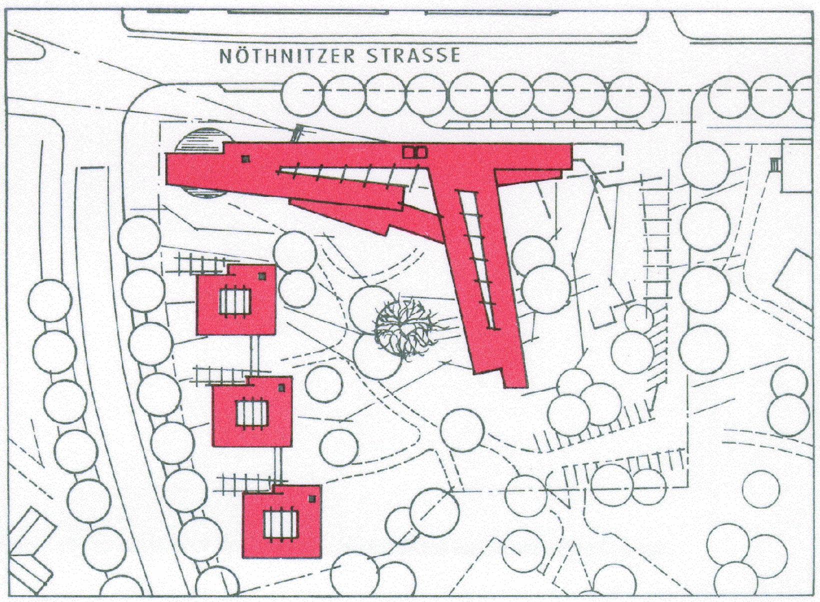
MAX-PLANCK-INSTITUT FÜR
PHYSIK KOMPLEXER SYSTEME
DRESDEN

1994 - 1995



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Cover: plan of the MPI for Physics of Complex Systems on Nöthnitzer Street.

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Wissenschaftlicher Tätigkeitsbericht
des Max-Planck-Instituts
für Physik komplexer Systeme
für den Zeitraum
vom 1. Januar 1994 bis zum 31. Dezember 1995

MAX-PLANCK-INSTITUT FÜR PHYSIK KOMPLEXER SYSTEME

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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. Die Räumlichkeiten in der Bayreuther Straße wurden von der Technischen Universität zur Verfügung gestellt. Gleichzeitig wurde mit der Planung und dem Bau eines Institutsgebäudes sowie dreier Gästehäuser begonnen. Bis Mitte 1997 sollen die Gebäude bezugsfertig sein. Da bis zum Einzug in den Neubau die Platzverhältnisse im Provisorium sehr begrenzt sind, ist ein kleiner Teil der Mitarbeiter zwischenzeitlich am MPI für Festkörperforschung in Stuttgart untergebracht. Zur Gewährleistung einer guten Zusammenarbeit und Kommunikation ist das Dresdner Institut mit seiner Stuttgarter Außenstelle über eine Videokonferenzschaltung verbunden, mit deren Hilfe Seminare von Dresden nach Stuttgart und umgekehrt übertragen werden können. Gegenwärtig zählt das Institut rund 77 Mitarbeiter und Doktoranden. Darunter befinden sich vier wissenschaftliche Nachwuchsgruppen.

Zu Hochschulen und außeruniversitären Forschungseinrichtungen des In- und Auslands 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 mit dem 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.

Es ist vorgesehen, daß im Endausbau das Institut aus drei theoretischen Abteilungen besteht. Daneben gibt es ein sehr umfangreiches Gästeprogramm, mit dessen Hilfe später drei- bis sechsmonatige Seminarveranstaltungen abgehalten werden sollen. Sie werden sich mit Themen auf dem Gebiet der Physik komplexer Systeme befassen, die sich in besonders starker Entwicklung befinden. In diesen Veranstaltungen wird der Nachwuchs der Hochschulen Gelegenheit erhalten, mit führenden Wissenschaftlern aus dem In- und Ausland zusammenzukommen. Neuentwicklungen sollen auf diese Weise früher als bisher sichtbar gemacht werden und junge Wissenschaftler sollen ermutigt werden, sich daran zu beteiligen.

Das Institutskonzept kann nur erfolgreich sein, wenn es von den Wissenschaftlern auch angenommen wird. Aus diesem Grund bemüht sich das Institut um Transparenz und Offenheit. Der Wissenschaftliche Beirat und das Kuratorium sind wichtige Gremien zur Förderung dieser Bemühungen.

Dresden, im Juni 1996 P. Fulde

Preface

The Max Planck Institute for Physics of Complex Systems was created by a resolution of the Senate of the Max Planck Society of November 1992. It is the third Max Planck Institute in former East Germany and the first 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. The building in Bayreuther Street was ceded by the University of Technology. Simultaneously the planning and construction of the institute's new building and of three guest houses was started. These buildings should be finished by mid 1997. Because of scarcity of space until completion of the new institute, a small number of co-workers is provisorily accomodated at the MPI for Solid State Research in Stuttgart. To ensure good communication and a cooperative work the institutes in Dresden and Stuttgart are connected through a video–conferencing system, with which seminars can be transmitted between both sites. At present the institute counts around 77 members including guests, Ph.D. students and four groups of young researchers.

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. With the Dresden University of Technology we are closely related through lectures and the participation in a Sonderforschungsbereich.

At its final stage, the institute is expected to consist of three theoretical groups. Additionally, the institute's concept includes a very large visitors program, within the frame of which we will organize seminars of three to six months duration. These will pick up subjects related to physics of complex systems which are in fast evolution. These seminar programs will give young scientists at the universities the possibility of finding contact to leading scientists at international level. In this way, new developments will be accessible at an earlier stage, which should encourage young scientists to take part on them.

The concept for the institute will be successful only if it is accepted by the scientific community. For this reason the institute makes great efforts to guarantee transparency and openness. The scientific advisory board and the board of trustees are important committees to promote these efforts.

Dresden, June 1996 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 zur Beschreibung elektronischer Korrelationen man auch die Wellenfunktion des Grundzustands eines Festkörpers mit derselben Genauigkeit beschreiben kann, wie es bisher für kleinere Moleküle der Fall war.

Das Arbeitsprogramm der Abteilung teilt sich auf in die Untersuchung schwach und stark korrelierter elektronischer Systeme. Bei den schwach korrelierten Systemen haben wir den Grundzustand der Elementhalbleiter sowie der III - V Verbindungen untersucht. Neben der Wellenfunktion wurde der Beitrag der Korrelationen zur Bindungsenergie, zum Kompressionsmodul sowie der Gitterkonstanten berechnet. Dasselbe gilt für Ionenkristalle wie MgO und CaO. In Zukunft sollen unsere Rechnungen auf Systeme mit d-Elektronen erweitert werden. Auch Metalle wollen wir behandeln, was die Modifikation etlicher rechnerischer Details erfordert, da für Metalle keine Wannier Orbitale konstruiert werden können. Neben den Rechnungen zum Grundzustand sollen auch Rechnungen zu angeregten Zuständen durchgeführt werden. Hierfür gibt es bereits Resultate für Valenzbänder, während solche für Leitungsbänder noch umfangreiche Arbeiten erfordern. Dies ist nicht überraschend, wenn man bedenkt, daß ein zusätzliches Elektron in einem Isolator oder Halbleiter ein völlig anderes Korrelationsloch mit sich führt als die bereits vorhandenen Elektronen.

Bei den stark korrelierten Elektronensystemen ist man für Festkörper noch auf Modelle angewiesen. Bei den Systemen mit schweren Fermionen hat sich das bisherige Bild insofern geändert, als es gelang, neben dem Kondo Effekt zwei weitere physikalische Mechanismen ausfindig zu machen, die zu schweren Quasiteilchen führen. So führt z. B. in $Nd_{2-x}Ce_xCuO_4$ der Zeeman Effekt und in Yb_4As_3 das Verhalten fast halbgefüllter Hubbard Ketten zu ähnlichen, niedrigliegenden Anregungen, wie wir sie seit etlichen Jahren für Kondo Systeme kennen. Auf einer größeren Energieskala läßt sich die spektrale Dichte von stark korrelierten Modellsystemen mit Projektionstechniken recht gut berechnen. Auch dieser Weg soll in Zukunkft ausgebaut werden.

Selbständige Nachwuchsgruppe "Nichtlineare Zeitreihenanalyse"

(Leiter: Dr. H. Kantz)

Die Nachwuchsgruppe Nichtlineare Zeitreihenanalyse nahm am 1. Januar 1995 ihre Arbeit auf. Ein wesentlicher Teil der Arbeit besteht in der Weiterentwicklung von Methoden zum Nachweis und zur Charakterisierung deterministischer Dynamik als Quelle von aperiodischem Verhalten, wie man es nicht nur in physikalischen Laborexperimenten, sondern in vielen Systemen unserer Umwelt beobachtet. Bei Zeitreihen, für die das mit heutigen Methoden schon gelingt, erlaubt es ein umfassendes Verständnis der zugrundeliegenden Dynamik über Modellbildung, quantitativer Charakterisierung, Kurzzeitvorhersage bis hin zur Chaos-Steuerung und -unterdrückung. Darüber hinaus ist nichtlineare Zeitreihenanalyse auch für Modellverifikation und Signalklassifizierung relevant. Neue Ergebnisse wurden erzielt bei der Rekonstruktion des deterministischen Anteils von Daten, die durch starkes Rauschen verunreinigt sind, beim Verständnis der Beschränkungen in der Analyse von skalaren Zeitreihen von Systemen mit vielen aktiven Freiheitsgraden und bei der Übertragung der Methoden auf Zeitreihen, deren Observable selbst Zeitintervalle repräsentiert. Weiterer Schwerpunkt ist das Studium von nichtlinearen Systemen, die mit stochastischen Prozessen wechselwirken, und von Systemen mit vielen aktiven Freiheitsgraden. Zu letzterem Aspekt gehören auch räumlich ausgedehnte Systeme, die als Modelle für homogene Medien und ihre Anregungen dienen können.

Nachwuchsgruppe "Quantenchemie"

(Leiter: Dr. M. Dolg)

Die Hauptforschungsgebiete der Quantenchemiegruppe sind die Effekte der Relativistik und der Elektronenkorrelation in Atomen, Molekülen und Festkörpern. Ein Interessengebiet ist die Anwendung von in der molekularen Quantenchemie bekannten Verfahren auf Problemstellungen aus dem Bereich der Festkörperphysik. Die Entwicklung und Implementierung neuer Methoden stehen jedoch ebenso im Mittelpunkt der Arbeiten.

