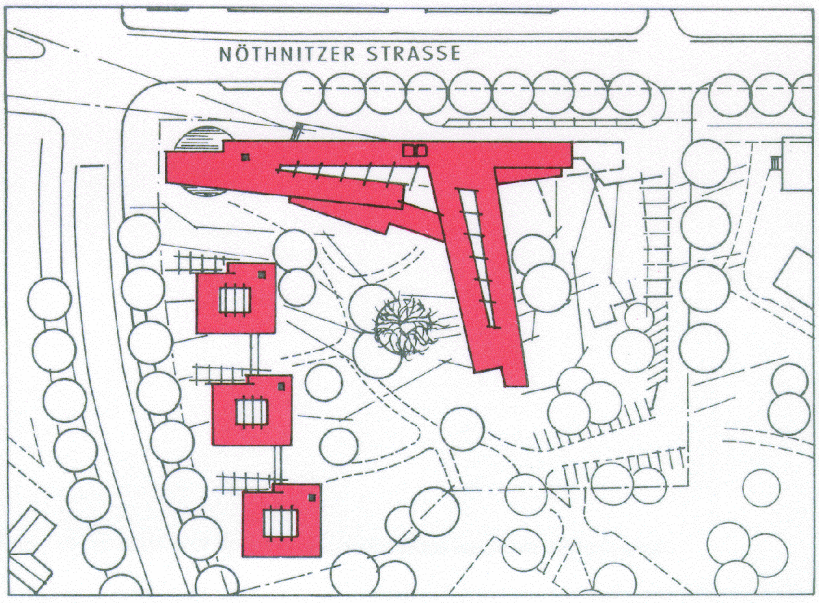
MAX-PLANCK-INSTITUT FÜR

PHYSIK KOMPLEXER SYSTEME

DRESDEN

1996 - 1997



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Wissenschaftlicher Tätigkeitsbericht

des Max-Planck-Instituts

für Physik komplexer Systeme

für den Zeitraum

vom 1. Januar 1996 bis zum 31. Dezember 1997

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Vorwort

Das Max-Planck-Institut für Physik komplexer Systeme wurde auf Beschluß des Senats vom November 1992 als drittes Max-Planck-Institut in den neuen Bundesländern und als erstes im Freistaat Sachsen gegründet. Als Sitz wurde Dresden ausgewählt, da hier mit der Technischen Universität und einer Reihe außeruniversitärer Forschungsinstitute das notwendige Umfeld vorhanden ist, welches für die erfolgreiche wissenschaftliche Arbeit eines Max-Planck-Instituts unverzichtbar ist.

Im Januar 1994 nahm das Institut seine Arbeit in Dresden auf. Die offizielle Institutseinweihung fand am 2. Mai 1994 in Anwesenheit des Präsidenten der Max-Planck-Gesellschaft, Herrn Professor Dr. H. Zacher, statt. Nach einer provisorischen Unterbringung in der Bayreuther Str. 40, der Liebigstr. 30 , Hübner Str. 27 und George Baehr Str. 20 konnten die Mitarbeiter Mitte 1997 das neue Institutsgebäude und die Gästehäuser in der Nöthnitzer Str. 38 in Betrieb nehmen. Die offizielle Einweihungsfeier fand am 22. September 1997 in Anwesenheit des Präsidenten der Max-Planck-Gesellschaft, Prof. Dr. H. Markl, sowie zahlreicher geladener Gäste statt. Das neue Gebäude wurde von den Architekten so konzipiert, daß die Kommunikation unter den Mitarbeitern auf vielerlei Weise gefördert wird. Die Arbeitsbedingungen werden allgemein als sehr gut angesehen. Entsprechend dem Institutskonzept wurde kurz nach Einzug in das neue Gebäude mit der Durchführung von Seminaren und Workshops begonnen. Im Anschluß an die Einweihungsfeier fand ein zweitägiges Symposium über Complexity in Physics statt. Dem folgten mehrtägige Workshops und mehrmonatige Seminare in kurzen zeitlichen Abständen.

Zu Hochschulen und außeruniversitären Forschungseinrichtungen des In- und Auslandes bestehen vielfältige Beziehungen und Verknüpfungen. So sind wir u. a. Partner im Netzwerk *Quantum Chemistry of the Excited State* der Europäischen Gemeinschaft sowie in einem INTAS Projekt *Collaboration with the International Center for Fundamental Physics in Moscow*. Besonders gute Beziehungen bestehen auch zum Minerva Center for Nonlinear Physics of Complex Systems am Weizmann Institut Rehovot sowie am Technion in Haifa. Mit der Technischen Universität Dresden sind wir über Lehrveranstaltungen und die Teilnahme an einem Sonderforschungsbereich eng verbunden.

Gegenwärtig arbeiten am Institut 112 Mitarbeiter einschließlich 11 Doktoranden. Vier wissenschaftliche Nachwuchsgruppen sorgen für die notwendige Breite des wissenschaftlichen Programms. Mit dem Aufbau der zweiten und dritten Abteilung soll noch in diesem Jahr begonnen werden. Der rege Zuspruch, den unser Gästeprogramm, die Seminare und Workshops finden, zeigt, daß unser Institutskonzept Akzeptanz gefunden hat. Um diese auch für die Zukunft zu sichern, streben wir ein hohes Maß an Transparenz und Offenheit, besonders gegenüber dem wissenschaftlichen Nachwuchs, an.

Dresden, im April 1998 P. Fulde

Preface

The Max Planck Institute for the Physics of Complex Systems was created by a resolution of the Senate of the Max Planck Society of November 1992. It was the third Max Planck Institute to be opened in former East Germany and the first one to be opened in the Free State of Sachsen. The location of Dresden was chosen because of the adequate surrounding given by the University of Technology and a series of non-university research institutions, which are essential for the successful scientific work of a Max Planck Institute.

The Institute started its activities in Dresden in January 1994. The official inauguration by the president of the Max Planck Society, Prof. Dr. H. Zacher, took place on May 2nd, 1994. Until the summer of 1997 the institute temporarily resided in Bayreuther Str. 40, Liebigstr. 30, Hübnerstr. 27 and George Baehr Str. 20. The members of the institute moved into the newly constructed building (including three guest houses) in Nöthnitzer Str. 38 in the summer of 1997. The official inauguration of the new buildings took place on September 22nd 1997 in the presence of the president of the Max Planck Society, Prof. Dr. H. Markl, and many invited guests. The new building was conceived by the architect in a way to stimulate and encourage the communication between scientists in many different ways. The working conditions are generally considered to be very good. In accordance with the concept of the institute the seminar and workshop program started in the new buildings. A symposium with a duration of two days took place right after the inauguration ceremony. Workshops of longer duration and seminars extending over several months followed.

The institute maintains relations and connections to universities and non-universitary research institutions inside Germany and abroad. We are participants in the European-Union-network on *"Quantum Chemistry of the Excited State"* and in the INTAS project *"Collaboration with the International Center for Fundamental Physics in Moscow"*, among others. Specially good relations also exist with the Minerva Center for Nonlinear Physics of Complex Systems at the Weizmann Institute in Rehovot and at the Technion in Haifa, Israel. We are closely related with the Dresden University of Technology through lectures and the participation in a Sonderforschungsbereich.

Currently there are 112 institute members including 11 PhD students. Four junior research groups guarantee the necessary broadness of the scientific program. The formation of the 2nd and 3d theoretical department will begin in 1998. The increasing interest in the guest program, which manages the seminars and workshops, shows that the concept of the institute is facing broad acceptance. To guarantee this also in the future, we aspire a high level of transparency and openness, especially towards the young members of the scientific community.

Dresden, April 1998 P. Fulde

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

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

Wegen ihrer gegenseitigen Coulombabstoßung bewegen sich Elektronen in einem Atom, Molekül oder Festkörper korreliert zueinander. Nur so läßt sich die Abstoßungsenergie soweit als möglich vermeiden. Das impliziert, daß die Wellenfunktion eines Elektronensystems eine komplexe Vielteilchenfunktion ist und nicht durch eine Slater Determinante darstellbar ist, wie es bei unkorrelierten Elektronen mit abgeschlossenen Schalen der Fall wäre. Eine parameterfreie, quantitative Beschreibung solcher Korrelationen, ihr Einfluß auf die Energie und die Wellenfunktion eines elektronischen Systems stehen im Mittelpunkt des Interesses unserer Abteilung. Dazu ist anzumerken, daß entsprechende Berechnungen für kleinere Moleküle seit Jahrzehnten ein zentrales Thema der theoretischen Chemie sind. Jedoch sind die dabei verwendeten Verfahren allgemein nicht auf unendliche, periodische Systeme, wie sie Festkörper darstellen, übertragbar. Vom physikalischen Standpunkt aus gesehen sollte es jedoch möglich sein, Moleküle und Festkörper mit den gleichen Verfahren zu beschreiben, denn das *Korrelationsloch*, welches ein Elektron mit sich führt, ist räumlich eng begrenzt. In der Tat hat sich gezeigt, daß bei Verwendung *lokaler* Operatoren verbunden mit einer Kumulantentechnik der Vielteilchen-Grundzustand eines Festkörpers mit ähnlicher Genauigkeit beschrieben werden kann, wie es bisher für kleine Moleküle der Fall gewesen ist.

Das Arbeitsprogramm der Abteilung teilt sich auf in das Studium schwach und stark korrelierter elektronischer Systeme. Die Arbeiten an schwach korrelierten Systemen konzentrieren sich auf Halbleiter und Isolatoren, für die der Grundzustand aber auch Valenzbänder mit Hilfe quantenchemischer Verfahren berechnet werden. Ein neu entwickeltes Hartree-Fock Programm für Festkörper, welches die Hartree-Fock Orbitale direkt in der Form lokalisierter Funktionen liefert, wird es in Zukunft ermöglichen, auch Anregungen in Leitungsbandzustände zu behandeln. Zuvor ist jedoch noch etliche Entwicklungsarbeit nötig. Die bisher aufwendigsten Grundzustandsrechnungen wurden für NiO sowie für Siliziumoberflächen mit ihren Rekonstruktionen durchgeführt.

Bei den Untersuchungen von stark korrelierten Festkörpersystemen ist man bisher noch auf Modelle angewiesen, obwohl auch hier ab initio Rechnungen basierend auf quantenchemischen Verfahren in den Bereich des Machbaren kommen. Besonderes Interesse galt dabei dem Phänomen der Elektronenkristallisation oder Ladungsordnung. Intermetallische Systeme seltener Erden sind hierfür gute Kandidaten, da die kinetische Energie durch Delokalisierung der $4f$ Elektronen, welche in Konkurrenz zur Coulombabstoßung der Elektronen steht, hier besonders klein ist. Mit Yb_4As_3 konnte ein überzeugendes Beispiel für Ladungsordnung gefunden werden. Hierbei kam es zu einer sehr guten Zusammenarbeit mit der Theoriegruppe der TU Dresden.

Selbständige Nachwuchsgruppe "Nichtlineare Zeitreihenanalyse"
(Leiter: Dr. H. Kantz)

In vielen Systemen, selbst wenn sie sehr einfachen Bewegungsgleichungen gehorchen, findet man komplexe Dynamik. Ziel der Zeitreihenanlyse ist es, ausgehend von zeitaufgelösten Beobachtungen dynamische Eigenschaften von Systemen zu charakterisieren und soweit als möglich zu verstehen. Die theoretisch fundierte Herleitung und Weiterentwicklung von Methoden zum Nachweis und zur Charakterisierung deterministisch chaotischer Dynamik als Quelle von aperiodischem Verhalten ist ein wesentlicher Teil der Arbeit dieser Nachwuchsgruppe. Wichtige Beiträge wurden zum Verständnis von Grenzen der Rekonstruierbarkeit von Zustandsvektoren aus skalaren Zeitreihen, zu Intermittenzphänomenen und zur Identifikation von Modellgleichungen aus Daten geleistet. Hochdimensionales Chaos in räumlich ausgedehnten Systemen und in Systemen mit zeitverzögerter Rückkopplung bildet ein weiteres Arbeitsfeld. Darüber hinaus werden konkrete nichtlineare Phänomene studiert, wie z.B. die Wechselwirkung von deterministisch chaotischen Prozessen mit stochastischen Prozessen. In den vergangenen zwei Jahre wurden eine Reihe von Anwendungen in Angriff genommen, die zum Teil in Zusammenarbeit mit experimentellen Gruppen stattfinden und zur Beantwortung physikalischer Fragestellungen führen sollen. Eines dieser Experimente ist die Stabilisierung (Chaos Kontrolle) von grünem Laser-Licht, das durch einen frequenzverdoppelnden Kristall von einem infraroten Nd:YAG Laser erzeugt wird, und am Lehrstuhl von Prof. Parisi an der Uni Oldenburg durchgeführt wird. Im Rahmen eines BMBF Projektes wird an der Entwicklung von Fehlerfrüherkennungverfahren für Elektromotoren gearbeitet, zu denen erste vielversprechende Ergebnisse vorliegen.

Nachwuchsgruppe "Quantenchemie"
(Leiter: Dr. M. Dolg)

Die Nachwuchsgruppe 'Quantenchemie' beschäftigt sich mit der quantitativen ab initio Berechnung der Eigenschaften von Atomen, Molekülen, Clustern, Polymeren und Festkörpern. Hierbei werden neben den Bindungsverhältnissen insbesondere auch die Beiträge der Relativistik und der Elektronenkorrelation untersucht und interpretiert.

Ein Hauptarbeitsgebiet der Gruppe, in Zusammenarbeit mit H. Stoll (Stuttgart), ist die Erweiterung der in der molekularen Quantenchemie bekannten Methoden auf Problemstellungen aus dem Bereich der Festkörperphysik, die mit anderen Verfahren nur schwer behandelbar sind. Hierbei stehen die Entwicklung und Implementierung neuer Methoden sowie deren exemplarische Anwendung im Vordergrund. Einen ersten Schritt zur ab initio Behandlung von elektronischen Korrelationen in unendlichen Systemen stellte die Formulierung und Implementierung eines in (lokalisierten) Wannier-Orbitalen arbeitenden Hartree-Fock-Programms dar. Zahlreiche Testrechnungen an ionischen und kovalenten Polymeren und Festkörpern zeigten die Gleichwertigkeit dieses Verfahrens zu den herkömmlichen mit (delokalisierten) Bloch-Orbitalen arbeitenden Methoden. Die im Institut bereits in der Vergangenheit sehr erfolgreich angewendete Inkrementenmethode soll schließlich ab initio Korrelationsrechnungen für Grundzustände unendlicher Systeme zulassen. Hierzu sind Coupled-Cluster Rechnungen in der Basis der selbstkonsistent erzeugten Wannier-Orbitale vorgesehen. Darüber hinaus soll versucht werden,

Korrelationsbeiträge auch in Bandstrukturrechnungen, die auf dieser Methode aufbauen, zu berücksichtigen.

Neben den Standardverfahren zur Korrelationsbehandlung, z.B. der Coupled-Cluster Methode, soll bei oben beschriebenem Zugang zu unendlichen Systemen auch die Quanten-Monte-Carlo Methode als Alternative eingesetzt werden. In den letzten Jahren wurde dieses Verfahren in der Gruppe insbesondere in Hinblick auf Rechnungen an endlichen Systemen (Atome, Moleküle, Cluster) mit schweren Atomen weiterentwickelt. Hierzu werden ebenfalls in der Gruppe entwickelte energie-konsistente relativistische ab initio Pseudopotentiale eingesetzt. Verfahren zur genauen Berechnung von Gesamtenergien, Feinstrukturaufspaltungen, Eigenschaften wie Polarisierbarkeiten und Dipolmomenten, sowie Ansätze zur Interpretation elektronischer Wellenfunktionen wurden entwickelt, implementiert und erfolgreich auf verschiedenste Atome, Moleküle und Cluster angewendet.

Die energie-konsistenten Pseudopotentiale der Dresdner und Stuttgarter Gruppe werden derzeitig im Rahmen eines DFG-Projekts weiterentwickelt. Ziel ist die effiziente Implementierung der Justierung an einer Vielzahl von Mehrelektronenzuständen im intermediären Kopplungsschema. Die Referenzdaten (Gesamt-Valenzenergien) sollen hierfür aus Dirac-Hartree-Fock Allelektronenrechnungen mit einem aus mehreren Konfigurationen bestehenden Ansatz für die Wellenfunktion gewonnen werden. Der zugrundeliegende Hamiltonoperator ist dabei der Dirac-Coulomb-Breit-Operator, wobei der Breit-Term sowie Korrekturen aus der Quantenelektrodynamik störungstheoretisch berücksichtigt werden. Die hervorragende Qualität solcher Pseudopotentiale wurde exemplarisch für einige schwere Elemente gezeigt. Ziel ist es, das entsprechende Justierverfahren zu einem Routineverfahren zu entwickeln und anschließend für insbesondere schwere Elemente einen Satz verbesserter Pseudopotentiale zu erzeugen. Im Falle der Lanthanoiden und Actinoiden wurden die für die vorhandenen Pseudopotentiale zur Verfügung stehenden Valenzbasissätze weiter optimiert. Testrechnungen an den ersten bis vierten Ionisierungspotentialen sowie d-f- bzw. f-d-Anregungsenergien stellen die derzeitig genauesten und umfassendsten Untersuchungen dieser Art für die f-Elemente dar. Die Methoden wurden u.a. auch auf organometallische Moleküle wie Cerocen oder Uranocen zur Untersuchung der elektronischen Zustände erfolgreich angewendet.

Als Alternative zu Pseudopotentialrechungen in Kombination mit wellenfunktionsorientierten ab initio Standardverfahren der Quantenchemie wurde auch die relativistische Dichtefunktionalmethode in der Gruppe weiterentwickelt und getestet. Ausgangspunkt ist hier der für das Allelektronensystem formulierte Dirac-Coulomb-Hamiltonoperator zusammen mit modernen gradientenkorrigierten Austausch- und Korrelationsfunktionalen. Die Ergebnisse für Atome und zweiatomige Moleküle der Lanthanoiden sind sehr vielversprechend. Derzeitig werden Untersuchungen an Verbindungen der superschweren Elemente in Zusammenarbeit mit W. Liu (seit 1.1.98 in Bochum) und P. Schwerdtfeger (Auckland, NZ) durchgeführt.

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

Die Arbeitsgruppe "Strukturbildung" beschäftigt sich in erster Linie mit der Modellierung und Analyse von Nichtgleichgewichtssystemen, deren Verhalten durch die Wechselwirkung von lokaler Dynamik und Transportprozessen bestimmt ist (Reaktions-Diffusions-Systeme). Dabei werden Modelle chemischer Reaktionen auf Katalysatoroberflächen in Zusammenarbeit mit experimentellen Gruppen in Berlin und Hannover untersucht. Dazu befassen wir uns mit der realistischen Beschreibung musterbildender biologischer Syteme (intrazelluläre Kalziumwellen, Aggregation des Schleimpilzes *Dictyostelium Discoideum*). Die angesprochenen Modelle werden dabei in Form von deterministischen, nichtlinearen partiellen Differentialgleichungen aus der Kenntnis der relevanten physikalischen, chemischen und biologischen Prozesse abgeleitet.

Neben direkten numerischen Simulationen liegt ein Schwerpunkt der Forschung auf der Entwicklung von Methoden zur Stabilitäts- und Bifurkationsanalyse nichtlinearer Wellen in einer und zwei Dimensionen. Diese Methoden sind für eine akkurate Beschreibung der Wechselwirkung von nichtlinearen Wellen sowie zum Verständnis von Welleninstabilitäten und Übergängen ins raumzeitliche Chaos notwendig.

Darüber hinaus werden Reaktions-Diffusions-Wellen in heterogenen Medien untersucht. Hier werden störungstheoretische Methoden zur Beschreibung der reduzierten Dynamik von Fronten und Pulsen angewendet und der Einfluß der Längenskala der Heterogenität erforscht. Ein anderes Projekt befasst sich mit Strukturbildung in Aktivator-Inhibitor-Modellen mit nichtlokaler Kopplung.

Weitere thematische Schwerpunkte liegen in der Untersuchung von Phasenübergängen in Nichtgleichgewichtssystemen (gerichtete Perkolation, Wachstumsmodelle) und von ungeordneten und fraktalen zellulären Strukturen (Mosaike) in verschiedenen physikalischen Anwendungen. Beide Ansätze werden auch auf musterbildende Systeme mit raumzeitlich chaotischer Dynamik anwenden.

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

Das Studium mesoskopischer elektronischer und optischer Systeme, insbesondere unter Verwendung von Methoden des "Quantenchaos", ist das zentrale Arbeitsgebiet dieser Gruppe. Mesoskopische Systeme sind typischerweise kleine, niedrig–dimensionale Objekte mit Größen im Nano- oder Mikrometerbereich, die aufgrund der sich über das System erstreckenden Phasenkohärenz der zugehörigen elektronischen Wellenfunktionen spezielle Quantenphänomene aufweisen. Derartige Interferenzeffekte -drücken sich zum Beispiel in der Leitfähigkeit, im Magnetismus und im Absorptionsverhalten aus.

Das Hauptaugenmerk der Arbeiten richtet sich auf ballistische Systeme, die dadurch ausgezeichnet sind, daß die elektronische Bewegung im wesentlichen durch Stöße an der Systemberandung determiniert ist. Diese Systeme werden durch zweidimensionale "Quantenbillards" modelliert. Ihre klassische Dynamik ist durch ihre Systemgeometrie

bestimmt und hat starken Einfluß auf die obenerwähnten mesoskopischen quantenmechanischen Eigenschaften.

Methoden des "Quantenchaos" und insbesondere semiklassische Verfahren bilden den Rahmen und das Werkzeug zur Untersuchung der Korrespondenz zwischen klassischer und Quantenmechanik, sowohl für integrable als auch chaotische Systeme. Dabei stehen Fragen, inwiefern der chaotische Charakter des Systems das mesoskopische Verhalten beeinflußt, sowie eine Vereinheitlichung der Theorien für ungeordnete und chaotische Systeme im Vordergrund. Quantenmechanische *ab–initio*–Rechnungen werden verwendet, um semiklassische analytische Näherungen zu überprüfen.

Gegenstand der Untersuchungen der Gruppe sind momentan: spektrale Korrelationsfunktionen chaotischer Quantenbillards, Transporteigenschaften von Quantenpunkten, Übergittern und Halbleiter-Supraleiter-Hybridstrukturen, thermodynamische Eigenschaften (wie Bahnmagnetismus und Dauerströme), die dynamische Antwort kleiner Teilchen auf äußere Felder (z.B. Polarisierbarkeit, Absorption), sowie die Streuung in starken, zeitabhängigen Feldern in Hinblick auf die Anwendung auf nichtlineare, frequenzabhängige Transportphänomene. Weitere Arbeiten der Gruppe befassen sich mit dem Übergangsregime zwischen ballistischer Bewegung einerseits, und diffusiver Dynamik in ungeordneten Systemen andererseits. Daneben ist die Berücksichtigung von Effekten elelektronischer Wechselwirkung in den Vordergrund getreten.

Neben den elektronischen Systemen werden auch mesoskopische optische Systeme mit Methoden der nicht-linearen Dynamik untersucht; insbesondere die Lichtausbreitung und Strahlungscharakteristik in kleinen optischen Kavitäten, die z.B. die Grundlage für Mikrolaser bilden.

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

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

The mutual Coulomb repulsion of electrons requires that electrons in an atom, molecule or solid move in a correlated fashion with respect to each other. This way the repulsive energy is kept as low as possible. As a consequence of these correlations the wavefunction of an electronic system is a complicated many-body function. It cannot be represented in the form of a single Slater determinant, as is the case for uncorrelated electrons in a closed shell system. A parameter free, quantitative description of correlations and of their influence on the wavefunction and energy of a system are at the center of the research interest of our department. It is well known that calculations of electron correlations for small molecules have been a main topic in quantum chemistry for several decades. However the methods employed there are generally not transferable to infinite, periodic systems such as solids. From a physical point of view it should be possible, though, to design methods and techniques which describe molecules as well ass solids because the *correlation hole* which an electron carries with it is a spatially

well confined object. Indeed, we can show that by applying *local* operators to describe the correlation hole one can construct the many-body ground-state wavefunction of a solid as accurately as for a small molecule.

The research program of our department is divided into two parts, one dealing with weakly correlated systems and the other with strongly correlated electrons. The work on weakly correlated systems focuses on semiconductors and insulators, for which we calculate the ground state as well as the valence bands with the help of quantum chemical methods. A newly developed Hartee-Fock program for the solid state, which yields Hartree-Fock orbitals explicitely in the form of localized functions, will allow to deal in the future also with excitations to conduction band states. However, this requires still a lot of future developments. The mostly involved ground-state calculations up to now were carried out for NiO and silicon surfaces with reconstructions.

As regards strongly correlated electron systems we still have to rely on simplified model Hamiltonians, although ab initio calculations based on quantum chemical methods are also becoming possible. The phenomenon of electron crystallization or charge ordering was of special interest here. Intermetallic systems with rare earth ions are good candidates, since the kinetic energy due to delocalization of $4f$ electrons, being in competition with the Coulomb repulsion of electrons, is especially small. A convincing example of charge ordering was established with Yb_4As_3. Herewith we had a very good collaboration with the theory group at the TU Dresden.

Independent Group of Young Researchers: "Nonlinear Time Series Analysis"

(Dr. H. Kantz)

Complex dynamics can be observed in many systems of physics and life-sciences. It is a goal of time series analysis to characterize and understand dynamical properties of systems by the study of observed data. An essential part of the research work of this group is the sound derivation and development of methods for the proof and characterization of deterministic chaos as the source of aperiodic time dependence of measurements. Relevant contributions of the last two years concern the understanding of folding effects in the embedding of scalar data, intermittency phenomena, and identification of model equations from data. Moreover, particular nonlinear phenomena were studied, such as the interplay between chaos and noise. Applications of time series methods, partly in collaboration with experimentalist are performed with the goal to approach issues of physical relevance. One of these experiments concerns the control of chaos in intensity fluctuations of green laser light, which is produced by an intra-cavity frequency doubling crystal from infrared light, and which is performed at the University of Oldenburg by Prof. Parisi. Failure detection by time series analysis of current measurements of induction motors is another application, which is funded by BMBF (German ministery for research and technology) and where first positive results are available.

Group of Young Researchers: "Quantum Chemistry"
(Dr. M. Dolg)

The group of young researchers 'Quantum Chemistry' works 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 are investigated and interpreted.

A major area of research, in collaboration with H. Stoll (Stuttgart), is the extension of methods well-known in molecular quantum chemistry to those problems in solid state physics, which are difficult to treat by other approaches. The development and implementation of new methods as well as their application to prototype systems are of primary interest. A first step towards an ab initio treatment of electron correlation in infinite systems is the formulation and coding of a Hartree-Fock method, which works in the basis of (localized) Wannier orbitals. Several test calculations for ionic and covalent polymers and solids demonstrate the equivalence of the method to common approaches based on (delocalized) Bloch orbitals. The method of increments was successfully applied to account for ground state properties of infinite systems and will allow to perform correlated calculations for ground states of infinite systems. In order to achieve this goal we plan coupled-cluster calculations in the basis of self-consistently determined Wannier orbitals. Moreover, starting from this approach we attempt to account for electron correlations also within band structure calculations.

Besides the standard methods treating electron correlation, e.g., the coupled-cluster approach, we plan to use the Quantum Monte Carlo technique as an alternative method for infinite systems. During the last years this approach was used and improved by the group for finite systems (atoms, molecules, clusters) with heavy atoms. In order to make these calculations feasible, energy-consistent relativistic pseudopotentials developed by the group have been used. Accurate algorithms for the calculation of total energies, fine structure splittings, properties like dipole moments and polarizabilities, as well as tools for the interpretation of electronic wavefunctions have been developed, implemented and successfully tested for various atoms, molecules and clusters.

The energy-consistent relativistic pseudopotentials of the Dresden and Stuttgart groups are currently improved within the framework of a project supported by the DFG. The goal is an efficient implementation of the adjustment to a multitude of many-electron states within the intermediate coupling scheme. The reference data (total valence energies) will be taken from Dirac-Hartree-Fock all-electron calculations with a multi-configurational ansatz for the wavefunction. The Dirac-Coulomb-Breit-Hamiltonian will be applied, where the contributions of the Breit term as well as other corrections from quantum electrodynamics will be considered by perturbation theory. The excellent quality of such pseudopotentials was demonstrated for several heavy elements. It is the goal to develop the method further in order to become a routine tool and thereafter to determine a set of improved pseudopotentials for heavy elements. For the lanthanides and actinides the valence basis sets for the existing pseudopotentials have been further optimized. Test calculations for the first to fourth ionization potentiasl as well as for d-f and f-d excitation energies are currently the most accurate and complete investigations of this kind for the f-elements. The methods have also been applied to investigate the electronic states of metal-organic molecules like cerocene and

uranocene.

The relativistic density functional approach was also tested and improved by the group as an alternative to pseudopotential calculations in combination with wavefunction-based standard quantum chemical methods . The starting point is the Dirac-Coulomb-Hamiltonian for the all-electron system and modern gradient-corrected exchange and correlation functionals. The results for atoms and diatomic molecules of lanthanides are very promising. Currently, in collaboration with W. Liu (since 1.1.98 in Bochum) and P. Schwerdtfeger (Auckland, NZ), molecules with superheavy elements are investigated.

Group of Young Researchers: "Pattern Formation in Reaction–Diffusion Systems"
(Dr. M. Bär)

The research group on "pattern formation" deals mainly with the modeling and analysis of nonequilibrium systems. The dynamics of these systems are governed by the interaction of local dynamics and transport processes (reaction-diffusion-systems). We investigate models of chemical reactions on catalytic surfaces in collaboration with experimental groups in Berlin and Hannover. Emphasis is laid also on the theoretical description of pattern formation in biological systems (intracellular calcium waves, aggregation of the slime mold *Dictyostelium Discoideum*). Deterministic nonlinear partial differential equations are derived from the knowledge of the underlying physical, chemical and biological processes.

Beyond direct numerical integrations of such models, tools of linear stability and bifurcation analysis are applied to nonlinear waves in one and two dimensions. These methods are essential for an understanding of interaction of waves, wave instabilities and transitions to spatiotemporal chaos.

Moreover, we study wave propagation and patterns in heterogeneous media. Perturbation theoretical methods are employed for that purpose to derive a reduced description of the dynamics of pulses and fronts. Another project focusses on the impact of nonlocal coupling on pattern formation in an activator-inhibitor model.

Finally, critical behavior and dynamics in statistical nonequilibrium systems (e.g. directed percolation, growth models) and properties of disordered and fractal mosaics are considered in various physical applications. Both approaches are also applied to the study of spatiotemporally chaotic patterns.

Group of Young Researchers: "Quantum Chaos and Mesoscopic Systems"
(Dr. K. Richter)

The main topic of this research group is the study of mesoscopic electronic and optical systems, using techniques of quantum chaos theory. Mesoscopic systems are typically small objects of reduced dimensionality (micro- or nanometer size) which, due to the phase–coherence of the electronic wavefunctions throughout the systems, exhibit peculiar quantum phenomena. Such interference effects, for instance, determine the conductance, magnetism or photoabsorption properties.

The main focus of the group is currently directed towards ballistic devices, where the motion of the electrons can be considered as nearly free between bounces off the system confinement potential. These systems are described in terms of two–dimensional electron "quantum billiards". Their classical dynamics is predominantly determined by the geometry and shape of the systems and has strong influence on the mesoscopic quantum properties mentioned above. Semiclassical methods and quantum chaos theory provide the framework and are used to investigate this relation between classical and quantum mechanics for chaotic as well as integrable devices. The question how the chaotic dynamics influences the mesoscopic quantum properties and a "unification" of theories for disordered and chaotic systems is in the center of present interest. *Ab–initio* quantum calculations are usually employed for testing the semiclassical analytical predictions.

Research interests of the group include: spectral correlations of chaotic billiards, transport properties of quantum dots, superlattices and semiconductor-superconductor hybrid structures, thermodynamic properties (orbital magnetism and persistent currents), the dynamic response of small particles to applied fields (e.g. the electrical polarizability), as well as techniques for scattering in strong time–dependent fields (in order to describe non–linear phenomena in frequency–dependent transport). Further work aims at the description of the cross-over regime between geometry–affected ballistic motion and diffusive dynamics in disordered systems. Furthermore, the study of interaction effects has recently come to the foreground.

Beside the electronic devices, mesoscopic optical systems are also investigated, in particular the propagation of light and the radiation characteristics in small resonant cavities which e.g. serve as a basis for microlasers.

Selection of Research Results

Towards An Ab Initio Description of the Solid State

A. Shukla, M. Albrecht, F. Schautz, M. Dolg,
P. Fulde and H. Stoll

The aim of this initiative is to understand the electronic structure of the solid state starting from first principles, employing wavefunction based methods. The choice of wavefunction-based methods is guided by our belief that in order to understand the phenomenon of electron correlation in all its complexity, one really needs to understand the many-particle wavefunction of the system. As many of the studies carried out in the institute reveal, important insights are gained even when one truncates an infinite solid to a finite cluster to make it accessible for study by traditional quantum-chemical methods. However, finite-size effects, which are difficult to quantify, generally accompany such an approach. Therefore, it is important from the outset to work with the infinite solid.

However, carrying over the wavefunction based quantum-chemical methods to describe an infinite solid is not an easy task. Firstly, one has to obtain the Hartree-Fock wave function of the system under consideration and then describe the electron correlations by considering virtual excitations from it. Both these tasks appear to be fraught with insurmountable problems considering the infinite number of degrees of freedom involved. In what follows, we will describe how one can circumvent this problem of "infinities" both at the Hartree-Fock and the correlation level.

