have arrived at a level which permits the (careful and not unrestricted) application to a large number of physical and non-physical systems. Since this expertise is hold by only a few research groups worldwide, it is natural to increase the availability of this knowledge by a school.

Concept
This school consisted of three building blocks: Lectures supplying the basic knowledge in linear and nonlinear time series analysis; focus talks and contributions by participants presenting particular applications and systems; tutor assisted computer labs for practical exercise with time series data and analysis software. Moreover, both the schedule (participants' presentations, computer labs, poster sessions) and the environment (all meals together, accomodation in the guest houses, nearby pubs, poster area, computers, discussion rooms being available all time) supported enhanced communication among the participants and between participants and tutors/lecturers.

Speakers
Distinguished researchers who have made the major substantial contributions to the field of nonlinear time series analysis could be gained as speakers. Peter Grassberger, Celso Grebogi and James Yorke as outstanding seniors, and James Theiler, Lenny Smith and Klaus Lehnertz as not less outstanding members of the younger generation.

Participants
Originally, about 20 to 30 participants were planned. However, we had about 120 applications before the deadline and about 30 more after the deadline. The selection of 48 of them (the maximum capacity of the guest houses) was difficult. A giudeline for the selection process was to achieve homogeneity in prior knowledge on nonlinear dynamics (i.e. not too advanced) but a large heterogeneity in the scientific background, coupled to a good coverage of countries of residence and a reasonable perspective that the newly attained knowledge will help the participants in their future research work. In numbers: Germans/ non-germans: 23 / 25; countries represented: 18; male/female: 40 / 8; physicists/ non-physicists by training: 35 / 13; current research fields: physics, mathematics, cardiology, neurosciences, geophysics, chemics, engineering, motor control of musicians.

Estimate of success
The high number of applications and the fact that nobody cancelled the participation speak for the popularity of the topic and the reputation of the speakers. The clear

impression is that this school was indeed very much apprechiated. Despite the density of the 10 days' program even on the last day the lectures were well attended. The computers were used during all times outside the official program, and the scientific communication among the participants was obviously extremely intense. The concept of the school, which massively exploited the local facilities (in particular the excellent computer equipment and computer installation, thanks to Hubert Scherrer and Helmut Deggelmann) and could not have been performed in a similar way elsewhere, should be adopted for other fields of research. The perfect assistance by the members of the visitors program, in particular by Katrin Lantsch, took most of the burden of organisation, such that this school was also a real pleasure for the scientific organizers.

Report on

Disordered Dynamical Systems

March 2 - April 9, 1998

Scientific director: G. Radons
42 participants

Main focus of the conference:

The goal of the meeting was to explore the possibilities of combining methods and knowledge from the field of disordered systems with recent approaches and advances in classical dynamical systems. Bringing together experts from both fields aimed at stimulating research on the interplay between chaos and quenched randomness, a challenge at the foundation of equilibrium a non-equilibrium statistical mechanics. Applications range from extended nonlinear systems with disorder in condensed matter physics to the dynamics of randomly coupled entities in biological systems such as the brain.

Most important participants:

International: H. van Beijeren (Utrecht), L.A. Bunimovich (Atlanta), P. Gaspard (Bruxelles), I. Kondor (Budapest), J.-M. Luck (Saclay), Ch.M. Newman (New York), C. Perez-Vincente (Barcelona), H. Posch (Vienna), I. Procaccia (Rehovot), B. Toth (Budapest)

National: T. Geisel (Göttingen), P. Hänggi (Augsburg), H. Horner (Heidelberg), K.W. Kehr (Jülich), A. Knauf (Leipzig, now: Erlangen), J. Krug (Essen), H. Rieger (Jülich, now: Saarbrücken), H. Spohn (München), D. Weiss (Regensburg), W. Zimmermann (Jülich, now: Saarbrücken)

Presentations of scientific newcomers:

Young scientist, who were accepted for participation, appeared on one hand as lively and interested discussion partners. On the other hand their presentations, mainly during the workshop, were on a high scientific level. Some of the foreign participants (e.g. from Iran, at that time scientifically isolated) were able to present themselves so convincingly that new scientific contacts with German researchers were established.

Scientific results of the conference:

One major general achievement of the Workshop and Seminar on Disordered Dynamical Systems was the exchange of scientific methods between the members of both

participating fields - disordered systems and nonlinear dynamics - and the initiation and advancement of research in the emerging field of disordered dynamical systems.

Report on

Recent Trends in Modern Physics and Chemistry

March 17, 1998

Scientific director: P. Fulde
15 participants

This one-day symposium was considered as a spin-off meeting to review some of the modern trends in the physics and chemistry of complex systems. The topics included solid state physics, quantum chemistry, atomic systems in laser fields, optical microresonators, complex fluids and nonlinear dynamics for data analysis, to name a few.

Report on

Fluctuations far from Equilibrium

April 19 - 23, 1998

Scientific directors: W. Ebeling, P. Hänggi, L. Schimansky-Geier
60 participants

This workshop has been devoted to a current topic in nonlinear statistical physics and biophysics. In particular, fluctuations far from equilibrium can induce noise induced transport. This latter phenomenon impacts many applications in physics, chemistry and biophysics. Novel ideas and approaches have been presented that boost the importance of nonequlibrium fluctuations to a level where noise must be considered as a source of order and organized complexity in its own right. Several lectures summarized the actual state of art of theory and experiment of noise induced order. A few biophysical situations were presented. as e.g.ion channels, muscle motion or neuronal activity. Lectures in this field were complemented by about 20 posters. A concept that met strong positive feedback was the organized session wherein the representatives of the posters could announce the highlight(s) of their work with a short oral presentation.

Some specific highlights of the conference were the lectures by J. Prost (Paris), P. Silberzan (Paris), T. Viscek (Budapest), P. Jung (Athens) and F. Marchesoni (Camerino) and the discussions following the talks in which N. van Kampen (Utrecht), P. Pechukas (Columbia) together with the three organizers engaged themselves actively. J. Prost looked at the application of simplified stochastic models for the function of muscles. P. Silberzan and T. Viscek discussed several experiments that demonstrate in situ the "force free", noise induced motion. P. Jung presented a survey of stochastic structures and its modeling in neuronal tissues. F. Marchesoni considered collective transport of elastic strings in solids such as the motion of connected balls in washboard like potentials (soliton dynamics in presence of noise and friction). P. Pechukas (Columbia) presented the state of the art for the propblem of activated escape over fluctuating

barriers. K. Sekimoto (Kyoto) and J. Parrondo (Madrid) addressed the issue of the "efficiency" of moelcular motors and Brownian motors.

Most interesting presentations were also given by young invited speakers. The lecture by P. Reimann (Augsburg) considered noisy coupled Brownian motors which collectively behaves bistable with a negative conductance. J. Garcia-Ojalvo (Barcelona) has reviewed phase separation induced by noise. The lecture of J. Vilar (Barcelona) presented new results of periodically driven systems with noise induced phases. J. Freund (Berlin) proved the efficiency of ratchets by comparing the mean flux of particles to the diffusive one.

The lectures and the poster presentations held at the workshop have proven the broad interest in and the vitality of the field of stochastic nonlinear dynamics. Several cooperations between groups working in this field (Augsburg-Madrid-Barcelona-Katowice, Berlin-Barcelona-Saratov) were intensified during the workshop.

Report on

Computational Approach to Electron Correlations in Solids

May 25 - 29, 1998

Scientific directors: M.I. Katsnelson, A.I. Lichtenstein
85 participants

General methods for accurate description of the electronic structure of materials with correlated electrons has yet to be developed. Such materials include the high-T_c and colossal magnetoresistance (CMR) materials, as well as the mixed-valence and heavy-fermion compounds. All these systems demonstrate essentially many-particle (correlation) features in their excitation spectrum and ground-state properties. The usual language of one-electron band theory appears to be inadequate to describe such features even qualitatively: e.g., the problem of Mott insulators, the heavy-fermion behavior in some rare-earth compounds, satellites and "mid-gap states" in electron spectra. Such effects as the metal-insulator transition, Kondo effect, and others, which helps to understand the basic physics in these strongly correlated materials, is usually considered in the framework of simplified models such as the Hubbard model, Anderson model, s-f exchange model and other correlation models. Nevertheless the complexity of the real crystals containing 10-15 different atoms per unit cell, interactions between electronic and lattice degrees of freedom demands a more detailed investigation of the energy spectra in such systems.

The main goal of this workshop was to collect experts in the many-body and LDA communities and discuss opportunities to combine "the best from both worlds" to investigate correlation effects in real systems.

An essential part of the program was devoted to discussions of the new development in the dynamical mean field theory: lectures by Gabriel Kotliar (New Jersey) , Walter Metzner (München) , Dieter Vollhardt (Augsburg), Antoine Georges (Paris) and others. The method provides a rather high accuracy for different many-particle models and seems to be very promising for the combinations with LDA and applications to real systems.

Different schemes of Quantum Monte Carlo (QMC) approach have been discussed by Shiwei Zhang (Williamsburg) with the detailed considerations of so called "sign-problem", Lubos Mitas (Urbana) with the review of recent applications of QMC to real systems (MnO, carbon and silicon clusters etc.), Martin Ulmke (Augsburg) - applications of QMC to the problem of disordered correlated systems.

Review of contemporary state of first-principle methods has been done in the lecture by Ole Krogh Andersen (Stuttgart). Eberhard Gross (Würzburg) and Lars Hedin (Stuttgart) discussed new development of the density functional theory (the optimized effective potential method and GW-approximation). Quantum chemical calculations of correlation effects in solids has been discussed by Beate Paulus (Dresden).