Die Gruppe befaßt sich mit der Entwicklung der Pseudopotentialmethode, einem in der Quantenchemie häufig eingesetzten Verfahren zur Berücksichtigung relativistischer Effekte und zur Verringerung des Rechenaufwandes für Systeme mit schweren Elementen. Zur Kalibrierung der Pseudopotentiale werden korrelierte, relativistische Allelektronenrechnungen an Atomen mit einem selbst erstellten Programm durchgeführt. Für benchmark-Untersuchungen an Atomen und kleinen Molekülen wurde eine effiziente Quanten-Monte-Carlo-Methode entwickelt, in der Pseudopotentiale und Spin-Bahn-Potentiale eingesetzt werden können.

Die Pseudopotentiale werden zur Untersuchung und Interpretation relativistischer Effekte in der Chemie schwerer Elemente eingesetzt, z.B. der Beiträge zur Lanthaniden- und Aktinidenkontraktion. Ungewöhnliche, durch Elektronenkorrelation bedingte elektronische Grundzustände wie z.B. in Cerocen werden ebenfalls untersucht.

In Festkörperrechnungen werden die Pseudopotentiale zur Berechnung der Grundzustandseigenschaften von ionischen und kovalenten Systemen eingesetzt. Die Korrelationsbeiträge werden hierbei mit der Methode der lokalen Inkremente berücksichtigt. Weiterhin wurde eine zum üblichen Hartree-Fock-Verfahren für Festkörper alternative Methode entworfen, die derzeitig programmiert wird.

Eine Methode zur Analyse von Multi-Konfigurationswellenfunktionen unter Verwendung lokaler Operatoren wurde entwickelt und implementiert. Eine erste Anwendung stellte eine Studie zur magnetischen Wechselwirkung von Übergangsmetallionen in Molekülkristallen dar. Das Verfahren wird auch zur Analyse und Interpretation von Korrelationseffekten in Modelsystemen mit Atomen aus der ersten und zweiten Hauptgruppe eingesetzt.

Nachwuchsgruppe “Strukturbildung in Reaktions-Diffusions-Systemen”

(Leiter: Dr. M. Bär)

Die Arbeitsgruppe “Strukturbildung” besteht seit November 1995 und beschäftigt sich mit der Modellierung und Analyse von Systemen, deren Verhalten durch Reaktions-Diffusions-Prozesse bestimmt ist. Dabei werden einfache Modelle chemischer Reaktionen in Lösungen und auf Katalysatoroberflächen sowie Amplitudengleichungen für die Umgebung charakteristischer Instabilitäten betrachtet. Die Modelle werden dabei in Form von partiellen Differentialgleichungen aus der Kenntnis der beteiligten physikalischen und chemischen Prozesse abgeleitet und anschließend in Abhängigkeit von den Kontrollparametern des Systems gelöst. Danach werden die gefundenen Muster quantitativ und qualitativ mit verfügbaren Experimenten verglichen. Wir interessieren uns insbesondere für Instabilitäten einfacher Muster, die zu komplizierten raumzeitlichen Strukturen oder gar raumzeitlicher chaotischer Dynamik führen. Dabei werden neben direkter numerischer Simulation der Gleichungen, auch Methoden der Kontinuation und Bifurkationsanalyse verwendet, um mögliche Lösungen der Reaktions-Diffusions-Gleichungen und ihre Stabilität zu berechnen. Darüber hinaus untersuchen wir Reaktions-Diffusions-Wellen in komplizierten Geometrien, wo Phänomene wie Beugung, Reflexion und randinduzierte Instabilitäten beobachtet werden. Einen weiteren Schwerpunkt bildet die Strukturbildung bzw. Wellenausbreitung in heterogenen Medien. Hier beobachtet man einen Übergang zu einem effektiven Medium, wenn die relevante Längenskala der Heterogenität kleiner wird als die typische Längenskala von Strukturen (Diffusionslänge). Zudem haben wir begonnen, den Einfluß raumzeitlicher Störungen und Rückkopplungen auf musterbildende Systeme zu untersuchen. Die letztgenannten Themen stehen in enger Beziehung zu Experimenten mit musterbildenden Reaktionen auf mikrostrukturierten Katalysatoroberflächen, wie sie in Berlin (Fritz-Haber-Institut) und an der Universität Hannover durchgeführt werden.

Nachwuchsgruppe “Quantenchaos und mesoskopische Systeme”

(Leiter: Dr. K. Richter)

Das Studium mesoskopischer elektronischer Systeme unter Verwendung von Methoden der Quantenchaostheorie ist das zentrale Arbeitsgebiet dieser Gruppe, die seit Januar 1996 besteht. Mesoskopische Systeme sind typischerweise kleine, niedrig–dimensionale Objekte, die aufgrund der sich über das System erstreckenden Phasenkohärenz der zugehörigen elektronischen Wellenfunktionen spezielle Quanteneffekte aufweisen.

Gegenstand der Untersuchungen der Gruppe sind Transporteigenschaften von Quantendots und Übergittern, thermodynamische Eigenschaften (wie Bahnmagnetismus und Dauerströme) sowie die dynamische Antwort kleiner Teilchen (z.B. die elektrische Polarisierbarkeit) auf äußere Felder.

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 wie Leitwert und Magnetismus. Die Quantenchaostheorie und insbesondere semiklassische Methoden bilden den Rahmen und das Werkzeug zur Untersuchung dieser Korrespondenz zwischen klassischer und Quantenmechanik für sowohl integrable als auch chaotische Systeme. Dabei stehen Fragen, z.B. wie der chaotische Charakter des Systems das mesoskopische Verhalten beeinflußt, im Vordergrund. Quantenmechanische *ab–initio*–Rechnungen werden verwendet, um semiklassische analytische Näherungen zu überprüfen.

Weitere Arbeiten der Gruppe zielen auf die Berücksichtigung der Streuung von Elektronen an Störstellen ab. Die Verknüpfung semiklassischer Methoden mit quantenmechanischer, diagrammatischer Störungstheorie dient als Zugang zur Beschreibung des Übergangsregimes zwischen ballistischer Bewegung einerseits, und diffusiver Dynamik in ungeordneten Systemen andererseits.

Ein weiteres, zukünftiges Ziel ist die Einbeziehung von Effekten aufgrund der Wechselwirkung der Elektronen in kleinen Systemen. Diese spielen z.B. für die dynamische Antwort eines Elektronengases auf äußere Felder eine Rolle. Daneben wurde ein Projekt begonnen mit dem Ziel der Entwicklung von Methoden (im Rahmen des Floquet–Formalismus) zur Behandlung von Streuung in starken, zeitabhängigen Feldern in Hinblick auf die Anwendung auf nichtlineare, frequenzabhängige Transportphänomene.

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 and 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 a 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. As regards weakly correlated systems we have investigated the ground state of the elemental semiconductors as well as of the III - V compounds. Not only the wavefunction was calculated for these systems but also the correlation energy contribution to cohesion, to the bulk modules and to the lattice constant. The same holds true for ionic crystals such as MgO and CaO. In the future we want to extend these calculations to d-electron systems. We also want to treat metals. Since for metals one cannot construct Wannier functions the technical details are different for calculations of these systems. In addition to ground-state calculations we plan to pursue calculations for excited states. While some results for valence bands are already available, computations for conduction bands still require considerable work. This is not too surprising in view of the fact that the correlation hole of an electron added to a semiconductor or insulator is quite different from that of the electrons already present.

As regards strongly correlated electron systems we still have to rely on simplified model Hamiltonians. Concerning heavy-fermion systems, our physical understanding of them has considerably broadened over the last few years. For a long time the Kondo effect was thought to be the only source of the large number of low lying excitations which result in the large effective quasiparticle mass. However, now we can identify two other physical origins of heavy-fermion behavior. One occurs in $Nd_{2-x}Ce_xCuO_4$ and is based on the Zeeman effect while the other is realized in Yb_4As_3 and is related to nearly half-filled one-dimensional Hubbard bands. When larger energy scales are considered, the spectral density of strongly correlated model systems can be determined quite well by applying projection techniques. We have plans for extending also this promising approach.

Independent Group of Young Researchers “Nonlinear Time Series Analysis”

(Dr. H. Kantz)

The Nachwuchsgruppe Nonlinear Time Series Analysis was founded in January 1995. Its main activity consists in the further development of methods to establish the presence and to characterize properties of deterministic chaotic motion as the main source of irregular, aperiodic behaviour, as it is found not only in many physical laboratory experiments but in many systems of the real world. For time series where this works successfully with present day methods one thus acquires an almost complete understanding of the underlying dynamics through modeling, quantitative characterization of chaotic properties, and short time predictions, culminating in chaos control and chaos suppression. Moreover, nonlinear time series analysis is relevant for model verification and signal classification. New results obtained in 1995 concern the reconstruction of the deterministic dynamical equations underlying very noisy chaotic data, the understanding of limitations in the analysis of systems with many active degrees of freedom on the basis of time series, and the application of current methods to data sequences which themselves represent time intervals. In addition to further elaboration of current techniques, emphasis is laid on the understanding of the interaction of chaotic deterministic dynamics and stochastic processes, and of systems with many degrees of freedom. Among the latter are spatially extended systems which are models for homogeneous media and their excitations.

Group of Young Researchers "Quantum Chemistry"

(Dr. M. Dolg)

The research activities of the quantum chemistry group are in the field of electron correlation effects and relativistic effects for atoms, molecules and especially solids. One of the major areas of interest of the group is to apply well-established methods of molecular quantum chemistry to problems in the field of solid state physics. Nevertheless, the development of new methods and the corresponding programs is also a main topic of the present research.

The group is concerned with the development of the pseudopotential technique, one of the most frequently used methods in quantum chemistry to incorporate relativistic effects into the calculations and to reduce the computational effort for systems containing heavy elements. Correlated relativistic all-electron calculations are performed with a self-developed program for atoms in order to calibrate the pseudopotentials. For benchmark studies of correlation effects in atoms and small molecules an efficient pseudopotential Quantum Monte Carlo scheme including spin-orbit coupling has been developed.

The pseudopotentials are used to evaluate and interprete relativistic effects in heavy element chemistry, e.g. contributions to the lanthanide and actinide contraction. Unusual correlation-induced electronic ground states as e.g. for cerocene are also studied.

In solid state calculations the pseudopotentials are applied to establish the ground state properties of covalent and ionic solids. Correlation contributions are evaluated using the method of local increments. The extension of this approach to excited states is under investigation. Moreover, an alternative scheme to the standard Hartree-Fock-approach to solids has been designed and is currently coded.

A scheme for the analysis of large-scale multi-configuration wavefunctions in terms of expectation values of local operators has been developed and implemented. A first application was the study and interpretation of magnetic interactions of transition metal ions in molecular crystals. The scheme is also used for the rationalization and interpretation of electron correlation effects in model systems containing first and second row atoms.