To tackle the problem of infinite number of degrees of freedom we must change our perception of how we visualize the electrons in a solid. Instead of viewing the electrons in a solid as being delocalized over the whole of the solid (itinerant electrons), we can view them as being pinned on to the individual atoms or bonds(localized electrons). The crystal orbitals that describe electrons in the itinerant picture are called Bloch orbitals while the simplest type of orbitals that can describe the electrons in a localized representation are called Wannier functions. While the Bloch-orbital-based representation is the most dominant one in solid-state physics, the Wannier-function-based point of view is much closer to the intuition of a chemist in that it amounts to seeing the infinite solid as a giant molecule. In the localized electron picture of the solid, one needs to describe only the electrons of one unit cell of the solid, with rest of the unit cells of the infinite solid being the copies of that cell. Thus, in order to obtain the Hartree-Fock wavefunction of the whole solid, one needs to solve the Hartree-Fock equations of the electrons of just one unit cell. Thus the problem of infinities is solved at the Hartree-Fock level.

The localized-electron picture helps to handle the problem of infinities at the correlation level as well. Here, one utilizes the fact that correlation effects are "local" in the sense that they are important only among the electrons which are nearby. Thus in the localized representation one can describe the correlations by means of a finite number of virtual excitations of the Hartree-Fock state in which one of the electrons involved will be in the reference cell and other ones could be in the reference cell or in a unit cell close by.

We have developed a Hartree-Fock approach that directly yields the Wannier functions of an infinite solid. Physically it employs an "embedded-cluster" picture of a crystalline

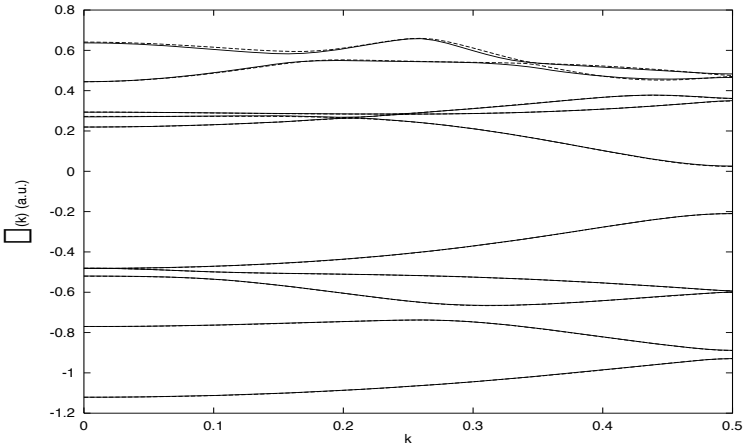

Figure 1: Band structure of t-PA obtained using our approach (solid lines) compared to that obtained using the CRYSTAL program (dashed lines). The experimental geometry and a 6-31G** basis set was used in both cases. Values of k (horizontal axis) are expressed in units of $\frac{2\pi}{a}$. The two sets of bands are essentially identical except for the top two conduction bands which are somewhat different.

solid. The main philosophy behind the embedded-cluster approach as applied to a perfect solid is that a solid can be seen as a central unit cell (called the "central cluster") embedded in the field created by the rest of the unit cells (called the "environment") which are identical to the central unit cell except for the fact that they are spatially separated from it by the multiples of the unit vectors of the crystal. Thus one solves the Hartree-Fock equations of this embedded cluster to obtain the Wannier functions of the electrons of the unit cell. These Wannier functions in turn are used to construct the orbitals of the rest of the solid, and the procedure is iterated till self consistency is achieved. The localization of orbitals is achieved by means of environment projection operators. The method and its computer implementation are discussed in detail in references [1] and [2].

In order to check the correctness of the procedure, it is very important to study a variety of systems by both our approach and a traditional Bloch-orbital-based Hartree-Fock approach as implemented, e.g., in the program called CRYSTAL [6]. In our previous papers, dealing with applications to three-dimensional ionic systems, we reported that we obtain results identical to those obtained by CRYSTAL program for quantities as diverse as total energy per unit cell, x-ray structure factors, Compton profiles, band structure, cohesive energies, bulk moduli, and lattice constants [1, 2, 3, 4]. Recently we have extended the approach to deal with one-dimensional periodic systems, and demonstrated it by applying to study the electronic structure of the model system composed of an infinite LiH chain, and of the real polymer *trans*-polyacetylene [5]. The application to *trans*-polyacetylene also happens to be the first application of our approach to a covalent system. We have also successfully applied the approach to polyethylene, and to several boron-nitrogen polymers. We plan to apply our approach to study the electronic structure of a variety of other polymers.

In Fig. (1) the Hartree-Fock band structure of *trans*-polyacetylene obtained by our approach is compared to the one obtained with the CRYSTAL program.

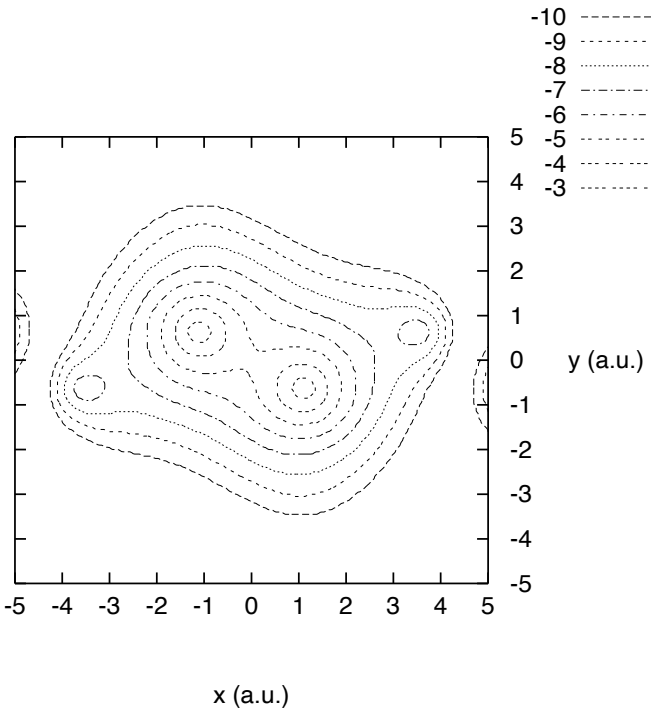

Figure 2: Contour plots of the charge density of the π-type valence Wannier function of the reference cell. Contours are plotted in the xy plane with $z = 0.25$ a.u. (x is the axis of the polymer). The magnitude of the contours is on a natural logarithmic scale. The two carbon atoms of the unit cell are located at the positions $(-1.11, 0.64, 0.0)$ a.u. and $(1.11, -0.64, 0.0)$ a.u. respectively. Clearly the dominant contours are surrounding the two carbon atoms of the reference cell indicating a covalent bond between them. Weaker contours due to the orthogonalization tails of the Wannier function extend up to nearest-neighbor carbon atoms and beyond. The rapidly decaying strength of the contours testifies to the localized nature of the Wannier function.

Fig. (2) presents the contour plots in the xy plane corresponding to the charge density of the Wannier function which describes the π electrons belonging to the reference unit cell of *trans*-polyacetylene. Clearly, the pictorial view of the covalent bond provided by the Wannier function—which obviously is impossible within a Bloch orbital picture—comes close to the intuition of a chemist.

Having established the correctness of the Wannier-function-based Hartree-Fock method, we are now prepared to study the electron correlations. The correlations will be included by considering local virtual excitations from the reference wavefunction, keeping the rest of the infinite solid frozen at the Hartree-Fock level. The computational scheme to be used for this will be the "incremental method" of Stoll [7]. In addition, we also plan to use this approach to study other local phenomena such as defects, impurities and excitons. Applications to study relativistic effects are also planned.

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Ab Initio Pseudopotential and Density Functional Studies of Lanthanide and Actinide Systems

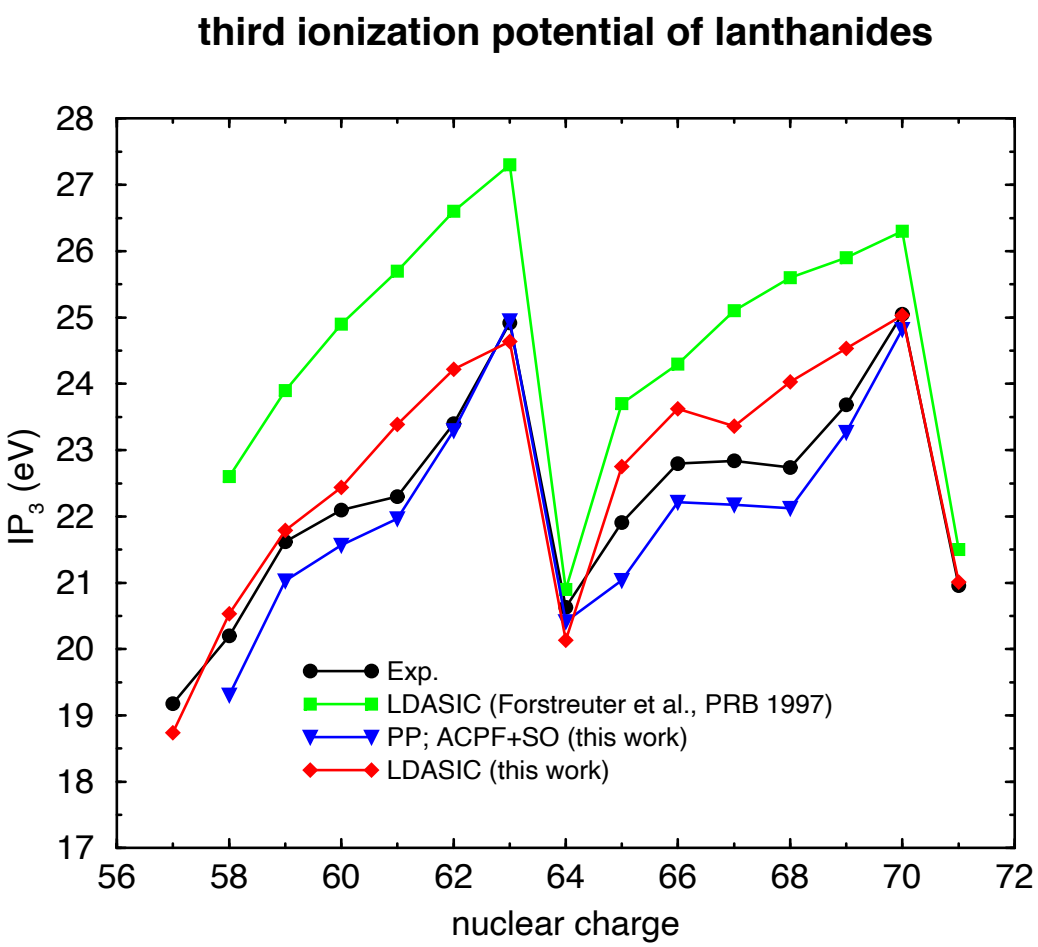
W. Liu, W. Küchle and M. Dolg

Accurate ab initio quantum chemical investigations of systems containing f-elements, i.e., lanthanides or actinides, face various severe difficulties: large differential relativistic and electron correlation effects, in many cases a quite high number of unpaired electrons in the (n-2)f, (n-1)d, ns and np valence shells and as a result an enormous number of low-lying electronic states which have, as a further complication, to be treated in an intermediate coupling scheme [1,2].

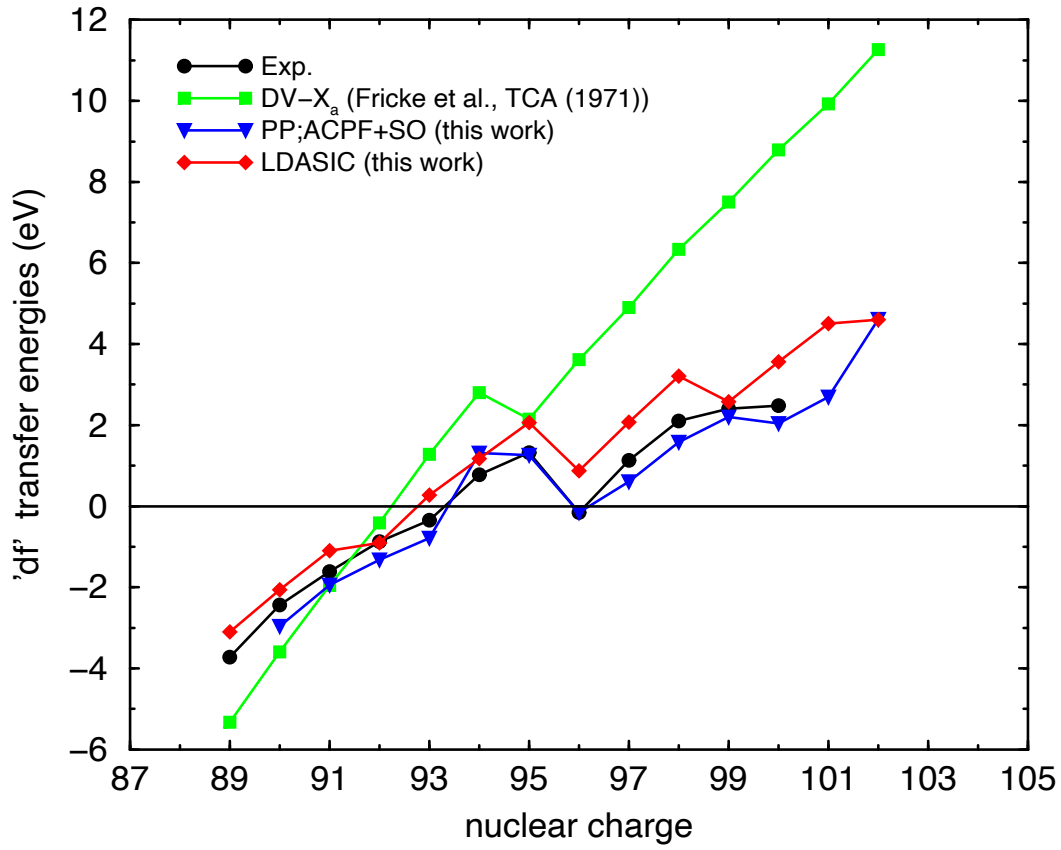
During the last decade, considerable progress has been made to treat quite accurately relativistic effects in chemistry: the development of all-electron Dirac-Hartree-Fock approaches based on the Dirac-Coulomb- or Dirac-Coulomb-Breit(Gaunt) Hamiltonian which do not suffer from variational collapse or finite basis set desease; subsequent correlation treatments which avoid the continuum dissolution or Brown-Ravenhall desease; computationally efficient no-pair theories where the charge degrees of freedom have been eliminated, e.g., the Douglas-Kroll-Heß or the Chang-Pelissier-Durand Hamiltonian; the elimination of the spin degrees of freedom from the Dirac-Coulomb Hamiltonian; the replacement of the divergent perturbation series based on the well-known Foldy-Wouthuysen transformation starting from the nonrelativistic one-component solution by the well-behaved so-called direct perturbation theory starting from the four-component nonrelativistic Levy-Leblond equation; last but not least, scalar-relativistic and relativistic ab initio pseudopotentials have been improved and still are the workhorse of relativistic quantum chemistry. Many nonrelativistic standard approaches for the treatment of electron correlations have been extended to the relativistic regime, i.e., (nonrelativistic) point group symmetry was replaced by (relativistic) double group symmetry. Nevertheless, due to the symmetry-lowering upon inclusion of spin-orbit coupling the computational effort for relativistic ab initio calculations will always be significantly higher than for corresponding nonrelativistic work. A very attractive alternative to the accurate but computationally demanding wavefunction-based approaches of quantum chemistry is offered by density functional theory. Much progress has been made in the development of reliable functionals for exchange and correlation, e.g., gradient corrections to the local density approximation. Some of the above mentioned relativistic approaches have been combined with modern density functional theory and now provide a quite successful alternative to the wavefunction-based investigations of heavy elements chemistry. Nevertheless, the main drawback of density functional theory is that a systematic improvement of the results is usually not possible, i.e., wavefunction-based ab initio approaches will remain quite valuable also in the future.

With the above described progress in the field of relativistic quantum chemistry it appeared timely to perform extensive test calculations of some of the new developed methods for systems with lanthanides and actinides. We choose the approaches which are in our opinion the most promising for the future: (a) relativistic energy-consistent ab initio pseudopotential theory combined with standard correlation treatments including corrections for spin-orbit coupling and (b) relativistic gradient-corrected density

functional theory based on the Dirac-Coulomb Hamiltonian. Excellent results were obtained in extensive test calculations for atomic ionization potentials as well as d-f- and f-d-excitation energies [3] (cf. figures) as well as for various diatomic molecules [4].



The ab initio pseudopotential approach was also used to investigate the electronic structure of *bis[8]annulene* complexes of selected lanthanides and actinides, as well as their anions [5]. The theoretically predicted electronic ground state of cerocene $Ce(C_8H_8)_2$, i.e., $e_{2u}(4f)^1\ e_{2u}(\pi)^3\ {}^1A_{1g}$ (cf. previous report 1994-1995), was confirmed by new experiments in 1996. The corresponding calculations for uranocene $U(C_8H_8)_2$ provide, thirty years after the first synthesis of the compound in 1968, a reliable picture of the low-lying electronic states and confirm the latest experimental ground state assignment. Work is ongoing for *[8]annulene* complexes, *bis[6]annulene* complexes and the related graphite intercalation compounds.



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Energy-consistent pseudopotentials for 5f-elements

W. Küchle and M. Dolg

Introduction

Currently the investigation of chemical compounds by the sophisticated methods of computational chemistry is limited by the computational resources. The demands in terms of computer time, disk space and computer memory are rapidly increasing with increasing size of the chemical system under consideration. The pseudopotential method provides a very successful way to circumvent this problem. Based on the fact that the chemical properties of an element are determined predominantly by its valence electrons, an efficient quantum chemical approach is to treat only these valence electrons in the calculation. In order to account for the interaction between the core electrons and the valence electrons an effective potential has to be introduced: the pseudopotential. The neglect of core electrons leads to a considerable reduction of the basis set that is needed to describe the molecular orbitals in quantum chemical calculations. Therefore, much larger systems are treatable while the accuracy of the calculations remains on the high standard of state-of-the-art all-electron methods.

For the heavy elements of the periodic table it is strictly necessary to account for the relativistic effects on the valence electrons in order to provide an accurate description of the chemical properties of those elements. The pseudopotential approach is an easy and reliable technique to include the major relativistic corrections in calculations on compounds containing heavy elements. In all-electron calculations the incorporation of relativistic effects is only possible at the cost of a considerably increased computational demand, sharpening the problem mentioned above. The pseudopotential method doesn't suffer from such a drawback. By adjusting the pseudopotential to relativistic data, scalar relativistic effects[1] are easily included in molecular calculations, without any additional cost[2] compared to nonrelativistic pseudopotential calculations. Spin-orbit effects can be taken into account by means of an additional spin-orbit potential.

Method

We use an atomic valence model Hamiltonian of the form

$$H = -\frac{1}{2}\sum_{i}^{val}\Delta_i + \sum_{i}^{val}U(r_i) + \sum_{i<j}^{val}\frac{1}{r_{ij}} \qquad (1)$$

[1]Scalar relativistic effects are essentially the relativistic contributions due to the mass-velocity and Darwin terms.

[2]Only for the construction of the pseudopotential, which has to be done only once, the effort is somewhat larger in the relativistic case.

including a semilocal pseudopotential

$$U(r_i) = -\frac{Q}{r_i} + \sum_{l=0}^{l_{max}} \sum_{k=1}^{k_l} A_{kl} e^{-\alpha_{kl} r_i^2} P_l. \tag{2}$$

where Q denotes the charge of the core, A_{kl} and α_{kl} are adjustable parameters and P_l represents the projection operator onto the Hilbert subspace with angular symmetry l.

The adjustment of the parameters A_{kl} and α_{kl} is essentially a four-step process:

- In the first step the valence energies of several low-lying electronic states of the neutral atom and singly positive ion are calculated using finite-difference all-electron Hartree-Fock calculations ($\rightarrow$ nonrelativistic pseudopotentials) or finite-difference all-electron Wood-Boring [1] calculations ($\rightarrow$ one-component quasirelativistic pseudopotentials). The use of finite-difference methods prevents any basis set dependence of the resulting pseudopotential and assures the high accuracy of the reference energies.

- In a second step the parameters A_{kl} and α_{kl} are adjusted in a least squares fit to reproduce the all-electron reference energies from step 1. If the core is choosen properly the resulting pseudopotentials are able to reproduce the reference data with an error of less than 0.1 eV.

- In a further step the accuracy of the pseudopotentials is tested for further excited states of the atom and ion. Usually the agreement between pseudopotential calculations and all-electron calculations is as good as for the reference states.

- In a last step the transferability of the pseudopotentials to molecular environments is tested. For this purpose the properties of experimentally well-investigated compounds are calculated.

For use of our quasirelativistic pseudopotentials within a two component formalism, additional spin-orbit operators of the form

$$U_{SO} = \sum_{l=1}^{l_{max}} \frac{2\Delta U_l}{2l+1} P_l \vec{l}\vec{s} P_l \tag{3}$$

have been generated. The difference ΔU_l of the radial parts of the quasirelativistic pseudopotentials for $j = l \pm \frac{1}{2}$, $U_{l,l+1/2}$ and $U_{l,l-1/2}$, may be written in terms of Gaussian functions [2]

$$\Delta U_l = \Delta A_l e^{-\alpha_l r^2} \tag{4}$$

The exponents α_l are usually set equal to the values of the corresponding pseudopotential parameters while the coefficients ΔA_l can be adjusted to reproduce the spin-orbit splittings obtained by first-order perturbation theory using the orbitals from a quasirelativistic all-electron calculation and a spin-orbit operator taken from the Wood-Boring

equation before averaging over j values. Alternatively an adjustment to spin-orbit splittings obtained by Dirac-Fock calculations can be performed.

Currently a complete set of both relativistic and nonrelativistic pseudopotentials with a [Kr] $4d^{10}$ $4f^{14}$ core (so called small-core pseudopotentials) for the 5f-elements actinium to lawrencium is available [3]. In addition another set of pseudopotentials with a larger [Xe] $4f^{14}$ $5d^{10}$ core (large-core pseudopotentials) has been adjusted recently [4].

Applications

In a recent study [5] of our group a thorough investigation of the actinide contraction, including a comparison with the well-known lanthanide contraction has been carried out. While the lanthanide contraction, i.e. the exceptionally large contraction of atomic and ionic radii throughout the lanthanide series, is well investigated both experimentally and theoretically, the experimental data for the actinide contraction is incomplete and the theoretical data is insufficient. Due to the fact that the transuranium elements have to be produced artificially with the last elements of the actinide series being available only in amounts of a few atoms, experimental ionic radii are available only up to einsteinium (Z=99) [6] up to now. A comparison of the ionic radii of Ac^{3+} and Es^{3+} shows a contraction of 18 pm. This value is 50% larger than the contraction of 12 pm for the corresponding lanthanide ions La^{3+} and Ho^{3+}. By extrapolating one obtains a total actinide contraction of 25 pm which has to be taken as an upper limit, since the contraction is larger at the beginning of the actinide series than at the end. Accounting for this fact by only extrapolating over the ionic radii of Pu^{3+} to Es^{3+} yields a contraction of 22 pm which is probably closer to the correct value. Theoretical investigations of Pyykkö [7] yielded a much larger value of 33 pm.

In our calculations we refer to the definition of Pyykkö, where the actinide (lanthanide) contraction Δ_{an} (Δ_{ln}) is given as

$$\Delta_{an} = r_{e,AcX} - r_{e,LrX} \tag{5}$$

$$\Delta_{ln} = r_{e,LaX} - r_{e,LuX} \tag{6}$$

where r_e denotes the equilibrium distance of the actinide (lanthanide) compound.

For the monohydrides, monofluorides and monoxides of lanthanum, lutetium, actinium and lawrencium quantumchemical investigations using several computational methods have been carried out. In the following discussion we refer to the results of MRACPF[3] calculations with additive inclusion of spin-orbit effects. The complete data and a more detailed discussion can be found in our original paper [5]. Table 1 shows the experimental bond lengths of the hydrides, fluorides and oxides of lanthanum and lutetium together with the calculated bond lengths of the corresponding actinide elements actinium and lawrencium. In agreement with earlier work of Wang and Schwarz [8] on the

[3]Multireference Averaged Coupled Pair Functional

Table 1: Bond lengths and corresponding lanthanide (Δ_{ln}) and actinide contraction (Δ_{an}) (in pm) of the monohydrides, monofluorides and monoxides of Lanthanum, Lutetium, Actinium und Lawrencium.

	experiment				relativistic			nonrelativistic		
	X=H	X=F	X=O		X=H	X=F	X=O	X=H	X=F	X=O
LaX	203.2	202.7	182.6	AcX	209.7	210.9	192.7	206.9	208.1	181.8
LuX	191.2	191.7	179.0	LrX	192.5	196.6	182.2	193.2	199.7	183.0
Δ_{ln}	12.0	11.0	3.6	Δ_{an}	17.2	14.3	10.5	13.7	8.4	-1.2

lanthanide contraction, the actinide contraction also depends strongly on the ligand. The contraction is large for "soft" bonds (small force constants) and small for strong bonds (large force constants). The actinide contraction turns out to be larger than the lanthanide contraction by 3.3 to 6.9 pm, which is due to the more diffuse character of the actinide 5f shell compared to the core-like lanthanide 4f orbitals. This causes a less efficient screening of the nuclear charge leading to a larger contraction of the valence shell. An important result of our investigation is the large relativistic effect on the actinide contraction. Relativity increases the radial contraction by 3.5 to 11.7 pm. In fact the actinide contraction of the oxides comes out as a purely relativistic effect. The reason for this unexpected result can be seen in the very short bond length of nonrelativistic AcO, which is a consequence of the strong π-π-interaction between the 5f-orbitals of actinium and the 2p orbitals of oxygen, even leading to a nonrelativistic actinide expansion.

Our current work is focused on a study of the properties of endohedral fullerenes. The compounds $U@C_{28}$ and $Ce@C_{28}$ are of special interest. The electronic ground states of these species are still unknown. Photoelectron spectra of the uranium compound indicate a U^{4+} valence state, which should correspond to a $5f^2$ configuration. However, a recent study of K. Zhao and R.M. Pitzer [9] proposed a $5f^1\ \pi^{*1}$ ground state configuration, 0.55 eV below the $5f^2$ configuration. The drawback of this study lies in the very small basis set applied for the carbon atoms (double zeta basis without polarization functions) and the very limited correlation treatment (singles spin-orbit CI with inclusion of a very limited number of double excitations). Since the relative energetic order of the U(5f) and C_{28} molecular orbitals is of primary importance for the proper description of the ground state it seems to be necessary to describe the carbon cage with a better basis set. In addition the uranium pseudopotential and basis set of our group may be able to yield more reliable results than the study above. In addition, a somewhat better correlation treatment is desirable, since the relative energetic order of the two configurations may strongly depend on electron correlation effects.

For $Ce@C_{28}$ the situation is similar, an earlier investigation by Rösch suggested a closed shell ground state. On the other hand a $4f^1\ \pi^1$ ground state has to be considered, since this ground state has been theoretically predicted [10, 11] and later experimentally observed [12] in the related compound $Ce[C_8H_8]_2$. The latter compound is unique due to the fact that the ground state is an open-shell singlet state and not a triplet as expected. A major topic of our study is to conclude whether such an anomality occurs

also in $Ce@C_{28}$.

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Quantum Monte Carlo Calculations for Atoms, Molecules and Clusters of Heavy Elements.

Heinz-Jürgen Flad, Friedemann Schautz, Yixuan Wang and Michael Dolg

Introduction

Electron correlation and relativistic effects play an important role in the chemistry and physics of heavy elements. Both effects are not additive for these elements and have to be treated on equal footing. This can be achieved for example by combining quantum Monte Carlo (QMC) methods [1] with relativistic pseudopotentials. Despite its success in condensed matter physics QMC does not belong to the well established methods in quantum chemistry. Nevertheless it provides a powerful tool for the investigation of electron correlation and it is worth the effort to study its applicability in this context. We have used the pure diffusion quantum Monte Carlo (PDMC) method of Caffarel and Claverie [2]. It is based on a generalization of the Feynman-Kac formula for the imaginary time Green's function, which allows importance sampling from a given trial wavefunction. The Schrödinger equation is treated using the so-called fixed-node boundary condition which means, that the nodes of the solution are the same as those of the trial wavefunction. The resulting energy is an upper bound of the exact ground state energy. An advantage of the PDMC algorithm is the straightforward calculation of expectation values of local operators and implementation of correlated sampling enabling the evaluation of small energy differences.

In all of our applications we have compared the QMC results with other *ab initio* methods using the same pseudopotentials and the best feasible basis sets. Only then it will be really possible to judge the quality of QMC results.

Atoms

The antisymmetry of fermionic wavefunctions represents a fundamental difficulty for quantum chemical applications of the QMC method. Using the fixed-node boundary condition requires a trial wavefunction which provides an accurate description of the nodes. For closed shell systems the nodes of the Hartree Fock (HF) solution are sufficient for most applications. On the contrary open-shell systems often are close to degeneracies which require a multi-reference treatment. Atoms provide a good starting point for a systematic investigation of this problem [3], which is of fundamental importance for systems containing heavy elements.

In order to achieve an accurate description of the fine-structure splittings of heavy elements it is necessary to take electron correlation into account. Atoms provide a good starting point for the incorporation of spin-orbit coupling into QMC calculations. Unfortunately substantial modifications in the whole QMC framework are required which have been done so far in nuclear physics only. The brute force approach used in nuclear physics is not suitable for quantum chemistry and we tried to develop a method which takes care of the peculiarities of electronic many-body systems.

Transition metal atoms

Due to the presence of an open 3d and a low lying 4p shell the atoms Sc, Ti, V, and Cr provide an interesting test system for the accuracy of the fixed-node approximation [4]. We have calculated excitation and ionization energies for several atomic states, including varying occupations of the 3d shell. The possibility of systematic improvements using multi-reference trial wavefunctions has been investigated in detail. Of special importance is the interaction between the 3p and 3d shells which have a strong radial overlap. This interaction decreases with increasing occupation of the 3d shell.

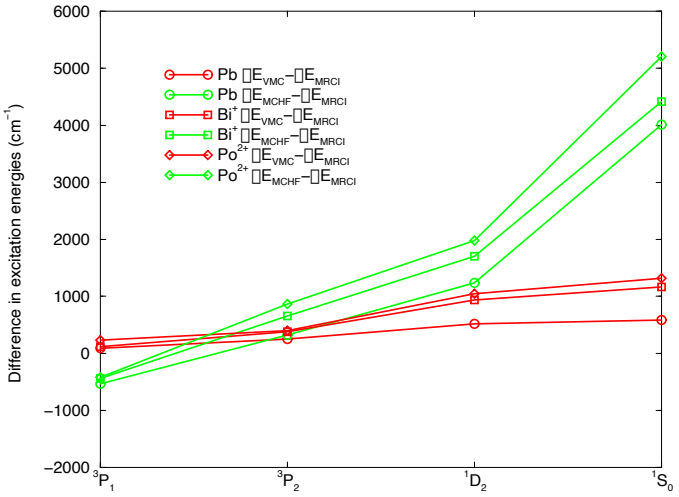

Figure 1: Difference in excitation energies (cm^{-1}) of variational quantum Monte Carlo (VMC), two-component multiconfiguration self-consistent field (MCHF) calculations with respect to multireference configuration interaction (MRCI) calculations.

Spin-orbit coupling

We are currently developing a method for the calculation of fine-structure splittings using variational quantum Monte Carlo [5]. The method uses an intermediate coupling

scheme for the antisymmetric part of the wavefunction which is multiplied by a symmetrical correlation factor. The correlation factor commutes with the total angular momentum operator and describes dynamical correlations through an explict dependence on the electron-electron distances. So far it has been applied to determine the influence of valence electron correlation on the total angular momentum eigenstates emerging from the $6s^2 6p^2$ valence configuration of Pb and the isoelectronic ions Bi^+ and Po^{2+}. The improvement due to the inclusion of dynamical correlation is shown in Figure 1.

Molecules

The application of QMC techniques to molecules containing heavy elements runs into similar difficulties as for atoms.

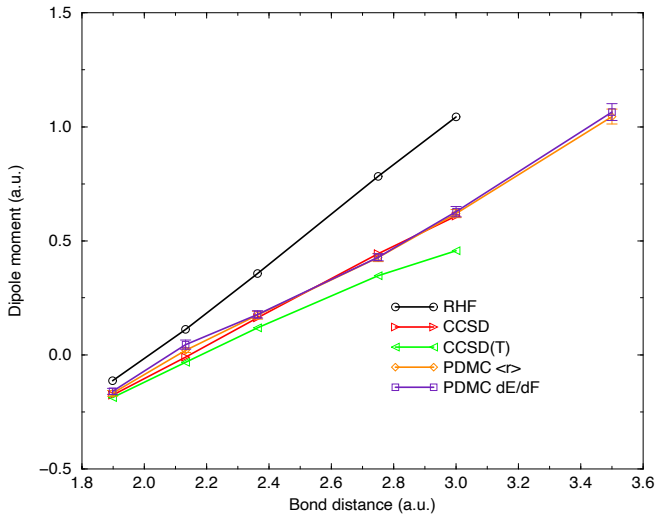

Figure 2: Dipole moment of CO from PDMC finite field and $< r >$ expectation value calculations compared to CCSD results.