Number of talks were devoted to investigations of electronic structures for interesting classes of materials, such as spin-ladders (Warren Pickett, Davis) , ytterbium pnictides (Helmut Eschrig, Dresden), fullerens (Olle Gunnarsson, Stuttgart) , CMR-manganites (Nobuo Furukawa, Zürich). Werner Hanke (Würzburg) discussed numerical results concerning SO(5) symmetry in high-T_c materials.

Two panel discussions devoted to the problems of magnetism and high-T_c superconductivity and poster session with 42 contributions were organized.

Report on

Small Scale Dynamics of Physico-Chemical Processes at Interfaces

June 15 - July 10, 1998

Scientific directors: M. Bär, Y. Kevrekidis, A. Thess
75 participants

Main focus

The workshop and seminar focussed on spatiotemporal dynamics at interfaces with particular emphasis on Marangoni effects and interfacial instabilities as well as chemical pattern formation. It brought together researchers from the fields of nonlinear dynamics, statistical physics, applied mathematics and engineering. The aspect of small scale dynamics had been addressed in several contributions dealing with microscopic models and experiments on nanostructures. Possible technological applications were highlighted in a special session during the workshop.

Participants and Contributions

85 scientists attended the program altogether, 76 (24) participants were present during the workshop (seminar). About 50 percent of the participants came from abroad. 32 (10) speakers had been invited for the workshop (seminar). A large number of applications has been taken into account in 10 short talks and 33 poster presentations. Topics and contributions can roughly be subdivided into experiments in Marangoni effects and interfacial instabilities (Linde, Adler, Schatz, Earnshaw, Bodouvis, Eckert), experiments in chemical pattern formation (de Kepper, Flesselles, Engel, Imbihl, Rotermund), systems involving hydrodynamics and chemistry (Troian, Müller, De Wit), nanostructures (Aksay, Pompe), small-scale modeling (Koplik, Kapral, Mikhailov), theory of reaction-diffusion systems (Meron, Barkley, Matkowsky), theory of thin films

and interfaces (Döring, Derby, Steen, Smith, Oron, Edwards) and last but not least applications (Marek, Meinköhn, Langbein).

Young Researchers

About 30 young researchers attended the program and presented 10 talk, 5 short talks as well as the majority of the posters. It is worth mentioning that the majority of the younger applicants had been working in universities and institutes in East Germany and Berlin.

Scientific Results

General - The workshop and seminar had intended to bring together scientists working experimentally and theoretically on instabilities and pattern formation in hydrodynamic and chemical systems and to compare methods and take on the challenges of small scale systems (below the micrometer scale). The exchange between the two communities proved very fruitful, various contributions showed that the coupling between chemical and hydrodynamical instabilities is a promising field of research. Another positive aspect was the good balance between experimental and theoretical contributions (16 talks each in the workshop) which lead to lively discussions and initiatives for collaborations.

Small Scale Dynamics - Various model approaches have been presented to address small-scale dynamics where fluctuations play an important role and macroscopic approach involving Navier-Stokes or reaction-diffusion equations may be invalid. These include molecular hydrodynamics, lattice-gas automata, active Brownian particles as well as stochastic partial differential equations obtained by coarse graining. Experiments on the nanoscale have so far not been able to detect nonequilibrium patterns. Here, the emphasis has been on the production of structured films or cluster arrays that are thermodynamically stable and are thus not dependend on particular dynamics. It remains an open question if the principles of pattern formation that are well established on the macroscopic scale above 1 μm will carry over to nanoscale structures.

Chemical Patterns - Experimentally, great progress has been made by the use of open reactors that mantain constant nonequilibrium conditions over a long time. Results on new phenomena such as spiral breakup, spiral interaction and pattern growth (fingering) and a large amount of quantitative results (phase diagrams) were reported at the conferences. Use of lithography has also lead to great progress in the study of patterns on catalytic surfaces. Theoretically, instabilities of simple patterns and issues of forcing and control as well as coupling to simple hydrodynamical instabilities have been reported and may stimulate new experiments.

Interfacial Instabilities and Marangoni Effects - Many talks have been devoted to this topic. Highlights include the discovery of square patterns in Marangoni convection, control of Marangoni convection in a liquid bridge, new instabilities in the spreading of films with surfactants. On the theoretical side, great efforts have been devoted to computational methods to deal with film rupture and other singularities in wetting and Marangoni problems. Further insight may come from techniques of model reduction and estimates on bounds of the heat transport. A project extending the latter approach to Marangoni convection has been started during the workshop.

Applications and Further Aspects - The applications include topics as diverse as technological applications of nonlinear dynamics in chemical reactors (reverse flow reactor, microreactors) and of thin film hydrodynamics, as well as experiments in microgravity

and ferrofluids. Finally, we have been positively surprised by the great number of applications *resp.* contributions from people working on problems outside the two main threads of the workshop. To name but a few: Pattern formation in polymer mixtures, simulations and experiments in crystal growth, patterns in geology and bioreactors. These aspects show a great future potential of the approaches discussed and made the meeting a very lively and enjoyable one.

Report on

Magnetism and Superconductivity in Highly Correlated Electron Systems

July 6 - 10, 1998

Scientific directors: P. Wölfle, G. Guentherodt, Y. Kuramoto, T. Fujita
58 participants

This 5th Bilateral German-Japanese Seminar on highly correlated electron systems focused on unusual collective phenomena in metallic compounds at low temperatures. New experimental results were presented and confronted with theoretical developments. The main topics discussed involved superconductivity in the cuprate compounds as well as in heavy fermion systems and magnetism in itinerant electron systems as well as those with local magnetic moments. Special attention was attached to orbital ordering and its interplay with spin ordering in compounds with several local orbitals. A further focus was the behavior of electrons and spins in reduced dimensions. The subject of quantum phase transitions at zero temperature and their influence on the strange metallic (non-Fermi liquid) behavior in a finite temperature range in the vicinity of a quantum critical point received much attention.

The program featured more than 40 talks, spanning a wide spectrum of topics in this field. After each talk, a discussion period of 5-10 minutes took place and was extensively used.

The meeting profited from the participation of internationally renowned scientists, Profs. Shiba, Kuramoto, Imada, Fukuyama, Ueda from the Japanese delegation and Profs. Vollhardt, Wegner, Lüthi, v. Löhneysen, Steglich, and others, from the German side. Among the about 50 participants, a sizeable fraction was younger than 30, several were Ph.D. students. Many of the younger people presented the results of their work in the poster sessions. The exchange of ideas and information on experiments and theory was very efficient.

The conference provided a forum to assess the status of the field, by allowing (i) exchange of the latest results, (ii) discussion of controversial subjects, (iii) agreement on questions already settled, (iv) identification of important new questions for future research. At the end of the conference many participants felt that the above goals had been met.

Report on

Dimension like Characteristics of Dynamical Systems

July 13 - 15, 1998

Scientific directors: M. Dellnitz, G. Keller, V. Reitmann
63 participants

The main concern of this workshop was a compact introduction into dimension like characteristics and multifractal analysis of dynamical systems. Starting from the central concept of Carathéodory dimension, the most important dimension like characteristics of sets and measures (Hausdorff dimension, capacity, entropies etc.) were derived (Ya. Pesin, J. Schmeling). Dimension like characteristics were discussed in a strong connection with invariant sets and invariant measures of dynamical systems. Efficient methods for estimating such characteristics mainly in terms of the singular values and the Lyapunov exponents were presented. Further the strong connection between different kinds of dimensions of an invariant sets and the parameters of a bifurcation was shown (V. Afraimovich, J. Muldowney). The estimates of dimension like characteristics from time series was discussed in terms of Lyapunov exponents. New embedding techniques as the Eckmann-Ruelle technique were presented (J. Yorke). Recent results concerning connections between projections, embeddings, and fractal dimension were also discussed (B.R. Hunt). Dimension estimates for global attractors of partial differential equations are based on a finite-dimensional approximation. The construction of inertial manifolds for certain types of differential equations was shown (E. Titi).

In the additional program of the workshop 15 participants presented posters. Further the use of the software package "Dynamics" was demonstrated by J. Yorke. For interested participants of the workshop there was organised a visit of the opera "Jenufa" by Leos Janacek performed at the Semper Opera House.

Report on

Physics of Turbulence

July 20 - August 7, 1998

Scientific directors: R. Friedrich, J. Peinke
68 participants

The goal of the seminar and the workshop was to give participants the opportunity to get a detailed overview on current research efforts in turbulence. The main topics covered in the seminar were: Selfsimilarity and turbulent fields (Yaglom), multifractal scaling behaviour (Ciliberto, Schertzer), cascades (Greiner, Naert), dynamics of coherent structures (Kwasniok, Comte, Couder, Clerx), dynamics of passive scalars (Pumir), bounds on turbulent transport (Busse) and fieldtheoretic methods (Procaccia, Falkovich). Furthermore, there were additional lectures on statistics (Honerkamp), synergetics (Haken) and the relationship between fincance and turbulence (Barndorff-Nielsen). During the subsequent international workshop scientists from all over the world as well as participants of the seminar presented recent results of their own activities. One of the major outcome of the seminar and workshop is the fact that young

german scientists working at different places used the opportunity to start a discussion about future common projects: The meeting has initiated interdisciplinary resarch activities on turbulence among physicists and engineers. Various common DFG-proposals are currently formulated.

Report on

DMRG and Other Advances in Numerical RG Methods

August 24 - September 18, 1998

Scientific directors: K. Hallberg, R. M. Noack, X. Wang
54 participants

Main Focus:

In recent years, the Density Matrix Renormalization Group became one of the most powerful methods for determining the low-energy properties of many quasi-one-dimensional strongly interacting systems. There have been important improvements to this technique, as well as extensions to different problems such as two-dimensional classical systems, quantum systems at finite temperature and the calculation of dynamical properties. The aim of the seminar was to provide a pedagogical introduction to the techniques for students and young researchers, as well as to provide an opportunity to work directly with the methods using the computational facilities at the Max-Planck-Institute in Dresden.