Group of Young Researchers "Pattern Formation in Reaction–Diffusion Systems"

(Dr. M. Bär)

The group on pattern formation started its work in November 1995 amd is concerned with the modeling and analysis of systems governed by reaction-diffusion processes. In particular, simple models stemming from chemical reactions in solution, gels and on catalytic surfaces as well as amplitude equations near characteristic dynamical instabilities are considered. One important aim is to derive realistic models from the knowledge of the underlying physics and chemistry, to solve these equations for different control parameter values and to compare the resulting structures qualitatively and quantitatively with available experimental data. In particular, instabilities of reaction-diffusion patterns leading to complex or even spatiotemporally chaotic patterns are studied. Besides direct simulation, here methods of continuation and bifurcation analysis are employed to find possible solutions and their stability. We also investigate waves and pattern in complicated geometries, where a variety of phenomena from boundary-induced instabilities to diffraction and reflection of reaction-diffusion waves are found. Moreover, we look at pattern formation and wave propagation in heterogeneous systems. Here,a transition to effective behavior is observed if the length scale of variation of parameter becomes smaller than the typical length scales of the pattern (diffusion length). Finally, we have started to look at the impact of spatiotemporal forcing and feedback on pattern forming systems. The latter subjects are in connection with experiments on pattern formation in various chemical reactions on microstructured surfaces that are carried out by research groups in Berlin (Fritz-Haber-Institut) and the University of Hannover.

Group of Young Researchers “Quantum–Chaos and Mesoscopic Systems”

(Dr. K. Richter)

The study of mesoscopic electronic systems, using techniques of the quantum chaos theory, is the main topic of this group, which started its activities in January 1996. These systems are typically small objects of reduced dimensionality which, due to the phase–coherence of the electronic wavefunctions throughout the systems, exhibit peculiar quantum effects. Transport properties of quantum dots and superlattices, thermodynamic properties (as orbital magnetism and persistent currents) and the dynamic response of small particles to applied fields (e.g. the electrical polarizability) are investigated.

The main focus of the group is currently directed to 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 (conductance, magnetism) 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. *Ab–initio* quantum calculations are usually employed for testing the semiclassical analytical predictions.

Further work aims at the inclusion of scattering of the electrons at impurities and an understanding of the transition regime between geometry–affected ballistic motion and diffusive dynamics in disordered systems by combining semiclassical and quantum diagrammatic perturbation theory. One future aim is the consideration of effects due to interactions between electrons in small samples, which, e.g. become important when considering the dynamic response to external fields. A further project is devoted to the development of techniques for scattering in strong time–dependent fields (based on the Floquet–formalism) in order to describe non–linear phenomena in frequency–dependent transport.

Selection of Research Results

From mixed valence to pseudo-one-dimensional spin chains in Yb_4As_3

B. Schmidt, P. Thalmeier and P. Fulde

Many Ytterbium (Yb) or Cerium (Ce) compounds show mixed-valent or heavy-fermion (HF) behaviour at low temperatures signified, e.g., by a strong enhancement of the linear specific-heat term and the Pauli susceptibility. Usually this behaviour is exhibited by intermetallic Ce- and Yb-compounds with metallic carrier densities. The origin of "heavy" effective electron masses is thought to result from an interplay of on-site $4f$ Coulomb repulsion and $4f$-conduction electron hybridization as described by the Anderson lattice model. In the HF limit one may view the heavy bands as coherent Bloch states emerging from local Kondo singlet–triplet excitations. There are also systems known that have thermodynamic properties like a metallic heavy fermion system but are insulators or semimetals. They are often referred to as Kondo insulators or low carrier Kondo systems, implying that the low energy excitations seen in e.g. the specific heat are of similar origin as in a Kondo lattice system.

Recently, a new class of low-carrier Rare Earth (R) compounds, the R_4X_3 pnictides $(X = \mathrm{As}, \mathrm{Bi})$ have been investigated experimentally in detail. These compounds have the cubic anti-Th_3P_4 structure at high temperatures, where the R-atoms are placed on $\langle 111 \rangle$-type space diagonals surrounded by the pnictogen (X) atoms (Figure 1, left). Thus the R-atoms form four parallel and interpenetrating families of rods oriented along the space diagonals (Figure 1, right).

In this class the semimetallic Yb_4As_3 compound was found to exhibit truly extraordinary behaviour which cannot be described within the Kondo-insulator scenario indicated above. It rather represents a new way of obtaining a HF ground state with very low carrier concentration. In fact the most striking aspect of this compound is the existence of a high linear specific-heat γ value of $200\,\mathrm{mJ/(molK^2)}$, while at the same time the free carrier concentration at low temperatures is only $7 \cdot 10^{18}\,\mathrm{cm^{-3}}$ corresponding to about $0.6 \cdot 10^{-3}$ carrier per Yb atom. The scenario proposed here basically corresponds to a transition from a high-temperature mixed valent state to a low-temperature low carrier state with pseudo-one-dimensional spin chain excitations and is described in the following.

1. *Charge ordering and the origin of low energy excitations*

Simple valence counting leads to the conclusion that on the average there is one $4f$ hole per formula unit. This means that one has one Yb^{3+} $(4f^{13})$ ion for three Yb^{2+} ($4f^{14}$, complete shell) ions. At high temperatures one therefore has a homogeneous mixed valent state with Yb^{2+} and Yb^{3+} states on the average distributed equally among the chains. The $4f$ holes can move and have an effective band width $\simeq 0.2\,\mathrm{eV}$ due to the hybridization with pnictogen (X) $4p$-states and thus contribute to transport properties. The number of carriers at high temperatures as inferred from the Hall constant R_H conforms whith the presence of one $4f$ hole per formula unit.

At room temperature the compound undergoes a (first-order) structural phase transition where the crystal shrinks along one of the space diagonals, thus leading to a trigonal

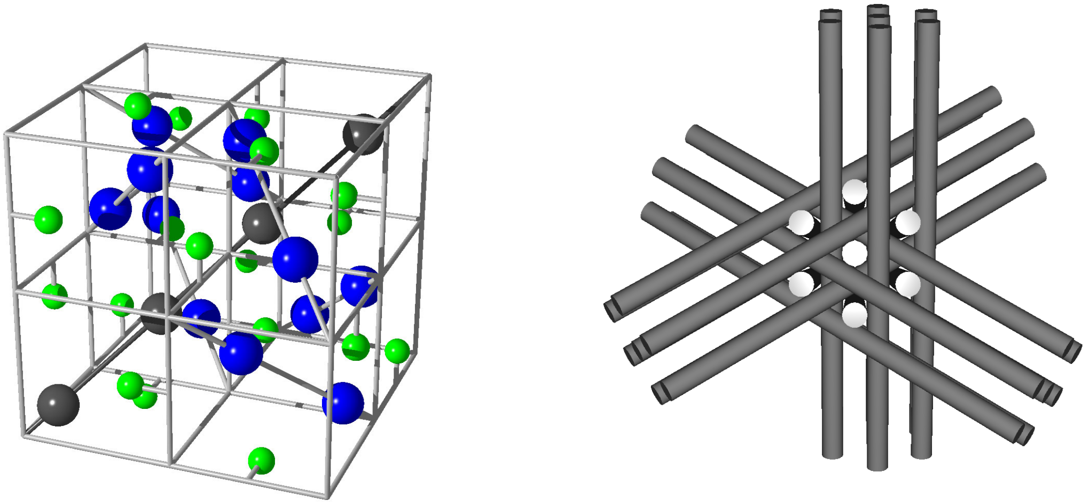


Figure 1: Left: Crystal structure of Yb_4As_3. The large balls depict the Yb-ions, small balls correspond to the As-ions. The four gray balls indicate the Yb-chain in the $\langle 111 \rangle$-direction. Right: Body-centred cubic rod structure. The $\langle 111 \rangle$-direction points perpendicular to the drawing plane.

low-temperature structure. This distortion is not accompanied by any modulation of the atomic positions, i.e., no superstructure peaks were observed, therefore it cannot be interpreted as a Peierls distortion. It is of a rather different origin: Because of the semimetallic carrier density long-range Coulomb interactions exist which favor *charge ordering* of $4f^{13}$ holes on the chains. Since the radius of Yb^{3+} is smaller than Yb^{2+} a trigonal distortion (shrinking) along $\langle 111 \rangle$ results. Naturally the four equivalent space diagonals lead to a domain formation in the low temperature phase. In an effective way the impact of long-range Coulomb interactions on lattice distortion may be described by a deformation-potential coupling to pseudo-one-dimensional Yb-hole bands, and the structural phase transition at T_c can be interpreted as a correlated-band Jahn Teller effect. The specification 'correlated' alludes to the essential mechanism that generates the low-temperature low energy excitations leading to the observed HF character of Yb_4As_3.

As seen in the inset of Figure 2, the distortion leads to a gradual filling of short chains with $4f^{13}$ holes whereas the long chains show carrier depletion. Because of the original one hole per formula unit one ends up with essentially half filled bands in the short chains at low temperature. Due to on-site Coulomb repulsion one has now a strongly correlated system which can effectively be described by a one-dimensional t-J model. The elementary excitations of this model are spinon excitations with an effective mass obtained in the saddle point approximation for nearly half filling as

$$\frac{m^*}{m_{\mathrm{b}}} = \frac{t}{\delta t + \frac{3}{4}\chi J}$$

where m_{b} is the bare mass, $4t$ the effective $4f$-band width ($\simeq 0.2\,\mathrm{eV}$) and δ the deviation from half filling. χ is a numerical constant close to one. Obviously, the spinon-band

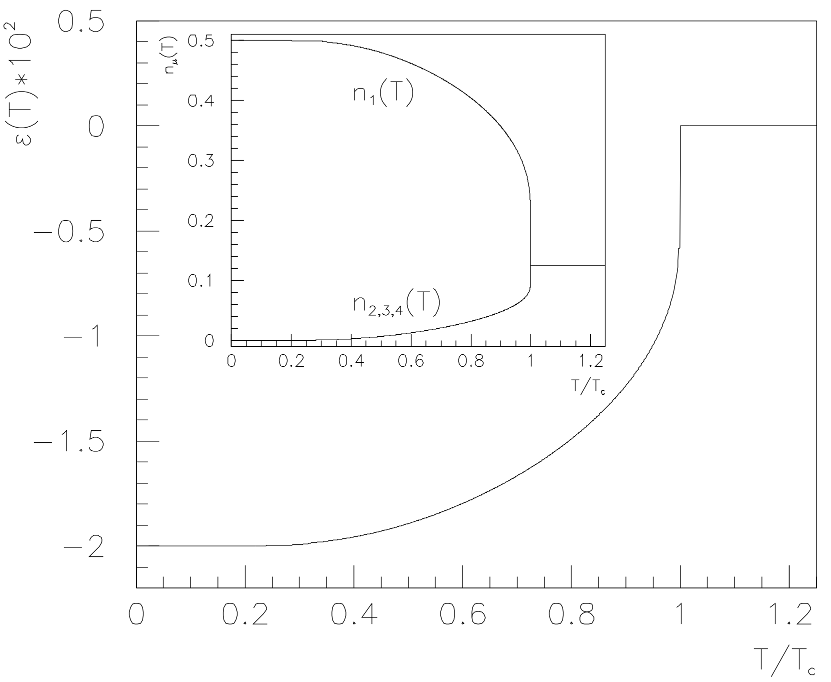


Figure 2: Temperature dependence of the strain order parameter $\epsilon_\Gamma(T)$. Inset: occupation numbers $n_\mu(T)$ of the four f-bands.

width is given by the exchange coupling along the chains which can be estimated to be $J \simeq 25\,\mathrm{K}$ in $\mathrm{Yb_4As_3}$. Since parallel chains are well separated from each other, the interchain coupling will be much lower. Thus the elementary excitations responsible for the low temperature anomalies in $\mathrm{Yb_4As_3}$ are pseudo-one-dimensional spin excitations and not the singlet-triplet excitations of a Kondo lattice.