For systems with a reasonably well defined HF ground state configuration sufficiently accurate results for the binding energy can be expected. We have done calculations for transition metal oxides ScO, TiO, VO and sulfides ScS, TiS, VS where we obtained a close agreement to coupled cluster single-double (CCSD) calculations. Beyond ground state energies there are a couple of interesting properties like dipole momenta and polarizabilities which are of great interest for molecules. The PDMC algorithm is especially advantageous for the calculation of these properties and we extended existing methods for calculations with pseudopotentials [6]. An example of such a calculation is shown in Figure 2 where we have calculated the dipole moment of CO for various internuclear distances, using PDMC and CCSD methods.

Van der Waals molecules

The weak bonding in van der Waals molecules is especially sensitive to electron correlation. We have studied the weakly interacting group 12 dimers [7, 6] Hg_2, Cd_2, and Zn_2 together with the Be_2 molecule. The QMC potential energy curves and static dipole polarizabilities show excellent agreement with CC calculations using large basis sets. In the case of Be_2 we have demonstrated the importance of a multi-reference trial wavefunction in order to get a bonding potential energy curve. To get an idea of the covalent contribution to the bonding we have also determined the charge fluctuations between the atoms from PDMC calculations. Figure 3 shows the interatomic charge fluctuations for the group 12 dimers which are mainly due to an overlap of the atomic orbitals already at the HF level. The effect of electron correlation is rather small.

Clusters

The encouraging results for the group 12 dimers suggest an extension of our calculations to larger clusters. Due to the change of the interaction from van der Waals to covalent and finally metallic bonding with increasing size, these clusters are of significant interest for theory and experiment. Most of the experimental [8] and theoretical [9] work

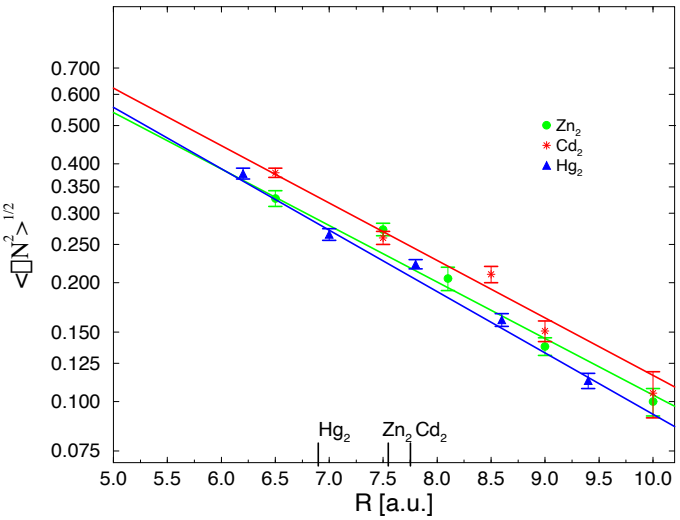

Figure 3: Interatomic charge fluctuations for Zn_2, Cd_2, Hg_2 from PDMC and HF calculations. The solid lines refer to HF.

has been done for Hg_n clusters. The theoretical work is based on model Hamiltonians which require some a priori knowledge of the type of bonding. We have performed *ab initio* calculations for small and medium sized Hg_n clusters [10] up to 15 atoms which do not require any prior assumptions on the type of bonding. A combined treatment

with QMC and CC methods was found to be especially useful. The application of QMC

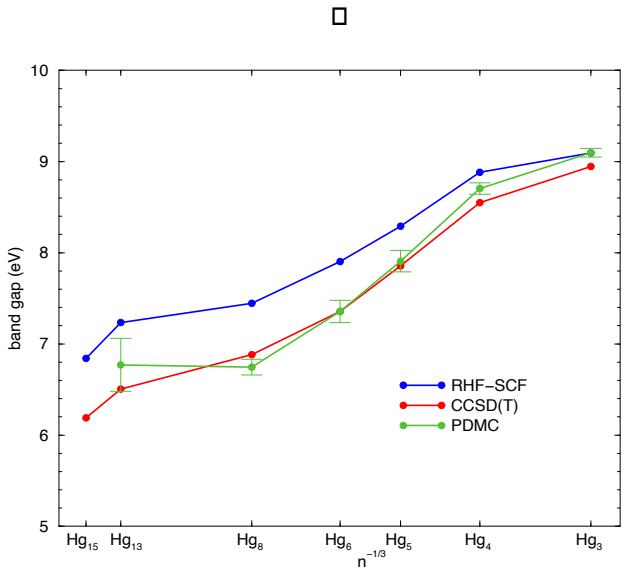

Figure 4: Band gap of Hg_n clusters.

methods permits a consistent treatment of electron correlation over a large range of cluster sizes. The calculated size-dependences of ionization potentials, electron affinities and cohesive energies reproduce the observed trends in experiments. A sensitive measure for the type of bonding is the 'band gap' of these clusters which is shown in Figure 4.

Comparative studies of X_n clusters $(X = Zn, Cd, Hg, Yb)$, $(n = 1, \ldots, 6)$

The previous studies on Hg_n clusters suggest an extension to the other group 12 elements Zn and Cd. In order to perform an analysis of the covalent contribution to the bonding we have calculated the electron localization function (ELF)[11]. An example is presented in Figure 5 which shows ELF together with the electron density on a section of Zn_4. Large ELF values correspond to covalent bonds and lone pairs. A systematic comparison of ELF in the interatomic regions of the clusters reveals qualitative trends in the covalent contributions which can be compared with trends in the cohesive energies or band gaps.

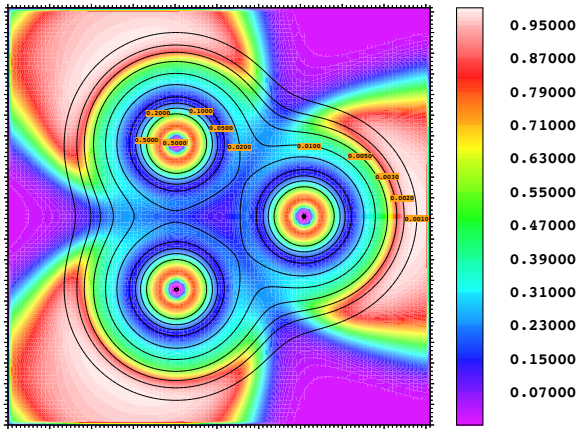

Figure 5: The electron localization function (colours) and electron density (contour lines) of Zn_4. The plot shows a section through three atoms of the tetrahedral structure.

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Semiclassical linear response: far–infrared absorption in ballistic quantum systems

Bernhard Mehlig and Klaus Richter

We provide a general semiclassical theory for calculating dynamical susceptibilities and transport coefficients within linear–response theory [1]. The semiclassical response functions are derived for quantum systems with internal ballistic dynamics at finite temperatures and finite frequencies. Such an approach is desirable since for instance, very recently, different experiments on dynamical properties of mesoscopic devices have been performed [2, 3].

According to linear–response theory, a susceptibility $\chi(\mu,\omega)$ is given by ($g_{\rm s}=2$)

$$\chi(\mu,\omega) = g_{\rm s}\left\langle \sum_{mn} \frac{|U_{mn}|^2[f(E_m)-f(E_n)]}{\hbar\omega - E_m + E_n + i\eta}\right\rangle , \tag{1}$$

where μ is the chemical potential, $U_{mn}=\langle\psi_m|\widehat{U}|\psi_n\rangle$, E_m and ψ_m are the eigenvalues and eigenfunctions of the unperturbed quantum system, and $\widehat{U}$ is an external or self–consistent perturbation, as discussed below. Finally, $f(E)=(\exp[\beta(E-\mu)]+1)^{-1}$ is the Fermi function, and $\langle\cdots\rangle$ denotes an average over weak disorder.

Generalizing a semiclassical approximation for sums over transition matrix elements [4, 5, 6] by including temperature and weak-disorder effects, the imaginary part, $\chi''(\mu,\omega)$, of $\chi(\mu,\omega)$ can be semiclassically evaluated. To leading order in β^{-1} and $\hbar^{-1}$ it consists of a dominant classical contribution and leading-order oscillatory corrections: $\chi''(\mu,\omega)\simeq\chi''_0(\mu,\omega)+\chi''_{\rm osc}(\mu,\omega)$. The classical part is of the form

$$\chi''_0(\mu,\omega) \simeq \hbar\omega\, g_{\rm s}\,\pi \int d\omega'\,\delta_\Gamma(\omega-\omega')\,C_0(\mu,\omega')\ . \tag{2}$$

Here, $\delta_\Gamma(x)$ is a Lorentzian window function of width $\Gamma=\hbar/2\tau_{\rm el}$ where $\tau_{\rm el}$ is the elastic scattering time. The function $C_0(E,\omega)$, is given in terms of the microcanonical phase–space average of the classical autocorrelations of $U(\mathbf{p},\mathbf{q})$ [4, 5, 6].

For chaotic systems, the oscillatory term can be semiclassically expressed in terms of a sum over contributions from (unstable) periodic orbits p of the system. The final result reads [1]

$$\chi''_{\rm osc}(\mu,\omega) = -\frac{2g_{\rm s}\Gamma}{\beta}\sum_{p\nu}\frac{w_p\alpha_{p\nu}}{\sinh(\pi T_p/\beta\hbar)}\frac{\exp(-\Gamma T_p/\hbar)}{(\hbar\omega-\hbar\omega_{p\nu})^2+(2\Gamma)^2} \tag{3}$$
$$\times\cos\left(\frac{S_p}{\hbar}-\frac{\pi}{2}\mu_p\right)\sin\left(\frac{\omega}{2}T_p\right)\left\{\cos\left(\frac{\omega}{2}T_p\right)+\frac{2\Gamma}{\hbar}\frac{\sin\left(\omega T_p/2\right)}{\omega-\omega_{p\nu}}\right\}\ .$$

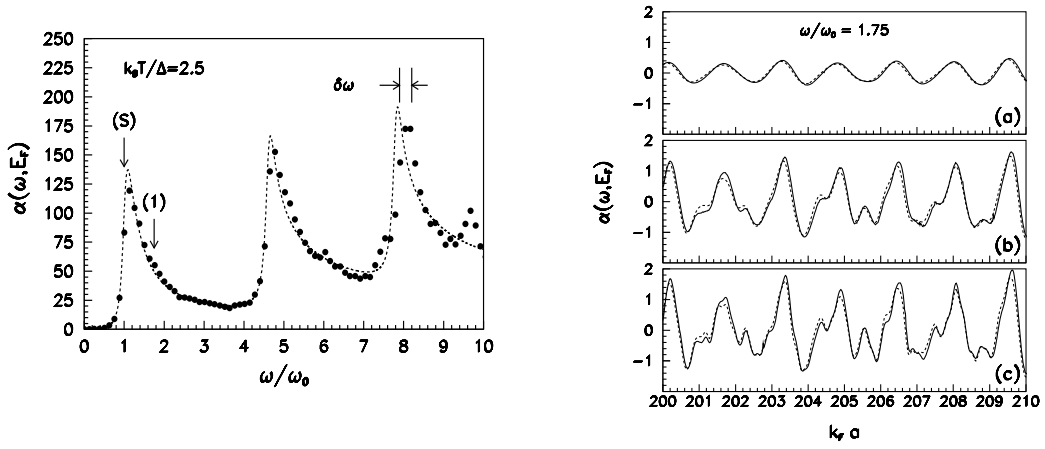

Figure 1: (left) Ensemble–averaged absorption coefficient $\overline{\alpha(\mu,\omega)}$ [arb. units]. The average was performed over samples with different sizes, with mean chemical potential $\overline{\mu}$. The temperature is $k_{\rm B}T/\Delta = 2.5$ and the disorder–related broadening $\Gamma/\Delta = 10$. The quantum–mechanical data are shown as dots ($\bullet$), while the semiclassical data (from Eq. (2)) are shown as a dashed line. The synchrotron resonance is indicated as *(S)*, while the frequency used in Fig. 2 is indicated by *(1)*.

Figure 2: (right) Quantum oscillatory contributions $\alpha_{\rm osc}(\mu,\omega)$ [arb. units] to the absorption coefficient (solid lines) as a function of $k_{\rm F}a$ for $\omega/\omega_0 = 1.75$ and for three different temperatures, $k_BT/\Delta = 20$ (a), 10 (b) and 5 (c). The frequency used is indicated by an arrow in Fig. 1. Also shown are the results of a semiclassical calculation, according to Eq. (3) (dashed lines), for the same parameters.

Here, S_p are the classical actions, μ_p the Maslov indices, T_p the periods, and w_p are the stability indices of the periodic orbits. The $\alpha_{p\nu}$ are the coefficients of a Fourier expansion of the classical autocorrelation functions (along periodic orbits): $C_p(E,t) = T_p{}^{-1}\int_0^{T_p} dt'\, U(t+t')U(t') = \sum_\nu \alpha_{p\nu}(E)\exp(i\omega_{p\nu}t)$, with $\omega_{p\nu} = 2\pi\nu/T_p$. Hence, those orbits contribute strongly whose eigenfrequencies $\omega_{p\nu}$ are in resonance with the external frequency ω.

As it stands, Eq. (3) refers to chaotic systems. However, a similar result holds for integrable systems where, roughly, the periodic orbits are replaced by tori and the autocorrelation functions are defined on rational tori.

Eq. (3) is the main result of our semiclassical approach. It provides a general means of calculating susceptibilities and transport coefficients in the semiclassical regime (large Fermi wave vector $k_{\rm F}$). In addition to the classical contribution, χ_0, Eq. (3) predicts characteristic oscillatory contributions due to quantum interference.

We emphasize that in order to obtain well–defined semiclassical results, it is essential to have $\Gamma \gtrsim \Delta$ (mean level spacing). For small Γ ($\Delta \lesssim \Gamma/\hbar \ll T_p^{-1}$) the (lowest–order) oscillatory periodic orbit contributions *vanish*. For very large Γ ($\Gamma/\hbar \gg T_p^{-1}$), on the

other hand, the contributions of long periodic orbits are exponentially damped. The same holds for large temperatures.

In the following we provide a specific example and use Eq. (3) to calculate absorption in conducting disks with ballistic internal dynamics. For time–dependent fields, screening due to electron interactions has to be taken into account. We calculate the absorption coefficient for radiation at frequencies the plasma frequency below ω_p using an approximate effective potential U related to the classical screening charge density in the static Thomas Fermi limit [7]. We thus neglect quantum corrections to the screening which are of higher order in $\hbar$. For the case of the circular disk of radius a the effective potential reads $U(\mathbf{r}) \sim E_0 r\cos(\varphi)\pi^{-1}(a^2-r^2)^{-1/2}$ in polar coordinates (r,φ).

The absorption coefficient is related to χ by $\alpha(\mu,\omega) = \omega/2\ \chi''(\mu,\omega)\, E_{\rm ext}^{-2}$ where $E_{\rm ext}$ is the external electric field. In the following we compare quantum results obtained for $\alpha(\mu,\omega)$ from Eq. (1) with the semiclassical theory Eq. (3). In keeping with the structure of Eqs. (2) and (3) we divide the absorption coefficient into a smooth and an oscillatory contribution, $\alpha(\mu,\omega) = \alpha_0(\mu,\omega) + \alpha_{\rm osc}(\mu,\omega)$.

Let us first consider the average absorption coefficient $\overline{\alpha(\mu,\omega)}$ of an ensemble of disks of different sizes. Since the oscillatory terms vanish upon averaging, only the classical contribution remains, $\overline{\alpha(\mu,\omega)} \simeq \alpha_0(\overline{\mu},\omega)$. Fig. 1 compares the quantum data with the classical result. We find excellent agreement with the classical expression calculated from $C_0(\mu,\omega)$ according to Eq. (2). We observe an average increase of the absorption linear in frequency and a series of resonances. The first resonance has a simple classical explanation. It is due to synchrotron motion of the electrons in phase with the external field.

We now turn to the behaviour of individual disks. According to Eq. (3) we expect to observe quantum oscillations superimposed onto a smooth classical background. In order to remove the classical background and to extract the oscillatory contributions, we have calculated the absorption at two different temperatures and plotted the difference. For $k_{\rm B}T/\Delta \simeq 50$ (where Δ is the mean level spacing), the oscillatory contributions are almost completely damped out. This corresponds to temperatures of about 1K in typical experimental setups. Fig. 2 (a–c) show the differences of quantum–mechanical absorption coefficients at $k_{\rm B}T/\Delta = 5, 10$ and 20 with the absorption at $k_{\rm B}T/\Delta = 50$, as a function of $k_{\rm F}a$. Also shown are the corresponding semiclassical results calculated from Eq. (3). The frequency is kept fixed at $\omega/\omega_0 = 1.75$, where $\omega_0 = v_{\rm F}/a$. For low temperatures we observe characteristic $k_{\rm F}$–oscillations. They arise as superpositions of quantum oscillations related to different periodic orbits since in billiard systems, $S_p(\mu)/\hbar = k_{\rm F}L_p$. Fig. 2 shows excellent agreement between the quantum data calculated from Eq. (1) and the semiclassical results from Eq. (3). This degree of agreement exists for a whole range of frequencies ω[1].

In summary, we have derived a semiclassical theory for dynamical susceptibilities of ballistic quantum systems. We have used our results to calculate the infrared absorption in conducting disks with ballistic dynamics. Our semiclassical results are in

excellent agreement with corresponding quantum calculations.

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Chaos and Interacting Electrons in Ballistic Quantum Dots

K. Richter, D. Ullmo, H.U. Baranger, F. von Oppen, and R.A. Jalabert

The connection between classical dynamics and wave interference has recently attracted attention in many fields of physics, including atomic, mesoscopic, and optical physics. A central question is to what extent the quantum properties of classically regular and chaotic systems differ. On the whole, this question has been addressed for non-interacting systems and very little is known about quantum chaos for interacting many-particle systems. Here we wish to address this issue and, in particular, to investigate the role of the classical dynamics of the corresponding non-interacting system in this context [1].

If the interactions are short-range and not too strong, the non-interacting classical dynamics may be important, and its role can be assessed with perturbation theory. This regime is physically relevant since it applies to a high density two-dimensional electron gas in which the quasi-particles interact weakly through the short-range screened Coulomb interaction. To be specific, we study the magnetic response of an ensemble of phase coherent, ballistic quantum dots formed from a two-dimensional electron gas. For the magnetic response, the high-density expansion (RPA) of the thermodynamic potential Ω has to be extended by including Cooper-like correlations, as carried out previously for disordered metals [2, 3, 4]. The perturbation expansion for the interaction contribution to Ω yields the magnetic susceptibility through $\chi \equiv (-1/a^2)\partial^2\Omega/\partial B^2$. ($a$ is the size of the microstructures, and B is the magnetic field which is assumed to be classically weak, i.e. cyclotron radius $\gg a$.) The dominant terms are shown in Fig. 1. The screened Coulomb interaction (wavy lines) is treated as local, $U(\mathbf{r}-\mathbf{r}') = \lambda_0 N(0)^{-1}\delta(\mathbf{r}-\mathbf{r}')$, with $N(0)$ the density of states and $\lambda_0 = 1$ identifying the order of perturbation. Straight lines represent the "free" finite-temperature Green function in the presence of the confining potential.

For instance, the first-order (Hartree-Fock) term and the complete "diagonal" or Cooper channel for the interaction contribution to Ω read, respectively,

$$\Omega^{(1)} = \frac{\lambda_0}{\beta}\mathrm{Tr}\left\{\Sigma_{\mathbf{r},\mathbf{r}'}\right\} \qquad , \qquad \Omega^{(D)} = \frac{1}{\beta}\mathrm{Tr}\left\{\ln[1+\lambda_0\Sigma^{(D)}_{\mathbf{r},\mathbf{r}'}]\right\} \ . \tag{1}$$

Here, the thermodynamical traces include a sum over Matsubara frequencies and refer to the spatial arguments of the particle-particle propagators $\Sigma_{\mathbf{r},\mathbf{r}'}$ which are composed of products of (finite-temperature) Green functions.

These expansions are particularly insightful when combined with a semiclassical approximation from which the connection to the nature of the classical dynamics can

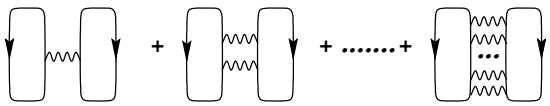

Figure 1: Leading Cooper-channel diagrams for the interaction contribution to the thermodynamical potential.

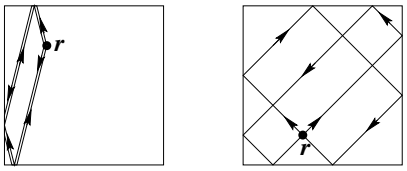

Figure 2: Typical pairs of real-space paths that contribute to the average susceptibility to first order in the interaction in the diagonal channel (left) and the non-diagonal channel (right).

be made. If the Green functions are semiclassically expressed in terms of sums over paths j with phases given by their classical actions S_j, $\Sigma_{\mathbf{r},\mathbf{r}'}$ is a sum over pairs of such trajectories joining $\mathbf{r}$ to $\mathbf{r}'$. To leading order, only those pairs contribute to the ensemble averaged susceptibility whose dynamical phases $\exp[iS_j(B=0)/\hbar]$ cancel while retaining a magnetic-field dependence. This is achieved by pairing each orbit j with its time reverse. The corresponding "diagonal" part $\Sigma^{(D)}$ of Σ then reads

$$\Sigma^{(D)}_{\mathbf{r},\mathbf{r}'} \simeq \frac{\hbar v_F}{\pi N(0)} \sum_{j:\mathbf{r}\to\mathbf{r}'} D_j \, \frac{R(L_j/L_T)}{L_j} \times \exp\left[\frac{i4\pi B A_j}{\phi_0}\right] . \qquad (2)$$

Here, the sum is over trajectories of length L_j enclosing an "area" A_j. The prefactor D_j includes the classical phase space density and Matsubara frequencies, and the function $R(x)$ accounts for temperature damping. It is exponential for trajectories longer than the thermal cutoff length $L_T = v_F\hbar/k_BT$ where $v_F = \hbar k_F/m$ is the Fermi velocity.

The trace in the first order term in Eq. (1) yields a sum over closed but not necessarily periodic trajectories. See, e.g. Fig. 2, left, for the case of a square microstructure. However, higher-order diagrams in the interaction (right equation in (1)) are essential in the diagonal Cooper channel, as known from the theory of superconductivity [2]. $\Sigma^{(D)}$ represents the building block for such higher order terms. Semiclassically, the n-th order contribution is given by a sum over closed trajectories visiting n (interaction) points in configuration space. $\Sigma^{(D)}$ has the nice property that all variations occur on classical scales: rapid oscillations on the scale of the Fermi wavelength λ_F have been washed out. The original interacting quantum problem becomes much simpler, involving only the "classical" operator $\Sigma^{(D)}$. Hence, we can discretize $\Sigma^{(D)}$ with mesh size larger than λ_F and then compute $\Omega^{(D)}$ efficiently.

We have performed this computation for the case of a square billiard. The dotted curve of Fig. 3 shows the temperature dependence of the susceptibility, $\chi(T)$, from the full Cooper channel. In this curve, we can distinguish three regimes. At low-temperature $\chi^{(D)}$ is *paramagnetic* and decays nearly exponentially. In the intermediate range, $\chi^{(D)}$ is small and *diamagnetic*. Finally, at high temperatures $\chi^{(D)}$ is again *paramagnetic*, but very small. This is naturally understood by associating each regime with an order

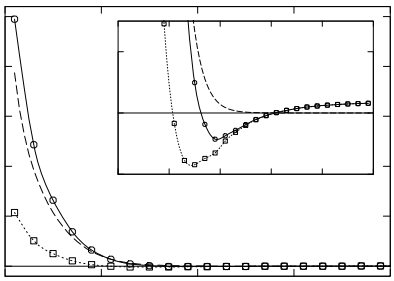

Figure 3: Temperature dependence of the zero-field susceptibility (solid line) for an ensemble of squares at $k_F a$=50. The contribution of the non-diagonal channel (dashed, family of orbits in Fig. 2, right) exceeds that of the diagonal Cooper channel (dotted) at low temperatures ($T_0/T = L_T/2a$).

in the perturbation series: the low-T part corresponds to the first-order term (orbits of the type in Fig. 2, left) which is exponentially suppressed when L_T becomes smaller than the shortest closed orbit. At this point the diamagnetic second-order term, due to closed paths of two trajectories connected by interactions, takes over. There is no minimum length of these paths, and hence this term is less rapidly suppressed by temperature. At even higher T once $L_T \ll a$, the third- and higher-order, bulk-like terms dominate.

A simple renormalization approach shows [1] that the higher order terms in the Cooper channel lead to a renormalized coupling constant: $\lambda_0 = 1 \to \lambda(a) \simeq 2/\ln(k_F a)$.

The diagonal channel is present independent of the nature of the classical dynamics, i.e. whether the non-interacting system is integrable or chaotic. However, as a peculiarity of integrable geometries, additional *non-diagonal* contributions to Ω, which do not exist in chaotic systems, survive the ensemble average. This non-diagonal contribution to $\chi(T)$ is shown in Fig. 3 as the dashed curve.

Non-diagonal terms stem from pairs of different periodic orbits of the same family (torus). Such orbits, which are shown in Fig. 2 (right) for the case of the square, have the same classical actions and hence the related dynamical phases cancel upon pairing them. Higher-order non-diagonal contributions are smaller by a factor $1/k_F a$ and can be neglected. Therefore, the first-order non-diagonal terms are *not* renormalized. Consequently, at low T, the diagonal contribution is *parametrically* smaller than the non-diagonal one by a factor $1/\ln(k_F a)$ because higher-order correlation terms reduce only the diagonal contribution.

Therefore, regular systems, for which there is a non-diagonal contribution, show a magnetic response logarithmically larger than generic chaotic systems, for which only the diagonal channel is open. Thermodynamic properties scale differently with Fermi energy for chaotic and regular systems. This correlation effect shows that the nature of the classical dynamics can have a substantial effect on the quantum properties of an

interacting system.

Specifically, the orbital magnetism is greatly enhanced over the Landau susceptibility by the combined effects of interactions and finite size. For comparison, we note that the non-interacting contribution obtained previously [5] is of the same order as the interaction contribution for integrable systems but smaller for chaotic ones. A related semiclassical approach can be adapted to diffusive dynamics [6] and yields the results of Ref. [4].

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Spectral correlations in chaotic systems with discrete translation invariance

T. Dittrich, B. Mehlig, H. Schanz and U. Smilansky

Spectral correlations in quantum systems with chaotic classical counterparts have been a focus of research since more than a decade. The simple universal behavior is modified notably in two cases: (i) when an additional symmetry is present and (ii) when the system is extended, i. e. when the time for ergodic coverage of the energy shell is not the only time scale in the classical evolution. In this contribution we summarize the semiclassical theory [1] for the spectral two-point correlations in a situation where both conditions are satisfied: We consider a chain of N identical chaotic unit cells with periodic boundary conditions, such that the full system shows a discrete translation invariance (fig. 1).

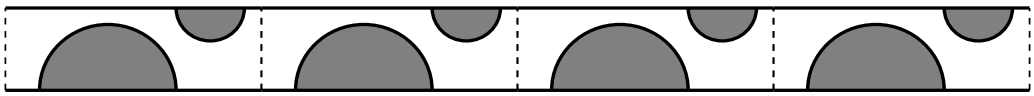

Figure 1: A quasi-one-dimensional chain of coupled chaotic billiards with periodic boundary conditions provides one example for the type of system studied in this contribution.

Before we outline our theory we would like to mention the important analogy between an extended periodic system and a single unit cell on a ring threaded by a magnetic flux. This analogy does not only extend the range of applicability of our semiclassical results, it also allows for a very detailed comparison to an earlier supersymmetric calculation [2].

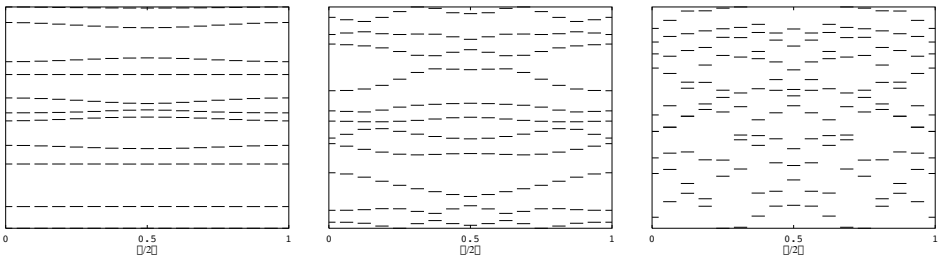

Figure 2: Discretized band spectra of a periodic chain with $N = 16$ unit cells. Shown are the levels as a function of the Bloch phase θ_n for 10 bands in the case of (a) low, (b) intermediate, and (c) high conductance. For low conductance the bands are flat and show little structure. For high conductance the bandwidth is of the order of the interband spacing and the correlation length inside the bands shrinks such that the bands can hardly be recognized, if the discretization is too coarse. Time-reversal symmetry of the Hamiltonian leads in this example to the reflection symmetry in the bands with respect to the center and the edges of the Brillouin zone.

In a system as the one displayed in fig. 1, the classical evolution is diffusive on time scales larger than the ergodic time of the unit cell. On time scales of the order of

the Thouless time the whole system is explored. This time represents a second important classical time scale. It can be combined with the mean level spacing to the dimensionless conductance, which is—apart from the number of unit cells N—the only free parameter in the theory to be presented. Because of the translation invariance, the spectrum consists of discretized energy bands whose precise form depends on the value of the conductance (fig. 2). Our aim is to determine the signatures of the band structure in the spectral two-point correlation function. It is convenient to work with the Fourier transform of the spectral correlator with respect to energy, the so-called form factor $K(\tau)$. The correlations are then represented as a function of time τ and the characteristic energy scale given by the mean level spacing is translated into a characteristic quantum-mechanical time scale, the Heisenberg time. We use a dimensionless time such that the Heisenberg time of the unit cell is unity and hence the Heisenberg time of the full chain is N. The main ideas needed to calculate the form factor semiclassically are due to Berry [3]: Using Gutzwillers trace formula [4], $K(\tau)$ is represented as a double sum over periodic orbits with period τ. The terms corresponding to orbits with different action contain a rapidly oscillating phase and can be neglected for $\tau < 1$ in a chaotic system with a single classical time scale.

In order to apply this so-called diagonal approximation to the extended and periodic system under consideration, we fold all periodic orbits back onto the unit cell. It is easy to see that the projections correspond to periodic orbits of the unit cell whose winding numbers are integer multiples of N, and that for a given τ most periodic orbits of the unit cell correspond to N orbits of the extended system which differ by a translation in space but are otherwise equivalent. These observations allow us to reduce the form factor for $\tau < 1$ to a single sum over periodic orbits of the unit cell which are selected by their winding number. Using certain ergodicity assumptions, the sum can in turn be related to the classical probability to stay in the same unit cell $P_0(\tau)$ after dimensionless time τ, as will be explicitly stated below. This connection between spectral correlations and the spatial extension of the system can be enhanced further: Using the additional information provided by the Bloch phases $\theta_m = 2\pi m/N$, $m = 0, \ldots, N-1$ labeling the levels in each of the bands, it is possible to introduce a form factor $\widetilde{K}_n(\tau)$ with a spatial argument n. While n appears quantum mechanically as the quantity complementary to the Bloch phase in a discrete Fourier transformation, $\widetilde{K}_n(\tau)$ contains, according to a semiclassical analysis analogous to the special case $n = 0$ described above, periodic orbits which wind $n + \mu N$ times around the unit cell in one period ($\mu = 0, \pm 1, \ldots$). Hence we call $\widetilde{K}_n(\tau)$ a winding-number-specific form factor. Semiclassically it is related to the coarse grained classical propagator $P_n(\tau)$ by

$$\widetilde{K}_n(\tau) = \gamma_n \tau P_n(\tau)\,. \tag{1}$$

The constant γ_n is unity unless there is time-reversal symmetry and the reversed orbit has the same winding number, which results in $\gamma_n = 2$ (e. g. $n = 0$ in a billiard chain). A relation in the form of (1) was first derived for extended but disordered systems [5]. When the classical diffusion propagator is inserted into (1), we obtain an explicit semiclassical expression of the form factor for $\tau < 1$, which remains to be extended beyond the region accessible to the diagonal approximation. Under certain assumptions about the shape of the bands, notably that they are not too flat (i. e. sufficiently large

conductance),

$$\widetilde{K}_n(\tau) = \frac{\gamma_n}{\tau} \sum_{\mu=-\infty}^{\infty} F\left(\frac{n-\mu N}{\tau}\right), \tag{2}$$

is derived for large time $\tau \gg 1$. Assuming that this scaling relation can be extended to $\tau \gtrsim 1$, the function F is determined by matching the form factor at the Heisenberg time term by term to the diagonal approximation.