Most important participants:

E. Carlon (Leuven, Belgium) A. Drzewinski (Warsaw, Poland) H. S. Krishnamurthy (Bangalore, India) M. A. Martin-Delgado (Madrid, Spain) T. Nishino (Kobe, Japan) S. Rommer (Goteborg, Sweden) U. Schollwöck (Munich, Germany) G. Sierra (Madrid, Spain) T. Xiang (Cambridge, UK) T. Costi (Karlsruhe, Germany) E. Jeckelmann (Irvine, USA) S. Liang (Ames, USA) S. Moukouri (Sherbrooke, Canada) I. Peschel (Berlin, Germany) S. Ramasesha (Bangalore, India) N. Shibata (Tokyo, Japan) S. R. White (Irvine, USA)

How did scientific newcomers present themselves:

The prospect of the conference was submitted by poster and e-mail to several places in different countries where research using similar methods was being performed. The Visitors Program worked in a very efficient way receiving and processing all the applications. We would like to point out that, although the scientific organizers where far apart (in Germany, Switzerland and Argentina), organization was possible, principally via e-mail, thanks to the experience and excellent predisposition of the secretaries and members of the Visitors Program of the MPI PKS in Dresden.

Scientific results of the Conference:

The experience of having both, a Workshop and Seminar simultaneously was very profitable. An introductory week helped young students to get acquainted with the methods. Then two weeks with first level talks on the latest advances on the subject followed, which also gave the opportunity to researchers working in the field to have an overview on the latest progresses on this matter. The last week was devoted to

hands-on work done by the students using the computing facilities at the MPI PKS. As an important outcome of the conference, the first book on Density Matrix Renormalization was published by Springer, as Lecture Notes in Physics ("Density Matrix Renormalization: A Numerical Method in Physics", I. Peschel, X. Wang, M. Kaulke and K. Hallbe rg eds., Springer,Heidelberg, Germany, 1999), intended to serve as a guide to newcomers and experts in the field.

Report on

Electronic and magnetic properties of novel transition metal compounds: from cuprates to titanates

October 5 - 30, 1998

Scientific directors: H. Eschrig, J. Fink
87 participants

The main focus of Workshop and Seminar was on the unconventional behavior of novel transition metal compounds. Their electronic and magnetic properties are characterized by the effects of strong electron correlations and low dimensionality. The contributions to the conference were equally distributed between experimentalists and theoreticians. A large part of it dealt with magnetic or superconducting cuprates, several talks were about manganites, but there were also many reports on vanadates or systematic treatments of transition metal compounds.

The Workshop started with a School with relatively long (up to three hours) tutorial lessons. High level speakers could be engaged for that purpose (like for instance S. Maekawa, G. Sawatzky, W. Hanke, D. Johnston or A. Aharony). In those lessons systematic, and more introductory treatments of several subtopics were given. On the contrary, during the following one-week scientific conference, each of the speakers concentrated on very actual and fresh results. For instance, two phase transition in NaV_2O_5 were reported (Ch. Geibel, C. Gros) and several proposals for charge order were given (P. Thalmeier). New results for other vanadates were presented as well (A. Loidl, W. Pickett, D. Khomskii). The strange electronic properties of underdoped cuprates (A. Chubukov, D. Hone) or of spin ladder systems (T.M. Rice) were treated in several talks. These strange properties can also be studied by introducing Zn impurities into high temperature superconductors (H. Alloul). It became clear that there are very interesting magnetic properties within the family of cuprates (A. Aharony, I. Meijer, S. Maleyev). The optical properties of manganites were analysed (P. Horsch) and charge-ordering was discussed (H. Hwang). During the conference two Poster Sessions were performed with a very good attendance.

The Workshop gave a good motivation for the following Seminar (October 19-30). The number of participants was less than during the previous conference but that gave the opportunity for intensive discussions. Everybody who wanted could present his own scientific results and there was one talk of one hour each day. That opportunity was especially chosen by scientific newcomers. The discussions helped to support existing collaborations or to create new ones.

Report on

From mesoscopic to microscopic quantum transport: new trends in theory and experiment

November 26-27, 1998

Scientific directors: K. Richter, D. Weiss
60 participants

Mesoscopic physics, as a young, interdisciplinary field in between condensed matter and atomic and molecular physics, is still rapidly progressing. The aim of this rather informal meeting was to bring together experts from different branches in mesoscopic quantum transport and related disciplines in order to discuss current progress and, in particular, to explore future trends and directions.

The topics of the meeting included on the one hand transport from mesoscopic scales (including superlattices, quantum billiards, quantum dots) to atomic scales (artificial atoms and molecules, point contacts, nano-tubes and -wires); on the other hand the question how to use quantum dots physics as a basis for quantum computing was discussed.

A major intention of the workshop was to intensify a real exchange between theory and experiment. Hence, the list of talks comprised an equal number of theoretical and experimental contributions. Besides leading senior researchers in the field, e.g. C. Beenakker, R. Jalabert, D. Loss, and G. Schön, the meeting served as a platform for many young people to present their work as invited talks. They outlined novel directions such as micromagnetism, nonlinear nanomechanics, and transport through break junctions, to name a few examples. The lectures were complemented by a an extended one-afternoon poster session, which allowed the other participants to present their work. With quantum transport from micron- to nanoscales and quantum computing as the two major subjects, the meeting certainly reflected two prominent and promising trends in future physics of coherent matter.

Report on

Beyond Quasiperiodicity: Complex Structures and Dynamics

Januar 11 - Februar 5, 1999

Scientific directors: U. Feudel, C. Grebogi, A. Pikovski
70 participants

The international workshop and seminar "Beyond quasiperiodicity: complex structures and dynamics" were aimed at the interdisciplinary aspects of complex almost-quasiperiodic phenomena in dynamical systems (strange nonchaotic attractors, synchronization phenomena, systems with fractal spectra), in condensed matter physics (localization phenomena, excitation in disordered lattices) as well as in the theory of quantum chaos (dynamical localization with respect to quasiperiodic excitation, anomalous diffusion in systems with fractal spectra). Especially the short workshop has found a very good response, and was attended by such famous scientists

as Ed Ott (Maryland), Kuni Kaneko (Tokyo), Jean Bellisard (Toulouse), Theo Geisel (Göttingen), Antonio Politi (Florence). Also young scientists got opportunities to present their works. During the extended seminar several selected topics have been a subject of lectures and discussions. As a result, several new collaborative projects have been started that already gave rise to several publications. The workshop/seminar definitely gave an impact in the studies of complex phenomena beyond quasiperiodicity, both in broadening the viewpoint and in deepening the research.

Report on

Cooperative Phenomena in Statistical Physics: Theory and Applications

February 7 - March 5, 1999

Scientific directors: M. Baake, U. Grimm, R. A. Römer, M. Schreiber
57 participants

It was the aim of this meeting to bring together researchers from statistical physics, mathematical physics, and mathematics, to exchange their views and join forces to treat various problems in the field of exactly solvable models and cooperative phenomena, and to study manifestations of different degrees of ordering in statistical systems, ranging from periodic via aperiodically ordered to disordered. Apart from the organizers, the workshop and seminar attracted a total of 57 participants from many countries and all continents, including a large fraction of students and young postdocs who attended the entire seminar or at least the major part of the four-week program.

The topics of the meeting included solvable lattice models, models of interacting electrons, self-organized criticality, growth models, random tilings, symmetries, and invariance principles. As part of the seminar, we had invited four colleagues to present short introductory courses into these topics. They were given by Paul A. Pearce (Melbourne) on solvable lattice models, by Manfred Scheunert (Bonn/Freiburg) on quantum groups, by Fabian H. L. Esler (Oxford) on correlated fermion models, and by Andreas Schadschneider (Köln) on self-organized criticality. These lectures were aimed particularly at the younger participants, who were also given the opportunity to present their own work in more specialized talks during the seminar and workshop, and in well-frequented evening poster sessions during the workshop.

The list of invited participants for the seminar was composed in such a way that smaller groups could form spontaneously for personal interaction and cooperation. Senior scientists (such as the above mentioned speakers and some others, e.g. Jean Bellissard, Robert V. Moody, and Vladimir Rittenberg) were asked to guide the research of younger participants in their field. This proved extremely successful and resulted in a number of research results and even publications that came out of the seminar.

In addition, the workshop provided an overview of current research trends, illuminating the central topics of the seminar in a broader perspective.

Report on

Statistical Physics of Neural Networks

March 1 - 26, 1999

Scientific directors: W. Kinzel, I. Kanter, M. Biel
45 participants

Models and methods of statistical physics may be used to account for cooperative effects in neural networks. This was the topic which gathered 45 scientists from e.g. Germany, Brazil, England, USA, Belgium, Denmark, Spain, France and Hungary. The aim was to report on new results from the research groups and to discuss common projects.

Each invited speaker was accompanied by a postdoc or PhD student. There were only a few invited talks which stimulated collaborations. This concept turned out to be very successful. During the seminar many new ideas were generated and expanded on. Many new collaborations were created. These led to partial results already during the seminar. Especially young scientists profited from the stimulating atmosphere and the excellent working conditions.

The seminar was used to present research in the field of the theory of neural networks. Such networks are trained using examples. After the training phase such networks not only correctly reproduce the examples, but they also show an overlap with the unknown rule, which was used to generate the examples. These new algorithms are thus trained to generalize. The generalization error, which is a function of the number of learned examples and the model parameters, may be computed using methods of statistical physics. Thus one arrives at an understanding of cooperative properties of those networks, which is important not only for the physics of complex adaptive systems, but also for neurobiology, informatics and engineering sciences.