The deviation from half filling enters only weakly into the effective mass in the above equation. Therefore one may say that thermodynamics (spin excitations) and transport properties (determinded by δ) are well decoupled in this system. According to low-temperature Hall measurements the carrier concentration corresponds to $\delta \simeq 0.6 \cdot 10^{-3}$ per Yb atom. What determines the deviation δ from half filling, i.e., from the insulating state? There are two possibilities: First, an intrinsic mechanism called ‘self-doping’ might exist where the hybridization of half-filled short chain states with split off empty long-chain states leads to a small deviation from half filling. This can be described within a slave-boson approach which leads to the conclusion that a threshold value for the interchain hybridisation is necessary to obtain a finite δ. Alternatively, the high-temperature valence might not exactly correspond to the ratio of $\mathrm{Yb^{2+}/Yb^{3+}} = 3:1$ leaving less than one hole per site in the short chains at low temperatures.

2. Spin-chain excitations and the field dependence of γ

The basic idea that pseudo-one-dimensional spin excitations are responsible for the high γ-value in $\mathrm{Yb_4As_3}$ was beautifully confirmed by recent inelastic neutron-scattering experiments of Kohgi et al. They show that the magnetic excitation spectrum is well described by one-dimensional spin wave excitations

$$\omega(q) = \frac{\pi}{2} J \sin(qd)$$

of des Cloizeaux and Pearson where q is the wave number in $\langle 111 \rangle$ direction and d the Yb-Yb distance along the chain. This also leads naturally to a linear specific heat for $k_{\mathrm{B}}T/J \ll 1$. From the maximum observed spin wave energy of $3.8\,\mathrm{meV} \approx 40\,\mathrm{K}$ at $q = \frac{1}{2}(\pi/d)$ one obtains $J = 25\,\mathrm{K}$ in good agreement with the estimate from the γ-coefficient.

However there is still one major observation to be explained within the spin-chain picture: Concerning the field dependence of γ in an applied field B one would expect deviations from $\gamma(B)$ of the order $(B/J)^2$, i.e., 10^{-2} at $4\,\mathrm{T}$ uniformly for all temperatures $k_{\mathrm{B}}T/J \ll 1$. Experiments by Helfrich et al. however revealed a quite different behaviour. Above $2\,\mathrm{K}$ changes in γ are indeed small. In contrast, at $0.5\,\mathrm{K}$ the field dependence of $\gamma(B)$ is dramatic. Already at $B = 4\,\mathrm{T}$ the γ-value is strongly suppressed in conflict with the above argument. This indicates that an additional energy scale much smaller than J ($25\,\mathrm{K}$) must be present in $\mathrm{Yb_4As_3}$.

The observation of a strong field dependence can be incorporated in the spin-chain model if one considers a small interchain coupling J' with $J'/J \ll 1$ to be present. This perturbation will immediately lead to anisotropy gaps in the spin-wave dispersion at zone-centre and boundary wave vectors. Furthermore, the gaps will strongly depend on the field strength and direction and a field dependence of γ will originate.

It is well known that in one dimension no long-range spin order is present. However, according to calculations for the $S = 1/2$ Heisenberg antiferromagnet, the spin-spin correlation function decays slowly, essentially as $\sim 1/r$ with distance r. Therefore it is possible to treat the excitations of the chain systems in spin-wave approximation, starting from a broken-symmetry ground state as long as J' is small enough so that the one-dimensional character is not perturbed too strongly. One then has to calculate the configuration of the six-sublattice antiferromagnetic structure (trigonal in-plane, stacked along chain) in the applied field parallel and perpendicular to the plane. Knowing the ground-state configuration it is possible to calculate the six excitation branches $\omega_\kappa(q, B)$ $(\kappa = 1 \ldots 6)$ which determine the low-temperature thermodynamics of the system.

The most important result is the appearance of anisotropy gaps at $q = 0, \pi/d$ which scale as $\Delta_{\mathrm{a}} \sim \sqrt{JJ'}$ and therefore may be appreciable despite $J'/J \ll 1$. These gaps also depend on field strength and field direction. As long as $T \gg \Delta_{\mathrm{a}}$ only insignificant field dependence of γ is expected—this corresponds to the dashed curve in Figure 3. Once the temperature is comparable to the anisotropy gaps, a strong field dependence of γ is observed which is most pronounced for transverse direction (Figure 3). This is in very good agreement with the experimental variation of γ obtained by Helfrich et al. From Figure 3 one deduces that $J'/J \simeq 10^{-4}$ so that the one-dimensional character of the spin-chain systems is indeed rather pronounced.

If J' is as small as obtained from $\gamma(B)$ one will not be able to observe the spin-wave gaps directly by neutron scattering. However, possibly they can be identified by magnetic-resonance experiments which measure the excitations at $q = 0$. This depends on whether the semimetallic conductivity in $\mathrm{Yb_4As_3}$ is small enough.

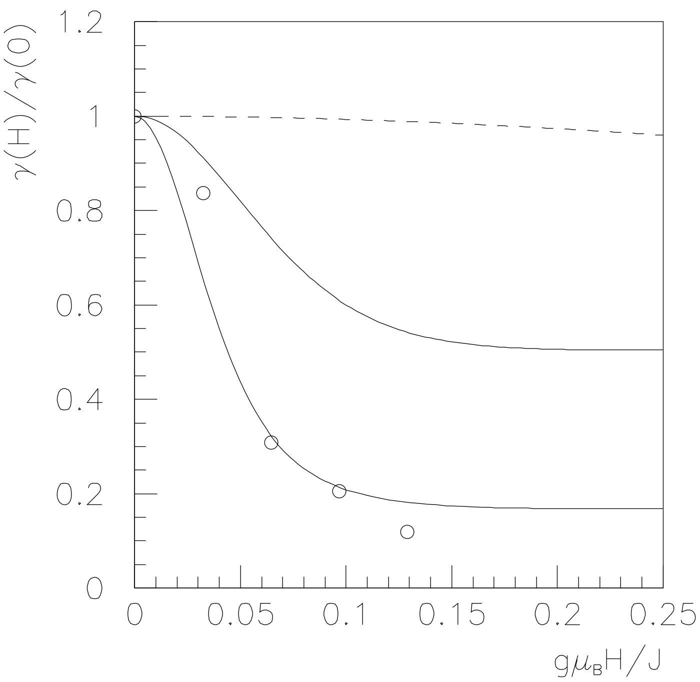


Figure 3: Magnetic-field dependence of the γ-coefficient. Bottom solid line: field applied perpendicular to the c-axis, top solid line: field parallel to the c-axis, both at $k_{\mathrm{B}}T = 0.02\,J \approx 0.5\,\mathrm{K}$. Dashed line: field dependence at $k_{\mathrm{B}}T = 0.2\,J \approx 5\,\mathrm{K}$. The open circles denote the data from Helfrich et al. The ratio J'/J of interchain- to intrachain-coupling is 10^{-4}.

Finally, the low-energy excitations have also been identified in anomalies in the elastic constants by Goto et al. There are well-founded reasons that this may also be explained in the present model.

Correlated Conduction Electrons with a Magnetic Impurity

T. Schork

For more than thirty years, intensive investigations have been performed on the behavior of magnetic impurities in metals (Kondo effect) [1]. By magnetic impurities we mean those impurities that have a localized, but otherwise free spin, e.g., atoms from the $3d$ transition series or $4f$ rare-earth elements. At high temperatures, their moment shows up in a Curie-type contribution to the magnetic susceptibility of the alloy. However, when the temperature is decreased below a characteristic value, the Kondo temperature T_K, the moment is screened and the impurity becomes effectively non-magnetic. At low temperatures a resonance at the Fermi level is formed (Abrikosov-Suhl resonance) which leads to Fermi-liquid behavior. The resonance width is given by the Kondo temperature which is often of order of meV and sets a new low-energy scale. Hence, e.g., specific heat and susceptibility are strongly enhanced compared to non-magnetic alloys. When the local moments form a lattice, the Kondo effect leads to quasiparticle excitations on an energy scale T_K. In thermodynamic properties, they can be characterized by a renormalized mass which is typically 10–1000 times that of free conduction electrons, hence the name "heavy fermions".

A few years ago, unusual heavy-fermion behavior was observed in the electron-doped cuprate $\mathrm{Nd_{2-x}Ce_xCuO_4}$ for $0.1 \lesssim \mathrm{x} \lesssim 0.2$ [2]. In the undoped system, a Schottky anomaly is found in the specific heat indicating that the Nd moments couple to the antiferromagnetically ordered $\mathrm{CuO_2}$ planes with a coupling constant of the order of 1 K. Upon doping a linear specific heat $C = \gamma T$ is observed with a large Sommerfeld coefficient $\gamma \simeq 4\mathrm{J}/(\mathrm{K}^2$ mole Nd). In the same temperature regime, the spin susceptibility is found to be temperature independent and similarly enhanced. These are characteristic features of heavy-fermion excitations. The energy scale of the excitations is of the order of 1 K as well. This energy scale cannot be explained by applying the usual theory of the Kondo effect. This is not too surprising since undoped $\mathrm{Nd_2CuO_4}$ is an antiferromagnetic charge-transfer insulator despite of one hole per unit cell and, hence, the Nd ions couple to a system of strongly correlated electrons rather than to free ones as is generally assumed.