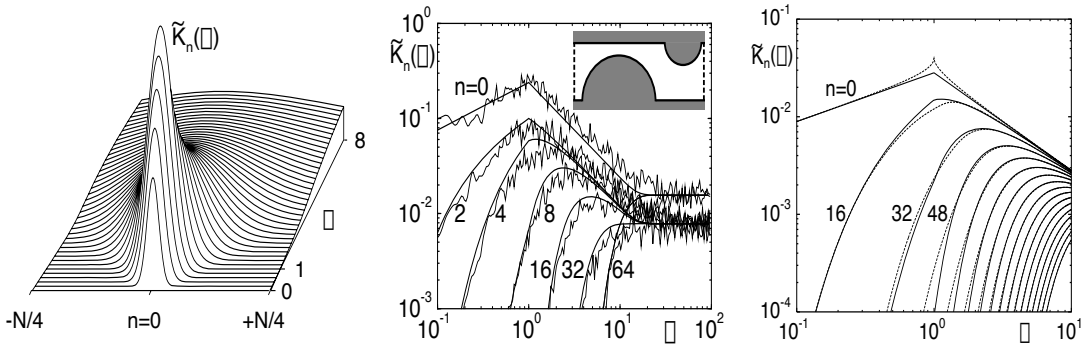

Figure 3: Winding-number-specific form factor for intermediate conductance: (a) The left panel shows the semiclassical theory as a time-dependent distribution in coarse-grained space. (b) Comparison of the semiclassical theory to a numerical calculation for a billiard chain with $N = 128$ unit cells, similar to fig. 1. The values of n are given next to the curves. (c) Comparison of the semiclassical theory for the limiting case $N \to \infty$ to an expression derived in Ref. [1] from the supersymmetric theory by Altshuler et al. Ref. [2]. The largest deviation is observed close to the Heisenberg time $\tau = 1$.

The form factor can now be interpreted in terms of the coarse-grained evolution of a wave packet which was initially centered at the origin. Here, we discuss the case of intermediate conductance (fig. 3). Up to the Heisenberg time the quantum evolution follows the classical diffusive spreading of the wave packet but for the additional factor τ. We assume that the classical diffusion is slow enough, such that the periodic boundary conditions are not yet important at the Heisenberg time. Then the form factor is an isolated peak centered at $n = 0$. If, on the other hand, the conductance is sufficiently large, the scaling function derived above predicts, for $\tau > 1$, a ballistic instead of a diffusive spreading of this peak, i. e. the width increases proportional to time while the maximum decays as $1/\tau$ such that the normalization is conserved. For very large time the wave packet reaches the boundary of the system and an equidistribution results.

Our theory was quantitatively verified by numerical computations (e.g. fig. 3b) and a comparison to a supersymmetric calculation in the limit $N \to \infty$ [2] (fig. 3c). The supersymmetric approach—where applicable—does not involve the approximations of the semiclassical treatment and is hence more accurate, in particular close to the Heisenberg time. On the other hand, the semiclassical calculation is simple and intuitive, and it yields a more explicit result which is better suited for a physical interpretation.

The behavior of the form factor can also be interpreted in terms of energy scales: At the Heisenberg time, all individual bands are resolved. With the normalization chosen, the form factor would be unity, if all levels were N-fold degenerate (flat bands). For

intermediate conductance (figs. 2b, 3), the band width equals the interband spacing. Still $K(\tau = 1)$ is of the order 1, because the levels clustered near the band edges—remnants of the van-Hove singularities for continuous bands—appear degenerate. With growing time, more and more levels are resolved, and the form factor decays to its asymptotic value $\sim 1/N$. Hence there is a maximum at $\tau = 1$. In contrast, for very large conductance the correlation length inside a band is smaller than the discrete sampling of the band by the Bloch phases (fig. 2c). In this case level clustering—and hence the maximum in the form factor—are absent.

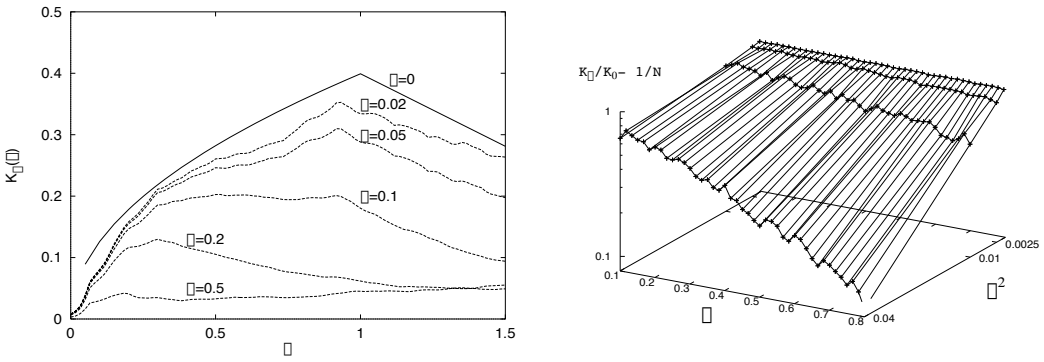

Figure 4: (a) Form factor for intermediate conductance and weak disorder compared to the semiclassical theory in the periodic case. The magnitude δ given next to the curves is proportional to the variation in the action of a periodic orbit due to the disorder. (b) Logarithmic plot of the relative suppression of the form factor in the semiclassical region. When allowance is made for the asymptotic constant $1/N$, the supression is exponential in τ and δ^2.

Another way to gradually destroy the level clusters at the band edges is to introduce weak disorder. Indeed the peak at the Heisenberg time disappears for growing disorder strength δ. This is shown in fig. 4a. An extension of the semiclassical theory predicts a suppression of the form factor in the region $0 < \tau < 1$, which is exponential both in τ and δ^2 [6]. Again, this is confirmed by numerical data (fig. 4b).

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Classical phase space structure in microcavities

Jens U. Nöckel

The study of optical processes in microcavities is a diverse and expanding field, extending from applied topics such as the design of novel microlasers and other optical devices to questions of more fundamental interest in non-linear optics and cavity QED. For an overview see Ref. [1].

In all of these areas, the key element is an extremely small resonator cavity in the size range of 1 to 1000 μm, at wavelengths from 0.1 to 10 μm. One of the most effective designs relies on *total internal reflection* as a means of confining the light. This is achieved when light rays circulate near the perimeter of some convex cross section of a dielectric body surrounded by a lower-index medium. The resulting resonator modes have a characteristic spatial intensity distribution concentrated near the dielectric interface, which in recognition of an analogous acoustic effect is referred to as the "whispering-gallery" (WG) phenomenon. The longest measured optical resonance lifetimes for such WG modes in clean glass microspheres are three orders of magnitude longer than can be achieved in microwave resonators with superconducting mirrors.

However, for technological applications such extreme lifetimes are useless, and prescriptions for degrading the resonator quality to some desired level are sought. For dielectric bodies with rotational symmetry, there furthermore exists no preferred emission direction, leading to isotropic emission in microlasers based on such cavities. Bothshortcomings can be addressed by turning to *asymmetric resonant cavities* (ARCs), convex but substantially deformed dielectric resonators for which the classical wave equation is nonseparable.

The significance of ARCs in the highly competitive field of microlaser development [2] has increased rapidly since their emission properties have been shown to be predictable largely relying on classical ray dynamics [3]. The ray dynamics of a generic ARC is partially chaotic and in fact represents a realization of a plane hard-wall billiard as long as no escape occurs. A semiclassical treatment is needed to connect the ray description with the discrete modes of the cavity. This makes ARCs a laboratory for the study of *quantum chaos*, similar to microwave resonators, however with an emphasis on novel questions aring due to the openness of the resonator, such as the lifetime and emission directionality of individual quasibound states.

A WG mode in a glass rod with a deformed cross section is shown in the inset to Fig. 1(a). Contrary to the results of an adiabatic approximation that is known to be exact in the ellipse billiard, emission here does not emanate tangential to the points of highest curvature. This is due to the KAM transition to chaos occuring in this oval shape. The Poincaré section (SOS) shows islands due to a stable periodic orbit intersecting the total-internal-reflection condition, $\sin\chi = 1/n$, which represents the lower bound on the angle of incidence χ allowing total internal reflection at the interface for refractive index n. A chaotically diffusing ray cannot enter the island, and hence

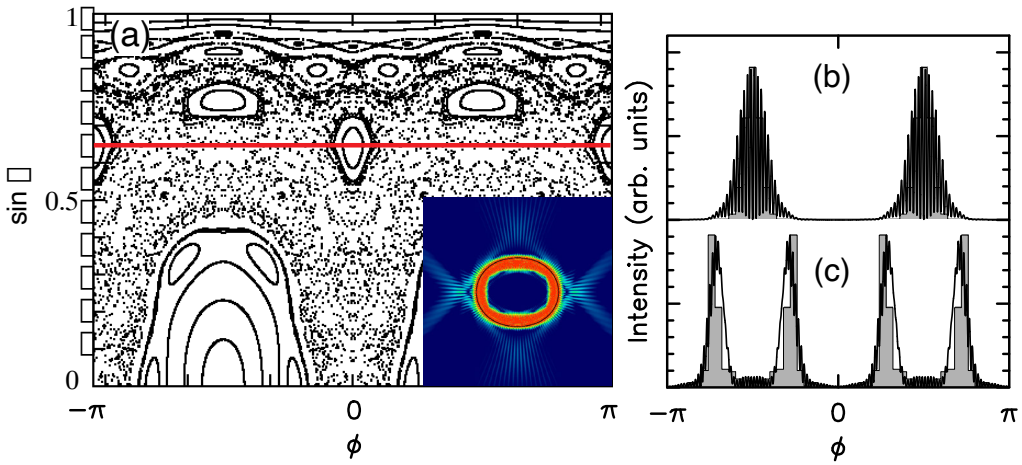

Figure 1: (a) Inset: TM polarized quasibound state wavefunction in a $\sim 10\%$ deformed ARC, $n = 1.54$. Main: Poincaré section for this cavity. Straight horizontal line indicates the classical escape condition. Farfield intensity patterns are shown in (b) for $n = 2$ and (c) for $n = 1.54$. Solid lines are wave results, histograms are ray simulations.

in this case is prevented from reaching the classical escape condition at the points $\phi = 0$ and π, which are the highest-curvature points. This *dynamic eclipsing* affects all WG modes for which classical ray diffusion as just described is the dominant escape mechanism, as opposed to the always-present tunneling. Ray and wave results agree very well at large deformations, whether the adiabatic approximation is valid [Fig. 1 (b)] or not [Fig. 1 (c)].

A cylindrical ARC shape has been combined with a quantum cascade heterostructure active region to create electrically pumped microlasers with an effective n of 3.3, a short diameter of $50\,\mu$ and long axes varying from $50\,\mu$ to $80\,\mu$, emitting at $\lambda = 5.2\,\mu$. The significance of phase space structure has been demonstrated in these devices [4]. At $\sim 15\%$ fractional deformation we find highly directional emission and an enhancement of the maximum emitted power by three orders of magnitude compared to circular resonators, but the dominant lasing modes are *not* of of the WG type. Instead, at $\sim 10\%$ to 12% deformation a crossover takes place from WG modes to bowtie-shaped bifurcations of the diametral "bouncing-ball" orbit, cf. Fig. 2. These orbits partially violate the total-internal-reflection condition but acquire higher reflectivity at higher deformation, until according to Fresnel's formula their lifetime in fact becomes long enough for lasing. This is substantiated by (1) excellent agreement of the laser mode spacings with semiclassical expectations, (2) a *decrease* of the laser threshold versus deformation above $\sim 12\%$, and (3) good agreement with numerically calculated intensity patterns.

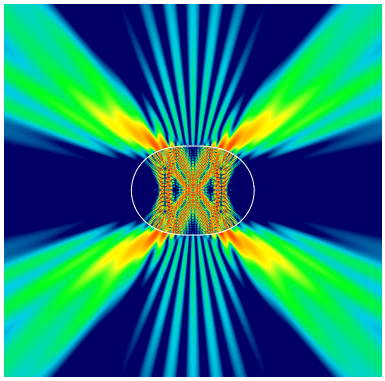

Figure 2: Bowtie mode in the 15% deformed "rounded-stadium" shaped microlaser.

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The transition from deterministic chaos to stochastic dynamics

Eckehard Olbrich

Although the first euphoria about explaining all kinds of observed irregular behaviour in time by deterministic chaos faded away, there is still a big interest in revealing the connections between chaos and randomness. While it is now a widespread belief that for a meaningful description of the most observed irregular time series from field measurements randomness is an irreducible ingredient, one can still ask for the origin of this randomness, at least if one believes in deterministic laws of nature. The most commonly known way to achieve stochastic output from a deterministic system in physics, is to increase the dimension to infinity. This is very intuitive: If the observed signal is composed of infinitely many degrees of freedom it becomes indistinguishable from a stochastic one. In this route to randomness essentially no nonlinearity and no chaos are involved.

But there is another route which is in some sense the counterpart to the route described above. If we parametrise deterministic dynamical systems by their dimension D (e.g. the dimension of the natural invariant measure) and their Kolmogorov-Sinai (KS) entropy h, which is a measure of their predictability, the case described above corresponds to $D \to \infty$ while $h = 0$. But also the limit $D = const$ and $h \to \infty$ produces dynamical systems whose output is indistinguishable from that of a stochastic one. The random number generators used mostly in computers can be related to this route of generating randomness. In some sense this is also not surprising, because the entropy h measures the predictability of the system, thus the system becomes unpredictable which is basically the indication of randomness.

From the point of view of time series analysis a contradiction still remains, namely: how do we usually identify the deterministic origin of a time series? We show that the points of the reconstructed attractor are restricted to a low dimensional manifold. However, if also a low-dimensional system can produce stochastic output in some limit, it seems not enough to show that a signal is low-dimensional to infer its deterministic origin.

To resolve this paradox we studied the so called dynamical systems of Langevin type (for a broad and detailed discussion see [1]), recently introduced in [2], which converge in an appropriate scaling limit to stochastic dynamics governed by a Langevin equation. The most comprehensively studied system of this type has the form

$$\begin{aligned} x_{n+1} &= T(x_n) \\ y_{n+1} &= \lambda y_n + \nu x_n \end{aligned} \tag{1}$$

with $\lambda = e^{-\gamma\tau}$ and $\nu = \sqrt{\tau}$. It is related to the solution of the ODE

$$\dot{Y} = -\gamma Y + L_\tau(t) \quad \text{with} \quad L_\tau(t) = \sqrt{\tau}\sum_n \delta(t - n\tau)x_n \tag{2}$$

by

$$Y(t) = e^{-\gamma(t-n\tau)}y_n \qquad n\tau \le t < (n+1)\tau\ . \tag{3}$$

Observing the process $Y(t)$ at a constant sampling rate Δt in the limit $\tau \to 0$ the observed process converges to a Langevin process, if the dynamics T of the x variable is sufficiently chaotic (strong mixing is a sufficient condition, see [2]). Let us choose

$$T(x) = 1 - 2x^2 \ . \tag{4}$$

The entropy h of the system (1) is equal to the entropy of T: $h = \ln 2$. In the $(\tau \to 0)$-limit [2] Eq.(1) generates an Ornstein-Uhlenbeck process for $\gamma > 0$ (i.e. $\lambda(\tau) = e^{-\gamma\tau}$, $\langle y^2 \rangle = \frac{1}{2\gamma}\langle x^2 \rangle = \frac{1}{4\gamma}$) and a Wiener process for $\gamma = 0$ ($\lambda(\tau) = \lambda = 1$, unbounded variance). The limit $\tau \to 0$ has to be performed in the following way: We have to observe $Y(t)$ with a constant sampling rate Δt but taking τ to zero. This means that we select t such that $Y(t) = y_n$. Taking into account Eq.(3) we choose Δt such that $Y(t + \Delta t) = y_{n+j}$ with $j = \Delta t/\tau$. Thus in the limit $\tau \to 0$ we have to enlarge the delay j for the delay embedding in such a way that

$$\Delta t = j\tau = const \ . \tag{5}$$

Thus, if we reconstruct the dynamics by delay embedding from a scalar measurement of $Y(t)$, observed with a sampling rate $\Delta = j\tau$, the reconstructed dynamics has the dimension $D = 2$ and the entropy $h = j \ln 2$. At first we studied what happens with the low dynamical manifold to which the dynamics is constrained in the limit $j \to \infty$. To allow the visualisation of the transition we chose a projection which led to a one dimensional constraint. First of all, Fig. 1 illustrates nicely the transition from a complicated, highly although nonlinearly correlated distribution of the increments towards a Gaussian shaped one, including the assymetries discussed in [3]. Second, we get an intuitive understanding of how the determinstc properties disappear: The 1-D graph representing the deterministic structure becomes the more complicated the larger the time lag j, so that it becomes increasingly difficult to resolve it. Thus we have a first solution of the paradox: The increase of the entropy causes stronger and stronger folding of the still low dimensional manifold, which disables us to resolve the low-dimensionality with a finite amount of data.
For a more quantitative analysis of this phenomenon we computed the correlation entropies h_m (see e.g. [4]), which can be used as an approximation for the KS-entropy of the system. The most relevant property of these entropies in this context is that they are independent of the resolution ϵ for a deterministic system, if the resolution is fine enough and the embedding dimension larger than the dimension of the attractor. For a stochastic system the asymptotic behaviour of these entropies can be estimated by using the continous entropies (cmp. e.g. [5]).

Fig. 2 shows the numerically computed correlation entropies h_m of the deterministic process $Y(t)$ from Eq. (3) with different τ, but $\Delta t = j\tau = 1$ remaining constant, compared with the entropies of the limiting stochastic process. We can identify a critical length scale where the determinism becomes visible, that is $h_m \approx const$ for $m > D$. This length scale becomes the smaller the larger j resp. the smaller τ. The convergence of the deterministic process to the stochastic one can be seen on the length scales larger than this critical one. For $j = 10$ there is no difference cognisable in the present calculation (we used 10^6 points), the deterministic region remains unresolved. On these length scales, the numerical results for the deterministic process are in excellent agreement with the differential entropies of the Ornstein-Uhlenbeck process, thus showing

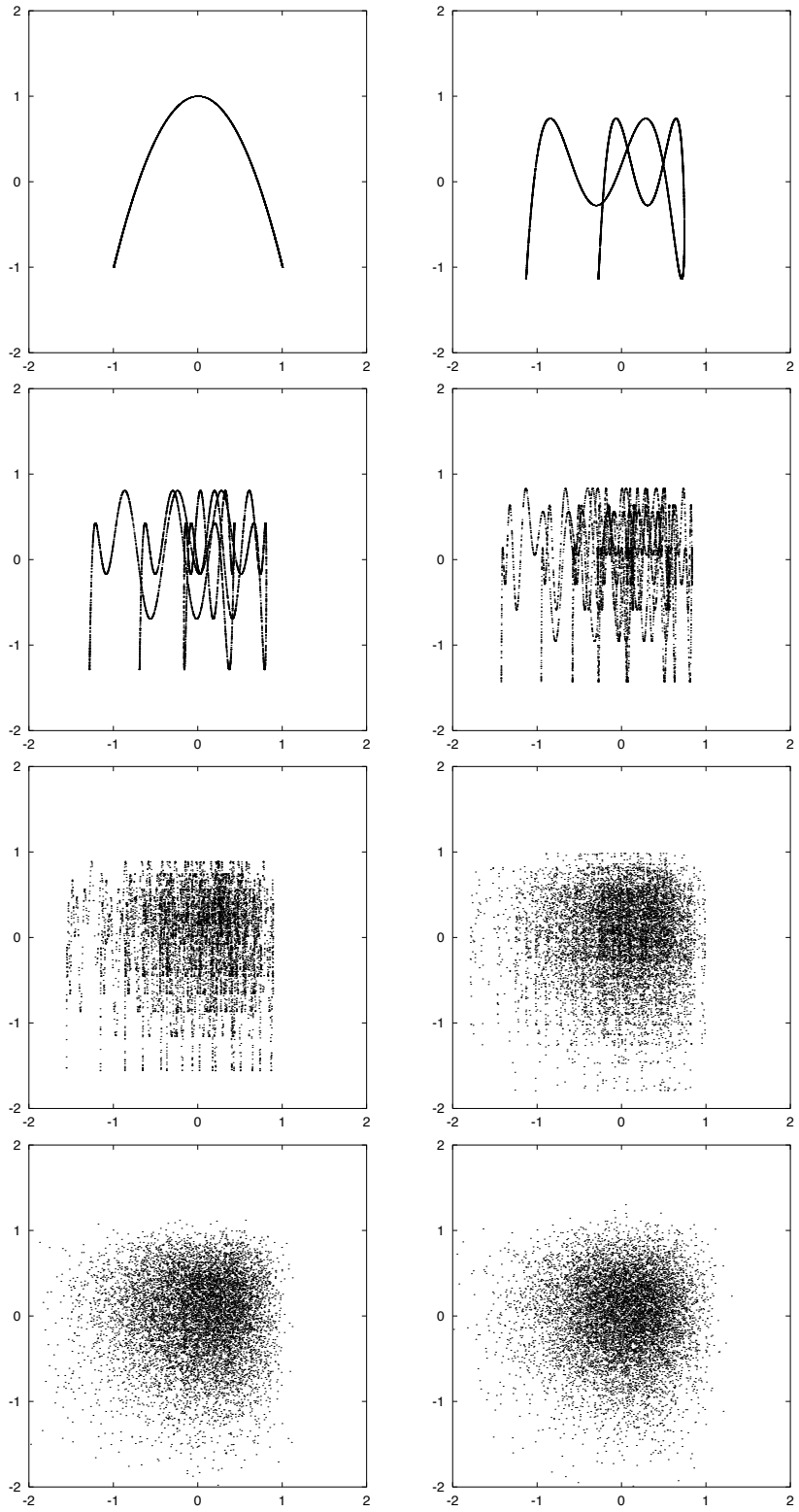

Figure 1: The graphs of the nonlinear constraints in a suitable projection, $y_{n+2j} - \lambda^j y_{n+j}$ vs. $y_{n+j} - \lambda^j y_n$ for $j = 1$ to 5, 7, 10 and 20. $\gamma = 0.1$ $j\tau = 1$.

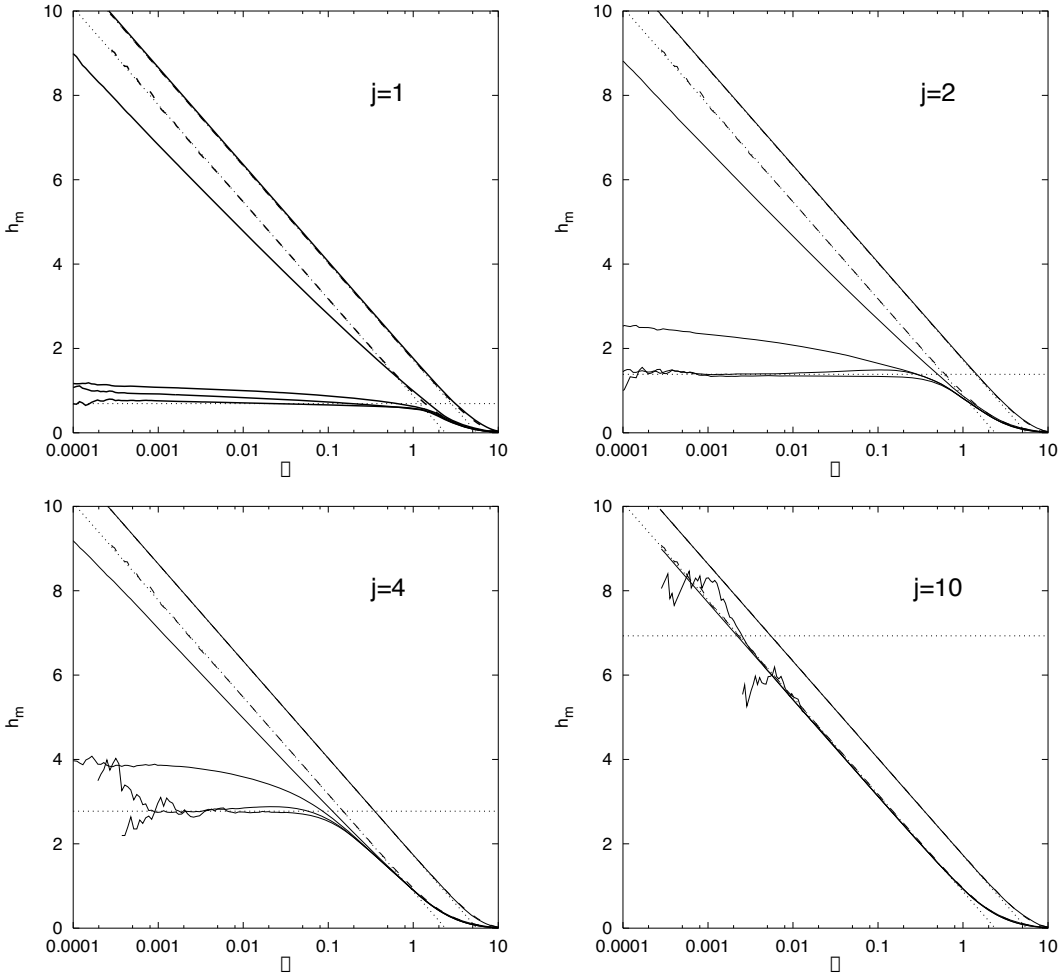

Figure 2: The differential correlation entropies h_m for m=0,1,2,3,4 as a function of ϵ for j=1,2,4,10; $j\tau$=1 (solid lines), and for the Ornstein-Uhlenbeck process (dashed), $\gamma = 0.1$. The dotted lines indicate the asymptotic behaviour of $h_0(\epsilon)$ and $h_1(\epsilon)$ for the Ornstein-Uhlenbeck process and the KS-entropy of the deterministic map.

that the correct stochastic properties are already present although on the small scales the deterministic properties are still visible. A rough estimation of the critical length scale, actually an upper bound, can be achieved by calculating the intersection point of the asymptotic behaviour of the conditional entropies of the stochastic process with that of the deterministic process $h_m \approx h = j \ln 2$. Thus we get for the critical length scale ϵ_c

$$\epsilon_c = \sqrt{\frac{\pi}{\gamma}(1 - e^{-2\gamma\Delta t})}\, e^{-j \ln 2} \; . \tag{6}$$

In the limit $h \to \infty$ this critical length scale will go to zero and therefore the signal will be indistinguishable from a stochastic one for all finite resolutions.

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Interactions and Collective Behaviour of Coherent Structures in Reaction-Diffusion Systems

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Spontaneous pattern formation has been observed in many physical, chemical and biological systems far from thermodynamic equilibrium. These systems often belong to the class of excitable media, where propagating pulses can be generated by exciting the medium with a sufficiently large local perturbation. In chemical systems, such excitations corresponding to concentration waves are often observed in catalytic reactions in solutions or on surfaces. In biology, two important examples are the propagation of electrical impulses in neurons and in the heart and aggregation processes of cells in colonies of amoebae. The latter is sometimes controlled by waves of chemical messenger substances which spread in the form of rotating spirals. In both cases, coherent structures - solitary pulses resp. spiral waves - transmit information. Here, the investigation of interactions between such coherent structures is reported. This study contributes to the understanding of complex patterns, which consist of ensembles of such dynamic, coherent structures (pulse trains resp. arrays of spiral waves). In particular, we present results concerning the interaction of pulses for a model excitable medium and study rotating spirals in a model of cell aggregation of the slime mold *Dictyostelium Discoideum.*

Excitable processes are well modelled by reaction diffusion equations. They consist of coupled, nonlinear partial differential equations, which describe the dynamics of continuous variables and which usually cannot be solved analytically. These variables are identified with concentrations in chemical reactions or densities of cells in aggregation processes. Many of these pattern-forming systems are of activator-inhibitor type, where spatiotemporal dynamics results from the interaction between a fast autocatalytic and diffusing substance, the activator, and a slow reacting inhibitor species.

The interaction of pulses and the resulting pulse dynamics were investigated in the case of a simple two-variable activator-inhibitor model for a chemical reaction in a one-dimensional ring (periodic boundary conditions)

$$\begin{aligned} \partial_t u &= \frac{1}{\epsilon} u(1-u)(u - \frac{b+v}{a}) + \partial_x^2 u, \\ \partial_t v &= f(u) - v, \end{aligned} \tag{1}$$

where $f(u)$ is a cubic function. The medium in a rest state, which is stable against small perturbations, until a pulse is excited. After passage of this pulse, a recovery time ("refractory phase") follows, in which the medium cannot easily excited be again. Because of this refractory phase, the velocity of a pulse decreases with the distance to its predecessor. Consequently, the velocity of a wavetrain decreases with the wavelength (normal dispersion). However, in new experiments concerning the catalytic reaction of CO and NO on a Pt-surface [1], the inverse behaviour has been found: Pulses get faster with decreasing distance (anomalous dispersion). As a consequence pulses can merge, annihilate each other or they can form stable bound pairs. Note, that for a

pair of pulses, anomalous (normal) dispersion corresponds to an attractive (repulsive) interaction.

To study interactions of pulses on a ring, reduced dynamics can be established. Here, only the influence of the interactions on the velocity of each involved pulse is considered. The interactions are determined by numerically computing the dispersion curve $c(d)$. The reduced dynamical equations can be derived asymptotically from perturbation theory assuming large interpulse distances [2]. Alternatively, one can use kinematical theory based on the knowledge of the dispersion curve $c(d)$. Equations for the positions $p_1, p_2 > p_1$ of a pair pulses read

$$\dot{p_1} = c(d_1), \tag{2}$$

$$\dot{p_2} = c(d_2) = c(L - d_1), \tag{3}$$

where $d_1 = p_2 - p_1$. In the case of a pair of pulses moving with equal speed and distances $d_1 = d_2$ on a ring, we transform the equations to a co-moving frame. Therein, a family of steady state solutions p_1^0, p_2^0 exists. Linearization of the reduced dynamics then yields the following evolution equations for perturbations δp_i of the steady state pulse positions $p_1 \circ, p_2 \circ$:

$$\dot{\delta p_1} = c'(d_1) \cdot (\delta \mathrm{p}_2 - \delta \mathrm{p}_1), \tag{4}$$

$$\dot{\delta p_2} = c'(d_2) \cdot (\delta \mathrm{p}_1 - \delta \mathrm{p}_2). \tag{5}$$

This leads to the eigenvalues

$$\lambda_1 = 0 \quad \text{and} \quad \lambda_2 = -(c'(d_1) + c'(d_2)) \tag{6}$$

with the respective eigenvectors

$$\vec{e}_1 = \begin{pmatrix} 1 \\ 1 \end{pmatrix} \quad \text{and} \quad \vec{e}_2 = \begin{pmatrix} -\frac{c'(d_1)}{c'(d_2)} \\ 1 \end{pmatrix}. \tag{7}$$

The eigenvector $\vec{e}_1$ corresponds to a shift of both pulses in the same direction. Due to the translational invariance of the system, the eigenvalue $\lambda_1 = 0$ equals here. The eigenvector $\vec{e}_2$ corresponds to a relative shift of pulse positions and thus yields a change in the interpulse distance. Thus, it is termed the "interaction" eigenvector with the "interaction" eigenvalue λ_2. The sign of λ_2 is given by the sum of the slopes of the dispersion curve at d_1 and d_2. For an equidistant pulse pair ($d_1 = d_2$), a negative (positive) slope yields instability (stability) against such a shift. A new branch of solutions with $d_1 \neq d_2$ (non-equidistant pair) can be easily obtained from the reduced pulse dynamics, if the dispersion curve is non-monotonous. Then, a given speed c corresponds to two or more distances d_i. To check the quality of the reduced equations, we computed interaction and -functions explicitly by numerical stability analysis.

Fig. 1 shows results of equidistant and nonequidistant pairs of traveling pulses in Eqns. (1) in the case of anomalous dispersion. The equidistant pulse pair (dashed red line in Fig. 1 (A)) is unstable and gets destroyed by pulse attraction. The new stable solution is given by the non-equidistant pulse pair (solid black line in Fig. 1 (A)).

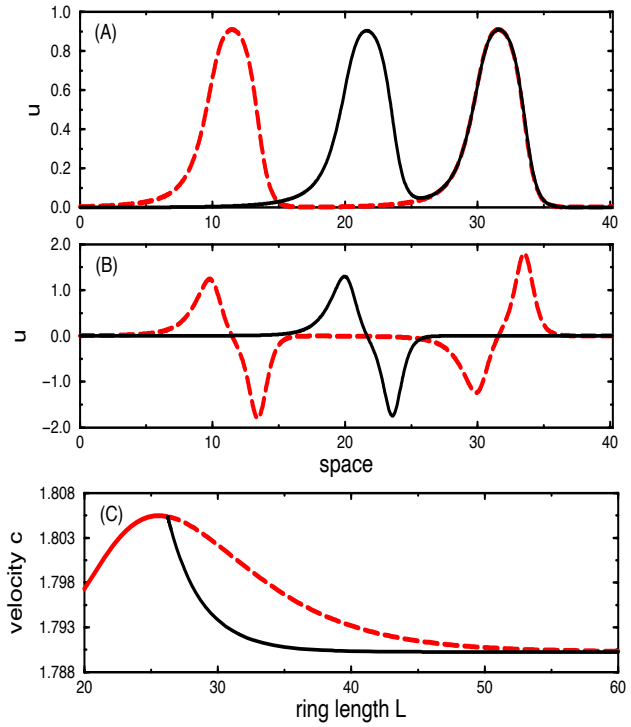

Figure 1: (A): Pair of pulses on a ring of length L. The solution with the pulse distance L/2 is unstable (red line). The black line shows a bound pair with a distance considerably smaller than L/2. (B): The interaction eigenmodes corresponding to the solutions in diagram (A). The black mode belongs to a negative and the red one to a positive eigenvalue. (C): The red curve corresponds to a branch of equidistant pulse pairs in a ring with length L, where the solid (dashed) line symbolizes stability (instability). It gives also the dispersion curve for pulse trains with pulse distance L/2. The black curve represents stable, non-equidistant pulse pair solutions.