A number of new results and approaches was discussed during the seminar. In the following we give a brief list of topics covered. For the first time it became possible to exactly compute properties of so-called support vector machines. These are nonlinear networks, which have been recently successfully used for applications. Many-layer networks, which are trained with the so-called back propagation algorithm, show up with a discontinuous phase transition into a configuration of high speciality upon increasing the number of examples. The relation between different learning algorithms and standard information theory (parameter estimation of Bayes) was obtained. New results were also found with respect to the analysis, prediction and generation of time series. One example is the exact computation of the properties of algorithms, which learn from each other. Methods of statistical mechanics were applied in game-theoretical problems for the first time. Models with a manifold of attractors and with cyclic attractors were discussed in connection to biological problems.

The seminar demonstrated, that the statistical physics of neural networks is a lively field of research. It generates many new results which are of interest for other research fields.

Report on

Dynamics of Complex Systems

March 30 - June 15, 1999

Scientific directors: Y. Alhassid, M. Wilkinson, B. Mehlig
120 participants

Structure of the seminar/conference

An international seminar *Dynamics of Complex Systems* took place from March 30 to June 15, 1999, at the Max Planck Institute for the Physics of Complex Systems. In connection with the seminar, a one-week conference was held from May 11 to May 15, 1999. The scientific directors of the seminar and conference were Yoram Alhassid (Yale), Bernhard Mehlig (Freiburg) and Michael Wilkinson (Glasgow).

Main focus of the seminar/conference

The seminar focused on various universal aspects in the dynamical properties of complex quantum systems beyond their spectral properties. These universal aspects are often exemplified by random matrix models. While earlier applications of random matrices often focused on single-particle dynamics, the seminar explored how the random matrix statistics might be modified in the presence of interactions.

Main participants

Mesoscopic Physics: Y. Avishai, C. Beenakker, Y. Blanter, J. Chalker, Y. Fyodorov, Y. Gefen, I. Lerner, C. Marcus, S. Mirlin, G. Montambaux, J.-L. Pichard, A.D. Stone

Nuclear Physics: S. Aberg, G. Bertsch, A. Bulgac, G.Mitchell, V. Zelevinsky

Physical Chemistry and Molecular Physics: S. Berry, R.D. Levine, W. H. Miller

Atomic Physics: J. M. Rost

Quantum Chaos: O. Agam, O. Almeida, D. Kuznezov, R. Prange, S. Tomsovic, D. Shepelyansky, N. Whelan

Scientific results in the broader sense

The seminar and conference brought together over 90 researchers from the condensed matter physics, nuclear physics, and physical chemistry communities. The scientific results of the program have been collected in a special issue of Physica E, due to appear in spring 2000.

Report on

Topological Defects in Non-Equilibrium Systems and Condensed Matter

June 7 - August 27, 1999

Scientific directors: L. Kramer, L. Pismen
105 participants

The main focus of the program

The program brought together scientists from the non-equilibrium physics community and equilibrium condensed matter physics community to discuss methods and tools of studies of dynamics of disordered media dominated by formation, motion and annihilation of topological defects. The applications included non-equilibrium patterns in fluid-mechanical, chemical and nonlinear optical systems, as well as dynamics of superfluids, superconductors, liquid crystals, ferromagnetic and cosmic strings. The program included the Workshop "Computer-aided analysis of dynamical structures and defects" (20 to 29 July) and four focus periods : "Topological Defects in Cosmology, Particle Physics and Condensed Matter"; "Optical Patterns and Defects"; "Ginzburg–Landau Equation and Beyond", "Properties and Dynamics of Defects in Liquid Crystals".

The most important participants Agnes Buka (The Hungarian Academy of Sciences, Budapest), Patricia Cladis (Advanced Liquid Crystal Technologies, Summit), Pierre Coullet (Universite de Nice, Valbonne), Ann-Christine Davis (Cambridge University), Willie Firth (University of Strathclyde, Glasgow), Shoichi Kai (Kyushu University, Fukuoka), Tom Kibble, FRS (Imperial College, London), Maurice Kleman (LMCP, Universite Pierre-et-Marie-Curie, Paris), Edgar Knobloch (University of California at Berkeley), Manfred Lücke (Universitaet des Saarlandes, Saarbruecken), Bernard Matkowsky (Northwestern University, Evanston), Michael Monastyrsky (Institute for Theoretical and Experimental Physics, Moscow), Alexander Nepomnyashchy (Technion, Haifa), Pawel Pieranski (Universite Paris-Sud, Orsay), Yves Pomeau (Ecole Normale Superieure, Paris) Nikolay Rosanov (Vavilov State Optical Institute, St. Petersburg), Maxi San Miguel (IMEDEA, Universitat de les Illes Balears, Palma de Mallorca), Victor Steinberg (Weizmann Institute of Science, Rehovot), Hans-Rainer Trebin (Universitaet Stuttgart), Valerii Vinokour (Argonne National Laboratory), Grigory Volovik (Helsinki University), Carl Weiss (Physikalisch-Technische Bundesanstalt, Braunschweig)

Scientific newcomers About 36 young researchers presented their talks at the seminar and workshop.

The scientific results of the conference in a broader sense The participants working in different branches of nonlinear physics exchanged computational programs and approaches to computer-aided analysis and lively discussed the talks, sometimes discovering that similar problems arise in different contexts. Some heavily discussed topics crossing the boundaries between scientific fields, which may find their way into the literature are: the role of topology, mechanisms leading to localized states, front propagation, spiral breakup scenarios, the gluing-bifurcation route to chaos, Maybe most importantly, new collaborations were established, and new projects started.

Report on

Linking Different Length and Time Scales in (Macro-)Molecular Systems

September 1 - October 31, 1999

Scientific directors: K. Kremer, H. Pleiner, B. Dünweg
80 participants

Structure and dynamics of complex fluids or "soft condensed matter" are typically determined by a rather complicated, and in most cases poorly understood, interplay of properties originating from different length and time scales. These scales typically span the range from $10^{-10}m$ to $10^{-6}m$ and $10^{-13}s$ to $10^{0}s$. Traditionally, the scientific progress has formed by specialized expertises suited for the phenomena occuring on one particular scale, such that the approaches of quantum chemistry and hydrodynamics (to just mention the extremes) have little in common, both with respect to methods and to language. Nevertheless, all communities are ultimately dealing with the same piece of matter. The organizers therefore believe that substantial progress in the future can be achieved if all the communities involved are brought in closer contact with each other, mutually benefitting from both the results and the methodological approaches of the others. This was the main purpose of the conference, which thus attempted to cover a very wide range of theoretical, simulational, and experimental soft condensed matter physics. Nevertheless, the conference could deal only with selected topics, as unmixing dynamics, rheology, surfactants, block copolymers, colloids, thin polymer films, (polymer) liquid crystals, gels, light scattering in dense systems, charged systems, proteins, and simulation methods, as coupling of algorithms (like elasticity theory vs. molecular dynamics, molecular dynamics vs. quantum mechanics), and new schemes like lattice Boltzmann. A selection of first–rate scientists was attracted to the conference; in order of appearance in the program: M. Cates, D. Roux, J. Fraaije, K. Winey, S. Hess, Y. Rabin, D. Weitz, U. Seifert, M. Fuchs, U. Suter, M. Doi, W. Paul, A. Gusev, C. Holm, K. Kawasaki, M.–W. Kim, J. Prost, J. Noolandi, P. Martinoty, D. Long, M. Allen, B. Erman, A. Grosberg, A. Torda, P. Pincus, A. Ajdari, J. Yeomans, F. Müller–Plathe, M. Parrinello, A. Panagiotopoulos, G. Maret. Altogether, there were more than 80 participants; many presented their research in 34 posters. There was a good chance for young researchers (which made up a substantial fraction) to get in contact with scientists of all ages from other groups; these opportunities were intensely taken advantage of. The conference was embedded in a more spezialized four–week seminar program, with typically some ten participants per week.

The organizers got very positive responses from the participants. Many people felt they had learnt quite a lot in a stimulating atmosphere of mutual exchange; this can clearly be said about the organizers, too. They view the meeting as a full success.

Report on

35. Symposium für Theoretische Chemie

TU Bergakademie Freiberg

September 12 - September 16, 1999

Scientific directors: M. Dolg, J. Fabian, H. Hartmann
160 participants

The 35th Symposium for Theoretical Chemistry took place September 12 - 16, 1999, at the Technical University Bergakademie Freiberg. The conference was organized by Dr. M. Dolg (Max-Planck-Institut für Physik komplexer Systeme, Dresden), Prof. Dr. J. Fabian (Technische Universität Dresden) and Prof. Dr. H. Hartmann (Fachhochschule Merseburg, Technische Universität Bergakademie Freiberg). The meeting was financially supported by the *Deutsche Forschungsgemeinschaft* and the *Staatsministerium für Wissenschaft und Kultus* of the state of Saxony. The symposium is annually taking place and the conference location changes regularly between Austria, Germany and Switzerland. The main topic of the meeting in 1999 were *relativistic effects and electron correlation effects in heavy-element chemistry*. The meeting is designed to bring together young researchers from the german speaking countries with internationally respected scientists of the field.

In total 153 participants, 108 of which hold a PhD degree, from 12 countries attended the meeting. 123 participants came from Germany, the others from Austria, Finland, France, Israel, Italy, New Zealand, Netherlands, Russia, Sweden, Slovakia and the United States of America. 12 internationally well-known scientists were invited to give lectures, i.e., Prof. Dr. B.A. Hes (Erlangen), Prof. Dr. U. Kaldor (Tel Aviv), Dr. T. Saue (Toulouse), Dr. Lucas Visscher (Amsterdam), Prof. Dr. E. J. Baerends (Amsterdam), Prof. Dr. N. Rösch (München), Prof. Dr. H. Schwarz (Berlin), Prof. Dr. W.H.E. Schwarz (Siegen), Prof. Dr. C. Teichteil (Toulouse), Prof. Dr. P. Schwerdtfeger (Auckland), Prof. Dr. W. Kutzelnigg. In addition 17 contributed talks, mainly given by young scientists, and 82 posters were presented.