Therefore, we investigate the influence of interactions among the conduction electrons on the Kondo effect. The Kondo effect is usually studied in the framework of the impurity Anderson model. We extend it by adding an on-site repulsion for the conduction electrons:

$$\begin{aligned} H &= \sum_{k\sigma} \epsilon_k c^\dagger_{k\sigma} c_{k\sigma} + \frac{U_c}{2} \sum_{i,\sigma\neq\sigma'} n^c_{i\sigma} n^c_{i\sigma'} \\ &\quad + \epsilon_f \sum_{\sigma} f^\dagger_\sigma f_\sigma + \frac{U_f}{2} \sum_{\sigma\neq\sigma'} n^f_\sigma n^f_{\sigma'} + V \sum_{k,\sigma} \left(c^\dagger_{k\sigma} f_\sigma + f^\dagger_\sigma c_{k\sigma} \right) \ . \end{aligned}$$

Here, c refers to conduction electrons, f to the impurity, and the other notation is standard. $\epsilon_f < 0$ and a large U_f ($= \infty$ in the following) ensure that a local moment is formed on the impurity site in the absence of the hybridization V.

For the case of uncorrelated conduction electrons, it has proven successful to generalize the model from the SU(2)-spin symmetry to SU(N), i.e., $\sigma = 1 \ldots N$, and to perform an expansion in $1/N$ [1]. To obtain a meaningful limit $N \to \infty$ in our case, not only the hybridization has to be scaled, $V \to V/\sqrt{N}$ [1], but also the Coulomb interaction of the conduction electrons, $U_c \to U_c/N$ (see also [3]). The scaling of U_c ensures that the diagrams which grow most rapidly in N, converge as $N \to \infty$.

We use the representation for the (impurity) partition function developed for strong local correlations [4]. It reduces to Brillouin-Wigner perturbation theory at $T = 0$. Starting from the Fermi sea, $|\mathrm{FS}\rangle$, ($f_\sigma^\dagger|\mathrm{FS}\rangle$) as unperturbed state, we find for the singlet (magnetic multiplet) ground-state energy

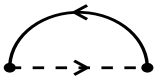
$$E_S = \Sigma_0(E_S) \qquad (E_M = \Sigma_f(E_M)) \ ,$$

where Σ_0 (Σ_f) denotes the self-energy of the f^0- (f^1)-configuration, resp. The Kondo resonance is found from the splitting of singlet and magnetic ground state as V is turned on.

The expansion of Σ in powers of $1/N$ is done in the standard diagrammatic way [1]: The f^0- (f^1)-configuration is denoted by a wavy (dashed) line and the conduction electrons by solid lines. Note that the interaction among the conduction electrons introduces a new vertex where two electrons scatter.

To order $1/N^0$, when neglecting trivial Hartree-type contributions, the correlations of the conduction electrons do not enter, and only the singlet energy is modified:

$$\Sigma_0^{(0)}(E_S) =$$



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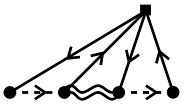
For a flat conduction band of width $2D$ and density of states ρ, the resulting Kondo temperature is given by the usual expression for free electrons

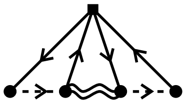
$$T_K^{(0)} = D \exp\left(\frac{\epsilon_f}{\rho V^2}\right) \ .$$

To order $1/N$, both singlet and magnetic energies are modified. However, the Hubbard interaction U_c affects only the singlet. To estimate the change of the Kondo temperature we consider lowest order in U_c, i.e., weak correlations. We find three contributions which differ in the time order of the interactions V and U_c:

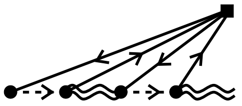
$$\Sigma_0^{(1a)}(E_S) =$$



$$\Sigma_0^{(1b)}(E_S) =$$



$$\Sigma_0^{(1c)}(E_S) =$$



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Note that corrections to the Kondo temperature occur already to first order in U_c, unlike the pure Hubbard model where the interaction does not enter until second order. This shows that the correlations renormalize the magnetic coupling to the impurity.

In the following we focus on the local moment regime defined by $J = -V^2/\epsilon_f \ll 1$. Here, $\Sigma^{(1c)} \sim J^0$ whereas $\Sigma^{(1a)}$, $\Sigma^{(1b)} \sim 1/J$. The different time orders of $\Sigma^{(1a)}$ and $\Sigma^{(1b)}$ correspond to different physical processes. In $\Sigma^{(1b)}$, the Hubbard interaction takes place while the system is in an (excited) f^0-configuration. This scattering of conduction electrons effectively shifts the impurity level resulting in a decrease of the Kondo temperature. In the Kondo limit ($\epsilon_f \rightarrow -\infty$) this process vanishes since the f^0-configuration becomes energetically unfavorable. In contrast, the impurity orbital is occupied in $\Sigma^{(1a)}$ when the conduction electrons scatter. This process could be viewed as a spin fluctuation in the conduction band. It yields an increase of the Kondo temperature.

These findings are illustrated in Fig. 1, where we present a numerical evaluation of $\Sigma_0^{(1a)}$ and $\Sigma_0^{(1b)}$ for different ϵ_f. The corresponding integrals were determined in the limit of infinite dimensions. The change of the Kondo temperature due to correlations is given by $\Delta T_K(U) = -(\Sigma_0^{(1a)} + \Sigma_0^{(1b)})$. We find an increase of the Kondo temperature when the interactions among the conduction electrons are turned on. Its magnitude depends strongly on the position of the impurity level, ϵ_f. For $\epsilon_f \rightarrow -\infty$, T_K is strongly enhanced due to spin fluctuations. When the impurity level moves into the band ($\epsilon_f \gtrsim -1$), correlations seem to be less important. However, the effective shift of the f-level due to the Hubbard interaction ($\Sigma^{(1b)}$) becomes more important, and the two contributions $\Sigma^{(1a)}$ and $\Sigma^{(1b)}$ partially compensate.

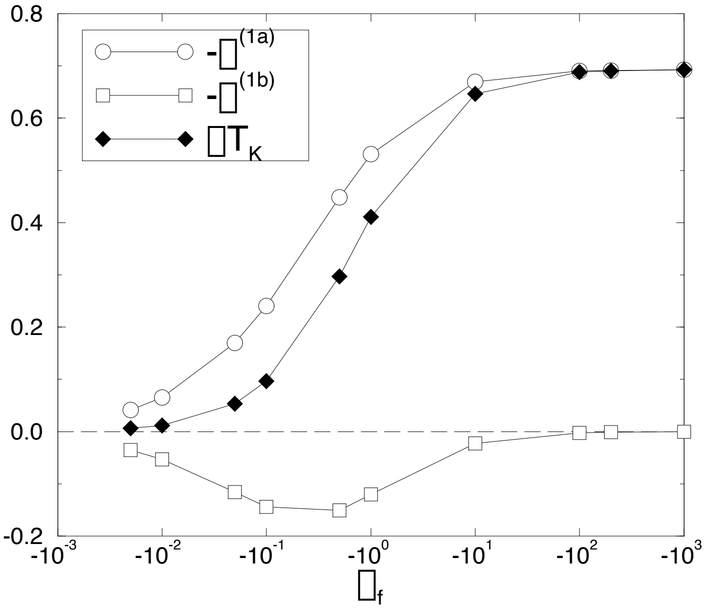

Figure 1: Change of the Kondo temperature to lowest order in U_c. Note that $T_K = T_K^{(0)} + \Delta T_K(U) = T_K^{(0)}\left(1 + \frac{1}{N}\frac{U}{J}t\right)$

Due to the scaling of U_c with respect to N, the kinetic energy of the conduction electrons and the Hartree contribution are of order N, whereas correlation effects enter to order N^0. Therefore, the starting point of our expansion is the Kondo effect for free electrons and our approach is limited to the weakly correlated case. Nevertheless, we find already to lowest order in U_c a large positive correction to the Kondo temperature. We conclude that correlations may strongly influence the low-energy scale.

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Dynamics of one–dimensional correlated electron systems

K. Hallberg and K. Penc

1. Density Matrix Renormalization Group Method (DMRG). The DMRG method is a powerful algorithm for calculating zero temperature properties of low dimensional systems. This technique leads to highly accurate results for much larger systems than those which can be solved by straightforward exact diagonalization. The DMRG allows for a systematic truncation of the Hilbert space by keeping the most probable states in describing a wave function (*e.g.* the ground state) of a larger system, instead of the lowest energy states usually kept in previous real space renormalization techniques. A general iteration of the method consists of: i)The effective Hamiltonian is defined for the superblock 1+2+1'+2' (a block is a collection of sites), where the blocks 1 and 1' come from previous iterations and blocks 2 and 2' are new added ones. It is diagonalized to obtain the ground state $|\psi_0\rangle$ (other states could be also kept: they are called target states). ii) The density matrix $\rho_{ii'} = \sum_j \psi_{0,ij}\psi_{0,i'j}$ is constructed, where $\psi_{0,ij} = \langle i \otimes j|\psi_0\rangle$, the states $|i\rangle$ ($|j\rangle$) belonging to the Hilbert space of blocks 1 and 2 (1' and 2'). The eigenstates of ρ with the highest eigenvalues (equivalent to the most probable states of blocks 1+2 in the ground state or in the chosen target state of the superblock) are kept up to a certain cutoff, keeping a total of m states per block. iii) These states form a new reduced basis to which all the operators have to be changed and the block 1+2 is renamed as block 1. iv) A new block 2 is added (one site in our case) and the new superblock (1+2+1'+2') is formed as the direct product of the states of all the blocks (the blocks 1' and 2' are identical to blocks 1 and 2 respectively). When more than one target state is used, *i.e* more than one state is wished to be well described, the density matrix is defined as:

$$\rho_{ii'} = \sum_l p_l \sum_j \phi_{l,ij}\phi_{l,i'j} \qquad (1)$$

where p_l defines the probability of finding the system in the target state $|\phi_l\rangle$ (not necessarily eigenstates of the Hamiltonian).

We want to calculate the following dynamical correlation function at $T = 0$:

$$C_A(\omega) = \sum_n |\langle\psi_n|A|\psi_0\rangle|^2\, \delta(\omega - (E_n - E_0)) = -\frac{1}{\pi} \lim_{\eta\to 0^+} \mathrm{Im} G_A(\omega + i\eta + E_0). \qquad (2)$$

where the summation is taken over all the eigenstates $|\psi_n\rangle$ of the Hamiltonian H with energy E_n, E_0 is the ground state energy and

$$G_A(z) = \langle\psi_0|A^\dagger(z - H)^{-1}A|\psi_0\rangle, \qquad (3)$$

The function G_A can be written in the form of a continued fraction with coefficients that are defined in a basis that tridiagonalizes H. Applying DMRG and keeping as target states the ground state and the first few of these basis functions, we can obtain an accurate description of the lowest-lying excitations with only a fraction of the total Hilbert space. To evaluate its performance we have used it to calculate the spin dynamics of the 1D antiferromagnetic Heisenberg model $H = \sum_{<ij>} \mathbf{S_i S_j}$:

$$S^{zz}(q,\omega) = \sum_n |\langle\psi_n|S^z_q|\psi_0\rangle|^2 \; \delta(\omega - (E_n - E_0)), \tag{4}$$

where $S^z_q = \sum_j e^{iqR_j} S^z_j$.