Fig. 1 (B) shows the $u-$components of the leading eigenmodes, where the red dashed curve represents the only mode with a positive eigenvalue λ_2 in the equidistant pair. Its antisymmetric shape corresponds to the eigenvector $\vec{e}_2$ of the reduced dynamics. The eigenfunction corresponding to $\vec{e}_2$ of the non-equidistant pulse pair (solid black curve in Fig. 1 (B)), on the other hand, has a negative eigenvalue and thus stabilizes the pulse pair. The destabilization near the maximum of the dispersion curve (red curve in Fig. 1 (C)), and the bifurcation of a non-equidistant pulse pair have been confirmed. The new branch is shown as solid black line. Fig. 2 shows a comparison of the eigenvalues (6) gained from reduced dynamics and the leading eigenvalues from numerical stability analysis. While the results show reasonable agreement in the case of the equidistant pulse pair, the prediction for the nonequidistant pairs are less satisfying. Thus, numerical stability analysis is essential to compute the stability of bound pairs.

under variation of the ring length The dispersion curve (red curve in Fig. 1 (C)) shows a transition from normal dispersion with a positive slope (red solid line) to anomalous dispersion with a negative slope (red dashed line). In the range of anomalous dispersion, a second branch of stable solutions corresponding to non-equidistant pulse

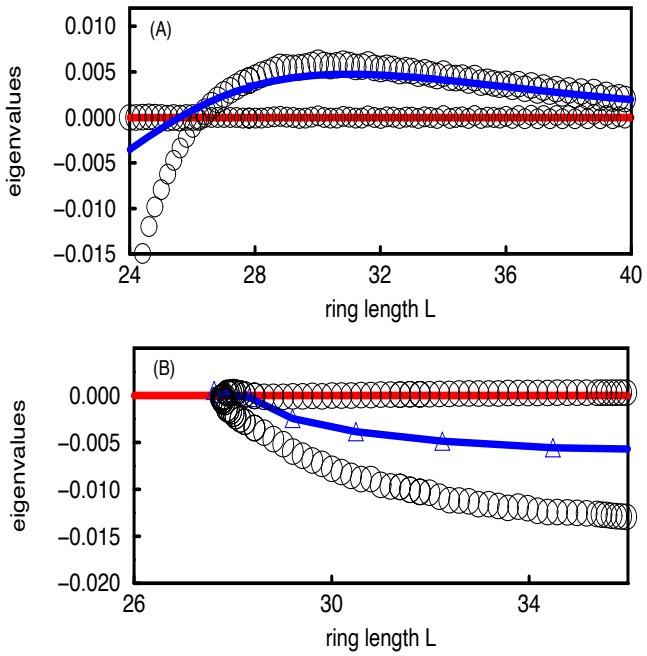

Figure 2: Comparison of the eigenvalues (4) of the reduced dynamics (blue and red lines) with results of numerical stability analysis (circles) for the case of equidistant (A) and non-equidistant (B) uniformly moving pulse pairs.

configurations exists (black curve in Fig. 1 (C)). In the case of very long systems, this branch represents a bound pair of pulses. Thus, bound pairs can be traced back to a pitchfork bifurcation near an extremum of the dispersion curve at finite wavelength. With the same methods bound states of three or more pulses have been calculated and their stability in dependence of the system parameters has been determined. Calculations with a more complicated and realistic model of the NO and CO reaction provide a qualitatively similar dispersion curve. There, pulses do not form bound states. Instead one of the pulses disappears as soon as it gets too close to the other one in agreement with laboratory experiments[1].

Rotating spirals are typical patterns in two dimensional excitable media. The aggregation process of the slime mold *Dictyostelium discoideum* is a widely discussed example for pattern formation in biological systems. The cells of a population of *Dictyostelium discoideum* spread on a substrate poor in nutrient and communicate by waves of cyclic adenosinmonophosphate (cAMP). This periodic stimulation with cAMP causes the cells to aggregate in the center of the pattern. At the same time, genes typical for the aggregation state are expressed. The wave patterns are expanding concentric rings, called target patterns. The target patterns break up and the free wave ends form spirals. The spirals compete for space and only a few governing a large area survive. Experiments show that the development of the pattern depends on the state of the aggregation process. The development of the pattern described before starts anew, if the pattern is extinguished by spraying of cAMP in an early state of aggregation.

Only target pattern arise, if the pattern is reset in a late state of aggregation. The target patterns do not break and hence spirals do not appear. These findings suggest that the development of the pattern could be determined by the development of the cells by expression of aggregation state genes. Furthermore, inhomogeneities of the cell density cannot be the reason for the break up of the target patterns, because they become stronger during aggregation. In cooperation with H. Levine, University of California San Diego, we generalized the Martiel Goldbeter model for wave propagation in *Dictyostelium discoideum* populations to include gene expression. That was done according to the aggregation gene network given in [4].

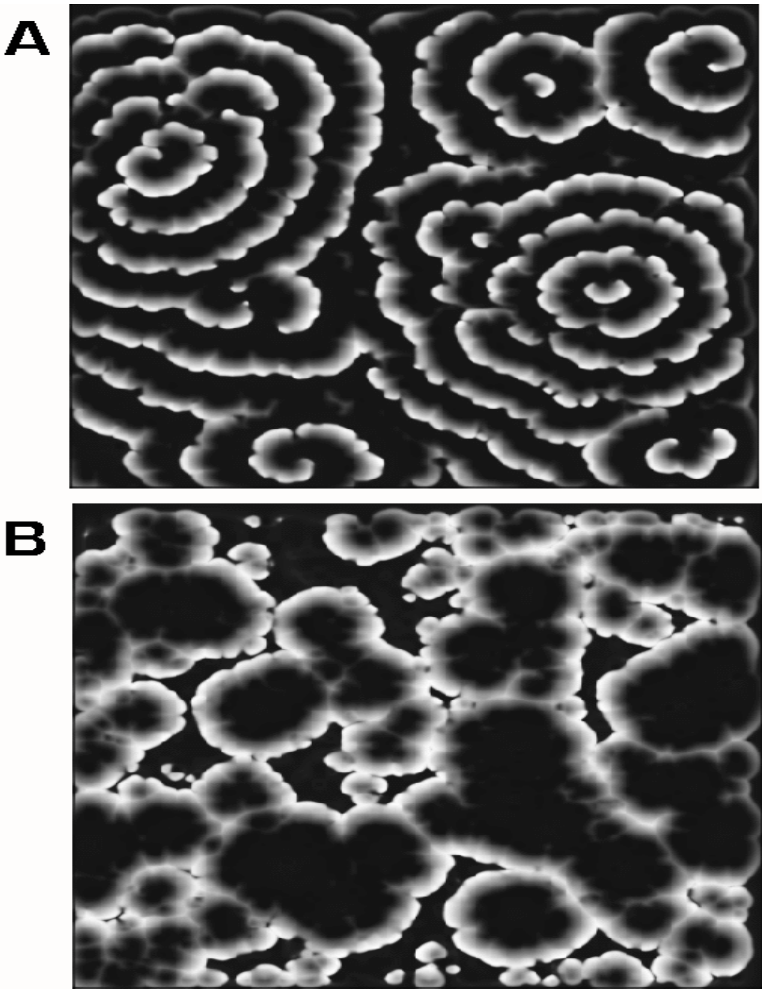

Figure 3: Simulation of the resetting experiment with *Dictyostelium discoideum*. Extinction of the patterns 2h after the onset of aggregation leads to re-appearance of spirals (A). Patterns fromed after an extinction 4h after onset of aggregation do not form spirals (B). Shown is the concentration of extracellular cAMP. Patterns were extinguished by setting the concentration of extracellular cAMP to a value ten times the typical value during pattern formation.

The generalized model reproduces the development of the patterns found in the experiments and suggests a simple explanation. Little developed cells are not able to relay the pulse of cAMP. They break up the target patterns. The following pattern competition turns out to be a consequence of the dependence of gene expression on the stimulation with cAMP. Areas already well developed have a higher pattern frequency

and hence a higher frequency of stimulation of the cells with cAMP. Therefore they develop even faster and conquer more space. Simulations of the resetting experiments reproduce the experimental findings. Target patterns do not break after extinction in a later state of aggregation because all cells are relay competent by then [5].

We presented two examples of interactions of coherent spatiotemporal structures. The application of bifurcation analysis to partial differential equations provides insight into the interaction of one- dimensional pulses and its consequences. The mathematical modelling of the gene expression during aggregation of *Dictyostelium discoideum* proved that simulations are a valuable tool of testing biological hypotheses.

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Different scales in disordered cellular structures - binary and fractal tessellations

G. Schliecker and H. Hinrichsen

Random cellular structures are often encountered in nature, as, for example in biological tissues, metallurgical aggregates and soap froths. Structurally, they are tessellations of space by cells, which are polygons in two dimensions. In addition to the naturally observed examples, the Voronoi construction, a generalization of the Wigner-Seitz construction, allows to generate such tessellations from sets of arbitrarily distributed points named generators: Each of the generators is assigned to a cell containing all points which are closest to it. Examples of generator sets may be randomly (Poissonian) distributed points or the centers of disordered arangements of discs in the plane. In most of the structures aforementioned, disorder and randomness are the rule rather than the exception.
Despite the fact that the molding forces are completely different, a huge variety of planar tessellations show a surprising similarity [1]. The cell shape distribution is denoted as $\{p_k\}$ where p_k is the probability that a randomly chosen cell has k sides (neighbours). In most natural structures, $\{p_k\}$ is a narrow distribution peaked at $k=6$, the average number of sides of the cells. Its shape is mainly characterized by its width, which can be interpreted as a measure of randomness. Correlations between neighbouring cells are often described by the quantity $km(k)$, the average total number of sides of the neighbours of a k-sided cell. Aboav's law [2] states that this quantity varies linearly in k – which is not obvious at all, but observed in most natural structures. The simplest quantity describing the correlations between shape and size of the cells is $\langle A\rangle_k$, the average area of an arbitrarily chosen k-sided cell. As pointed out first by Lewis [3], $\langle A\rangle_k$ usually increases linearly with k. Deviations from Lewis' law so far have been restricted to cells with only few neighbours whereas for large k the linear law appeared to be asymptotically valid. These laws have been confirmed in detailed experimental studies of the Voronoi-tessellations of mono-size disc arrangements on an air table at various densities [4]. So far, all these structures are characterized by one typical scale, mainly the mean size of a cell. The question arises, how the universal properties are affected in tessellations, in which a unique typical scale does not exist.

The tessellations of arrangements of discs with *two different sizes* offer an excellent example for cellular structures with two typical scales. Experimental studies show that not only the metrical, but as well the topological properties of the corresponding tessellations change drastically. At high packing fraction, one observes bimodal cell shape distributions, and $km(k)$ for the whole tessellation is no longer linear. The experimental results imply that Aboav's law holds instead for the neighbours of each species separately. As a consequence of the different length scales, Lewis' law does not hold. These effects are less pronounced when the density is reduced, and for vanishing density the patterns of the two species become indistinguishable [5].
Formulating a theoretical model for these structures, the elementary processes by which the structures are successively modified, have to be identified. The evolution in time

is governed by the rules under which these processes occur. In two-dimensional systems of moving discs, the neighbour-switching is the dominant process. As shown in Fig. 1, the cells containing the black discs share one side in the left configuration, but not in their displaced positions on the right. It turns out that the possibility for such processes is restricted.

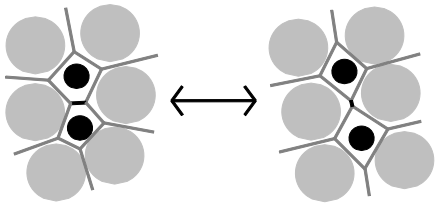

Figure 1: Neighbour switching in a binary packing of discs.

In fact, the topological properties of mono-size disc assemblies on the air table are very similar to those of a simple topological model for random tessellations [6]. The solution of this model coincides with the statistical equilibrium properties of dynamical networks represented in Fig. 2a, in which the neighbour-switching is restricted to the dashed edges.

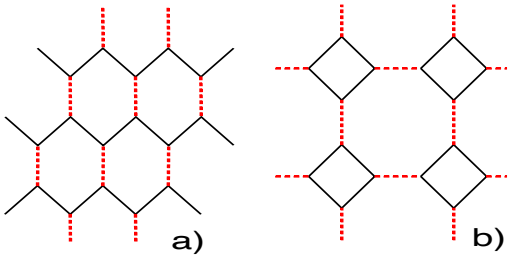

Figure 2: Ordered structures of the topological model for simple (a) and binary (b) random tessellations.

The probability for the flip of a randomly chosen dynamical edge is weighted with p if it is in the position of Fig. 2a and with $1-p$ for the reverse process. A comparision between the properties of this model and the experiment allows the interpretation of the parameter $w = |1-2p|$ as a measure of the packing fraction. Moreover, applying the same dynamical rules to the binary structure in Fig. 2b, the experimentally observed changes of the topological properties are reproduced: one obtains bimodal cell shape distributions, whereas Aboav's law for the correlations between neighbouring cells holds for each species separately. The binary character of the tessellation is reduced with increasing disorder [7]. The metrical properties of binary cellular structures cannot be studied by means of this topological model. The topological quantities of various *fractal* structures show an algebraic behaviour [8]. Less is known about the relation between topological and metrical properties in scale-invariant mosaics. For this purpose Voronoi tessellations of intermittent particle distributions with algebraic long-range correlations that are generated by planar stochastic point processes are studied numerically [9]. As an example point distributions generated by a directed percolation process in 2+1 dimensions [10, 11] are considered. In directed percolation – interpreted as a time-dependent stochastic process – particles on a lattice either produce an offspring or self-destruct. Depending on the rates of offspring production and self-destruction the process exhibits a phase transition from a fluctuating active phase into an absorbing state. Directed bond percolation [10] is controlled by a single parameter, namely the percolation probability p. Below a critical threshold $p < p_c$ the system approaches the absorbing state in exponentially short time whereas for $p > p_c$ a fluctuating stationary state exists on the infinite lattice. Close to criticality such a stationary process evolves through configurations that are characterized by spatially intermittent patterns with long range correlations [12]. The Voronoi construction is applied to spatial configurations (snapshots) of active particles generated by an almost critical stationary directed bond percolation process.

As shown in Fig. 3, such a tessellation appears to be very different from ordinary cellular structures. The reason is that the generators approximate a fractal set, apart from lower and upper cutoffs due to system size and lattice spacing. In contrast to natural cellular structures their Voronoi tessellations are expected to be invariant under rescaling.

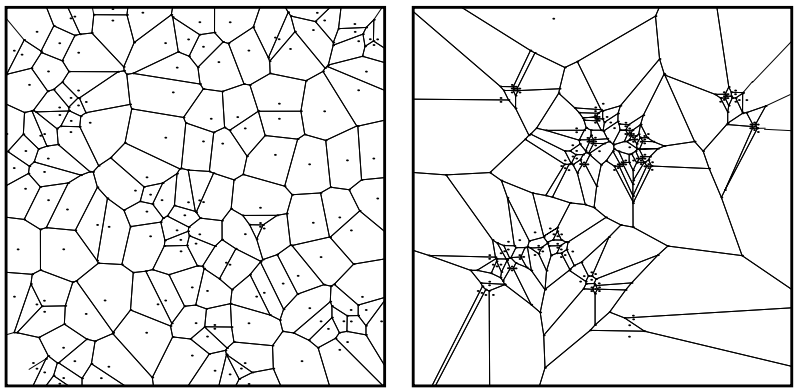

Figure 3: Voronoi tessellations for a Poissonian distribution of points (left) and for a point set generated by an almost critical directed percolation process (right).

Consequently, the curve for the normalized average area of k-sided cells, $\langle A\rangle_k/\langle A\rangle$, shows an untypical behaviour as it increases significantly faster than in cellular structures without scale invariance (see Fig. 4). It neither resembles Lewis' law nor a quadratic behaviour that has been discussed in the context of a perimeter law for metallurgical grain structures. In fact, it turns out that $\langle A\rangle_k/\langle A\rangle$ increases algebraically.

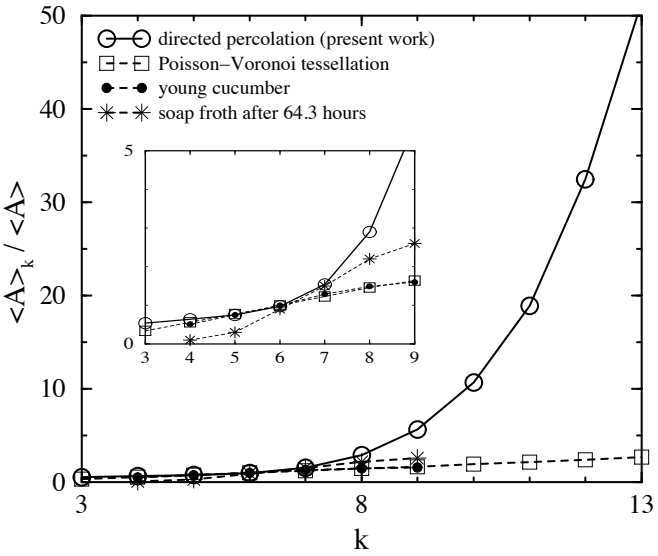

Figure 4: Normalized average area of k-sided cells in comparison with various ordinary structures. The inset shows a magnification for small values.

The cell topology, i.e., the number of neighbours, k, can be regarded as an additional quantity for the description of a directed percolation process in more than one spatial dimension. In order to find an appropriate scaling relation, we conjecture that the cell topology exhibits scaling properties similar to those of distances and densities. This means that the corresponding scaling regime is restricted to $k < \kappa$, where κ diverges close to the transition as $\kappa \sim (p - p_c)^{-\tau}$. Here κ limits the scaling regime of edge numbers similarly as the spatial correlation length $\xi_\perp$ limits the scaling regime of distances in the active phase. In the scaling regime we therefore expect the probability distribution $P(k, A)$ for cells with topology k and area A to obey the scaling form

$$P(k, A) \sim A^{2+(\tau-\beta)/d\nu_\perp}\, \Phi(kA^{-\tau/d\nu_\perp}), \qquad (k < \kappa, A < \xi_\perp^2) \tag{1}$$

where $\Phi(z)$ is a universal scaling function, and β and $\nu_\perp$ are the scaling exponents of the stationary particle intensity and the spatial correlation length. In order to verify

this scaling relation, the exponent τ is estimated numerically by data collapse. Our best estimate is $\tau = 0.20(4)$. This result should not depend on the specific choice of the dynamics (e.g., bond or site percolation). Rather we expect τ to be a universal exponent characterizing the directed percolation universality class in $2+1$ dimensions.

To summarize, tessellations without a unique typical scale are charcterized by topological and metrical properties that are significantly different from those of most natural cellular structures. The Voronoi construction and its generalizations offer further insight into the structures of disordered systems. These tools of stochastic geometry may also facilitate the characterization of irregular patterns in dissipative systems, as e. g. defect patterns in electroconvection in liquid cristals and spiral defect chaos in chemical reactions.

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Analysing time delay feedback systems from scalar measurements

Rainer Hegger

One of the biggest challenges in nonlinear time series analysis is the exploration of high dimensional chaos. The reason why this is rather difficult is related to the problem of reconstruction of state spaces from scalar data. It can be shown that the lengths of the time series needed grow exponentially with the product of the dimension of the chaotic attractor and the system's entropy [1]. This requirement sets a limit due to experimental possibilities as well as to numerical ones. One important class of high dimensional systems is that of spatially extended systems given by partial differential equations. Their phase spaces are infinite dimensional and therefore the dimensions of the attractors are not restricted at all. Another class with similar properties is that of time delay feedback systems, which is believed to be ubiquitous e.g. in physical and biological systems. In the following we discuss equations of motion of the form

$$\dot{\vec{x}}(t) = \vec{f}(\vec{x}(t), x^l(t-\tau_0)) \qquad \vec{x} \in \mathbf{R}^d \;, \tag{1}$$

where the l-th component is fed back with a time delay τ_0. Due to this fact the phase space is the direct product of $\mathbf{R}^d$ with the space of all differentiable functions from the interval $[-\tau_0, 0]$ to $\mathbf{R}$ and is thus infinite dimensional.

Besides the practical problem that the attractor can be very high dimensional, there is the theoretical problem that the system is non autonomous, in the sense that it is nonlocal in time. This makes a straightforward application of the embedding theorems [2, 3] impossible. Recently we proposed a method which overcomes both problems [4]. If we describe the system with vectors formed with the $2d+1$ coordinates

$$(\dot{\vec{x}}(t), \vec{x}(t), x^l(t-\tau_0)) \;, \tag{2}$$

Eq. (1) defines d contraints. This means that these vectors are always restricted to a $(d+1)$–dimensional manifold $\mathcal{M}$. This property is independent of the dimension of the attractor. If we could reconstruct this manifold, we were able to investigate the system in a rather low dimensional space. In a typical experiment, only a single observable is recorded as a function of time. In such a case, we first have to reconstruct the vectors in Eq. (2). To do this we make use of the ideas of Casdagli [5] for so called input–output systems. He treated systems of the form

$$\vec{x}_{n+1} = \vec{f}(\vec{x}_n, \epsilon_n) \tag{3}$$

where ϵ_n is an arbitrary input. He argues that a simultaneous measurement of one component x_n^i and ϵ_n makes it again possible to reconstruct the non observed components of $\vec{x}$. We use this property in the following way:
Let $\{y_n\}_{n=1}^N$ be the measured time series. Suppose the y_n are the $x^l(t_0 + n\Delta t)$ from Eq. (1) or an invertible function of it. This means that we have access to both, a

system's actual state and the input variable, which is the delayed observation. We construct $(2m)$–dimensional delay vectors of the form

$$\vec{v}_n(\tau_0) = \left(y_n, y_{n-1}, \ldots, y_{n-m+1}, y_{n-\tau_0}, \ldots, y_{n-\tau_0-m+1}\right) \ , \tag{4}$$

where we assume that the delay time τ_0 is an integer multiple of the sampling time Δt. If $m > 2d$ this provides a diffeomorphic representation $\tilde{\mathcal{M}}$ of $\mathcal{M}$ and with $\hat{\dot{y}}_n$ being an estimate of $\dot{y}$ we can model $\tilde{\mathcal{M}}$ through

$$\hat{\dot{y}}_n = g(\vec{v}_n(\tau)) \ . \tag{5}$$

Usually we do neither know g nor τ_0. Both can be determined simultaneously, choosing an ansatz $\tilde{g}_{\vec{p}}$ for g and using a likelihood scheme for estimating the parameters $\vec{p}$ and τ_0.

Once we know g and τ_0 we can study the properties of the system. For example, we can calculate the first $k = \tau_0/\Delta t$ Lyapunov exponents [6].

Let $\vec{z}_n = (y_n, \ldots, y_{n-\tau_0-m+1})$ be $(k+m)$–dimensional delay vectors. With them we can write the Jacobian of the system as

$$J_{ij} = \left(\frac{\partial \vec{z}_{n+1}}{\partial \vec{z}_n}\right)_{ij} = \begin{cases} \frac{dy_{n+1}}{dz_j} & : \quad i = 1 \\ \delta_{i(j+1)} & : \quad i \neq 1 \end{cases} \tag{6}$$

to iterate the dynamics in tangent space. This gives the first Lyapunov exponents.

To test the methods we used a two dimensional model derived from the Mackey–Glass equation. It is given by

$$\begin{aligned} \dot{x_1}(t) &= \frac{a x_1(t-\tau_0)}{1 + x_1^{10}(t-\tau_0)} + x_2(t) \\ \dot{x_2}(t) &= -\omega^2 x_1(t) - \rho x_2(t) \ , \end{aligned} \tag{7}$$

In Fig. 1 we show the two dimensional delay embedding of the time series data obtained from the original attractor (left plot) and of the one (right plot) obtained from an integration of the fitted Eq.(5). One sees a very good agreement. Fig. 2 shows the estimate of the first 10 Lyapunov exponents. Also there the results of the model match the exact results extremely well.

The application of the above described methods to experimental systems is in progress. There is a close collaboration between our group and the group of Prof. F.T. Arecchi from the *Istituto Nazionale die Ottica* in Florence, where a CO_2 laser experiment with time delayed feedback is operated.

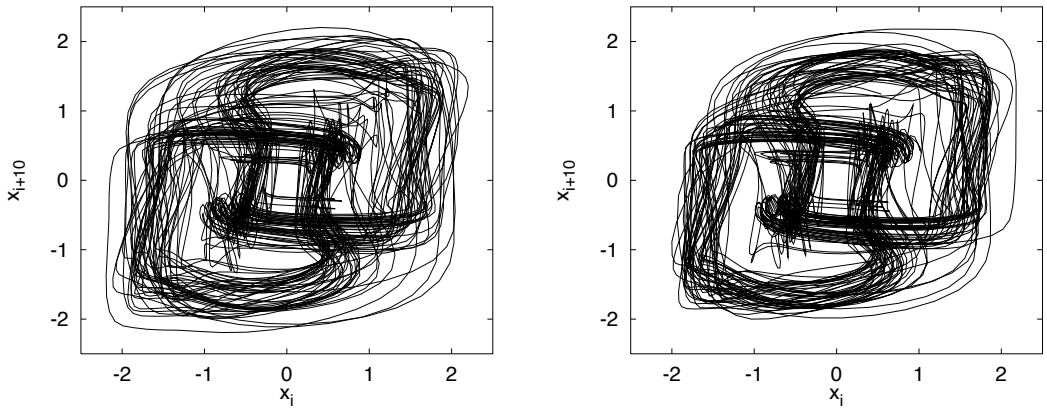

Figure 1: Two dimensional projection of the original attractor (left plot) and the modelled one (right plot). The parameters of Eq. (7) were: $a = 3$, $\omega^2 = 2$, $\rho = 1.5$ and $\tau_0 = 5$. The embedding was done with $m = 2$, which is considerably smaller than even the Kaplan–Yorke dimension which turns out to be ≈ 6.5.

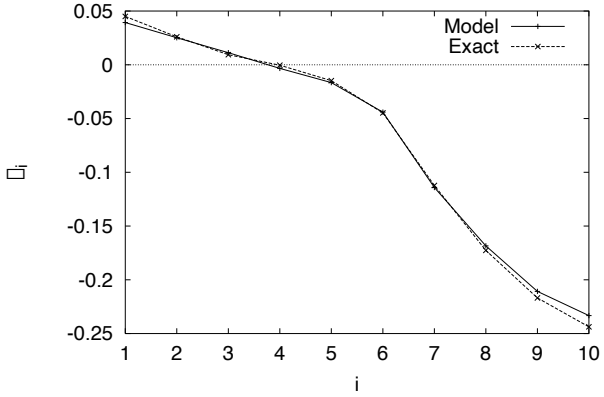

Figure 2: The first 10 Lyapunov Exponents for the reconstructed equation (5) for data from the the system Eq.(7). Also shown are the first 10 Exponents calculated from the exact Jacobians in the original state space.

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Properties of the lowest energy excitations of one-dimensional strongly correlated electrons

Konstantin Kladko

Low-energy excitation spectra of correlated systems have long been in the centre of theoretical condensed matter research (see [1] and references therein). In 1932 Hans Bethe proposed his Ansatz method [2] for correlated wave functions, that was then used to solve many one-dimensional quantum and also two-dimensional classical models. Using the Bethe Ansatz (BA) method des Cloizeaux and Pearson [3] derived the energy of low lying $S = 1$ (triplet) states of the spin-1/2 antiferromagnetic Heisenberg model (AFHM). The spectrum of the excitations was found to be $E_t(k) = 1/2J\pi \mid \sin k \mid$. $E_t(k)$ is a π-periodic function of k. des Cloizeaux and Pearson assumed the excitations $E_t(k)$ to be the elementary excitations of the system, therefore assigning to an elementary excitation spin 1. Later investigations [4] have shown that the spectrum of [3] was incomplete. The problem was finally clarified by Faddeev and Takhtajan in Ref. [5]. It was shown that all excitations of the spin-1/2 AFHM are superpositions of spin-1/2 elementary excitations (called kinks or spinons). For periodic rings having odd/even number of sites only odd/even number of kinks are possible in the system. Energies and momenta of many-kink states add, as for independent particles. The dispersion relation of a kink is $1/2J\pi \sin k$, with $0 \leq k \leq \pi$. The Brillouin zone is therefore only half of the original one.

For the ferromagnetic case the one magnon spectrum of the one-dimensional spin-1/2 ferromagnetic Heisenberg model (FHM) has the form $2J(1-\cos k)$, possessing a gap at nonzero k and not being π-periodic. Careful analysis shows that one-magnon states are not the lowest energy states of the system. It was shown using Bethe Ansatz [6], that the elementary excitations of the system (excitations having one quantum number) are magnons and strings. Strings are complexes of $2M + 1$ spins, having the dispersion relation $J\frac{2}{2M+1}(1 - \cos k)$ The lowest bound for the excitation spectrum is formed, when M goes to infinity. Therefore the spectrum is gapless for all wavevectors k. As will be shown below, this property characterizes *all* Heisenberg-like one-dimensional models (integer spin or half-integer spin) which are magnetic in the thermodynamic limit.

Let us prove that the π-periodicity of the lowest-lying excitations is a model independent feature and holds for all one-dimensional isotropic Heisenberg models having a half-integer value of the spin per unit cell, and for all one-dimensional isotropic Hubbard models with an odd number of electrons per unit cell. The only necessary condition is that the interaction is short-ranged enough, namely that it falls off more rapidly as $1/r$.

Consider a one-dimensional half-integer spin Heisenberg model on a periodic ring having $2N$ sites:

$$H = J\sum \mathbf{S}_n \cdot \mathbf{S}_{n+1} = J\sum \left[S_n^z S_{n+1}^z + \frac{1}{2}\left(S_n^+ S_{n+1}^- + S_{n+1}^+ S_n^- \right) \right]. \qquad (1)$$

Consider an eigenstate $\mid \psi_k \rangle$ of H, having wave vector k and energy E

$$T \mid \psi_k \rangle = e^{ik} \mid \psi_k \rangle, \quad H \mid \psi_k \rangle = E \mid \psi_k \rangle. \qquad (2)$$

Here T is the translation operator, $n \to n+1$. Let us write the state $\mid \psi_k \rangle$ as a linear combination of $S^z_{\text{full}} = 0$ spin configurations

$$\psi_k = \sum_\sigma A_\sigma \mid \sigma \rangle. \qquad (3)$$

Any $S^z_{\text{full}} = 0$ configuration is characterized by $2NS$ numbers $x_1 \le x_2 \le x_3 ...$ showing the positions of fictitious particles, each of them increasing S^z on a given site by one. The vacuum of the system is assumed to have all spins down. Since the system is periodic, the x's are defined only $mod\ 2N$. Consider the state

$$\psi_{k+\pi} = \sum_\sigma e^{\frac{2\pi i}{2N}(x_1+x_2+...)} A_\sigma \mid \sigma \rangle. \qquad (4)$$

Adding $2N$ to any of the x's does not change $\psi_{k+\pi}$. Therefore the mentioned freedom of defining the x's is satisfied. If the operator T acts on the state $\psi_{k+\pi}$, then all x's are incremented by 1. Therefore an additional phase factor $e^{i\pi 2S} = e^{i\pi}$ is acquired (2S is odd), and the state $\psi_{k+\pi}$ has a wave vector $k+\pi$. In the same fashion the state

$$\psi_{k-\pi} = \sum_\sigma e^{-\frac{2\pi i}{2N}(x_1+x_2+...)} A_\sigma \mid \sigma \rangle \qquad (5)$$

has a wave vector $k-\pi$. Note that $k+\pi$ and $k-\pi$ are the same wave vectors since they differ by 2π.

Taking the thermodynamic limit one finds

$$\begin{aligned} \langle \psi_{k+\pi} \mid H \mid \psi_{k+\pi} \rangle - \langle \psi_k \mid H \mid \psi_k \rangle = 2N\frac{J}{2}(e^{-\frac{2\pi i}{2N}} \langle \psi_k \mid S_{n+1}^+ S_n^- \mid \psi_k \rangle + \\ e^{\frac{2\pi i}{2N}} \langle \psi_k \mid S_n^+ S_{n+1}^- \mid \psi_k \rangle - -\langle \psi_k \mid S_{n+1}^+ S_n^- \mid \psi_k \rangle - \langle \psi_k \mid S_n^+ S_{n+1}^- \mid \psi_k \rangle) = \\ iJ\pi \left(\langle \psi_k \mid S_n^+ S_{n+1}^- \mid \psi_k \rangle - \langle \psi_k \mid S_{n+1}^+ S_n^- \mid \psi_k \rangle \right). \end{aligned} \qquad (6)$$

In exactly the same way

$$\begin{aligned} \langle \psi_{k-\pi} \mid H \mid \psi_{k-\pi} \rangle - \langle \psi_k \mid H \mid \psi_k \rangle = \\ -iJ\pi \left(\langle \psi_k \mid S_n^+ S_{n+1}^- \mid \psi_k \rangle - \langle \psi_k \mid S_{n+1}^+ S_n^- \mid \psi_k \rangle \right). \end{aligned} \qquad (7)$$

Note that the expressions (6), (7) differ by sign. Therefore one of the states (4), (5) has the expectation value of energy lower or equal than the state $\mid \psi_k \rangle$. In other words, having some excitation at the wave vector k one can always construct an excitation at the wave vector $k+\pi$ having less or equal energy.

Let us now take ψ_k to be a minimum energy excitation for a given value of the wave vector k. As has been proven there exists an excitation with a wave vector $k+\pi$ having the energy less or equal to the energy of ψ_k. Therefore: $E_{low}(k) \geq E_{low}(k+\pi)$. But we could have also started from the state $k+\pi$ to show that $E_{low}(k+\pi) \geq E_{low}(k)$. Therefore $E_{low}(k) = E_{low}(k+\pi)$, so the spectrum of the lowest energy excitations is π-periodic.