For the first time the *Hans G. A. Hellmann-Award* for a young german-speaking scientist was awarded by the *Arbeitsgemeinschaft Theoretische Chemie*. The price winner was Dr. Willem Klopper (Utrecht), who made important contribution of the field of accurate correlated calculations, i.e., r_{12}-dependent wavefunctions.

Abstracts of all talks and poster presentations are available on the internet under http://www.mpipks-dresden.mpg.de/∼stc99.

Report on

Non-Fermi Liquids

September 29 - October 1, 1999

Scientific directors: S. Hüfner, H. v. Löhneysen, P. Wölfle
53 participants

The concept of the Fermi liquid is one of the cornerstones of solid state physics. In short it describes a system of interacting electrons in a metal by a system of independent particles with renormalized properties. This obviously makes a complicated many body problem tractable. With the advent of the high-temperature superconductors, speculation has increased whether metallic systems occur with such strong deviations from the Fermi-liquid behaviour that they should be rather called non-Fermi liquids. There are basically two broad classes of systems on which the investigations of non-Fermi liquid behaviour has focused. One encompasses the heavy-fermion compounds near the quantum critical point at a magnetic instability where their thermodynamic properties exhibit strong deviations from ordinary Fermi-liquid behaviour, or metals with impurities with an internal degree of freedom coupled strongly to conduction electrons. The second class of systems is derived from the old theoretical finding by Tomonaga and Luttinger, namely that in a one-dimensional interacting electron gas Fermi-liquid theory breaks down (leading to, e.g., spin charge separation in the excitation spectrum). Prototype materials are all systems that are quasi one-dimensional, like the carbon nanotubes, special organic or inorganic materials, quantum wires, or edge states in the quantum Hall effect.

The three-day workshop on Non-Fermi liquids brought together about 70 experimentalists and theorists from a wide variety of fields, all being concerned with different types of non-Fermi-liquid behaviour. That was the main object of the workshop and it worked out surprisingly well. We had 25 invited lectures, well balanced between experimental and theoretical talks, and on one evening a lively poster session with 20 posters. Different communities learned how the new phenomena manifest themselves in very different materials and different types of experiments, from macroscopic thermodynamic and transport measurements to microscopic measurements such as neutron scattering. In contrast to the concept of the Fermi liquid, no similar generally and, in principle, simple concept of a "non-Fermi liquid" exists. This, however, as far as the organisers are concerned, is a very gratifying result, because it shows that here is a field of exciting new phenomena, which invites new efforts to come to a unified understanding of this fascinating subject. We are grateful to the Max-Planck-Institut für Physik komplexer Systeme for giving us the opportunity for holding this workshop, for its hospitality and the superb organization, and last but certainly not least for the generous support allowing the participation of physicists from many different countries.

Report on

Atomphysik '99

November 25 - 27, 1999

Scientific director: J.- M. Rost
54 participants

The two and a half day meeting brought together experimental and theoretical groups working in the area of atomic physics all over Germany,
e.g. from Berlin (TU, FU, Fritz-Haber-Institut, Hahn-Meitner-Institut, Max-Born-Institut), Bielefeld (Uni), Darmstadt (GSI), Dresden (TU), Freiburg (Uni), Frankfurt (Uni), Giessen (Uni), Halle (MPI für Mikrostrukturphysik), München (TU).
Each group was encouraged to participate with several, in particular younger researchers. This concept was well accepted and led to a high scientific level accompanied by lively discussions including fresh questions.

The talks reflected the broad activity of the atomic physics community. Experiments were reported from major facilities worldwide, from accelerator based physics to processes involving synchrotron radiation. A half day focus was devoted to electron correlation in intense laser fields. Exciting new data on the recoil momentum of the ionized atoms was presented[2] and the participants tried to assess its relevance for the mechanism of multiple ionization in intense fields, still under discussion.

Another highlight were two discussions held in parallel on "'The many-body problem in atomic dynamics" (J. Ullrich) and "'Time and measurement in Quantum Mechanics" (J. S. Briggs).
We hope and are almost certain that the lively discussions and atmosphere has given all participants and in particular the young Diploma and Ph. D. students a stimulus for their own work well into the future.

[2]Rottke H. et al.: Momentum distributions of Ne^{n+} ions created by an intense ultrashort laser pulse. Phys. Rev. Lett. **84**, 447 (2000).

Report on

Diffraction: Theory and Practice

December 19 - 21, 1999

Scientific directors: D. Joseph, U. Grimm, M. Baake
33 participants

The last symposium at the MPIPKS in 1999 brought together 33 researchers from both sides, theory and experiment. It was organized by Dieter Joseph, Michael Baake, and Uwe Grimm. The aim was to provide a discussion forum about the different problems of the field for specialists and newcomers. The program consisted mainly of longer plenary talks devided into an introduction for non-specialists and a state of the art part. The length of the talks gave enough time for questions and detailed discussions. Both, the speakers and the audience, used this freedom.

Michael Baake (Tuebingen) discussed the current state of knowledge about the question: "Which state of matter diffracts". Although this question was posted (by Bomberi and Taylor) already in 1985 a possible answer is far more complicated than expected. Afterwards, Veit Elser (Cornell) gave an intuitive approach to the diffraction properties of random tiling structures and Moritz Hoeffe (Tuebingen) showed diffraction properties of several examples, with focus on the diffuse background. Conradin Beeli (Zuerich) gave a review about electron microscopy. After an introdution to several technical aspects, he focused on the achievements and the problems of electron imaging. Eveline Weidner (Muenchen) gave the introduction to the different aspects of X-ray scattering. Afterwards Fritz Frey (Muenchen) spoke about what we know and what we can do with X-ray scattering concerning the structure analysis of quasicrystals. Marc de Boissieu (Grenoble) summarized the knowledge about neutron scattering, the state of the art and the problems. These sessions were brought into one line by the speakers so that the audience could follow the advantages and disadvantages of the different techniques. Stephen Pennycook (Oak Ridge) spoke about Z-contrast imaging in general and its application to aperiodic crystals in particular. He outlined its potential power but he also clearly marked the possible pitfalls. Afterwards, Veit Elser gave an overview about his method of phase-reconstruction called "Principle of Minimum Charge" that can become an alternative approach in structure analysis. The end of the program was a talk of Dr. Takakura (Tsukuba) about "Modelling and Structure Refinement of Quasicrystals".

All talks were embedded into lively discussions. Although no direct solution to the announced problems were found, the meeting provided a basis for intense collaboration of the participants in the future.

Beteiligung an Drittmittelprojekten

Participation on third-party funds

DFG Projekte

DFG funding

- DFG Forschergruppe “Nanostrukturierte Funktionselemente in makroskopischen Systemen”, Project C2: “Wachstum, Strukturbildung und Transport in nanostrukturierten Systemen”, Dr. Markus Bär, Heiko Kühne
- DFG-Schwerpunktprogramm “Quasikristalle: Struktur und physikalische Eigenschaften” (SPP 1031), Projekt: “Cluster- und Supercluster-Strukturen in Quasikristallmodelle”, Dr. Dieter Joseph
- DFG Projekt "Ballistischer Transport im Rahmen der Fredholm-Theorie", Dr. Klaus Richter
- DFG Schwerpunkt "Relativistische Effekte in der Chemie und Physik schwerer Elemente", Projekt Sto 305/1-3, Bernhard Metz, Prof. Michael Dolg
- Kooperationsprojekt der DFG "Complex systems in condensed matter physics - strong correlation and disorder", Prof. Peter Fulde

Sonderforschungsbereiche

- SFB 256 "Nichtlineare partielle Differentialgleichungen" an der U. Bonn, Dr. Andreas Deutsch
- SFB 276 "Korrelierte Dynamik hochangeregter atomarer und molekularer Systeme", Prof. Jan-Michael Rost
- SFB 393 "Numerische Simulationen auf massiv parallelen Rechnern", TU Chemnitz, Dr. Bernhard Mehlig
- SFB 463 "Seltenerd-Übergangsmetallverbindungen: Struktur, Magnetismus und Transport", TU Dresden, Prof. Peter Fulde

BMBF Projekte

BMBF funding

- BMBF-Förderung: Mitgliedschaft im Kompetenzzentrum "NanOp" für die Nanostrukturen in der Optoelektronik, Dr. Jens Nöckel
- BMBF Projekt:" 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
- BMBF:"Fehlerfrüherkennung durch Zeitreihenanalyse", Dr. 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, Thema ”Nichtlineare Methoden zur Last- und Energieangebotsprognose in lokalen Energiesystemen, insbesondere bei Windenergie und Photovoltaik”, Mario Ragwitz, Dr. Holger Kantz

- BMBF: ”Nichtlineare Methoden zur Last- und Energieangebotsprognose in lokalen Energiesystemen, insbesondere bei Windenergie und Photovoltatik, Dr. Holger Kantz

EU Projekte
EU funding

- EU-Förderung: (INTAS-Network) “Periodically Driven Zero-Dispersion Systems”, Dr. Klaus Richter

- EU-Förderung: Participant in the COST P5 Initiative “Mesoscopic Electronics”, Dr. Klaus Richter

- EU-Netzwerk: (CERION/ ESPRIT IV) Participant of the “Canadian European Research Initiative on Nanostructures”, Dr. Klaus Richter