In Fig. 1 we show the dependence of the spectra with m for 24 sites as compared to the exact diagonalization results. The spectra correspond to $m = 100$ (0.3% of the total Hilbert space), $m = 150$ (0.7%) and $m = 200$ (1.4%). From here it can be seen that by keeping more states the spectrum converges rapidly to the exact one. The inset shows the size dependence of the first three excited energies.

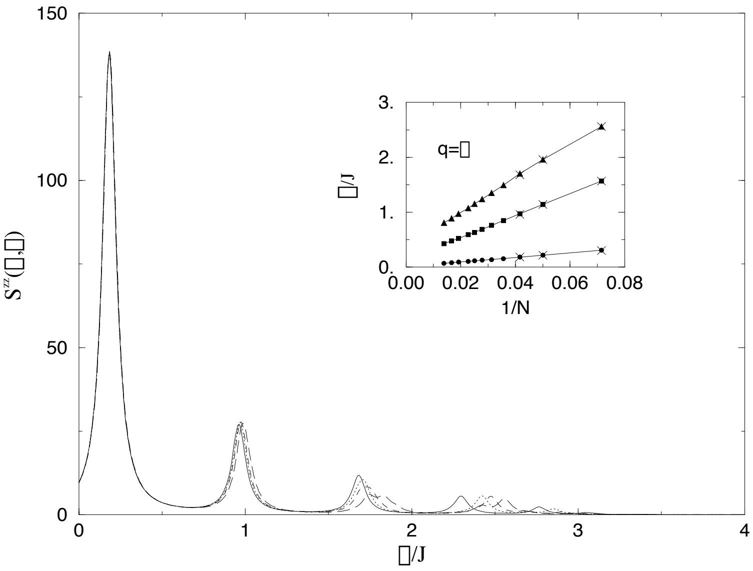

Figure 1: Spectral densities for $q = \pi$ and $N = 24$. Full line: exact result. The rest are calculated using DMRG method with $m = 100$ (long-dashed line), $m = 150$ (dashed line) and $m = 200$ (dotted line). Inset: Size dependence of the first three excited energies at $q = \pi$ up to $N = 72$. The crosses are exact results.

This method is quite general and it can be applied also to fermionic systems. An underlying advantage is that it is also convenient when states with a definite momentum are wanted.

2. Spectral functions of the one–dimensional Hubbard model. The Hubbard model describes electrons on a lattice with hopping integrals t and on–site repulsion U, and it can be viewed as a generic microscopic model of strongly correlated electron systems. In spite of its simplicity and the availability of an exact solution by Bethe Ansatz, the dynamical properties, like the one-particle spectral functions, are not fully understood yet. The low energy behavior can be described in terms of the Luttinger liquid theory, and higher energy range is accessible only by numerical methods (exact diagonalization of small clusters and Quantum Monte Carlo, both of them having their limitations).

We used the combination of analytical and numerical techniques to calculate the spectral functions in the limit of large U repulsion. The calculation is based on the Ogata-Shiba wave function, where the charge and spin degrees of freedom factorize and which is exact in the limit of $U \to +\infty$. Due to the factorization, the spectral function simplifies into a convolution of a charge part which describes the energy scale of order of t and can be calculated analytically , and into a spin part with typical energies of t^2/U and can be calculated numerically using exact diagonalization and DMRG.

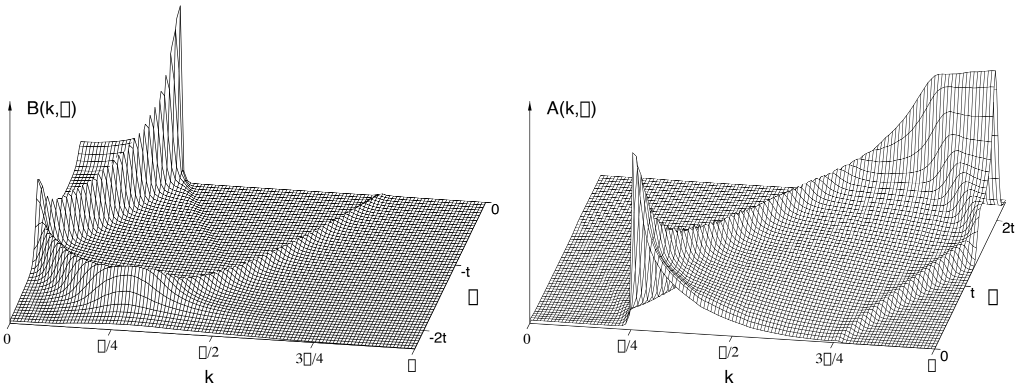

Figure 2: The photoemission $B(k,\omega)$ and inverse photoemission $A(k,\omega)$ spectra of the quarter filled large–U Hubbard model.

The resulting spectral function is very rich in structure (see Fig. 2) : for low energies ($|\omega - \varepsilon_F| < t^2/U$) we recover the Luttinger liquid properties, while for intermediate energies ($|\omega - \varepsilon_F| \sim t$) there is a well defined band that crosses the Fermi energy at $3k_F$. We interpret this feature as a shadow band coming from the spin fluctuations that diverge at $2k_F$. The shadow band should be in principle observed by the photoemission experiments with present resolution.

Formally Tetravalent Cerium and Thorium: Quantum Chemical Study of the Cerocene $Ce(C_8H_8)_2$ and Thorocene $Th(C_8H_8)_2$ Ground States

M. Dolg and P. Fulde

Both, the lanthanide element Cerium (^{58}Ce) and the actinide homologue Thorium (^{90}Th) posess four valence electrons, i.e. they may formally occur as tetravalent elements in chemical compounds. However, large differences are present between the lanthanide and actinide series due to shell structure effects as well as relativistic effects. The 4f-shell of the lanthanides has no core shell of the same angular quantum number to be orthogonal to and therefore is especially compact and energetically rather low-lying in energy. This so-called missing primogenic repulsion for the 4f-shell already causes a significant difference between the 4f-element Ce and the 5f-element Th at a nonrelativistic level of theory (fig. 1, left side). In addition, relativistic effects become more important with an increasing nuclear charge and tend to destabilize and expand especially the f-shells (fig. 1, right side). Whereas in case of Ce the 4f-shell is still energetically well separated from the 5d- and 6s-valence shells, the 5f-, 6d- and 7s-shells of Th are almost degenerate.

As a consequence of these effects derived at an effective one-particle level of theory, different electronic ground states arise for the Ce and Th atoms: disregarding relativistic effects both elements have a ground state configuration with two electrons in the f-shell (fig 2, left side), however a relativistic treatment yields a $4f^15d^16s^2$ ground state configuration for Ce in contrast to the $6d^27s^2$ ground state configuration of Th (fig. 2, right side), a picture which is in qualitative agreement with experimental findings despite the lack of electron correlation in the calculations.

The differences between Ce and Th present at the atomic level also affect the chemical behaviour of these elements. In simple diatomic molecules like the monoxides CeO [1] and ThO [2] one finds the ground state configurations $\phi_{4f}^1\sigma_{6s}^1$ and σ_{7s}^2, respectively, which are described here under the assumption of a purely ionic charge distribution $M^{2+}O^{2-}$.

In organometallic systems like the bis-cyclooctatetraene sandwich compounds of Ce and Th, i.e. cerocene $Ce(C_8H_8)$ and thorocene $Th(C_8H_8)$, the exceptional stability of the Ce 4f-shell also causes fundamental differences: whereas in the ground state of thorocene indeed a Th^{4+}-ion is complexed by two aromatic $C_8H_8^{2-}$-rings, a situation with a Ce^{3+}-ion possessing a 4f-shell occupied by one electron and ligand systems $C_8H_8^{1.5-}$ having a hole delocalized over both rings appears to be by far more favourable [3]. It was argued by Neumann and Fulde in 1989 [4] on the basis of semiempirical estimates and later confirmed by Dolg et al. in 1991 [5] by means of rigorous ab initio investigations that cerocene despite the open-shell character of the ground state configuration, still has a singlet ground state. This unusual ground state is induced by configuration interaction between the low-lying $4f^1\pi^3$ configuration corresponding to a formally trivalent Ce and the high-lying $4f^0\pi^4$ configuration corresponding to a formally tetravalent Ce. At the moment there is no experimental evidence in disagreement with this interpretation. The simple picture of tetravalent Ce in cerocene thus has to be revised.

Table 1: Ground states of X, XO und $X(C_8H_8)_2$ (X=Ce,Th).

system	symmetry	Ce		Th	
X	K_h	$4f^1 5d^1 6s^2$	$^1G_4$	$6d^2 7s^2$	$^3F_2$
XO	$C_{\infty v}$	$\phi^1_{4f}\sigma^1_{6s,6p}$	$^3\Phi_4$	σ^2_{7s}	$^1\Sigma^+$
$X(C_8H_8)_2$	D_{8h}	$e2u^1_{4f}e2u^3_{\pi}$	$^1A_{1g}$	$e2u^4_{\pi}$	$^1A_{1g}$

The results obtained so far for the ground states of Ce and Th systems are summarized in table 1. Current investigations indicate that the findings for cerocene and thorocene are typical for the electronic situation of the other lanthanide and actinide bis-cyclooctatetraene complexes [6].

The calculations summarized here have been performed using energy-consistent pseudopotentials for Ce [7] and Th [2], which on one hand replace the core-electron system and reduce the computational effort and on the other hand allow for a convenient inclusion of the major relativistic effects into quantum chemical calculations. The standard treatment consists of a scalar-relativistic self-consistent field or multi-configuration self-consistent field calculation with a subsequent treatment of correlation effects at the configuration interaction level. Spin-orbit effects, which are especially important for the excited states, have been derived from limited configuration interaction calculations in the intermediate coupling scheme. Cerocene and thorocene are the largest f-element systems studies so far by purely ab initio methods.