Inclusion of more than nearest-neighbour interactions or next order terms like $\left(\mathbf{J}_n \cdot \mathbf{J}_{n+1}\right)^2$ does not change the proof . Any one-dimensional half-integer spin per unit cell Heisenberg Hamiltonian having spherical symmetry will posses features proven above. One can also note that the full spherical symmetry is not necessary. The only facts really used were that the Hamiltonian is symmetric with respect to rotation around the z-axis, and that the lowest energy excitations can be chosen to have $S^z_{\text{full}} = 0$. As long as this is satisfied the spectrum of the lowest energy excitations is π-periodic.

Similar considerations can be used for any isotropic one-dimensional extended Hubbard model having odd number of electrons per unit cell (then $x_1 \leq x_2 \leq x_3 ...$ are the positions of spin-up electrons). The results obtained are similar - the spectrum of the lowest energy excitations is π-periodic and the spin current is zero. For rational fillings the spectrum will be $2k_f$-periodic, where k_f is the Fermi wave vector .

So far we used the subspace $S^z_{\text{full}} = 0$ for our derivations. Consider now a Heisenberg model, where one of the (possibly many) ground states is magnetic in the thermodynamic limit, i.e. $\lim_{N\to\infty} S_{\text{full}}/2N \geq M > 0$, where S_{full} is the spin of the ground state. Then for fixed N S^z_{full} of the ground state can be chosen to be between $-2MN$ and $2MN$. Let us choose the ground state to have $S^z_{\text{full}} = C$, and write it in a linear combination of $S^z_{\text{full}} = C$ configurations. Let us now consider the state

$$\mid \psi' \rangle = \sum_{\sigma} e^{G\frac{2\pi i}{2N}(x_1+x_2+...)} A_\sigma \mid \sigma \rangle \tag{8}$$

where $x_1, x_2, ...$ are again the positions of the $2NS + 2C$ fictitious particles. G is an integer number. The wave vector of the state $|\psi' >$ differs from the wave vector of the ground state by $2\pi G(S + C/N)$. Choosing different (allowed) values of C and G, one can show after a careful analysis, that there is no gap at any value of k in the thermodynamic limit. This result does not depend on whether the spin is half-integer or integer. Therefore if the system is magnetic in the thermodynamic limit, the spectrum is gapless for any k. A similar result can be obtained for one-dimensional extended Hubbard models.

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Energy thresholds for discrete breathers in one-, two- and three-dimensional lattices

S. Flach, K. Kladko and R. S. MacKay

Recently progress has been achieved in the understanding of localized excitations in nonlinear lattices. Discrete breathers (DBs) are time-periodic, spatially localized solutions of equations of motion for classical degrees of freedom interacting on a lattice [1, 2]. Nowadays it is known that the reason for the generic existence of DBs is the *discreteness of the system* paired with the *nonlinearity* of the differential equations defining the evolution of the system [3]. Thus one can avoid resonances of multiples of the discrete breather's frequency Ω_b with the phonon spectrum Ω_q of the system [4]. If the coupling is weak the phonon spectrum consists of narrow bands. The nonlinearity and the narrowness of the phonon bands allows for periodic orbits whose frequency and all its harmonics lie outside the phonon spectrum. For some classes of system, existence proofs of breather solutions have been published [5, 6, 7].

For generic Hamiltonian systems, periodic orbits occur in one-parameter families, and discrete breathers are no exception. In many cases, the energy can be used as parameter along the family, but as is well known, the energy can have turning points along a family of periodic orbits. Mathematically, such a turning point in energy is called a *saddle-centre periodic orbit.*

The main message of this paper is that in 3D lattices, a turning point (in fact, minimum) in energy is almost inevitable for discrete breather families.

One important property of DBs is their generic existence for weak enough coupling, independent of the lattice dimension [5]. This means that DBs are not just a 1D curiosity but could be interesting from the point of view of applications. The experimental detection of DBs requires some additional knowledge about their properties. In this contribution we give heuristic arguments that the energy of a DB family has a positive lower bound for lattice dimension d greater than or equal to some d_c, whereas for $d < d_c$ the energy goes to zero as the amplitude goes to zero, and we confirm these predictions numerically. The critical dimension d_c depends on details of the system but is typically 2 and never greater than 2. Furthermore, for $d > d_c$, the minimum in energy occurs at positive amplitude and finite localisation length. Consequently experiments could be designed to look for activation energy thresholds for localized excitations.

Let us consider a d-dimensional hypercubic lattice with N sites. Each site is labeled by a d-dimensional vector $l \in Z^d$. Assign to each lattice site a state $X_l \in R^f$, where f is the number of components and is to be finite. The evolution of the system is assumed to be given by a Hamiltonian of the form

$$H = \sum_l H_{loc}(X_l) + H_{int}(X_l, \{X_{l+s}\}), \tag{1}$$

where H_{int} depends on the state at site l and the states X_{l+s} in a neighbourhood. We assume that H has an equilibrium point at $X_l = 0$, with $H(\{X_l = 0\}) = 0$.

DB solutions come in one-parameter families. The parameter can be the amplitude (measured at the site with maximum amplitude), the energy E or the breather frequency Ω_b. It is anticipated that the amplitude can be lowered to arbitrarily small values, at least for some of the families for an infinite lattice. In this zero amplitude limit, the DB frequency Ω_b approaches an edge of the phonon spectrum Ω_q. This happens because the nonresonance condition $\Omega_q/\Omega_b \neq 0, 1, 2, 3, ...$ has to hold for all solutions of a generic DB family [4]. In the limit of zero amplitude, the solutions have to approach solutions of the linearized equations of motion, thus the frequency Ω_b has to approach some Ω_q, but at the same time not to coincide with any phonon frequency. This is possible only if the breather's frequency tends to an edge Ω_E of the phonon spectrum in the limit of zero breather amplitude. If we consider the family of nonlinear plane waves which yields the corresponding band edge plane wave in the limit of zero amplitude A, then its frequency Ω will depend on A like

$$|\Omega - \Omega_E| \sim A^z \tag{2}$$

for small A, where the "detuning exponent" z depends on the type of nonlinearity of the Hamiltonian (1), and can be calculated using standard perturbation theory.

It is tempting to check then whether the breather appears through a bifurcation from a periodic orbit which is a normal mode of the linearized equations of motion for any system with finite N. Band edge plane waves of the linearized equations of motion can be continued to non-zero amplitudes for the general nonlinear system. The stability analysis of these periodic orbits yields the possibility of tangent bifurcations (collision of Floquet multipliers at +1) if some algebraic inequalities of the expansion coefficients of H in (1) are met [8]. It has been also shown that the orbits which bifurcate from the plane wave are not invariant under discrete translations and have the shape of discrete breathers [8]. It has been conjectured that the new bifurcating orbits *are* discrete breathers. Subsequently it was successfully explained why discrete breathers exist or not for certain models by analyzing the above-mentioned algebraic inequalities [8].

The above-mentioned analysis of stability of band edge plane waves was carried out for systems with detuning exponent $z = 2$ and large N. The critical amplitude A_c of the plane waves at the bifurcation point depends on the number of lattice sites as $A_c \sim N^{-1/d}$ [8]. We see that the amplitudes of the new orbits bifurcating from the plane wave become small in the limit of large system size. If the energy of the system is given by a positive definite quadratic form in the variables X in the limit of small values of X it follows for the critical energy of the plane wave at the bifurcation point [8]

$$E_c \sim N^{1-2/d} \quad . \tag{3}$$

Result (3) is surprising, since it predicts that for $z = 2$ the energy of a DB for small amplitudes should diverge for an infinite lattice with $d = 3$ and stay finite (nonzero) for $d = 2$, whereas if $d = 1$ the breather energy will tend to zero (as initially expected) in the limit of small amplitudes and large system size. The whole construction depends

on the validity of the assumption that the new periodic orbits bifurcating from the plane wave through the above-mentioned tangent bifurcation are indeed DBs.

It is not known how to prove this assumption. But we can estimate the discrete breather energy in the limit of small amplitudes and compare the result with (3). Define the amplitude of a DB to be the largest of the amplitudes of the oscillations over the lattice. Denote it by A_0 where we define the site $l = 0$ to be the one with the largest amplitude. The amplitudes decay in space away from the breather center, and by linearising about the equilibrium state and making a continuum approximation, the decay is found to be given by $A_l \sim CF_d(|l|\delta)$ for $|l|$ large, where F_d is a dimension-dependent function

$$F_1(x) = e^{-x} \quad , \quad F_3(x) = \frac{1}{x}e^{-x} \tag{4}$$

$$F_2(x) = \int \frac{e^{-x\sqrt{1+\zeta^2}}}{\sqrt{1+\zeta^2}} d\zeta \quad , \tag{5}$$

δ is a spatial decay exponent to be discussed shortly, and C is a constant which we shall assume can be taken of order A_0. To estimate the dependence of the spatial decay exponent δ on the frequency of the time-periodic motion Ω_b (which is close to the edge of the linear spectrum) it is enough to consider the dependence of the frequency of the phonon spectrum Ω_q on the wave vector q when close to the edge. Generically this dependence is quadratic $(\Omega_E - \Omega_q) \sim |q - q_E|^2$ where $\Omega_E \neq 0$ marks the frequency of the edge of the linear spectrum and q_E is the corresponding edge wave vector. Then analytical continuation of $(q - q_E)$ to $\mathrm{i}(q - q_E)$ yields a quadratic dependence $|\Omega_b - \Omega_E| \sim \delta^2$. Finally we must insert the way that the detuning of the breather frequency from the edge of the linear spectrum $|\Omega_b - \Omega_E|$ depends on the small breather amplitude. Assuming that the the weakly localized breather frequency detunes with amplitude as the weakly nonlinear band edge plane wave frequency this is $|\Omega_b - \Omega_E| \sim A_0^z$. Then $\delta \sim A_0^{z/2}$.

Now we are able to calculate the scaling of the energy of the discrete breather as its amplitude goes to zero by replacing the sum over the lattice sites by an integral

$$E_b \sim \frac{1}{2}C^2 \int r^{d-1} F_d^2(\delta r) \mathrm{d}r \sim A_0^{(4-zd)/2} \quad . \tag{6}$$

This is possible if the breather persists for small amplitudes and is slowly varying in space. We find that if $d > d_c = 4/z$ the breather energy diverges for small amplitudes, whereas for $d < d_c$ the DB energy tends to zero with the amplitude. Inserting $z = 2$ we obtain $d_c = 2$, which is in accord with the exact results on the plane wave stability [8] and thus strengthens the conjecture that discrete breathers bifurcate through tangent bifurcations from band edge plane waves. Note that for $d = d_c$ logarithmic corrections may apply to (6), which can lead to additional variations of the energy for small amplitudes.

An immediate consequence is that if $d \geq d_c$, the energy of a breather is bounded away from zero. This is because for any non-zero amplitude the breather energy can not be zero, and as the amplitude goes to zero the energy goes to a positive limit ($d = d_c$)

or diverges ($d > d_c$). Thus we obtain an energy threshold for the creation of DBs for $d \geq d_c$. This new energy scale is set by combinations of the expansion coefficients in (1). If $z = 2$ with $|\Omega - \Omega_E| \sim \beta A^2$ for the nonlinear plane waves, and the energy per oscillator $E \sim gA^2$ and the spatial decay exponent δ is related by $|\Omega_b - \Omega_E| \sim \kappa\delta^2$, then the energy threshold E_{min} is of the order of $\kappa g/\beta$, and the minimum energy breather in 3D has spatial size of the order of the lattice spacing, independently of κ, g and β. One should allow for a factor of $(2+d)$ for underestimating the true height of the minimum and the contributions of nearest neighbours.

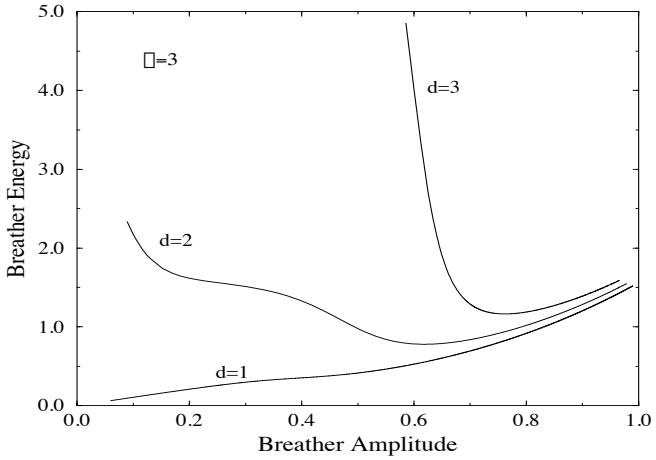

Figure 1: Breather energy versus amplitude for the DNLS system in one, two and three lattice dimensions. Parameters $C = 0.1$ and $\mu = 3$ for all cases. System sizes for $d = 1, 2, 3$: N=100, N=25^2, N=31^3, respectively.

To confirm our findings, we performed numerical calculations. First we study the discrete nonlinear Schrödinger (DNLS) equation

$$\dot{\Psi}_l = \mathrm{i}(\Psi_l + |\Psi_l|^{\mu-1}\Psi_l + C \sum_{m \in N_l} \Psi_m), \tag{7}$$

where N_l denotes the set of nearest neighbours of l. The detuning exponent z is easily seen to be $\mu - 1$. Making the substitution $\Psi_l = A_l \mathrm{e}^{\mathrm{i}\Omega_b t}$ we solve the algebraic equations for the real amplitudes A_l. Numerically this is implemented by considering the case of large breather amplitude A_0 first. Then the breather is essentially given by $A_0 \approx (\Omega_b - 1)^{1/(\mu-1)}$ and $A_{l\neq 0} = 0$. Next we define a functional G which is the sum over the squares of differences between left hand and right hand parts of all algebraic equations for the amplitudes. This functional is minimized by gradient descent, where the initial guess is the large amplitude approximate solution. Finally the frequency Ω_b is varied in small steps and the breather solution is traced. In Fig.1 we show the resulting breather energy as a function of the amplitude A_0 for $\mu = 3$ and $d = 1, 2, 3$. The results are in full accord with the predictions. For $d = 3$ the above estimate of the minimum energy yields a value of 0.2 with $\beta = g = 1$ and $\kappa = C = 0.1$. The mentioned factor $(2+d) = 5$ accounts for the deviation from the true value of 1. Fig.2 in [9] shows the amplitude distribution of the discrete breather with minimum energy in the (x, y)-plane crossing the breather center for $d = 3$. The minimum energy breather is strongly

localized - its spatial width is only few lattice spacings. In Fig.2 we show results for

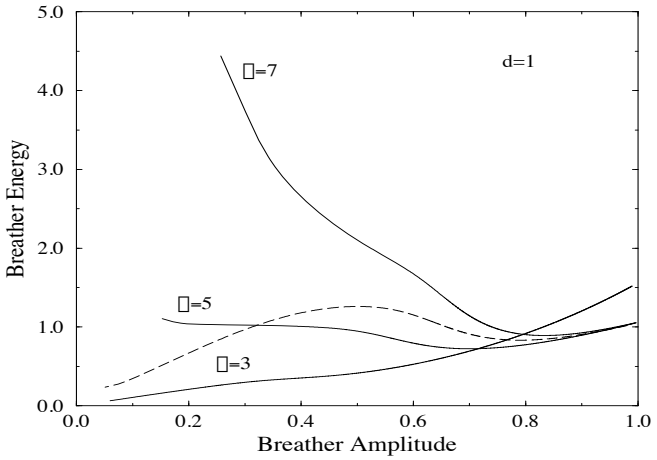

Figure 2: Breather energy versus maximum amplitude for the DNLS system in one lattice dimension and for three different exponents $\mu = 3, 5, 7$ (solid lines). The system size is $N = 100$ and the parameter $C = 0.1$. The dashed line is for the modified system (cf. text).

$d = 1$ and $\mu = 3, 5, 7$. Again we find full agreement. Note that even one-dimensional lattices exhibit positive lower bounds on breather energies if $\mu \geq 5$.

To demonstrate that the numerical results are not an artefact of the DNLS case, we also studied the d-dimensional nonlinear Klein-Gordon lattice $\ddot{U}_l = -U_l - U_l^\mu - C\sum_{m\in N_l}(U_l - U_m)$. The detuning exponent z is given by $\mu - 1$ for μ odd and $2\mu - 2$ for μ even. Again the discrete breather with large amplitude is essentially an on-site excitation and given by $\ddot{U}_0 = -U_0 - U_0^\mu$ and $U_{l\neq 0} = 0$. The equations of motion are integrated numerically for a given set of initial conditions $\{U_l(t=0), \dot{U}_l(t=0)\}$ over the breather period $T_b = 2\pi/\Omega_b$. The functional $G = \sum_l \left((U_l(T_b) - U_l(0))^2 + (\dot{U}_l(T_b) - \dot{U}_l(0))^2\right)$ is minimized with respect to the initial conditions using gradient descent. This method allows us to perform a reliable numerical calculation of DBs in 3-dimensional arbitrary lattices. The result in Fig.4 of [9] for $\mu = 3$ and $d = 3$ is again in full accord with the predictions.

We can predict that a modified DNLS system with an additional term $v_{\mu'}|\Psi_l|^{\mu'-1}\Psi_l$ can exhibit complex curves $E_b(A_0)$. For example, for $d = 1$, $\mu = 7$, $\mu' = 3$ and $v_{\mu'} = 0.1$, the $E_b(A_0)$-dependence will be nearly identical to the case $v_{\mu'} = 0$ already considered, if the amplitude A_0 is not too small. Then $E_b(A_0)$ will show a minimum at a non-zero value of A_0. For small A_0 however the energy of the breather will ultimately decay to zero, so the curve has a maximum for smaller amplitudes! The dashed line in Fig.2 shows the numerical calculation, which coincides with our prediction.

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Konferenzen, Workshops und Symposien 1996-1997

Conferences, Workshops and Symposia 1996-1997

Report on

"Chaos and disorder in spatially extended systems"

February 15 - February 22 , 1996

Scientific directors

H. Kantz (Max-Planck-Institut für Physik komplexer Systeme),
R. Livi (Diparimento di Fisica, Universität Bologna)

18 participants

During the last two decades nonlinear dynamics developed into a rapidly evolving field of research. At present, complex dynamics in low-dimensional systems is fairly well understood. However, there are even more systems which possess both a *high-dimensional* phase space and a *high-dimensional* attractor. Perhaps the most important ones are spatially extended systems. They possess spatial translational invariance, their number of degrees of freedom is proportional to the physical size of the system, and the individual degrees of freedom are allocated to points in space. Such systems can exhibit space-time chaos. Prominent examples are hydrodynamical turbulence and reaction-diffusion systems. Despite many efforts undertaken about a decade ago, up to now the understanding of such systems in the chaotic regime is quite limited. Currently it is time to start a new attempt, which is reflected by many new activities in this field.

Concept and main results

On this small workshop outstanding researchers in this area met in order to review the present state of knowledge and to get an overview over current research activities. Relevant and tractable issues and open problems were pointed out. As a result, it was agreed on applying for funding for a research network in the framework of the EU program "Training and Mobility of Researchers", and the reserach program was outlined.
Every participant gave a talk. There was much time for informal discussions, and a small number of computers was available for numerical work. Round-table discussions on selected focus issues were organized. Young scientists from the institute had the opportunity to get insight in this field of research, to learn about recent developments, and to be confronted with ongoing research and open issues.

The following topics were addressed:
partial differential equations, coupled map lattices, cellular automata,
Lyapunov analysis, dimensional analysis, local approaches
space-time intermittency, synchronization effects, collective behaviour,
correspondence to surface growth phenomena and percolation.

Topics of round table discussions:
- usefulness and perspectives of dimension analysis
- characteristic quantities for spatiotemporal disorder
- what is "disorder without chaos"?

- local approaches? time series analysis?
- open systems
- relevance and physical meaning of couped map lattices and cellular automata

Participants
Participation was possible only by invitation.

16 participants from outside the institute, 4 Germans, 1 Canadian, 1 Israelian, others: EU members.
Professional status of the participants:
Young generation at senior level (professors or senior researchers)

List of participants

Markus Bär (Dresden), Franco Bignone (Firenze), Tomas Bohr (Copenhagen), Hugues Chaté (Saclay, France), Bernard Derrida (Saclay, France), Rudolf Friedrich (Stuttgart), Holger Kantz (Dresden), Raymond Kapral (Toronto), Roberto Livi (Firenze), Robert S. MacKay (Cambridge), David Mukamel (Weizmann), Arkady Pikovsky (Potsdam), Antonio Politi (Firenze), Harald Posch (Wien), Stefano Ruffo (Firenze), Thomas Schreiber (Wuppertal), Ruedi Stoop (Zuerich), Angelo Vulpiani (Roma)

Holger Kantz

"International Symposium on Electron Correlations in Solids"

April 12, 1996

Scientific director
P. Fulde (Dresden)
140 participants

"International Workshop on Superconducting State with Modulated Order Parameter"

June 17 - June 20, 1996

Scientific directors
H. Eschrig (TU Dresden), D. Rainer (Bayreuth), F. Steglich (Darmstadt)

33 participants

A couple of decades ago, by theoretical reasoning P. Fulde and R.A. Ferrell and independently A.I. Larkin and Y.N. Ovchinikow conjectured that in a type-II superconductor at temperature well below Tc and with an applied magnetic field close to the upper critical one, free energy could be gained by a certain spatial order parameter modulation. This predicted phase obtained in the literature the name Fulde-Ferrell-Larkin-Ovchinikow state (FFLO state). In recent years, experimentalists have found irregularities, sometimes called peak effects, in the magnetic response of a variety of superconductors ranging from V_3Si through the high-Tc cuprates to various heavy-fermion superconductors. Some experts conjectured that these phenomena might be fingerprints of the FFLO state.

Independently of this conjecture, the initiators of the reported international workshop, F. Steglich, D. Rainer and H. Eschrig, found it just timely to organize a small high-level meeting of the very experts in the world, both experimentalists and theoreticians, on phenomena presumably related to superconducting order parameter modulations, in Dresden in 1996. The workshop was held in Dresden, 3-6 June 1996. The number of active participants was limited to about 30, by invitation of some 15 leading experts and encouraging each of them to suggest one of their younger colleagues. The organizational work and the infrastructure as well as very substantial financial support was provided by the Max-Planck-Institute for Physics of Complex Systems, Dresden. Of course, the lecture hall was open to the local graduate students.

Considering the program, the list of speakers (8 from Germany, 4 from Europe, 6 from the U.S. and 7 from Japan) and the lively and extended discussions, the workshop was a full success. The topic of the workshop was nearly completely covered considering actual activities. Order parameter modulation, order parameter mixing, interaction with vortices and anomalous pinning staggered pairing, strong correlation in supersolids, layered systems, d-wave pairing, quantum oscillations in the mixed state, peak effects of magnetisation, peculiarities in magnetocaloric and elastic properties were subjects addressed. On purpose we did not plan proceedings, and as a result we had reports of very fresh results, occasionally delivered the previous day by FAX from the laboratory.

The central result of the workshop was a negative statement, although decisive: The anomalies seen in various experiments cannot be indicative of the FFLO state for a number of reasons. However, on the phenomenological level, a leap ahead was made by comparison of measurements and intensive discussion between the active laborato-

ries. There remains a lot to investigate until the experimentally discovered effects are understood, and the participants left with new enthusiasm, new ideas, and with words of high estimation of the workshop.

Helmut Eschrig

Report on

"International Workshop on Non-Pertubative Approach to Chaos in Mesoscopic Systems and Localization"

August 11 - September 7, 1996

Scientific director
V. Fal'ko (Oxford U.)
Advisory Board: B. Altshuler (Princeton), K. Efetov (Stuttgart),
H. Weidenmüller (Heidelberg)

40 participants

The international workshop 'Non-Perturbative Approach to Chaos in Mesoscopic Systems and Localization' was held at the MPI-PKS from 11 August untill 7 September, 1996. The main topics which was in the focus of this meeting was the rapidly expanding applications of the supersymmetric non-linear sigma-model and the random matrix theory methods to the problems of quantum chaos, mesoscopics and localization in the quantum Hall effect regime. This workshop has taken place at such a lucky stage in the mesoscopics and the localization theory when a series of long-standing problems have been solved exactly, or were in the progress of successful development, and the first ideas of a 'grand unification' between the semiclassical theory of quantum chaos and the quantum transport in disordered systems were flying in the air. As a result, the Dresden meeting has given a push to the whole progression of similar events devoted to this growing field (Lorentz Institute - Leiden 1997, Newton Institute - Cambridge 1997, SISSA - Trieste 1998). The use of non-perturbative methods in the theory of quantum chaos has become since then a common tool to calculate the statistical properties and spectral correlations in disordered conductors and model chaotic billiards, and the sigma model has found its broader applications in the field theory prototype of the turbulence.

The aim of this meeting was not limited only by conferencial activities and exchange of opinions, which were, nevertheless intensive and, sometimes, quite hot. One of the ideas of it was to promote a productive cooperation between theorists from different institutions and countries on the hospital ground of a new-born institute, and to stimulate new collaborations between participants. The working groups of young bright theorists participating to this meeting (O.Agam, A.Altland, R.Baranger, C.Bruder, U.Eckern, Y.Fyodorov, R.Jalabert, A.Macedo, C.Mudry, F. von Oppen, K.Richter, B.Simons, R.Smith) were gathered around leading specialists in the field, such as J.Alhassid, C.Beenakker, J.Chalker, K.Efetov, A.Finkelshtein, Yu.Gefen, S.Hikami, D.Khmelnitskii, I.Lerner, J-L.Pichard, A.Pruisken, M.Zirnbauer, F.Wegner, H.Weidenmuller. Many of those for whom this meeting was one of the first experiences of this kind, as A.Andreev, G.Hackenbroich, E.MacKann, B.Muzykantskii, and Yu.Oreg have since then proved their high qualification in theoretical physics. The workshop seminars and lectures were both of special and introductory type, accessible to the staff of MPI-PKS and visitors from Dresden University and Chemnitz University.

Report on

"Workshop on Stochasticity and Structure Formation"

October 7 - October 11, 1996

Scientific directors

U. Behn, A. Küehnel, K. Schiele (Leipzig)

58 participants

From October 7 to October 11 1996 the University Leipzig was hosting a workshop of the Max Planck Institute for Physics of Complex Systems (Dresden) on stochasticity and structure formation. The scientific coordinators of this event were Prof. Dr. U. Behn, Prof. Dr. A. Kühnel and Dr. K. Schiele (Institut für Theoretische Physik und Naturwissenschaftlich-Theoretisches Zentrum der Universität Leipzig). Dr. I. Allekotte was taking care of the organizational work on behalf of the MPI.

The subject of the workshop was a recent and rapidly evolving field: the physical description of complex systems of inanimate and animate nature. This aspect showed up in the strong resonance to the invitations of approximately 25 leading experts from Europe and Overseas. The spectrum of topics was deliberately broadened in order to bring together colleagues which would not usually meet during more specialized events. There were approximately 60 colleagues from 8 European countries, the USA, Japan, New Zealand and Israel participating in the workshop. The workshop was opened by Prof. Dr. Peter Fulde, who informed about the aims and scientific profile of the newly established institute in Dresden.

We want to highlight the following topics from a total of about 40 talks.

Structure formation in spatially extended systems. About one third of the workshop program was devoted to this topic. Friedrich Busse (University Bayreuth) is one of the pioneers of the experimental and theoretical studies of structure formation, who opened the workshop with the talk "'Experiments and theory of time dependent convection in a rotating layer"'. The afternoon session of the first day was devoted to Prof. Busse, who turned 60 not long ago. During this session his students and friends gave talks, like Agnes Buka (Budapest) on "'Pattern forming instabilities in liquid crystals"', Werner Pesch (Bayreuth) "'Spirals in Rayleigh-Benard convection"', Ingo Rehberg (Magdeburg) "'Structure formation in complex fluids: Experimental results"' and finally Alan Newell (Warwick) with his talk on "'Natural patterns"'. Also the talks of Lorenz Kramer (Bayreuth) "'Convection instabilities in systems with spontaneously broken anisotropy"', Siegfried Grossmann (Marburg) "'Turbulence"', Tamas Tel (Budapest) "'Pattern formation in chaotic advection"', Alexander Groismann (Rehovot) "'Solitary vortices in visco-elastic Couette flow"' and Stefan C. Müller (Magdeburg) "'Reaction- diffusion structures under external constraints"' should be mentioned with respect to this.

Noise induced phenomena. A second complex was devoted to the study of qualitatively new phenomena induced by stochasticity. Here we want to mention the talks by Christian Van den Broeck (Diepenbeek) "'On the origin of noise induced phase transitions"', Jaume Masoliver (Barcelona) "'The escape problem for inertial processes"', Florence Baras (Brüssel) "'Stochastic description of periodic phenomena"', Franz J. Elmer (Basel) "'Noise induced pattern switching in parametrically excited spin waves"' and Günter Radons "'Localization of chaotic motion by quenched disorder"'. Interesting problems of nonlinear dynamics were dealt with in the talks of Jürgen Kurths (Potsdam) "'Phase synchronization of chaotic oscillators"' and Slava Priezzhev (Dubna) on "'Self-organized criticality in self-directing walks"'.

Yet another highlight were biologically motivated problems. Talks were given by Frank Moss (St. Louis) "'Stochastic resonance in visual image perception"' , Leo van Hemmen (München) "'Is brain tissue an excitable medium?"', Kim Sneppen (Kopenhagen) "'Punctuated equilibria in Evolution"', Werner Ebeling (Berlin) "'Dynamic models of evolution processes in continuous and discrete spaces"', Kunihiko Kaneko (Tokio) "'Isologous diversivication theory for the formation of biological society"', Hans-Peter Herzel (Berlin) "'Stochastic models of DNA"', Walter Zimmermann (Jülich) "'On patterns in inhomogeneous convection, microtubuli-polymerisation and biomembranes"' and by the psychologist Hans-Georg Geißler from Leipzig on "'Hypotheses on quantal time structures in brain functioning"'.

As can be already seen from the abovesaid, those different topics were interconnected. This made the discussion and the scientific exchange very fruitful. Of course people from Leipzig and colleagues from the MPI used the chance, to present own results in the talks of Heidrun Amm, Ulrich Behn, Jens Emmerich, Adolf Kühnel, Karen Lippert, Reinhard Müller, Heiko Patzlaff, Ralf Stannarius (all from Leipzig) and Markus Bär and Holger Kantz (both from Dresden). Thanks to the engagement of Dr. Allekotte and his colleagues from Dresden as well as to the engagement of Gertraud Eichel, Daniela Schmidt and the graduate students Micaela Krieger and Thomas John the organization of the meeting was done very neatly and smoothly. A large part of the participants was very impressed by the scientific level of the meeting.

Ulrich Behn, Adolf Kühnel, Konrad Schiele

Report on

"Localization in Nonlinear Lattices"

April 7 - April 11, 1997

Scientific directors

S. Flach (Dresden), R. S. MacKay (Cambridge)

36 participants

The workshop held in Dresden at the Max Planck Institute for Physics of Complex Systems aimed to bring together researchers working on discrete breathers, attract experimentalists carrying out (or who could carry out) experiments related to the creation and detection of discrete breathers, and stimulate new ideas in this young field of research.

The main topics of the workshop were
(i) localized vibrations of classical Hamiltonian lattices,
(ii) quantum breathers and bound states of phonons,
(iii) breathers in non-Hamiltonian networks.

This workshop was the first one devoted specifically to discrete breathers. The need of such a forum reflected itself in the strong response to the invitations of experts from Europe, USA, Japan and Australia. Instead of the initially expected 20 participants the final number of participants grew up to 36. Practically all groups working in this field were presented. However the workshop character was not lost. There was enough time for discussions and work. The facilities of the MPI - several workstations - were heavily used.

The talks can be roughly splitted into several parts.

Introductory talks. David Campbell (Urbana) gave an introductory lecture on the search for breathers in continuum theories, which led to the observation that breathers are structurally stabilized by using a spatial lattice. S. Takeno (Osaka) gave a review of his work on classical and quantum breathers.

Rigorous results on existence and properties of breathers. Talks were given by D. Bambusi (Milano), C. Baesens (Cambridge), J.-A. Sepulchre (Cambridge).

New analytical and numerical results on breathers in Hamiltonian lattices were reported by J. C. Eilbeck (Edinburgh), M. Johannson (Lyngby), S. Aubry (Saclay), S. Flach (Dresden), T. Cretegny (Lyon), J. B. Page (Tempe), R. Livi (Florence), R. Dusi (Stuttgart), K. Kladko (Dresden), M. Spicci (Dresden) and J. L. Marin (Saragoza).

Results on quantum lattices were presented by A. Bishop (Los Alamos), A, Kosevich (Kharkov), V. Fleurov (Tel Aviv), M. Wagner (Stuttgart), A. Mayer (Regensburg), V.

Tognetti (Florence), M. Salerno (Salerno) and D. Ellinas (Heraklion).

Finite temperature studies and noinhamiltonian lattices were covered by talks of M. Peyrard (Lyon), Yu. Kivshar (Canberra), L. M. Floria (Zaragoza) and M. Abel (Potsdam).

Most importantly experimental results were presented by A. J. Sievers (Ithaca), K. K. Lehman (Princeton), F. Fillaux (Thiais), P. Jakob (Munich) and H. van der Zant (Delft).

The results of this meeting will be published soon in a special issue of Physica D.

The meeting has already triggered some recent developments in the field. Extending previous work the problem of acoustic breathers (breathers in the presence of acoustic phonon modes) was studied for a simple 2d lattice (Flach/Kladko/Takeno, PRL 1997) and for a class of models with harmonic coupling (Aubry), with the outcome that breathers do exist, but their spatial decay is modified, and most of the details of MacKay's general treatment of breathers in systems with Euclidean invariance have now been worked out.