- EU-Förderung (Marie Curie Training Site) ”Physics of Complex Systems”, Prof. Jan-Michael Rost

- Node of the EU TMR Network ”Quantum Chemistry of the Excited State”, Prof. Peter Fulde, Prof. Michael Dolg, Dr. S. Pleutin

Andere
Others

- German-Israeli Foundation (GIF), Grant for Feasibility Study, 10/99 - 10/00, “Pattern Formation in Catalysis”, Dr. Markus Bär

- Indirekte Drittmittel durch Stipendienaufenthalte (DAAD, spanisches Ministerium für Bildung, Socrates), Dr. Holger Kantz

- Verbundprojekt im Rahmen des Programms Technische Anwendungen von Erkenntnissen der Nichtlinearen Dynamik , Thema ” Theoretische Konzepte zur Fehlerfrüherkennung durch Zeitreihenanalyse”, Dr. E. Olbrich, Dr. Holger Kantz

Beantragte Drittmittelprojekte
Project applications

- DFG Sachbeihilfe "Experimentelle und theoretische Untersuchung von räumlich lokalisierten Anregunge in nichtlinearen Gittern", Dr. Sergej Flach
- Volkswagen-Stiftung: Projekt "Molekularsieblaser-Konglomerate im Infraroten", Dr. Klaus Richter
- EU-TMR-Network: "Mathematical Modeling and Simulations for the Improvement of Cancer Therapies", Dr. Andreas Deutsch
- EU-Förderung (Marie Curie Training Site) "Physics of Complex Systems", Prof. Jan-Michael Rost
- Subcontractor of EU-IHP Network "Localization by Nonlinearity and Spatial Disceteness and Energy Transfer, in Crystals, Biomolecules and Josephson arrays.", Dr. Sergej Flach
- EU-Förderung (Marie Curie fellowships):
"Nanostructure and Electronic Transport", Dr. Markus Bär, MPI Dresden.
- EU-Förderung: (INTAS-Netzwerk)
"Nonlinear Transport and Optical Effects in Carbon Nanotubes", Dr. Klaus Richter

Stipendien
Stipends

- Humboldt Stipendium - Gastwissenschaftler (Dr. Oleg Yevtushenko) "Regular and Stochastic Dynamics of Spatially periodic magnetic fields", April 1997-März 1998

Industriekooperationen

Cooperations with Industry

Group: "Nonlinear Time Series Analysis"

Within the framework of funding from the BMBF on failure prediction there was a fruitful cooperation with the Siemens-division SCR in Princeton, USA. A smaller project on quality control for electrically operated sunroofs of cars was conducted in cooperation with Carl Schenk AG, Darmstadt. The German patent for the noise reduction algorithm for human voice was accepted (December 1999) and its application in Europe, the US, and Japan is submitted.

Patente und Lizenzen

Patents and licences

- US-Patent, eingereicht am 21. April 1998:
  "Solid state laser for operation in librational modes".
  Beteiligte: Lucent Technologies (F.Capasso, A.Y.Cho, J.Faist, C.F.Gmachl, D.L.Sivco), Yale University (E.E.Narimanov, A.D.Stone) und MPIPKS (J.U.Nöckel).

- Erfingungsmeldung eingereicht am 19. November 1998
  "Rauschunterdrückung auf Sprachsignalen mit Methoden der nichtlinearen Zeitreihenanalyse"
  Beteiligte: Dr. Hegger, PD Dr. Kantz, L. Matassini

- Erfindungsmeldung eingereicht am 1. November 1999
  "Adaptive Regelung zur Leistungsstabilisierung frequenzverdoppelter Festkörper-Laser"
  Gemeinschaftserfindung: MPI (Tobias Letz)/DaimlerChrysler

Vorlesungen an Universitäten

Lectures at Universities

Wintersemester 97/98

"Strukturbildung in Physik, Chemie und Biologie"
M. Bär, TU Dresden

"Nichtlineare Dynamik wechselwirkender Vielteilchensysteme"
S. Flach, TU Dresden

"Allgemeine Relativitätstheorie"
H. Hinrichsen, FU Berlin

Sommersemester 98

"Quantenmechanik II"
H. Hinrichsen, FU Berlin

"Einführung in die Nichtgleichgewichtsstatistik"
W. Just, TU Darmstadt

"Nichtlineare Dynamik"
H. Kantz, Uni Wuppertal

"Theoretische Festkörperphysik"
G. Schliecker, FU Berlin

Wintersemester 98/99

"Turbulenz"
W. Just, TU Darmstadt

"Quantenchaos"
J. Nöckel, TU Dresden

"Ordnung und Unordnung in dynamischen Teilchenmodellen"
M. Or-Guil u. H. Hinrichsen, TU Dresden

Sommersemester 99

"Hydrodynamische Turbulenz"
H. Kantz, Uni Wuppertal

"Spezielle und allgemeine Relativitätstheorie"
G. Schliecker, FU Berlin

Wintersemester 99/2000

"Niedrigdimensionale Systeme und Mikrostrukturen"
K. Richter, Uni Augsburg

"Spezielle Relativitätstheorie"
M. Sieber, Uni Ulm

Berufungen

Appointments

- Prof. Dr. Michael Dolg hat einen Ruf auf eine Professur an die Universität Bonn angenommen.
- Prof. Dr. G. Zwicknagl hat einen Ruf auf eine Professur an die Universität Braunschweig angenommen.

Habilitationen

Habilitations

Flach, S.: Localization in nonlinear lattices without disorder.
Dresden 1998

Richter, K.: Semiclassical Theory of Mesoscopic Quantum Systems
Augsburg 1998

Hinrichsen, H.: Critical Phenomena in Nonequilibrium Systems.
Berlin 1999

Mehlig, B.: Chaos und Unordnung: Fluktationen in komplexen Systemen
Chemnitz 1999

Deutsch, A.: Cellular Automata and Biological Pattern Formation.
Bonn 1999

Dissertationen

Dissertations

Gorin, T.: Statistische Streutheorie für reguläre Quantensysteme
Dresden 1998

Kalvoda, S.: Lokale elektronische Korrelationen in Gadoliniumnitrid und anderen periodischen Systemen.
Dresden 1998

Kladko, K.: Correlations and nonlinearity in solid state physics.
Dresden 1998

Wenschuh, U.: Mikroskopische Theorie phononischer Zerfallsprozesse in Halbleitern - von Anharmonizitäten zu Meßgrößen.
Stuttgart 1998

Güttler, S.: Theoretische Konzepte der Zeitreihenanalyse und Anwendungen auf die Signalklassifikation in technischen Systemen.
Wuppertal 1999

Henseler, M.: Theoretische Konzepte der Zeitreihenanalyse und Anwendungen auf die Signalklassifikation in technischen Systemen.
Dresden 1999

Kilian, R.: From Cuprates to Manganites: Spin and Orbital Liquids.
Dresden 1999

Persson, E.: Resonance trapping - a relastic effect?
Dresden 1999

Schmüser, F.: Analytische Beiträge zum Raum-Zeit-Chaos: von gekoppelten Abbildungen zum Isingmodell.
Wuppertal 1999

Utzny, C.: Pattern dynamics in heterogeneous media
Dresden 1999

Auszeichnungen

Awards

Prof. Dr. Peter Fulde
Honorary doctoral degree of the University of Waterloo (Canada), 1998
Corresponding member of the Sächsische Akademie der Wissenschaften zu Leipzig, 1998

Dr. Konstantin Kladko
Nichtlinearitäten und starke Korrelationen in der Festkörperphysik
Otto-Hahn-Preisträger 1999

Dr. Jens W. Nöckel
Dissertation:"Ausstrahlungs-Eigenschaften asymmetrischer dielektrischer Resonatoren mit chaotischer Strahlendynamik"
"Award for Outstanding Doctoral Thesis Research" 1999

Dr. Christian Rödenbeck
Beste Promotionsarbeit auf dem Gebiet der Zeolithforschung
Preis der Federation of European Zeolithe Associations 1999

Öffentlichkeitsarbeit

Public Relations

Open House Day

On **November 7th, 1998** we opened the doors for all interested citizens of Dresden to visit our institute. In talks, video shows and poster presentations our scientists conveyed the importance and fascination of their research to a broad audience. The resonance was very good, about 200 interested people participated the event.
Topics covered included:

- Computer experiments in scientific fields like "Pattern Formation", "Nonlinear Time Series Analysis"
- Short lectures about the scientific work at the institute
- A Lecture for high school students on "The physics of baloons"
- Physical experiments

Journal "Kontakt"

We participate in the editorial board of the alumni journal "Kontakt" (with Technische Universität Dresden, Forschungszentrum Rossendorf e.V., Institut für Festkörper- und Werkstofforschung 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 MPIPKS.

"Wissenschaft im Rathaus"

The MPIPKS, the TUD (university) and the city of Dresden have launched a series of public lectures (about 3 per year) labeled "Wissenschaft in Rathaus":

- 23. February 1999
  Prof. Dr. Klaus von Klitzing (Nobelpreis 1985), Max-Planck-Institut für Festkörperforschung, Stuttgart,
  "Vom Urmeter zur Atomuhr"
  about 300 participants

- 22. September 1999
  Prof. Dr. Elsässer, Max-Planck-Institut für Astronomie, Heidelberg
  "Auf den Spuren des Urknalls - Bau und Entwicklung des Universums"
  about 500 participants

- 24. November 1999
  Prof. Dr. Klaus Hahlbrock, Max-Planck-Institut für Züchtungsforschung, Köln
  "Gentechnik - Für oder Wider die Natur"
  about 250 participants

Lectures for high school students

- Prof. Dr. Martienssen (Uni Frankfurt) gave a lecture on "Gesetz und Zufall in der Natur. Würfelt Gott doch?" to an audience of about 500 high school students on September 17th, 1999. Due to the large number of participants we rented a lecture hall of the TUD.