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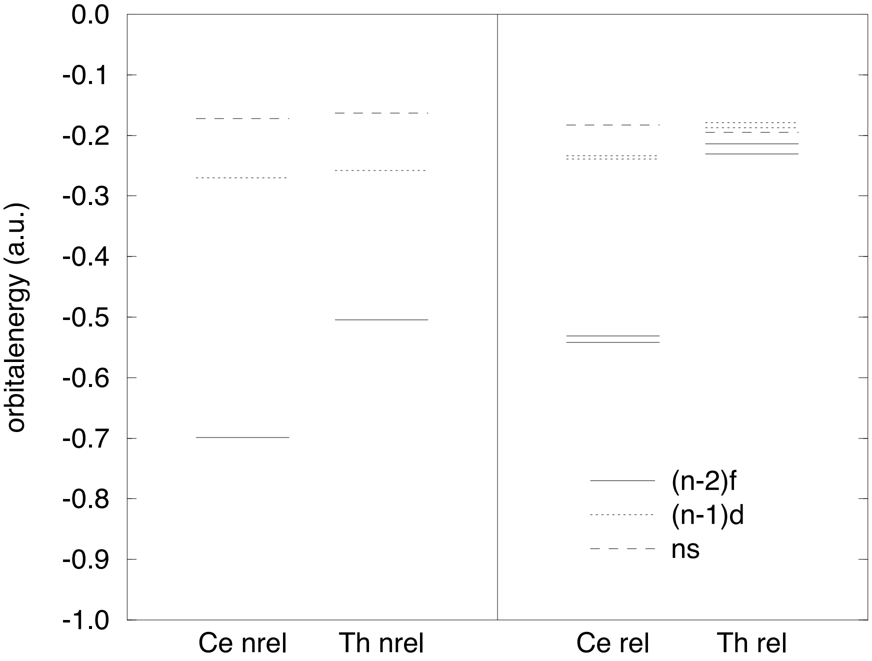

Figure 1: Orbital- and spinorenergies (a.u.), respectively, for the $(n-2)f^1(n-1)d^1ns^2$ configurational average of Ce (n=6) and Th (n=7) from Hartree-Fock and Dirac-Hartree-Fock calculations.

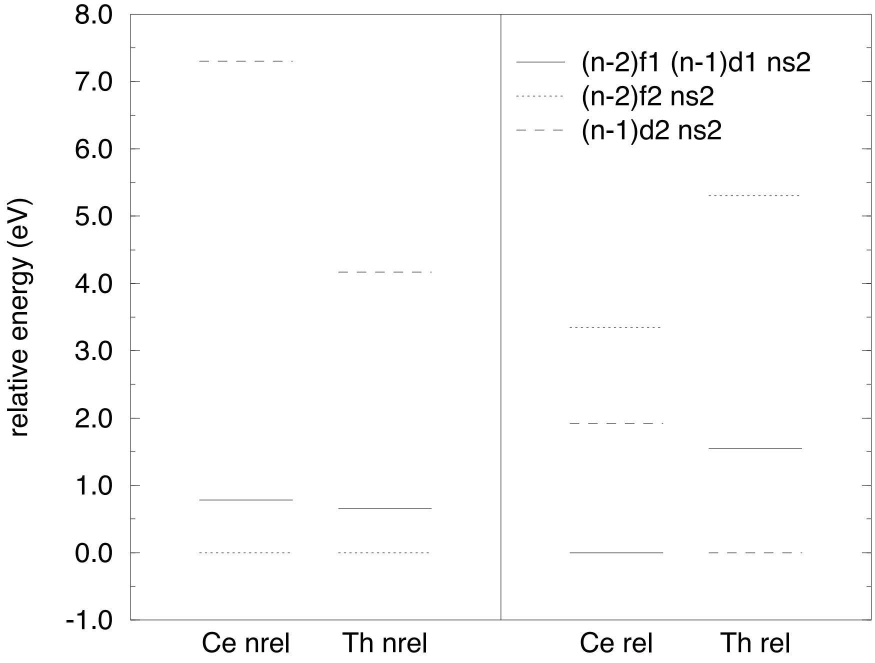

Figure 2: Relative energies (eV) of the $(n-2)f^1(n-1)d^1ns^2$, $(n-2)f^2ns^2$ and $(n-1)d^2ns^2$ configurational averages of Ce (n=6) und Th (n=7) from Hartree-Fock and Dirac-Hartree-Fock calculations.

Quantum Monte Carlo Calculations for Heavy Elements

H.-J. Flad

The calculation of electron correlation is a central topic in quantum chemistry. Despite of the significant successes obtained by standard quantum chemical methods like configuration interaction and coupled-cluster, it is still profitable to study more unconventional methods like quantum Monte Carlo (QMC) (for a comparison of QMC and standard methods see e.g. [1]). This method has been proven useful for an accurate treatment of electron correlation in atoms and molecules [2, 3]. However up to now most applications were concerned with systems containing only light main group elements. Only a few applications to transition metals have been reported in the literature [4, 5, 6]. Therefore an extension of the range of applications of the QMC method for heavy-element systems seems to be timely. In order to include relativistic corrections in the Hamiltonian and to obtain sufficiently small statistical errors, it is necessary to replace the core electrons by relativistic pseudopotentials [7, 8, 9, 10, 11]

In our QMC studies we focus our attention on typical problems which arise in connection with heavy elements. Currently we are studying the structure and physical properties of Hg clusters which show some characteristic variations of properties with the cluster size. Electron correlation is of central importance for a quantitative understanding of these systems which suggests an application of QMC methods. To get a reasonable estimate of the accuracy of our calculations, we have carried out extensive conventional *ab initio* and QMC calculations for the Hg atom and dimer [12]. The dimer is interesting for its own due to its very weak bond which is a pure correlation effect and the importance of relativistic effects. We obtained good agreements with experiment for the bond and ionization energy and for the vibrational frequency. Based upon these results we have attained to an approach which enables accurate calculations for small and medium cluster sizes.

Another problem is the treatment of spin-orbit coupling which has so far not been incorporated in QMC calculations for atoms and molecules. Up to now only scalar relativistic effects have been taken into account in QMC calculations. This is often not sufficient for heavy elements where spin-orbit effects become significant. In some cases it may be appropriate to treat electron correlation and spin-orbit coupling separately, but in general it would be desirable to treat both effects on the same footing. We study an approach [13] for the combined treatment of both effects within variational Monte Carlo (VMC) calculations. This means, that electron correlation is described by a correlation factor which depends explicitly on the electron-electron distances and is symmetric with respect to the electron coordinates [14]. The final wave function consists of a product of the correlation factor and an eigenfunction of the total angular momentum in a convenient coupling scheme. VMC means that one calculates the energy expectation value for such a wave function, where the spin-orbit operator has been taken from a relativistic pseudopotential. Energy differences between different states are calculated using a correlated sampling method which allows a very accurate determination of energy differences.

A fundamental feature in the application of QMC methods to large systems or systems containing heavy elements is the fixed-node approximation [15]. It permits an exact stochastic solution of the Schrödinger equation within a supplementary boundary condition. This boundary condition is given by the nodal structure of a trial wave function and the stochastic solution is forced to have the same nodes. The resulting energies are upper bounds of the exact ground state energies. Therefore it is necessary to find a trial wave function with a nodal structure close to the exact one. This problem is still not solved satisfactory when near degeneracies become important, which would require a complete active space treatment in the standard approaches. Transition metals provide numerous examples for systems which behave in this manner. We have focused our attention on 3d-elements where we have studied the fixed node errors for atoms and small molecules. In some cases HF and small MCSCF wave functions give only a poor description of the nodal hypersurface. To get a better understanding of this problem, we have carried out some systematic studies for the atoms B to F which show similar near degeneracy effects but the number of important configuration state functions is much smaller than for atoms with open d-shells [16].

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Ab-initio calculation of correlation energies by means of increments

K. Doll, B. Paulus, M. Dolg, H. Stoll, P. Fulde

Ab-initio calculations for solids are most often performed using density functional theory (DFT)[1]. However, the many-body wavefunction can not be obtained from this method and a systematic improvement seems to be a difficult task. Hartree-Fock (HF) calculations with an exact treatment of the exchange can nowadays be routinely performed with the program package CRYSTAL[2]. But since correlation effects are not included, the results (e.g. for ground state properties) still show a significant deviation from the experimental values. For molecules quantum chemical methods such as configuration interaction and coupled cluster approaches have been developed for determination of correlation energies. These calculations are of high quality, but the computational effort increases strongly with the system size (power laws roughly $\sim N^3$ ... N^7 hold). However, with a recently proposed incremental scheme [3] it has been shown that the methods of quantum chemistry can be applied to solids.

The idea of this method is to decompose the correlation energy in local increments. In a first step, localized orbitals have to be created. One-body correlation energy increments $\Delta\epsilon_i$ are then calculated by correlating one single group of orbitals (e.g. one localized bond in the case of semiconductors or a group of atom-centered orbitals in the case of ionic solids). Two-body increments $\Delta\epsilon_{ij}$ are next determined by considering two groups of orbitals:

$$\Delta\epsilon_{ij} = \epsilon_{ij} - (\Delta\epsilon_i + \Delta\epsilon_j),$$

where ϵ_{ij} is the correlation energy of the joined system $\{ij\}$. Higher order increments are defined in an analogous way, for example for the three-body increments one has

$$\Delta\epsilon_{ijk} = \epsilon_{ijk} - (\Delta\epsilon_i + \Delta\epsilon_j + \Delta\epsilon_k) - (\Delta\epsilon_{ij} + \Delta\epsilon_{jk} + \Delta\epsilon_{ki}).$$

The correlation energy of the solid is finally obtained by adding up all the increments:

$$E^{\mathrm{corr}}_{\mathrm{bulk}} = \sum_i \Delta\epsilon_i + \frac{1}{2!}\sum_{i,j}\Delta\epsilon_{ij} + \frac{1}{3!}\sum_{i,j,k}\Delta\epsilon_{ijk} + \ldots.$$

It should be mentioned that a formal derivation of this equation is also possible using the framework of projection technique.
The idea is now to neglect higher orders of increments. This only works if increments up to, say, three-bond increments are sufficient and if the increments decrease rapidly with increasing distance between localized orbitals. These conditions have been shown to be well met in all the materials that we have examined, provided that the correlation method used is size-consistent. We have performed our correlation calculation with the different coupled cluster approaches of the program package MOLPRO94[4].

We have applied the method of increments to four elementary semiconductors with diamond structure, to twelve III-V compounds with zincblende structure and to two ionic solids with NaCl structure, namely MgO and CaO. Since dynamical correlation is a local effect, the increments should be fairly local entities. We use this property

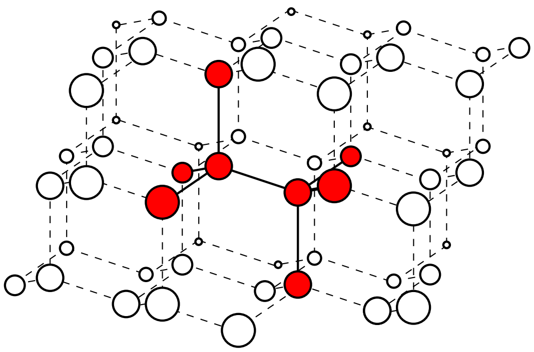

Figure 1: One of the clusters (red atoms) within the diamond structure used in the correlation calculation.