Investigations of the existence of slowly moving breathers in an adiabatic approximation are being carried out (MacKay), but there are strong restrictions on the existence of exact moving breathers.

There are plans (both experimental and theoretical, e.g. Floria, Ustinov, van der Zant) to study further the properties of breathers in Josephson ladders.

Prompted by the report of Jakob on breathers in interacting dipole systems, Baesens and MacKay have extended their proofs of localization of breathers from exponentially decaying interaction to algebraically decaying interaction.

It is a great pleasure to thank (also on behalf of the participants) the MPIPKS Dresden for hosting the workshop in such a perfect way. The support and advice of Prof. P. Fulde, Dr. I. Allekotte, Mrs. I. Schmidt and Mrs. K. Lantsch are gratefully acknowledged.

S. Flach, Dresden

Report on

"From Correlated Electrons to the Quantum Mechanics of Complex Systems "
Symposium in honor of Martin C. Gutzwiller

June 23 - June 25, 1997

Scientific directors
Eckhardt (Marburg), E. Heller (Harvard), K. Richter (MPI Dresden)

84 participants

Complex behaviour manifests itself in a variety of quantum systems ranging from interacting many particle systems, in particular correlated electrons in condensed matter, to low-dimensional systems with only a few strongly coupled degrees of freedom. This gives rise to classically chaotic behaviour in the latter which makes them ideal candidates for the study of quantum chaos. Both the physics of correlated electrons and quantum chaos have evolved into rapidly developing fields. The conference successfully aimed to promote the use of concepts from quantum chaos and non-linear dynamics in many-body physics and lead to an intensive exchange of ideas between the two related, but usually disjunct, communities.

The conference covered topics from condensed matter theory as well as atomic and mesoscopic physics, where the latter could be viewed as an interface for a mutual transfer of methods and ideas from many body physics and quantum chaos. Twenty plenary talks covered a broad spectrum ranging from arithmetic billiards via microwave cavities, quantum chaos in natural and "designer" atoms (quantum dots), random matrix theory to strongly correlated electrons in solid state systems.

The meeting which was attended by 84 participants brought together nearly all researchers who have made major contributions to the development of quantum chaos, including M.V. Berry, E. Bogomolny O. Bohigas, P. Cvitanović, E. Heller, F. Haake, M.C. Gutzwiller, U. Smilansky, and F. Steiner, to name only a few. Furthermore experts of correlated electrons included e.g. K.-A. Chao, Y. Kakehashi, and D. Vollhardt.

The conference, which was the first one in the institute's new building, was held in honour of Martin Gutzwiller who has significantly advanced the areas of both correlated electrons and quantum chaos. The Symposium received an additional special tone through historical remarks by M. Dresden, M.V Berry and M.C Gutzwiller.

The plenary lectures were complemented by a large poster session which allowed young researchers to present and discuss their work in the community.

K. Richter, Dresden

Report on

"German-Israeli meeting of young researchers: From Quantum to Classical Mechanics of Complex Systems"

June 26 - June 27, 1997

Scientific director
K. Richter

38 participants

This meeting was intended to support and to bring together young researchers up to the post-doc level and to give them the opportunity to present their recent work to an international audience of experts in the field, including several senior researchers.

38 theoretical physicists from Canada, England, France, Germany, Israel and the USA participated in this meeting. The travel expenses of the participants from Israel were partly covered by Minerva funds.

The workshop focussed on problems in Classical and Quantum Chaos, as well as Mesoscopic Physics, with an emphasis on advanced semiclassical approaches. The four sessions during the two days were devoted to four topics of current interest in the field of quantum chaos: Quantal-classical duality and the semiclassical trace formula, quantum chaos in systems with spatial symmetries, novel techniques for periodic orbit quantization, and quantum dynamics in mixed phase space. These topics represented a natural extension of the preceding conference "From Correlated Electrons to the Quantum Mechanics of Complex Systems" at the Max-Planck Institute.

The concept of the meeting was to have a limited number of longer oral presentations, which deal in more detail with new analytical and numerical techniques and methods, or the derivation of novel interesting results. The rather informal character of this meeting lead to extended, lively and sometimes rather controversial discussions and stimulated an exchange of ideas between the participants. The special character and atmosphere developed during this workshop was appreciated by all participants.

K. Richter, Dresden

Report on

"International Workshop on Novel Physics in Low-Dimensional Electron Systems"

July 28 - August 8, 1997

Scientific director
T. Chakraborty(Madras)

105 participants

The international workshop was held during July 28 - August 8, 1997, almost immediately after the new building of the institute was opened. A major goal of the meeting was to discuss the most recent developments in the field of quantum Hall effects (integral and fractional), quantum dots, quantum rings and other mesoscopic systems like narrow channel systems, double-layer, double-dot systems, etc. Most of the invited speakers were the leading experts in the field. The poster presentations were largely by younger scientists.

Ever since the discovery of the quantum Hall effects more than fifteen years ago, there has been an almost unending series of theoretical and experimental challenges and triumphs in the field. This meeting was perhaps the first major event in the fields of quantum Hall effect and quantum dots where almost all major contributors were present. In a meeting of this kind the participants therefore had a unique opportunity to interact and benefit from the up-to-date talks and posters presented during the two weeks. In quantum Hall effects, the prominent speakers included: B.I. Halperin (Harvard), F.D.M. Haldane (Princeton), J.P. Eisenstein (Caltech), S. Barrett (Yale), R. Willett (Bell Laboratories), A. Pinczuk (Bell Laboratories), S. Das Sarma (Maryland), J.K. Jain (Stony Brook), N. Read (Yale), J. Smet (MPI, Stuttgart), G. Ernst (MPI, Stuttgart), W. Dietsche (MPI, Stuttgart), D. Yoshioka (Tokyo). The themes of all those talks were current topics like, edge states physics, Coulomb drag in Coulomb coupled systems, problems of the half-filled Landau level, spin-texture excitations, composite fermions, etc. Puzzling experimental results like anomalies in the surface acoustic wave measurements on a two-dimensional system with periodic density modulation was discussed in this meeting and are still open problems. Similarly, discrepancies in different measurements of spin-texture excitations discussed by various speakers in the meeting remain, as yet, unresolved.

In the fields of quantum dots and other mesoscopic systems, the prominent speakers included, H. Aoki (Tokyo), R. Ashoori (MIT), S. Tarucha (NTT, Japan), J. Kotthaus (Munich), L. Kouwenhoven (Delft), P. McEuen (Berkeley), A. Plaut (Exeter, UK), D. Heitmann (Hamburg), etc. Here the major topic of discussion was the electronic properties of quantum dots, in particular, the energy spectra in the presence of a magnetic field.

The 105 registered participants were from Germany (37), US (29), Sweden (5), Japan (5), UK (5), Belgium (4), Russia (3), Israel (3), Finland (3), Switzerland (2), Italy (2), The Netherlands (2), Iceland (1), India (1), Spain (1), France (1), and Canada (1). A large group of participants from MPI, Stuttgart, headed by Prof. Klaus von Klitzing made major contributions through talks, posters and discussions.

The proceedings of the meeting was published in the international journal **Physica E**, vol. 1, p. 21-326 (1997) (North-Holland), within four months after the meeting was concluded.

Tapash Chakraborty

Report on

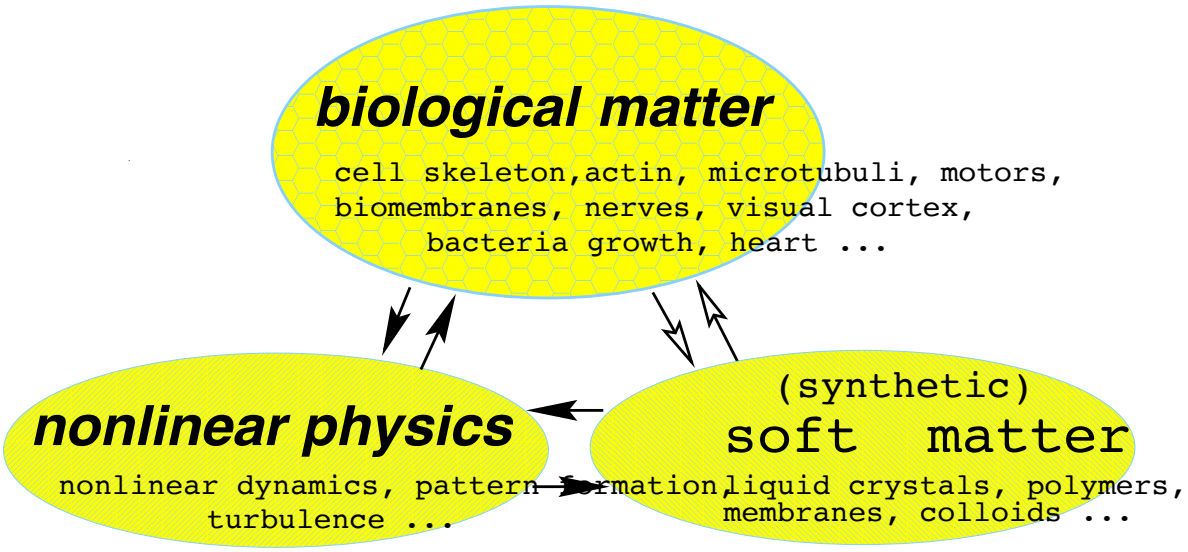
Workshop and Seminar on "Pattern Formation in Complex Fluids and Biology"

August 30 - December 5, 1997

Scientific director
Walter Zimmermann, Jülich

80 participants

It is commonly recognized that the physics of complex soft matter and nonlinear physics are two rapidly developing major branches of modern physics. Physics of soft matter deals mainly with the complex nature of thermal equilibrium states occurring in (synthetic) materials with several internal degrees of freedom, such as liquid crystals, polymers, colloids etc.. This part of research has recently been extended from synthetic to living matter, a trend which is also found in Germany (open arrows in Figure).



Nonlinear dynamics and pattern formation consider driven non-equilibrium systems and strive towards an understanding and classification of the complexity of motion (dynamics) and the complexity of patterns.

A more recent development is research on complex soft matter far from equilibrium, such as driven liquid crystals (films) and flow of polymer solutions etc. (horizontal solid arrows). Most selforganization phenomena in biology occur also far from thermal equilibrium. The large number of internal degrees of freedom in combination with the complex nonlinear dynamics leads to a great and yet unexplored variety of phenomena in these systems. Moreover, research on microtubule polymerization, collective behavior of molecular motors, microtubuli-motor interactions etc. recently reached a semi-quantitative experimental level and hence became susceptible to the concepts of physics. On the other hand their understanding often requires new physical approaches

for their description (solid arrows).

Experienced researchers such as F.H. Busse, P. Fromherz, P.C. Hohenberg, J. Howard, A. Libchaber, H. Müller-Krumbhaar, J. Prost, E. Sackmann, K. Simons, V. Steinberg agree that a stronger interplay between research on nonlinear physics and biological materials as well as synthetic soft matter would bear an enormous potential and it would be timely to have a workshop bringing together scientists from the fields shown in the Figure.
Fortunately several distinguished researchers participated as speakers in this interdisciplinary workshop and seminar: G. Ahlers, A. Ajdari, I. Aranson, D. Bensimon, E. Ben Jacob, D. Bonn, E. Bodenschatz, E. Brener, H.R. Brand, F.H. Busse, H. Cháte, P. Cladis, S. Chu (*Nobelpreis 1997*), T. Duke, J. Fineberg, H. Flyvbjerg, P. Fromherz, L. van Hemmen, T. Geisel, G. Gerisch, R. Goldstein, U. Kaupp, T. Kawakatsu, J. Käs, P. Kolodner, L. Kramer, A. Libchaber, S. Loewel, H. Levine, A.C. Newell, M. Matsushita, C. Misbah, S.C. Müller, G. Oster, A. Panfilov, P. Pelce, W. Pesch, H. Pleiner, J. Prost, I. Rehberg, E. Sackmann, J. Shapiro, J.V. Small, V. Steinberg, S. Tabeling, A. Arneodo, C. Weijer, L. Wolpert.

The workshop and seminar had many highlights. Last but not least the later Nobel Laureate 1997, Steven Chu, fascinated with his report about recent observations of the dynamics of single DNA molecules in flow. The observation of "Molecular Individualism" (P.G.deGennes, 1997) is a key experiment for a future understanding of the macroscopic (nonlinear) dynamics of viscoelastic polymer solutions. During the workshop round table discussions formed spontaneously. Lively discussions and interactions took place in small groups in the entrance hall, on the terrace, in the seminar rooms etc. during the whole time.

Additionally to the plenary talks some 50 high quality poster contributions were presented by young researchers as well as senior scientists. Discussions at the posters always lasted long into the night. Many participants expressed their appreciation that this workshop exposed them to novel developments, especially in neighboring fields.

Several collaborations were initiated at this meeting, so the aim of promoting the communication across scientific borders was met. Many participants of the three-month seminar praised the inspiring atmosphere at the institute, including the enjoyable and fruitful excursions in small groups on the weekends.

Last but not least I should mention the assistance of the members of the visitors program, who took most of the burden of the organization and made this meeting a real pleasure for the organizer.

Walter Zimmermann

Report on

Korrelationstage 1997

October 1 - October 4, 1997

Scientific director
H. Keiter (Dortmund)

150 participants

With more than 150 participants, 39 talks, 23 short talks and more than 60 poster contributions all important german groups working in the fields of High-T_c superconductivity and heavy fermion systems were present, including additional ones from neighbouring countries. The spectrum of the talks ranged from material science to mathematical physics. Fundamental theoretical problems like 1) mechanisms of itinerant ferromagnetism (D. Vollhardt), 2) crystallization of electrons under unifying considerations into a Wigner crystal, Mott-Hubbard transitions and Jahn-Teller effects (P. Fulde), 3) metal-insulator transitions (P. van Dongen), 4) non-Fermi liquids (K. Schönhammer, P. Wölfle), 5) Berry phase in the double exchange of manganites (E. Müller-Hartmann) were discussed as well as new experiments (G. Czjzek, V. Müller, Ch. Geibel, A. Loidl, H. von Löhneysen). Lots of talks were devoted to current numerical methods and their applications (W. Hanke, H. Eschrig, B. Paulus). During both symposia on spin-Peierls systems (B. Lüthi) and on quantum Hall effects (W. Weller) the different aspects of these complicated phenomena were considered. It was shown by several contributions, that the physics of one-dimensional systems and their models can give concrete hints for more general systems (A. Klümper, J. Zittartz, H. Mütter). E.g. these models have been applied to traffic problems (A. Schadschneider).

The success of the meeting was largely due to the rigorously enforced limitations on the length of talks, leaving about one third of the total talk time for discussions. These discussions were used during all talks. It turned out to be of advantage to shift the poster session into the morning hours: the participants were fresh and open for discussions. There were several new agreements on collaboration with the young participants playing an important role. The young participants have presented themeselves very well, where we noticed a shift towards concrete materials (like the spin-Peierls systems $CuGeO_3$, the Kondo insulator $CeNiSn$, the antiferromagnetic cuprates Ca_2CuO_3, Sr_2CuO_3 etc) as compared to previous Korrelationstage meetings.

With this richness of presented material it is rather subjective to make a scientific judgement. Progress was reported also on the understanding of pseudogaps in High-T_c materials (H. Monien), in the numerics of density functional methods as well as of simulations. The role of phonons in highly correlated systems was emphasized in several contributions (e.g. W. Weber, W. Brenig, H. Fehske).

New numerical methods like the 'loop algorithm' (H. G. Evertz), the parallelization of configuration interaction methods (W. Wenzel) and density matrix renormalization group will repay the expectations most probably only in the future.

H. Keiter (Dortmund))

Vorlesungen an der TU Dresden

Lectures at TU Dresden

"Elektronische Korrelationen in Molekülen und Festkörpern"

P. Fulde; Wintersemester 1995/96

"Ausgewählte Themen der Festkörperphysik"

P. Fulde; Sommersemester 1996

"Elementare Rechenmethoden der Physik"

J. Rau; Wintersemester 1996/97

"Transporttheorie"

J. Rau; Sommersemester 1997

"Ausgewählte Themen der Festkörperphysik"

P. Fulde; Sommersemester 1997

"Non-linear dynamics of many particle systems"

S. Flach (MPI Dresden); Herbst 1997; Vortragsreihe

"Strukturbildung in Physik, Chemie und Biologie"

M. Bär, (MPI Dresden; Herbst 1997; Vortragsreihe

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Habilitationen

Habilitations

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Stuttgart 1997

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Doll, K.: Berechnung von Korrelationsenergien von ionischen Festkörpern.
Dresden 1996

Fischer, K.: Eine neue Methode zur Berechnung der Energieskalen von Metallen mit Störstellen.
Dresden 1996

Schmidt, B.: Theorie des Halbmetalls Yb_4As_3.
Dresden 1996

Blawid, S.: Ein Modell des halbmetallischen Verhaltens in Seltenerd-Verbindungen.
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Jaeger, L.: Wechselwirkung deterministischer chaotischer Systeme mit stochastischen Störungen und Modellbildung in der nichtlinearen Zeitreihenanalyse.
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Dresden 1997

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Tran, M.T.: Eine selbstkonsistente Inkrementenmethode und ihre Anwendung auf Kondogitter Systeme.
Dresden 1997

Diplomarbeiten

Diploma

Letz, T.: Lyapunov-Exponenten und Expansionen auf endlichen Längenskalen.
Dresden 1997

Auszeichnungen

Awards

Nöckel, Jens: Henry-Prentiss-Becton Prize, 1997

Schanz, Holger: Humboldt-Preis der Humboldt Universität Berlin, 1997

Vorträge und Seminare in Dresden 1996 - 1997

Seminar talks given in Dresden 1996 - 1997

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14.10.97	A New Type of Spontaneous Spatiotemporal Disorder in Coupled Oscillators	Prof. Y. Kuramoto, Kyoto
14.10.97	Complex Structures and Chaos in the Complex Ginzburg-Landau Equation for Anisotropic System	Prof. L. Kramer, Bayreuth
15.10.97	Asymmetric Vortex Structures (Resonances, Mean Flow etc)	Prof. L. Pismen, Haifa
15.10.97	Modeling Collective Excitations in Cortical Tissue	Prof. L. van Hemmen, Garching
15.10.97	Weak Turbulence in Low Prandtl Number Fluids	Dr. H. Xi, Ohio
15.10.97	Strukturbildung in Physik, Chemie und Biologie	Dr. M. Bär, Dresden
16.10.97	Selforganized Molecular Networks	Prof. A. Mikhailov, Berlin
17.10.97	Spin and Orbital Excitation Spectrum in the Kugel-Khomskii Mode	Dr. G. Khaliullin, Dresden
17.10.97	Dynamics of Fragmenting Hot Drops	Dr. C. Dorso, Buenos Aires
21.10.97	Electronic and Transport Properties of a Chiral Carbon Nanotub	Dr. O. Yevtuschenko, Dresden

Termin	Thema	Vortragender
21.10.97	Competition Between Singlet Formation and Magnetic Ordering in Kondo Lattice Systems	Dr. T. M. Tien, Dresden
28.10.97	Contrasting Effects of Magnetic Field on Thermo- dynamic and Resistive Transitions in High-Tc Cuprates	Dr. V. Kabanov, Dubna
04.11.97	Pattern Formation of Cracks Induced by Dessication Proces	Dr. T. Mizuguchi, Kyoto
04.11.97	The Photochemical Behaviour of Rh(III) Doped into AgCl lattice	Dr. C. Ribbing, Leuven
05.11.97	The Contribution of Reflexes to Physiological Tremor	Dr. J. Timmer, Freiburg
06.11.97	Chemisorption at an Electrochemical Interface: Electronic Structure of a Copper Layer on Gold Electrode	Dr. A. K. Mishra, Madras
06.11.97	Dynamical Density Response in 1D Mott-Hubbard and Charge-Transfer Insulator	Dr. W. Stephan, Dresden
07.11.97	The Discovery of Fractional Shot Noise - Direct Observation of Laughlin's Fractionally Charged Particles	Dr. S. Ketterman, Dresden
11.11.97	Super-Interference Phenomena in the Solid State; Canalized States in Thin Films and Contact States in Compound Solid	Prof. E. Solovyev, Skopje
13.11.97	Fluctuations in Vesicles	Prof. E. Kats, Moskau
14.11.97	The Mathematics and Physics of Finance	Dr. P. Kornilovitch, Dresden
17.11.97	Excitations from a Filled Landau Level in the 2D Electron Gas and Electron-Phonon Inelastic Scatterin	Dr. S. Dickmann, Moskau
18.11.97	Tunneling in Intense Laser Fields	Dr. M. Wagner, Hitachi
18.11.97	Screening of Magnetic Impurities in d-Wave Superconductors	C. Cassanello, Köln
20.11.97	Spatio-Temporal Patterns in Dispersed Two-Phase Flows	Dr. M. Göz, Halle-Wittenberg
20.11.97	Dissipation in Granular Materials	S. Dippel, Duisburg
21.11.97	Dynamics of Particles in Fluids	Dr. S. Schwarzer, Stuttgart
24.11.97	Entropies in Time Series Analysis - Part 1: Theory	Dr. E. Olbrich, Dresden
26.11.97	Bound States in Generalized Ginzburg-Landau Equations	Prof. B. Malomed, Tel Aviv

Termin	Thema	Vortragender
26.11.97	Theory of the X-Ray Spectra of TM, RE, and AC Ions in Solids	Prof. N. Kulagin, Kharkov
26.11.97	Mechanism of Exchange Interactions Between f-Ions in Clusters and Insulating Compounds:Direct Calculations of Exchange Spin Hamiltonians	Dr. V. S. Mironov, Moskau
27.11.97	Novel Nonequilibrium Critical Behavior Induced by Unidirectional Coupling of Stochastic Processes	Dr. H. Hinrichsen, Dresden
27.11.97	Nonlinear Effects in High-T_c Superconducting Microwave Resonators	Dr. T. Dahm, Dresden
02.12.97	Noise-Induced Synchronous Neuronal Oscillations	Dr. C. Kurrer, Paris
02.12.97	Metamagnetism in $CeRu_2Si_2$	F. Bagehorn, Dresden
03.12.97	Instabilities and Pattern Formation in Blood Circulation	Dr. G. Guria, Moskau
04.12.97	The Kondo Box - Transport through an Ultrasmall Metallic Grain with a Kondo Impurity	J. v. Delft, Karlsruhe
05.12.97	Simplest Possible Self-Organized Critical System	Dr. A. Valleriani, Dresden
09.12.97	Multi-Band Gutzwiller Wave Functions for General On-Site Interactions: Correlated Band Structures and Itinerant Ferromagnetism	Dr. F. Gebhard, Grenoble
11.12.97	The Magneto-Impurity Theory of Colossal Magneto-Resistance Material	Prof. E. Nagaev, Moskau
12.12.97	A New Statistical Estimate for the Information Dimension	G. Keller, Erlangen
12.12.97	Phase Transition in Human Behavior	Dr. M. Greiner, Dresden
16.12.97	Connection between Integrability of the Hamiltonian and of the S-matrix	Dr. C. Jung, Mexico
17.12.97	Aspects of the Study of Solid Surfaces by Photo-Electron Diffraction and Holographic Methods	Dr. M. Alaga-Bogdanovic,Belgrade
18.12.97	Zero-Dispersion Phenomena, or Could One Find a Harmony in Nonlinear Deterministic and Noisy Dynamics?	Dr. S. Soskin, Kiev

Vorträge und Seminare in Stuttgart 1996–1997

Seminar talks given in Stuttgart 1996-1997

Termin	**Thema**	**Vortragender**
11.01.1996	Introductions to Random Matrix Theory and its Applications	H.-J. Flad, Stuttgart
19.01.1996	(Non)Fermi liquid behavior of Stuttgart	D. Kveshchenko, NORDITA
13.02.1996	New phases in an extended Hubbard model explicitly including atomic polarizablities	J. van den Brink,Groningen
12.03.1996	Canted Spin Order and Localized States in the Three-Band Hubbard Model	M. Letz, Stuttgart
22.03.1996	Hawking Process in Solids: Relaxation Jumps of a Strong Vibrations	V. Hizhnyakov, Estonia
04.04.1996	Characterization of Quantum Chaos	S. Kettemann, Stuttgart
10.04.1996	Characterization of Quantum Chaos part II	S. Kettemann, Stuttgart
26.04.1996	An Introduction to phase coherent transport in mesoscopic superconductor	C.J. Lambert,Lancaster
03.05.1996	Percolation and Transport in Hierchical Random Networks	A.N. Samukhin, Petersburg
04.06.1996	Magnetic and Single-Particle Properties of the $t-J$ Model	T. Pruschke, Regensburg
19.06.1996	Quantization of Sinai's Billiard - A Scattering Approach	H. Schanz, Berlin
02.07.1996	Nonequilibrium Kondo Physics in Point Contacts and Tunnel Junctiuons	M. Hettler, Florida
09.07.1996	Macroscopic Quantum Tunneling of a Bose Condensate	H. Stoof, Utrecht
22.08.1996	Interacting electrons near filling factor one in the Quantum Hall Regime	M. Kasner, Stuttgart
27.09.1996	Magnetische Anregungen in Kupraten mit Seltenen Erden	G. Zwicknagel, Stuttgart
16.10.1996	From mixed valence to pseudo-one-dimensional spin chains in Yb_4As_3	B. Schmidt, Dresden

Termin	Thema	Vortragender
11.11.1996	Pyridine-Based Light-Emitted Polymers: Photophysics and Devices	A.J. Epstein, Ohio
19.11.1996	New family of exactly solvable 1D frustrated quantum spin models	A.A. Ovchinnikov, Moscow
11.03.1997	Tunneling into a quantum dot and the Kondo Physics: A tutorial	Y. Gefen, Rehovot
12.05.1997	Critical behavior of weakly disordered anisotropic spin systems in two dimensions in two dimensions	B.N. Shalaev, St. Petersburg
23.05.1997	Attenuation of surface acoustic waves	A. Knäbchen, Rehovot
06.06.1997	The Selfvonsitency Theory of Phase Transitions	D.I. Uzunov, Sofia
04.07.1997	Two dimensional quantum Heisenberg antiferromagnet: the continuum limit	S. Villain-Guillot, Paris

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Amtszeit bis 31.12.2000

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Stand: März 1998

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Deutsche wissenschaftliche Mitarbeiter 1996–1997 (inkl. Gastwissenschaftler und Doktoranden)

W = Wissenschaftler
D = Doktorand

Name	Zeitraum	W/D	Arbeitsthema
Abel, Markus	04/97	W	Localization in a sympletic coupled map system
Albrecht, Martin	6/96	D	Elektronische Korrelationen in Halbleitern
Altland, Alexander	8/96	D	Non-perturbative approach to chaos in mesoscopic systems and locization
Baer, Markus	11/95	W	Pattern formation
Bagehorn, Frank	4/97-12/97	W	Elektronische Korrelationen
Beck, Christian	11/96-12/96	W	Raumzeitliches Chaos
Blawid, Stefan	seit 3/1997	W	Berechnung von Eigenschaften stark korrelierten Elektronen
Blawid, Stefan	3/94-02/97	D	Berechnung von Eigenschaften stark korrelierten Elektronen
Bode, Mathias	6/96-7/96	W	Musterbildung in komplizierten Geometrien
Bode, Mathias	10/97-11/97	W	Hierarchische Systeme
Bolte, Jens	6/97	W	Global statics of quantum energies
Brenig, Wolfram	2/97-3/97	W	Elementare Anregung zu niedrigdimensionalen Spinsystemen
Bruder, Christoph	8/96-9/96	W	Non-perturbative approach to chaos in mesoscopic systems and localization
Bulla, Ralf	seit 9/97	W	Elektronische Korrelationen
Bünner, Martin	5/97-9/97	W	Nichtlineare Zeitreihenanalyse
Dahm, Thomas	seit 11/97	W	Elektronische Korrelationen
Deutsch, Andreas	9/97	W	Strukturbildung in komplexen Flüssigkeiten
Dippel, Sabine	11/97	W	Granulare Medien
Dittes, Frank Michael	1/97-3/97	W	Offene Quantensysteme
Dittrich, Thomas	6/96-2/98	W	Quantenchaos
Dolg, Franz Michael	seit 2/94	W	Quantenchemie
Doll, Klaus	3/95-2/96	D	Elektronische Korrelationen in Molekülen und Festkörpern
Doll, Klaus	3/96 -10/97	W	Quantenchemie
Drasdo, Dirk	9/97	W	Strukturbildung in komplexen Flüssigkeiten
Eckern, Ulrich	8/96	W	Non-perturbative approach to chaos in mesoscopic systems and localization

Name	Zeitraum	W/D	Arbeitsthema
Eckhard, Bruno	6/97	W	Wissenschaftliche Leitung des Symposiums
Egger, Reinhold	7/97-8/97	W	Novel physics in low-dimensional electron systems
Ernst, Gabriele	7/97-8/97	W	Novel physics in low-dimensional electron systems
Falcke, Martin	seit 6/97	W	Strukturbildung
Fischer, Kurt	10/94-10/97	W	Elektronische Korrelationen
Flach, Sergej	seit 9/94	W	Discrete breathers
Flad, Heinz-Jürgen	7/1994	W	Quantenchemie
Frauenkorn, Helge	10/97-11/97	W	Strukturbildung in komplexen Flüssigkeiten
Frey, Erwin	9/97	W	Pattern formation in complex fluids
Friedrich, Rudolf	9/97	W	Vorbereitung Workshop: Die Physik der Turbulenz
Gade, Renate	10/94-03/97	W	Quanten-Hall Effekt
Greiner, Martin	seit 9/97	W	Turbulenz
Güttler, Stefan	seit 4/96	D	Fehlerfrüherkennung mit nichtlinearer Zeitreihenanalyse
Hackenbroich, Gregor	9/96	W	Non-perturbative approach to chaos in mesoscopic systems and localization
Hallberg, Karen	7/97-8/97	W	Anwendung der Dichtematrix-Renommierungsgruppen-Methode
Hegger, Rainer	8/95	W	Nichtlineare Zeitreihenanalyse
Heid, Rolf	1/97	W	Gitterdynamik
Henseler, Michael	3/96	D	Nicht störungstheoretische Behandlung zeitabhängiger Streusysteme
Hetzel, Ralf	2/97-4/97	W	Elektronische Korrelationen
Hinrichsen, Haye	5/97	W	Phasenübergänge
Höfer,Thomas	12/96-10/97	W	Strukturbildung
Hüpper, Bruno	6/97-6/97	W	Semiclassical cross section
Jaeger, Lars	2/95-5/97	D	Signaturen nichtlinearer Dynamik in Zeitreihen
Jaeger, Lars	6/97-11/97	W	Nichtlineare Zeitreihenanalyse
Jakob, Peter	4/97	W	Localization and relaxation effects of weakly interacting dipoles
Just, Wolfram	seit 5/97	W	Nichtlineare Zeitreihenanalyse
Kalvoda, Simon	7/95	D	Untersuchung korrelierter Elektronensysteme im Hinblick auf die High-Tc-Supraleitung

Name	Zeitraum	W/D	Arbeitsthema
Kantz, Holger	seit 1/95	W	Nichtlineare Zeitreihenanalyse
Karshenboim	11/97-12/97	W	Theoretische Kernphysik
Kasner, Marcus	7/96-12/96	W	Elektronenkorrelation im starken Magnetfeld
Keller, Joachim	2/96	W	Stark korrelierte Elektronensysteme
Kettemann, Stefan	3/96-1/98	W	Elektronische Korrelationen
Khalilov, Samed	7/97- 12/97	W	Spinfluktuationen in itineranten Ferromagneten
Kilian, Rolf	7/96	D	Untersuchung des Effekts magnetischer Störstellen in Systemen mit korrelierten Leitungselektronen
Klemm, Thomas	10/96	W	Elektronische Korrelationen
Koepernik, Klaus	11/1996	W	Elektronische Korrelationen
Kohler, Sigmund	6/97	W	Quantum Chaos / Dissipation
Kornilovitch	3/97- 2/98	W	Monte-Carlo simulation von Elektron-Phonon Wechselwirkung
Kramer, Lorenz	10/97	W	Structurbildung in komplexen Flüssigkeiten
Kruse, Karsten	6/97	W	What determines the spreading of a wave packet
Küchle, Wolfgang	seit 1/97	W	Quantenchemie
Kurrer, Christian	11/97-12/97	W	Nichtlineare Dynamik und statische Physik Neuronaler Systeme
Lehner, Christoph	1/94-1/97	D	Die spektrale Dichte eines valenzfluktuierenden Systems
Lehner, Christoph	1/97-4/97	W	Elektronische Korrelationen
Letz, Martin	9/95-8/96	W	Elektronische Korrelationen
Letz, Tobias	11/96-2/98	W	Nichtlineare Zeitreihenanalyse
Main, Jörg	6/97	W	Periodic orbit quantization by harmonic inversion
Malek, Jiri	4/97-12/97	W	Wechselwirkung zwischen Elektronen und Breathers
Mallwitz, Steffen	7/95-6/96	D	Starke Korrelationen in f-Elektronensystemen
Mallwitz, Steffen	7/96-3/97	W	Elektronische Korrelationen
Massoth, Michael	2/95-7/98	D	Behandlung elektronischer Korrelationen mit quantenmechanischer Genauigkeit
Mayer, Andreas	4/97	W	Quantum aspects of self-localized solutions in discrete systems
Mehlig, Bernhard	seit 3/94	W	Quantenchaos
Mertins, Frank	4/96	W	Elektronische Korrelationen