Haushalt des Instituts

Budget of the Institute

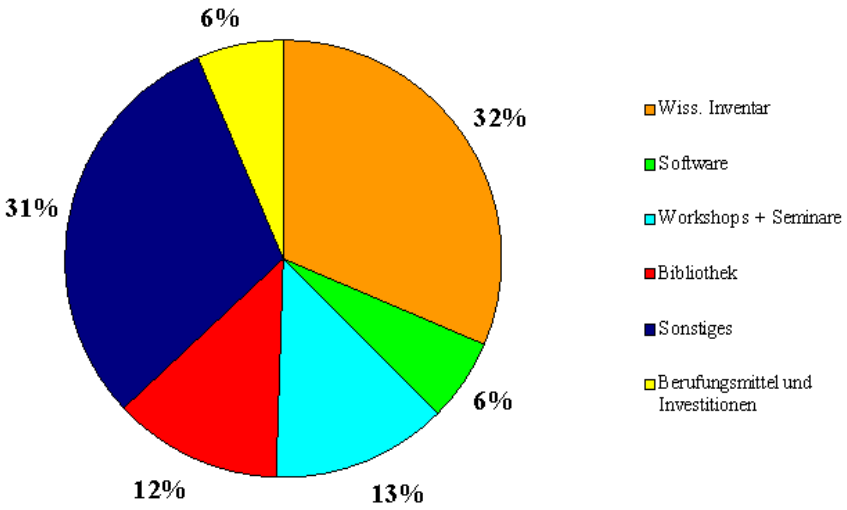

Figure 1: *Forschungshaushalt 1998, (Gesamtetat 2,98 Mio DM)*

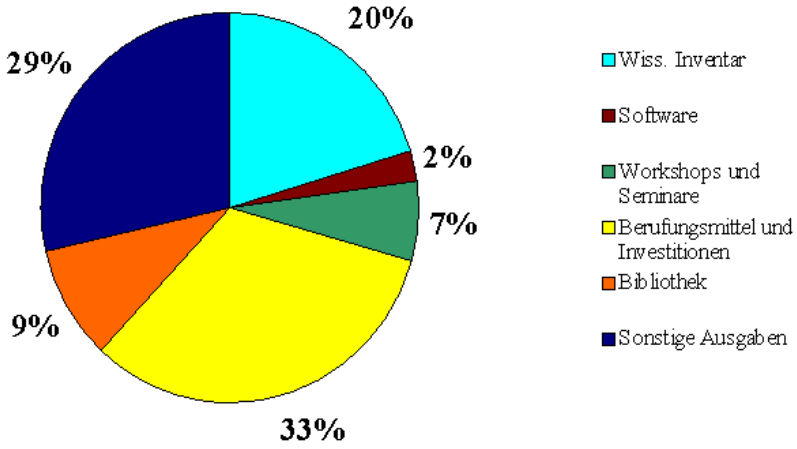

Figure 2: *Forschungshaushalt 1999, (Gesamtetat 4,4 Mio DM)*

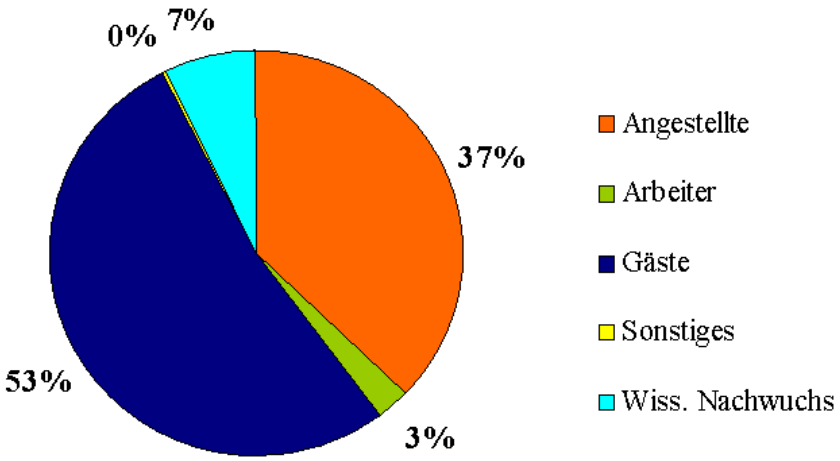

Figure 3: *Personalausgaben 1998, (Gesamtetat 7,08 Mio DM)*

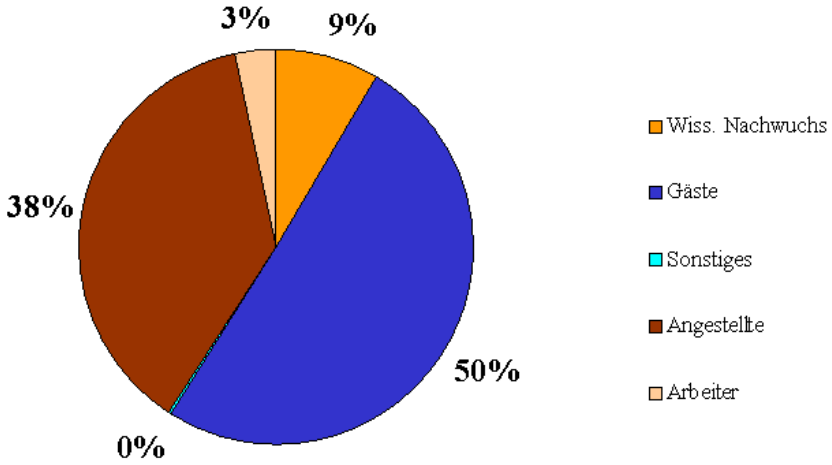

Figure 4: *Personalausgaben 1999, (Gesamtetat 8,4 Mio DM)*

Apparative und räumliche Ausstattung

Equipment und premises

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 most of the computer servers are located in server rooms. At present the institute has approximately 60 computers (100 cpu's), where most of the servers are interconnected by an ATM network. The computers range from 1 to 4 cpu's and are equipped with up to 16 GBytes of memory and 300 GBytes of disk space. Most of the computers are forming a network queuing cluster in order to guarantee the highest possible throughput, the average cpu usage always being as high as 90% during the last years. Apart from the homogeneous unix cluster there are about 15 PCs, mainly for the administration, the secretaries and the library. Also a number of laptops is available which are mostly running the linux operating system.

Since our institute hosts workshops and seminars throughout the year, a separate cluster is operated for the participants of those meetings. This cluster offers approximately 30 terminals. The separation from our main cluster was mainly necessary in order to guarantee a smooth operation of both clusters.

Our computer facilities also include various software tools necessary for a theoretically oriented institute in physics research as well as printing services up to A0 sized posters, dial-in access to our cluster and backup and archiving of user data. Of course email, web and other services are also made available by our servers. The institute is connected to the 'Deutsches Forschungsnetz' using a bandwidth of 2 MBit/s. At irregular intervals talks and courses, mainly on special software programs are held at our institute.

The computer department is run by three full-time employees and a student who is working part-time at irregular intervals.

Library

The library of the institute collects literature corresponding to the research fields of the departments. It is a special library for reference only. The library is always accessible for all members including guests.

For scientists from outside usage is possible if the office of the library is occupied (8.00 a.m. to 4.00 p.m.)

The librarian is Heidrun Näther.

The library is located on the ground floor (205 m^2) and the basement (142 m^2).

In the library there are 8 reading desks and a space with armchairs for discussion of the users. There are several national and international newspapers and magazines available.

The journal volumes are arranged in alphabetical order. The old volumes (typically from before 1980) are stored in the basement. The most recent issues can be found the users in special boxes.

A special copy machine only for books and journals is available, a scanner is part of the equipment.

The monographs are arranged in systematical order. A computer to use the online catalogue is also available.

The www-homepage of the library informs on the actual service system (access to electronical journals, databases, standardized supply of the Max-Planck-Society).

At the moment we have about 2000 monographs (1998: 1732; 1999: 1962) and 66 scientific journals (1998: 59; 1999: 66) The journal collection now contains 9000 bound volumes (1998: 7614 ; 1999: 8924).

Books or references not available in the library can be ordered through the inter-library lending (copy or original).

The librarian ordered 1430 monographs and references (1998: 640 ; 1999: 790). The library management system Bibliotheca 2000 of the B.O.N.D. GmbH was installed and used for one year.

Guest houses

The Max Planck Institute for the Physics of Complex Systems provides accommodations in its own three guest houses located just behind the institute. The guest houses comprise 40 residential units.

Guest House no. 1

The guest house no. 1 has twenty single rooms and five double rooms. All units are furnished and have their own bathroom and telephone. Some units have a balcony. The guest house offers a fully-equipped communal kitchen for guests and two meeting rooms. A television set with German and English channels is available in the lounge. There are also bookshelves with a good selection of books and newspapers in German and English.

Guest House no. 2

The guest house no. 2 has ten fully-furnished one-bedroom apartments. All apartments have television connection ports and telephones. Some apartments have a balcony. Each apartment consists of a living room, bedroom, bathroom, and kitchen. A washing machine and tumble dryers are available in the basement, which is accessible from all three guest houses.

Guest House no. 3

The guest house no. 3 has ten fully-furnished two-bedroom apartments. Like in the guest house no. 2 all units have their own television connection ports and telephones. Some apartments have a balcony. The apartments consists of a living room, two bedrooms, bathroom, and kitchen.

Rooms and apartments are regularly cleaned (including towels and bed linen). The institute provides free of charge rental service for TV sets, radios, alarm clocks, etc.