Name	Zeitraum	W/D	Arbeitsthema
Mirbach, Bruno	11/96	W	Mesoskopische Systeme
Mödl, Martin	8/95-7/96	W	Quantenchemie
Müller, Hans-Walter	8/97-10/97	W	Oberflächenwellen in komplexen Flüssigkeiten
Müller-Gerking, Johannes	9/97-10/97	W	Strukturbildung in komplexen Flüssigkeiten
Nöckel, Jens-Uwe	seit 8/96	W	Quantenchaos
Olbrich, Eckehard	seit 12/97	W	Nichtlineare Zeitreihenanalyse
Or Guil, Michal	seit 1/97	W	Strukturbildung
Paulus, Beate	seit 1/96	W	Elektronische Korrelationen
Peinke, Joachim	9/97	W	Organisation des Workshops: Die Physik der Turbulenz
Peschel, Ingo	4/97	W	Statistische Physik
Peschel, Ingo	8/97-9/97	W	Statistische Physik
Pietig, Rainer	seit 12/97	W	Elektronische Korrelationen
Rau, Jochen	seit 10/96	W	Transporttheorie
Richter, Klaus	seit 1/96	W	Quantenchaos und mesoskopische Systeme
Rössler, Ulrich	11/96-12/96	W	Semiclassical approach to dynamical response
Rost, Jan-Michael	3/97	W	Review on Helium
Rzehak, Roland	8/97-9/97	W	Strukturbildung in komplexen Flüssigkeiten
Saalmann, Ulf	seit 11/96	W	Offene Quantensysteme
Schanz, Holger	seit 12/96-	W	Quantenchaos
Schautz, Friedemann	seit 2/97	D	Korrelierte Rechnungen für die elektronische Struktur von Festkörpern
Schliecker, Gudrun	seit 10/97	W	Strukturbildung
Schmüser, Frank	3/96	D	Übergang von effektiv niedrigdimensionaler Dynamik zu hochdimensionalem Chaos
Schomerus, Henning	6/97	W	Semi classical spectra from periodic-orbit clusters in amixed phase space
Schöne, Michael	5/97-7/97	W	Elektronische Korrelationen
Schork, Thomas	7/93-9/97	W	Elektronische Korrelationen
Schröder, Ulrich	9/97	W	Struktur und Dynamik von Halbleiteroberflächen
Schwarz, Ulrich	4/97	W	Localization in nonlinear lattic
Sieber, Martin	6/97	W	Semiclassical interpretation of the mass asymmetry in nuclear fission

Name	Zeitraum	W/D	Arbeitsthema
Sinde, Erik	seit 4/97	D	Nichtlineare Zeitreihenanalyse
Stephan, Walter	1/96-3/98	W	Korrelierte Elektronensysteme
Stoll, Hermann	seit 11/96	W	Quantenchemie
Tanner, Gregor	3/97	W	Review on Helium
Tanner, Gregor	6/97	W	Qantum manifestations classical intermittency
Taut, Manfred	1/97-4/97	W	Gitterdynamik
Thalmeier, Peter	seit 9/94	W	Schwere Fermionen
Timmer, Jens	11/97	W	Zeitreihenanalyse
Torcini, Alessandro	10/97	W	Strukturbildung in komplexen Flüssigkeiten
Utzny, Clemens	4/96	D	Musterbildung in komplizierten Geometrien und heterogenen Medien
Van Oppen, Felix	8/96-9/96	W	Non-perturbative approach to chaos in mesoscopic systems
Van Oppen, Felix	7/97-8/97	W	Novel physics in low-dimensional electron systems
Vietze, Knut	10/97	D	Beschreibung des Elektronensystems in endohedralen Seltenerd-Fullerenen
Vojta, Matthias	3/96-7/96	W	Elektronische Korrelationen
Vojta, Matthias	5/97-9/97	W	Elektronische Korrelationen
Waalkens, Holger	6/97	W	Elliptic quantum billiards
Wackerbauer, Renate	11/96	W	Nichtlineare Zeitreihenanalyse
Wagner, Max	4/97	W	Quantum aspects of self-localized solutions in discrete systems
Wegner, Franz	8/96-9/96	W	Non-perturbative approach to chaos in mesoscopic systems and localization
Weinmann, Dietmar	6/97	W	Level statistics for a few interacting particles in disordered systems
Weniger, Ernst	4/97-5/97	W	Konvergenzbeschleunigung und Summation spezieller Funktionen
Wenschuh, Ullrich	7/95-8/96	D	Theorie der Phononen-Dynamik in Halbleitern fern vom thermodynamischen Gleichgewicht
Wenschuh, Ullrich	seit 9/96	W	Theorie der Phononen-Dynamik in Halbleitern fern vom thermodynamischen Gleichgewicht
Wirzba, Andreas	6/97	W	Quantum mechanics and semiclassics of N-disk scattering systems

Name	Zeitraum	W/D	Arbeitsthema
Ziegler, Klaus	seit 7/95	W	Elektronische Korrelationen
Zimmermann, Walter	9/97-12/97	W	Strukturbildung in komplexen Flüssigkeiten und biologischen Systemen
Zirnbauer, Martin	8/96	W	Non-perturbative approach to chaos in mesoscopic systems and localization
Zülicke, Ulrich	7/97-8/97	W	Novel physics in low-dimensional electron systems
Zwicknagl, Gertrud	7/96-12/97	W	Elektronische Korrelationen

Ausländische Gastwissenschaftler und Doktoranden 1996 - 1997

W = Wissenschaftler
D = Doktorand

Name	Land	Zeitraum	W/D	Arbeitsthema
Abramson, Giullermo	Argentinien	11/97	W	Selbstorganisation in Evolutionsmodellen
Abusch-Magder, David	USA	8/97	W	Novel physics in Low-dimensional electron systems
Agam, Oded	Israel	8/96-9/96	W	Non-perturbative approach to chaos in mesoscopic systems
Agam, Oded	Israel	6/97	W	Field theory approach to quantum chaos
Ahlers, Günther	USA	9/97	W	Strukturbildung in biologischen Systemen
Akera, Hirothi	Japan	7/97-8/97	W	Novel physics in Low-dimensional electron systems
Alhassid, Yoram	Israel	8/96-9/96		Non-perturbative approach to chaos in mesoscopic systems and localization
Allekotte, Ingomar	Argentinien	8/93-10/97	W	Leiter Gästeprogramm
Andreev, Anton	Russland	8/96-9/96		Non-perturbative approach to chaos in mesoscopic systems and localization
Antoni, Mikael	Frankreich	7/96-	W	Self consistent study of N-Body Hamiltonian systems
Antonov, Victor	Russland	10/97-12/97	W	First principle Untersuchungen der elektronischen Struktur
Aoki, Hideo	Japan	7/97-8/97	W	Novel physics in Low-dimensional electron systems
Aronson, Igor	Israel	10/97	W	Strukturbildung in komplexen Flüssigkeiten
Arrachea, Liliana	Argentinien	11/97-2/98	W	Stark korrelierte Systeme
Ashoori, Raymond	USA	7/97-8/97	W	Novel physics in Low-dimensional electron systems
Aubry, Serge	Frankreich	4/97	W	Breather mobility
Ausländer, Ohir	Israel	6/97	W	Exact eigenfunctions of a chaotic system
Baesens, Claude	Belgien	4/97	W	Exponential localization in networks with exponentially decaying interactions

Name	Land	Zeitraum	W/D	Arbeitsthema
Bala, Jan	Polen	7/96-12/96	W	Stark korrelierte Elektronensysteme
Bala, Jan	Polen	8/97-9/97	W	Starke Korrelationen in Hochtemperatur-Supraleitern
Bambusi, Dario	Italien	4/97	W	Are breathers in hamilton networks of oscillators attractive
Bangia, Anil	Indien	3/96-4/96		Bifurcations in reaction-diffusion systems
Baranger, Harold	USA	8/96		Non-perturbative approach to chaos in mesoscopic systems and localization
Beenakker, Carlo	Niederlande	8/96		Non-perturbative approach to chaos in mesoscopic systems and localization
Bishop, Alan	USA	4/97	W	Classical and quantum localization and decay in nonlinear lattices
Bogdan, Mikhail	Ukraine	8/97-11/97	W	Soliton coherent structures in low-dimensional systems
Bonesteel, Nick	USA	7/97-8/97	W	Novel physics in Low-dimensional electron systems
Borkowski, Lech	Polen	6/96		Magnetische Verunreinigungen in gap-losen Fermionensystemen
Boschee, Mathias	Frankreich	seit 2/97	S	Elektronische Korrelationen
Butcher, Paul	Großbritanien	7/97-8/97	W	Novel physics in Low-dimensional electron systems
Cafiero, Raffaelo	Italien	1/97-	W	Selbstorganisierte Kritikalität und fraktales Wachstum
Campbell, David	USA	4/97	W	4 Theory: still a few kinks in the system
Canals, Benjamin	Frankreich	seit 12/97	W	Unordnungseinfluß in Quantenspinflüssigkeiten
Capezzali, Massimiliano	Italien	9/97-10/97	W	Stark korrelierte Elektronensysteme
Castella, Herve	Schweiz	10/97-	W	Ultraschnelle Phänomene in Halbleitern
Chakraborty, Tapash	Indien	5/97-	W	Niedrigdimensionale Elektronen-systeme
Chalker, John	Großbritanien	8/96		Non-perturbative approach to chaos in mesoscopic systems and localization

Name	Land	Zeitraum	W/D	Arbeitsthema
Chattopadhyay, Tapan	Indien	8/95-2/98	W	Röntgenmessung an Einkristallen
Choquard, Phillippe	Schweiz	4/97	W	Dynamische Systeme und Statistische Mechanik
Christiansen, Freddy	Dänemark	5/96-	W	Chaos und Quantenchaos in niedrigdimensionalen Systemen
Cohen, Avraham	Israel	3/97-5/97	W	Dauerströme in mesoskopischen Systemen
Cohen, Avraham		6/97	W	Persistent currents in continuous one-dimensional disordered rings
Cohen, Doron	Israel	6/97	W	Quantal classical duality and the semiclassical trace formula
Conti, Sergio	Italien	7/97-8/97	W	Novel physics in Low-dimensional electron systems
Cooper, Nigel	Großbritanien	7/97-8/97	W	Novel physics in Low-dimensional electron systems
Creagh, Stephen	Irland	6/97	W	Tunneling in chaotic systems
Cretegny, Thierry	Schweiz	4/97	W	Plane wave scattering by breathers
Davies, Mike	Grobritanien	2/97	W	nonlinear dynamics
De Los Rios, Paolo	Italien	11/96-10/97	W	Statistische Mechanik von ungeordneten Systemen
Deo, Shingha	Indien	7/97-8/97	W	Novel physics in low-dimensional electron systems
Dorozhkin, Sergei	Russland	7/97-8/97	W	Novel physics in Low-dimensional electron systems
Dotsenko, Alexander	Russland	6/97-	W	Hochtemperatur Supraleitung
Duke, Thomas	Großbritanien	8/97-9/97	W	Pattern formation in complex fluids
Dusi, Roberto	Italien	4/97	W	On the wing behaviour of the overtones of self-localized
Dyugaev, Alexander	Russland	4/97-6/97	W	Magnetic properties of superconductors
Dyugaev; Alexander		8/97	W	Magnetische Verunreinigung in Metallen
Efetov, Konstantin	Russland	1/95-4/97	W	Mesoscopic systems
Eilbeck, I. Chris	Großbritani	4/97	W	Longitudinal breathers in 1-D and 2-D

Name	Land	Zeitraum	W/D	Arbeitsthema
Ellinas, Demosthenes	Griechenland	4/97	W	q-Symmetries, site-entanglement and semiclassics in quantum models
Epstein, Arthur	USA	11/96		Photophysics of Pyridin-based polymers
Falko, Vladimier	Russland	7/96-9/96	W	Non-perturbative approach to chaos in mesoscopic systems and localization
Fazekas, Patrik	Ungarn	6/97-7/97	W	Applications of the Gutswiller variational method for the correlated two-band models
Ferell, Richard	USA	9/97	W	Supraleitung mit moduliertem Ordnungsbarometer
Fillaux, Francois	Frankreich	4/97	W	Inelastic neutron scattering studies of quantum breathers
Finkelstein, Alexander	Israel	8/96	W	Non-perturbative approach to chaos in mesoscopic systems and localization
Fishman, Shmuel	Israel	12/96	W	Fredholm-Theorie und Quantenchaos
Fleurov, Victor	Israel	2/96-3/96	W	Chaos-assisted tunneling
Fleurov, Victor		8/96-9/96		Quantum Breathers
Fleurov, Victor		4/97		Tunneling in the nonintegrable trimer-a step towards quantum breathers
Fleurov, Victor		8/97		Quantum Breathers
Floria, Luis Mario	Spanien	4/97	W	Localization in Josephson junctions ladders and other forced-damped physical systems
Fogler, Michael	Russland	7/97-8/97	W	Novel physics in low-dimensional electron systems
Frustaglia, Diego	Argentinien	8/97-	D	Strukturbildung und komplexe Systeme
Fyodorov, Yan	Russland	9/97		Non-perturbative approach to chaos in mesoscopic systems and localization
Gangardt, Dimitry	Israel	6.97	W	Semiclassical desription of interacting electrons
Garanin, Dimitry	Russland	12/97-	W	Magnetische Systeme

Name	Land	Zeitraum	W/D	Arbeitsthema
Gefen, Yuval	Israel	8/96-9/96		Non-perturbative approach to chaos in mesoscopic systems and localization
Geller, Michael	USA	7/97-8/97	W	Novel physics in low-dimensional electron systems
Giaquinta, Antonio	Italien	6/97-7/97	W	Nonlinear time series analysis from experiment
Ginzburg, Ilya	Russland	11.97	W	Kernkollisionent
Goldberg, Bennett	USA	7/97-8/97	W	Novel physics in low-dimensional electron systems
Goldhaber-Gordon, David	USA	7/97-8/97	W	Novel physics in Low-dimensional electron systems
Grimaldi, Claudio	Italien	2/94-3/97	D	
Gurian, George	Russland	11/97-12/97	W	Strukturbildung in komplexen Flüssigkeiten
Ha,Zachari	USA	7/97-8/97	W	Novel physics in low-dimensional electron systems
Hallberg, Karen	Argentinien	8/94-2/97	W	Elektronische Korrelationen
Hallberg, Karen		7/97-8/97		Anwendung der Dichtematrix-Renommierungsgruppen-Methode zu stark korrelierten Elektronensystemen
Halperin, Bertrand	USA	7/97-8/97	W	Novel physics in low-dimensional electron systems
Hayne, Manus	Großbritanien	7/97-8/97	W	Novel physics in Low-dimensional electron systems
Hikami, Shinobu	Japan	8/96		Non-perturbative approach to chaos in mesoscopic systems and localization
Hoang, Anh Tuan	Vietnam	4/95-4/96		Elektronische Korrelationen
Hong, Gongy	China	seit 10/97	W	Chemie der f-Elemente
Huang, Gouxiang	China	11/95-2/96	W	Nichtlineare Anregungen in Systemen kondensierter Materie
Huang, Gouxiang		5/97-7/97		Nichtlineare Anregungen in stabilen und instabilen Medien
Igarashi, Yun Ichi	Japan	4/96	W	Schwere Fermionen
Igarashi, Yun Ichi		7/96-8/96		Schwere Fermionen
Igarashi, Yun Ichi		7/97-8/97		Stark korrelierte Elektronensysteme
Inomata, Akira	Japan	6/97	W	Gutswillers trace formula in super-symmetric quantum mechanics

Name	Land	Zeitraum	W/D	Arbeitsthema
Ivanov, Vladimir	Russland	11/97	W	Theoretische Kernphysik
Jain, Jainendra	Indien	7/97-8/97	W	Novel physics in low-dimensional electron systems
Jaklic, Janez	Slowenien	2/97-6/97	W	Eigenschaften der Kondo-Gitter
Johansson, Magnus	Schweden	4/97	W	Dynamics of breathers in DNLS
Jug, Giancarlo	Italien	8/97	W	theoretical research at the frontiers of many-body Physic
Kabanov, Victor	Russland	10/97-11/97	W	Magnetfelddefekte beim Supraleitungsübergang
Kaga, Hiroyuki	Japan	7/96-8/96	W	Magnetic Properties of the Hubbard-Model
Kagalovsky, Victor	Israel	7/97-8/97	W	Novel physics in Low-dimensional electron systems
Kagan, Yuri	Russland	9/97	W	Kondensation wechselwirkender Bosonen
Kakehashi, Yoshiro	Japan	4/96		Magnetische Momente in Übergangsmetallsystemen
Kaplan, Lev	USA	6/97	W	Weak quantum ergodicity
Karlhede, Aners	Schweden	7/97-8/97	W	Novel physics in low-dimensional electron systems
Karshenboim Savely	Russland	11/97-12/97	W	Theoretische Kernphysik
Karshenboim, Savely		2/97-4/97		Relativistische und QED-Effekte in atomaren Systemen
Kashinje, Stanslaus	Tanzania	10/96-9/97	W	Heavy Fermions in strongly correlated electron systems
Kats, Efim	Russland	10/97-12/97	W	Physik der weichen Materie
Katsnelson, Mikhail	Russland	10/96-11/96		Stark korrelierte Elektronen-systeme
Kawakatsu, Toshiro	Japan	8/97-9/97	W	Pattern formation in complex fluids
Kessler, David	Israel	8/97-9/97	W	Pattern formation in complex fluids
Khalilov, Samed	Russland	7/97-12/97		Spinfluktationen in itineranten Ferromagneten
Khaliullin, Giniyat	Russland	10/96-	W	Stark korrelierte Elektronen-systeme
Khalilov, Samed	Russland	7/97-12/97		Spinfluktationen in itineranten Ferromagneten

Name	Land	Zeitraum	W/D	Arbeitsthema
Khaliullin, Giniyat	Russland	10/96-	W	Stark korrelierte Elektronen-systeme
Khmelnitskii, David	Russland	8/96	W	Non-perturbative approach to chaos in mesoscopic systems and localization
Kinaret, Jari	Finnland	7/97-8/97	W	Novel physics in low-dimensional electron systems
Kivshar, Yuri	Australien	4/97	W	Nonlinear surface and impurity modes
Kladko, Konstantin	Russland	8/95-	D	Elektronische Korrelationen
Koga, Mikoto	Japan	1/97-9/97	W	Schwere Fermionensysteme
Kornilovitch, Pavel	Russland	3/97-2/98	W	Monte-Carlo Simulation von Elektron-Phonon Wechselwirkung
Kornilovitch, Pavel		1/97	W	Elektronenkorrelationseffekte in Hochtemperatursupraleitern
Korolev, Andrei	Russland	2/96-3/97	W	Exziton Zustände in stark korrelierten Systemen
Kossevich Arnold	Ukraine	4/97	W	Semiclassical quantization of magnetic solitons
Kossevich, Arnold		11/96-12/96		Nichtlineare Dynamik der kondensierten Materie
Krasovsky, Igor	Ukraine	seit 8/97	W	Bloch-Elektron im magnetischen Feld
Kukushkin, Igor	Russland	7/97-8/97	W	Novel physics in low-dimensional electron systems
Kuramoto, Yoshiki	Japan	10/97	W	komplexe Dynamik großer Systeme gekoppelter Oszillatoren
Kyung, Bumsoo	Korea	7/96-	W	Normal state of high Tc superconductors
Leadbeater, Mark	Großbritanien	10/96-	W	Mesoscopic phenomena in normal metal superconductor hybribrid structures
Lehmann, Kevin	USA	4/97	W	Localized vibrations in polyatomic molecules
Leininger, Thierry	Frankreich	10/96-8/97	W	Kopplung von Elektronen-Korrelation und Relativistischen Effekt
Lejnell, Kennet	Schweden	7/97-8/97	W	Novel physics in Low-dimensional electron systems

Name	Land	Zeitraum	W/D	Arbeitsthema
Lepri, Stephano	Italien	2/97-	W	Chaos in räumlich ausgedehnten Systemen
Lerner, Igor	Russland	8/96		Non-perturbative approach to chaos in mesoscopic systems and localization
Li, Yanmin	China	8/96-9/96	W	Jahn-Teller-Effekt vs. elektronischen Korrelationen
Lilliehöck, Daniel	Schweden	7/97-8/97	W	Novel physics in Low-dimensional electron systems
Lipa, Peter	Österreich	4/97	W	Translationsinvarianz in turbulenten Kaskadenmodellen
Liu, Wenjan	China	9/95-12/97	W	Quantenchemische Untersuchungen an Verbindungen
Liu, Yu-Liang	China	7/96-1/98	W	Stark korrelierte Elektronensysteme und Quanten-Hall-Effekt
Livi, Roberto	Italien	4/97	W	Heat conduction in anharmonic chains
Loos, Daniel	Schweiz	8/97	W	Novel physics in low-dimensional electron systems
Lozovik, Yurij	Russland	7/97-8/97	W	Novel physics in low-dimensional electron systems
Macedo, Antonio	Brasilien	8/96	W	Non-perturbative approach to chaos in mesoscopic systems and localization
MacKay, Robert	Großbritanien	4/97	W	Leitung des Workshops LNL
Maki, Kazumi	Japan	4/96	W	Supraleitung mit unkonventioneller Paarung
Maki, Kazumi		6/96	W	D-wave Supraleitung
Maki, Kazumi		5/97	W	D-wave superconductivity
Maki, Kazumi		9/97	W	Unkonventionelle Supraleiter
Maksym, Piotr	Großbritanien	8/97	W	Novel physics in low-dimensional electron systems
Malek, Jiri	Tschechien	9/96-12/96	W	Electron-phonon coupling in strongly correlated systems
Malek, Jiri		4/97-12/97	W	Wechselwirkung zwischen Elektronen und Breathers
Malomed, Boris	Israel	11/97	W	Strukturbildung in komplexen Flüssigkeiten
Manfra, Michael	USA	7-97-8/97	W	Novel physics in low-dimensional electron systems
Marin, Jose Luis	Spanien	4/97	W	Numerical calculations of breathers

Name	Land	Zeitraum	W/D	Arbeitsthema
Marsili, Matteo	Italien	8/97	W	Stochastische Dynamik in der Spieltheorie
Martinez, Gerardo	Brasilien	7/97-8/97	W	Systeme korrelierter Fermionen
Matsushita, Mitsugu	Japan	9/97	W	Pattern formation in complex fluids
Mc Cann, Edward	Großbritanien	3/96-2/97	W	Elektronische mesoskopische Systeme
Meron, Ehud	Israel	9/97	W	Strukturbildung in komplexen Flüssigkeiten
Meservey, Robert	USA	4/96	W	Tunneln zwischen Ferromagneten
Mikhailov, Sergey	Russland	seit 5/97	W	Kollektive Anregungen
Mila, Frederic	Frankreich	5/97	W	New aspects of the 1D-2D cross-over: persistent currents
Miller, Daniel L.	Israel	6/97	W	Quantal-classical duality and the semiclassical trace formula
Mishbah, Chaouqi	Frankreich	8/97-10-97	W	Strukturbildung in komplexen Flüssigkeiten
Mishra, Ashok Kumar	Indien	9/97-11/97	W	Stark korrelierte Systeme
Misiak, Mikolaj	Polen	9/97	W	B-Meson Physics
Mizuguchi, Tsuyoshi	Japan	11/97	W	Strukurbildung in komplexen Flüssigkeiten
Mudry, Christopher	USA	8/97	W	Non-perturbative approach to chaos in mesoscopic systems and localization
Muldoon, Mark	USA/Irland	3/97	W	Nichlineare Rauschunterdrückung
Muzykantskii, Boris	Russland	8/97	W	Non-perturbative approach to chaos in mesoscopic systems and localization
Nefiedov, Andrei	Russland	9/97	W	Quantum electrodynamical effects in mulitcharged ions
Nepomnyashchy, Alexander	Israel	9/97-10/97	W	Nicht-potentiale Effekte bei Strukturbildung
Nicola, Ernesto Miguel	Italien	seit 3/96	D	Instability of reaction-diffusion waves and transition to spatiotemporal chaos
Niemelä, Kari	Finnland	2/97-8/97	W	Novel physics in low-dimensional electron systems
Nieuwpoort, Willem	Niederlande	4/97-6/97	W	Ab-inito quantum chemical approaches
Nifosi, Gerardo	Italien	8/97	W	Novel physics in low-dimensional electron systems
Oreg, Yuval	Israel	8/96	W	Non-perturbative approach to chaos in mesoscopic systems and localization

Name	Land	Zeitraum	W/D	Arbeitsthema
Orgad, Dror	Israel	8/97	W	Novel physics in low-dimensional electron systems
Ovchinnikov, Alexandre	Russland	11/96-12/96	W	Frustrierte eindimensionale Quantenspinsysteme
Ovchinnikov, Yuri	Russland	6/96	W	Nichttriviale Lösungen der Landau-Ginzburg Gleichung
Ovchinnikov, Yuri		4/97-6/97	W	Magnetic properties of Superconductors
Ovchinnikov, Yuri		8/97	W	Magnetische Verunreinigung in Metallen
Paalanen, Mikko	Finnland	8/97	W	Novel physics in low-dimensional electron systems
Page, John	USA	4/97	W	Optical creation of instrinsic localized modes
Penc, Karlo	Ungarn	9/95-9/97	W	Stark korrelierte Elektronensysteme
Perlov, Alexander	Ukraine	10/97-4/98	W	Magnonenspektren und Magnetismus bei endlichen Temperaturen
Persson,Emil	Schweden	11/96-12/97	W	...
Peyrard, Michel	Frankreich	4/97	W	Mechanism for the localization of thermal energy in nonlinear lattices
Pichard, Jean Louis	Frankreich	8/96	W	Non-perturbative approach to chaos in mesoscopic systems and localization
Pichaureau, Paul	Frankreich	6/97	W	Ballistic transport in integrable cavities
Pietiläinen, Pekka	Finnland	8/97	W	Novel physics in low-dimensional electron systems
Pinczuk, Aron	Argentinien	7/97	W	Novel physics in low-dimensional electron systems
Pismen, Leonid	Israel	10/97	W	Strukturbildung in komplexen Flüssigkeiten
Plaut, Annette	Großbritanien	8/97	W	Novel physics in low-dimensional electron systems
Pleutin, Stephane	Frankreich	seit 11/97	W	Quantum chemistry of the excited State
Prigodin, Vladimir	Russland	1/95-5/97	W	Mesoskopische Systeme
Primack,Harel	Israel	6/97	W	Accuracy of trace formula in two and three dimensions
Priusken, Adrianus	Niederlande	8/96	W	Non-perturbative approach to chaos in mesoscopic systems and localization
Pumir, Alain	Frankreich	9/97	W	Strukturbildung in komplexen Flüssigkeiten

Name	Land	Zeitraum	W/D	Arbeitsthema
Quinn, John	USA	7/97	W	Novel physics in low-dimensional electron systems
Read, Nicholas	Großbritanien	8/97	W	Novel physics in low-dimensional electron systems
Robin, Jean Marc	Frankreich	seit 2/97	W	Starke Korrelationseffekte in Elektron-Phonon Systemen
Rosciszewski, Krzysztof	Polen	4/96	W	Intra-atomic correlation energy in molecules
Rosciszewski, Krzysztof	Polen	7/97-10/97	W	Elektronenkorrelation in Molekülen und Festkörpern
Sachrajda, Andrew	Kanada	8/97	W	Novel physics in low-dimensional electron systems
Salerno, Mario	Italien	4/97	W	SO(4) invariant basis functions for strongly correlated fermi systems
Sauer, Timothy	USA	4/97	W	Nichtlineare Zeitreihenanalyse
Sepulchre, Jaques-Alexander	Belgien	4/97	W	Stability of discrete breathers
Serbo, Valery	Russland	11/97	W	Kernkollisionen
Serhan, Mohammed	Jordanien	2/96-8/97	W	Wechselwirkung einer magnetischen Verunreinigung mit korrelierten Leitungssystemen
Shabaev, Vladimir	Russland	6/97-7/97	W	Nuclear recoil corrections
Shankar, Ramachandra	Indien	7/97-8/97	W	Novel physics in low-dimensional electron systems
Shen, Shun-Qing	China	5/95-2/97	W	Supercoreductivity and magnetism in Hubbard-Model
Shi, Fajian	China	8/95-1/97	W	Quantenchemie
Shiina, Ryosuke	Japan	6/97-7/97	W	Quadrupolar ordering in CeB6
Shukla, Alok	Indien	6/95-12/97	W	Quantenchemie
Sievers, Albert	USA	4/97	W	Search for instrinsic localized modes in crystals
Simons, Ben	Großbritanien	8/96- 9/96	W	Non-perturbative approach to chaos in mesoscopic systems and localization
Smilansky, Uzy	Israel	5/97	W	Quantum chaos on graphs
Smith, Robert	Großbritanien	8/96-9/96	W	Non-perturbative approach to chaos in mesoscopic systems and localization
Spicci, Mauro	Italien	4/97-3/98	W	Diskrete Breathers in nichtlinearen Gittern
Stafford, Charles	USA	8/97	W	Novel physics in low-dimensional electron systems
Steinberg, Vicror	Israel	9/97	W	Pattern formation, turbulence
Stern, Ady	Israel	7/97-8/97	W	Novel physics in low-dimensional electron systems
Subrahmanyam, Vemuru	Indien	9/95-8/96	W	Antiferromagnetism

Name	Land	Zeitraum	W/D	Arbeitsthema
Sütö, Andreas	Ungarn	10/97	W	Strukturbildung in komplexen Flüssigkeiten
Tachiki, Masashi	Japan	5/96-6/96	W	Supraleitende Eigenschaften von stark korrelierten Elektronen-systemen
Takeno, Shozo	Japan	4/97	W	Nonlinear localized modes
Tejedor, Carlos	Spanien	7/97-8/97	W	Novel physics in low-dimensional electron systems
Thang, Nguyen Toan	Vietnam	10/97-11/97	W	Stark korrelierte Elektronen-systeme
Tien, Tran-Minh	Vietnam	1/94-11/97	D	Elektronische Korrelationen
Tien, Tran-Minh	Vietnam	seit 12/97	W	Elektronische Korrelationen
Tognetti, Valerio	Italien	4/97	W	Thermodynamics of two- dimen-sional quantum antiferromagnets by effective potential approach
Torcini, Alessandro	Italien	12/96	W	Phasenübergänge und Transport in Hamiltonschen Systemen
Torcini, Alessandro	Italien	10/97	W	Strukturbildung in komplexen Flüssigkeiten
Ulloa, Sergio	Mexiko	7/97-8/97	W	Novel physics in low-dimensional electron systems
Uzunov, Dimo	Bulgarien	4/97-7/97	W	Statistische Physik komplexer Systeme kondensierter Mater
Valleriani, Angelo	Italien	seit 11/96	W	Quantenfeldtheoretische Metho-den in der statistischen Mechanik
Van der Zant, Herre	Holland	4/97	W	Josephson junction arrays as model systems
Van Hecke, Martin	Holland	10/97	W	Lokale Strukturen in raumzeitlicher intermittency
Van Hemmen, Leo	Niederlande	10/97	W	Strukturbildung in komplexen Flüssigkeiten
Van Oosten, Toni	Holland	7/96-8/97	W	Magnetic inter-actions in cuprates by ab initio quantum chemistry
Vega Sanchez, Jose Luis	Spanien	seit 11/96	W	Conductance in nanowires
Vignale, Giovanni	Italien	7/97-8/97	W	Novel physics in Low-dimensional electron systems
Villain-Guillot, Simon	Frankreich	seit 10/97	W	Feldtheorie in niedrige Dimensionen
Walker, Paul	Großbritanien	4/96- 5/96	W	Mesoskopische Systeme
Wang, Xiaoqun	China	2/94-2/96	W	Thermodynamik eindimension-aler Quantensysteme mit der DMRG-Methode
Wang, Xiaoqun	China	4/97	W	Thermodynamik eindimension-aler Quantensysteme mit der DMRG-Methode

Name	Land	Zeitraum	W/D	Arbeitsthema
Wang, Yxuan	China	7/97	W	Quantum chemistry
Weijer, Cornelis Jan	Niederlande	9/97	W	Pattern formation in complex fluids
Whelan, Niall	Irland	6/97	W	Complex periodic orbits and tunneling between chaotic wells
Willett, Robert	USA	7/97-8/97	W	Novel physics in low-dimensional electron systems
Wolf, György	Ungarn	12/97-2/98	W	Untersuchung von Hadron-Kern und Kern-Kernstößen
Wolf, Wilfried	Österreich	5/97-4/98	W	Strukturbildung
Xi, Haoven	China	10/97	W	Strukturbildung in Systemen fernab vom Gleichgewicht
Xie, Qian	China	9/96-12/97	W	Embedded-Cluster approach to defects in solids
Yacoby, Amir	Israel	7/97-8/97	W	Novel physics in low-dimensional electron systems
Yan, Dadong	China	seit 11/97	W	Stark korrelierte Systeme
Yaresko, Alexander	Ukraine	10/97-4/98	W	First principle Untersuchungen der anisotropen Austauschkopplung in Ce
Yoshioka, Daijiro	Japan	7/97-8/97	W	Novel physics in low-dimensional electron systems
Yu, Ming	China	4/95-3/97	W	Quantum chemistry
Zevin, Vilen	Israel	7/96-8/96	W	Schwere Fermionensysteme
Zhang, Guoping	China	5/96-7/97	W	Quantum chemistry
Zimmermann, Martin	Argentinien	4/97-9/97	W	Pulse bifurcations in reaction-diffusion-equations