Wissenschaftlicher Beirat
Scientific Advisory Board

Gemäß der Institutssatzung besteht für das Max-Planck-Institut für Physik komplexer Systeme ein wissenschaftlicher Beirat. Der Beirat berät die Institutsleitung bei den Forschungsvorhaben. Er beurteilt die allgemeine Aufgabenstellung des Instituts, die wissenschaftliche Bedeutung und die Erfolgsaussichten von Forschungsvorhaben sowie die Zusammenarbeit innerhalb des Instituts, mit den Hochschulen, mit anderen Forschungseinrichtungen und mit der Industrie. Der wissenschaftliche Beirat nimmt zu den von der Institutsleitung im Jahresbericht vorgelegten Ergebnissen und Forschungsprogrammen Stellung und erstellt in der Regel alle zwei Jahre für den Präsidenten der Max-Planck-Gesellschaft einen Bericht über die wissenschaftliche Arbeit des Instituts.
Zur Zeit sind folgende Damen und Herren Mitglieder des wissenschaftlichen Beirats:

Aharony, A.
Professor Dr.
School of Physics & Astronomy
Tel Aviv University
Tel Aviv 69978
Israel

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
Professor Dr.
Universität Essen
Universitätsstraße 2
45141 Essen

Heller, E. J.
Professor Dr.
Lyman Laboratory of Physics
Harvard University
Cambridge, MA 02138
USA

Lhuillier, J. C.
Professor Dr.
Physique Théoretique des Liquides
Université Pierre & Marie Curie
4, Place Jussieu
F-75252 Paris Cedex 05

Peyerimhoff, S. D.
Professor Dr.
Lehrstuhl für Theoretische Chemie
Universität Bonn
Wegelerstraße 12
53115 Bonn

Tosatti, Erio
Professor Dr.

SISSA
International School for
Advanced Studies
Via Beirut n. 2-4
34013 Trieste
ITALY

Wegner, F.
Professor Dr.

Institut für Theortische Physik
Universität Heidelberg
Philosophenweg 19
69120 Heidelberg

KURATORIUM
Board of Trustees

Für das Max-Planck-Institut für Physik komplexer Systeme wurde satzungsgemäß ein Kuratorium gebildet, welches mit den Direktoren den Haushaltsvoranschlag, den Jahresbericht und den Haushaltsbeschluß des Vorjahres berät. Das Kuratorium soll das Institut in wichtigen Fragen beraten und die Verbindung zu den an der Forschung des Instituts interessierten Kreisen fördern.
Im Berichtszeitraum waren folgende Herren Mitglieder des Kuratoriums:
Amtszeit bis 31.12.2000

Eggers, Harald	Geschäftsführer Siemens Microelectronics Center GmbH & Co. OHG Scharfenberger Strase 66, 01139 Dresden
Eschelbacher, Hans C. Dr.-Ing.	Ministerialdirigent im Bundesministerium für Bildung Wissenschaft, Forschung u. Technologie Heinemannstrase 2, 53175 Bonn
Freiesleben, Hartwig Professor Dr.	Dekan Fachrichtung Physik Technische Universität Dresden Zellescher Weg 16, 01062 Dresden
Junker, Frank Dr.	Mitglied des Vorstandes König & Bauer AG Friedrich-List-Str. 47-49 01445 Radebeul
Mehlhorn, Achim Professor Dr.	Rektor der Technischen Universität Dresden Mommsenstrase 13, 01069 Dresden
Meyer, Hans-Joachim Professor Dr.	Staatsminister im Sächsischen Staatsministerium für Wissenschaft und Kunst Archivstrase 1, 01097 Dresden
Müller, Horst Dr.	Mitglied des Vorstandes Dresdner Bank AG Jürgen-Ponto-Platz 1 60329 Frankfurt/Main
Schmidt, Joachim, MdB Dr.	Vorsitzender der CDU-Landesgruppe Sachsen Erbische Str. 5, 09599 Freiberg
Wagner, Herbert Dr.	Oberbürgermeister der Landeshauptstadt Dresden Dr.-Külz-Ring 19, 01067 Dresden

Mitarbeiter am Max-Planck-Institut für Physik komplexer Systeme

Stand: März 2000

1.	Planstelleninhaber	**38**
1.1	Wissenschaftliches Personal	
	Wissenschaftliche Mitglieder	2
	Wissenschaftliche Mitarbeiter (einschließlich vier Nachwuchsgruppen)	17
1.2	Mitarbeiter in technischen Berufen	5
1.3	Verwaltungs- und Infrastrukturmitarbeiter	14
2.	Wissenschaftliche Mitarbeiter, finanziert aus Drittmitteln	**2**
3.	Doktoranden	**27**
3.1	Deutsche Doktoranden (MPG Mittel)	20
3.2	Ausländische Doktoranden (MPG Mittel)	5
3.3	Doktoranden (Drittmittel)	2
4.	Gastwissenschaftler	**41**
4.1	Deutsche Wissenschaftler	10
4.2	Ausländische Wissenschaftler (MPG Mittel)	31

Veröffentlichungen 1998/99

Publications 1998/99

Publications 1998

Abel, M., S. Flach and A. Pikovsky: Localization in a coupled standard map lattice. Physica D 119, 4 – 21 (1998).

Abel, M. and M. Spicci: Nonlinear localized periodic solutions in a coupled map lattice. Physica D 119, 22 – 33 (1998).

Abramson, G. and D. H. Zanette: Globally coupled maps with asynchronous updating. Physical Review E 58, 4454 – 4460 (1998).

Albrecht, M., P. Reinhardt and J.-P. Malrieu: Ab initio correlation to the Hartree-Fock quasi band-structure of periodic systems employing Wannier-type orbitals. Theoretical Chemistry Accounts 100, 241 – 252 (1998).

Albrecht, M., A. Shukla , M. Dolg, P. Fulde and H. Stoll: A Hartree-Fock ab initio band-structure calculation employing Wannier-type orbitals. Chemical Physics Letters 285, 174 – 179 (1998).

Aligia, A.A., E. Gagliano, L. Arrachea and K. Hallberg: Superconductivity with s and p symmetries in an extended Hubbard model with correlated hopping. The European Physical Journal B 5, 371 – 378 (1998).

Alon, U., M.R. Evans, H. Hinrichsen and D. Mukamel: Smooth phases, roughening transitions, and novel exponents in one-dimensional growth models. Physical Review E 57, 4997 – 5012 (1998).

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Antoni, M., Y. Elskens and D.F. Escande: Explicit reduction of N-body dynamics to self-consistent particle-wave interaction. Physics of Plasmas 5, 841 – 852 (1998).

Antoni, M., Y. Elskens and C. Sandoz: Weak turbulence and structure evolution in N-body Hamiltonian systems with long-range force. Physical Review E 57, 5347 – 5357 (1998).

Antoni, M. and A. Torcini: Anomalous diffusion as a signature of a collapsing phase in two-dimensional self-gravitating systems. Physical Review E 57, R6233 – R6236 (1998).

Antonov, V.N., A.N. Yaresko, A. Ya. Perlov, P. Thalmeier and P. Fulde: Electronic structure of low-carrier Yb_4As_3 and related compounds. Physical Review B 58, 9752 – 9762 (1998).

Arrachea, L. and A.A. Aligia: Does long-range antiferromagnetism help or inhibit superconductivity? Physica C 303, 141 – 150 (1998).

Bala, J. and A. M. Oles: Dependence of photoemission spectra on the charge-transfer gap in CuO_2 planes. Physical Review B 58, 9408-9414 (1998)

Bünner, M. J. and W. Just: Synchronization of time-delay systems. Physical Review E 58, R4072-R4075 (1998)

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Cafiero, R., A. Gabrielli and M.A. Muñoz: Disordered one-dimensional contact process. Physical Review E 57, 5060 - 5068 (1998).

Cafiero, R., P. De Los, F. M. Dittes, A. Valleriani and J.L. Vega: Power-law behavior in a nonextremel Bak-Sneppen model. Physical Review E 58, 3993 – 3996 (1998).

Cafiero, R., V. Loreto and P.P. Prosini: Anisotropy and non-universality in kinetic roughening. Europhysics Letters 42, 389 - 394 (1998).

Cafiero, R., A. Valleriani and I.L. Vega: Damage-spreading in the Bak-Sneppen model without noise. The European Physical Journal B 4, 405 – 408 (1998).

Caldarelli, G., R. Cafiero and A. Gabrielli: Dynamics of fractures in quenched disordered media. Physical Review E 57, 3878 – 3885 (1998).

Castella, H. and J.W. Wilkins: Splitting of the excitonic peak in quantum wells with interfacial roughness. Physical Review B 58, 16186 – 16193 (1998).

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Chattopadhyay, T. , K.D. Liss and T. Brückel: Incommensurate-commensurate lock-in phase transition in $EuAs_3$. Journal of Magnetism and Magnetic Materials 177, 1058 – 1060 (1998).

Cohen, A. , K. Richter and R. Berkovits: Spin and interaction effects on charge distribution and currents in one-dimensional conductors and rings within the Hartree-Fock approximation. Physical Review B 57, 6223 – 6226 (1998).

Cretegny, T., S. Aubry and S. Flach: 1 D phonon scattering by discrete breathers. Physica D 119, 73 – 87 (1998).

Cretegny, T., R. Livi and M. Spicci: Breather dynamics in diatomic FPU chains. Physica D 119, 88 – 98 (1998).

Dahm, T., R.B. Hammond, D. J. Scalapino, J.R. Schrieffer, E.R. Soares and B. A. Willemson: Intrinsic limits on the q and intermodulation of low power HTS microstrip resonators. Journal of Applied Physics 84, 5662 – 5667 (1998).

Dahm, T., D. Manske and L. Tewordt: Collective Modes in High-Temperature Superconductors. Physical Review B 58, 12454 – 12458 (1998).

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