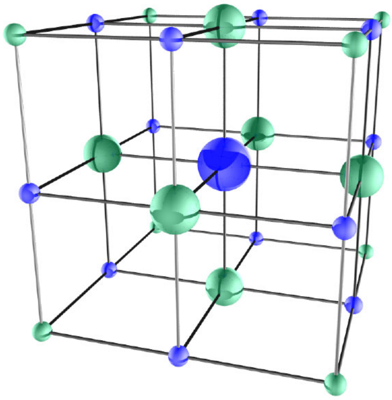

Figure 2: MgO; Central atom (large sphere) is a fully correlated oxygen, surrounded by Mg pseudopotentials (mediumsize spheres) and point charges (small spheres).

to calculate the correlation energy increments in finite clusters. A possible choice of clusters is shown in Fig. 1 for the diamond structure, in Fig. 2 for the NaCl structure. To discuss the influence of the electron correlations we need reliable Hartree-Fock ground state energies for these solids. We use the program package CRYSTAL92 to perform the Hartree-Fock calculations. At the Hartree-Fock level we obtain only 50-70% of the experimentally determined cohesive energy. Adding the correlation contribution to the cohesive energy we reach about 93% of the experimental value (for some results see Table I). This shows that we can calculate the main part ($\approx 85\%$) of the correlation energy of the solid. The missing part is mainly due to basis set defects. Only minor errors are due to the truncation in the incremental scheme ($\leq 2\%$).

Another aspect of our work is the influence of electron correlations on lattice constants (for some results see Table I). In the case of the semiconductors, Hartree-Fock overestimates the lattice constant by 1-2%. A main reduction is due to core polarization which we include by a core polarization potential. In the valence electron system interatomic correlations (due to correlations in the bonds) increase the lattice constant, while intraatomic correlations (due to correlations in the atom) decrease it. We have seen these opposite trends for all the semiconductors. For solids from lighter atoms like diamond, the interatomic part predominates, for solids from heavier atoms the intraatomic one. In the case of ionic solids, the van der Waals-type of correlation leads to a reduction of the lattice constant. A contribution in the opposite direction comes from the intraatomic correlation of the oxygen ion. The excitation energies for an oxygen ion embedded in the crystal are higher than for the hypothetical free ion and therefore correlations are less important at a shorter lattice constant.

These results show that the method of increments provides an *ab initio* scheme to calculate the correlation energies of solids with quantum chemical accuracy. We have

	$E_{\text{coh}}^{\text{HF}}$	$E_{\text{coh}}^{\text{HF+corr}}$	$E_{\text{coh}}^{\text{exp}}$	a_{HF}	$a_{\text{HF+corr}}$	a_{exp}
Si	-0.227 (66%)	-0.325 (94%)	-0.344	5.499 (+1.2%)	5.426 (-0.1%)	5.432
GaAs	-0.130 (53%)	-0.228 (93%)	-0.246	5.755 (+1.8%)	5.647 (-0.0%)	5.649
CaO	-0.279 (68%)	-0.380 (93%)	-0.409	4.864 (+1.3%)	4.801 (-0.0%)	4.803

Table 1: Cohesive energies per unit cell in a.u. (percentages of the experimental value are given in parentheses). Lattice constants in angstroms (deviations from experiment are given in parentheses). Hartree-Fock (HF) values are obtained within a basis set of double zeta quality plus one polarization function, the correlation calculation was performed within a basis set of triple zeta quality plus three polarization functions.

presented here the application to elementary and cubic III-V semiconductors as well as to ionic compounds. We have found a very good agreement with experiment and a deeper understanding of the influence of electron correlations on ground state properties.

In the future we want to brigde the gap between covalent and ionic bound solids by applying the method of increments to II-VI semiconductors. On the other hand we want to expand the scheme to systems with stronger correlations such as NiO.

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Universal and non-universal aspects of complex quantum spectra

B. Mehlig

Universal aspects. It has been known for a long time that complex quantum spectra exhibit universal statistical properties. Experimentally, complex quantum spectra arise in many different cases, such as disordered metals, the Hydrogen atom in a strong magnetic field and generally in systems whose classical limit is chaotic. For these systems, random matrix theory provides a unifying description. Consider, for example, a classically chaotic Hamiltonian system with Hamilton function $H(\boldsymbol{p},\boldsymbol{q})$. The corresponding quantum system has energy levels E_α and eigenfunctions $|\psi_\alpha\rangle$ determined by the stationary Schrödinger equation $\widehat{H}|\psi_\alpha\rangle = E_\alpha|\psi_\alpha\rangle$. According to the Wigner-Dyson hypothesis, the distribution function $P(\Delta)$ of nearest-neighbour spacings Δ, for instance, should have the universal form $P(\Delta) = \pi/2\,\Delta\exp(-\pi/4\,\Delta^2)$. Fig. 1(a), for example, shows $P(\Delta)$ together with numerical data obtained by quantizing a classically chaotic system (the spectrum is unfolded such that the mean level spacing $\langle\Delta\rangle$ is unity).

A more stringent test of universality is provided by the sensitivity of the quantum levels (or the eigenfunctions) with respect to changes of the boundary conditions[1] or with respect to changing an external parameter[2]. In the case of the Hydrogen atom, this could be the magnetic field, it could be shape fluctuations of a small metal particle or a magnetic flux threading a disordered metal. In general, the Hamilton operator of such a system is written as $\widehat{H} = \widehat{H}_0 + \widehat{H}_1(X)$, where X is the external parameter. The influence of the external parameter X upon the spectrum is characterized by the derivatives $\partial E_\alpha/\partial X$ of the energy levels $E_\alpha(X)$ with respect to the parameter X. The parametric dependence of complex spectra can be modeled by a diffusion process of random matrices in a fictitious time related to the parameter X. In this way it is possible to derive universal spectral correlation functions, such as for instance,

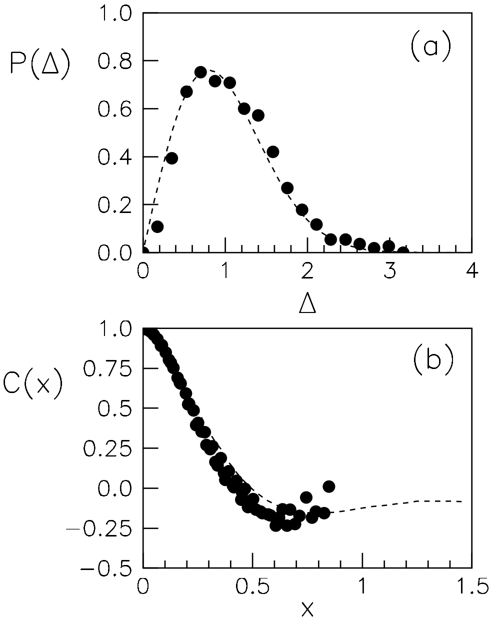

Figure 1: (a) Nearest-neighbour spacing distribution function $P(\Delta)$. (b) Correlation function $C(x)$.

$$C(X) = \Big\langle \frac{\partial E_\alpha(0)}{\partial X}\frac{\partial E_\alpha(X)}{\partial X}\Big\rangle. \tag{5}$$

In Fig. 1(b) the correlation function $C(x)$ is shown. Also shown are numerical data pertaining to a quantum system with a classically chaotic limit. The parameter X has been rescaled according to $x = X\sqrt{C(0)}$ in order to obtain a universal function (note that the mean level spacing is taken to be unity).

Non-universal aspects. As it stands, the Wigner-Dyson hypothesis applies to chaotic systems provided phase space is uniformly chaotic. In this case, the quantum wavefunctions are Gaussian random functions of the coordinates $\boldsymbol{q}$. This implies in particular that the distribution of quantum-mechanical matrix elements such as $\langle\psi_\alpha|\partial\widehat{H}_1/\partial X|\psi_\alpha\rangle$ will also be Gaussian, as required for the universal form of $C(x)$.

However, most experimentally realizable systems, such as, e. g. the Hydrogen atom in a strong magnetic field are mixed systems: their phase space is not uniformly chaotic. The presence of stable islands, in particular, causes deviations from the universal behaviour. In the following it will be discussed how non-universal features arise from classical periodic orbits. This discussion serves as an application of the semi-classical theory of matrix elements[3], which has recently been applied to chaotic billiards[4] and the Hydrogen atom in a strong magnetic field[5].

Here we consider an electron moving in a domain D with specular reflection from the boundary. The shape of the boundary can be varied and is characterized by a deformation parameter X, such that for $X = 0$ the boundary is a circle.

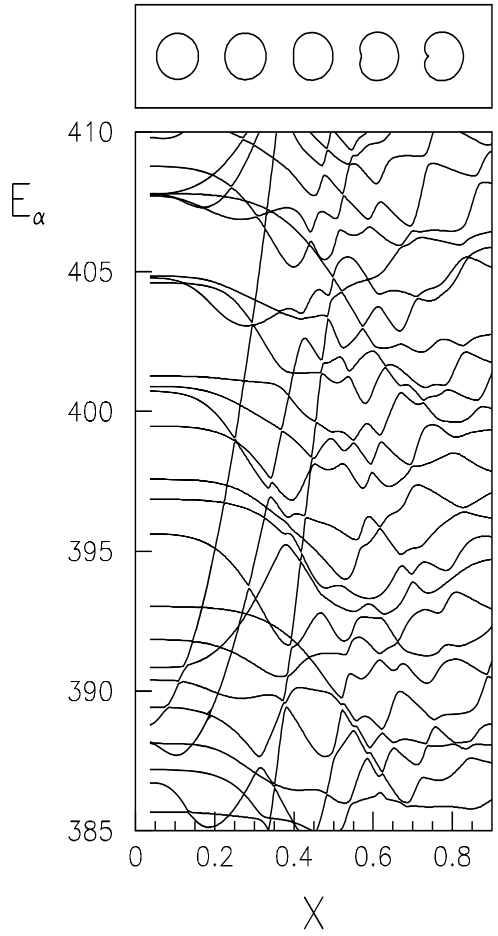

Figure 2: (top) Family of "billiards". (bottom) Quantum spectrum as a function of the deformation parameter X.

As X is increased from zero, the shape changes as shown in Fig. 2 (top) and the classical mechanics undergoes a transition from integrable to chaotic motion. Such "billiard" models are not only of interest theoretically. They may be thought to model electronic motion in a small metal particle or a quantum dot. Fig. 2 shows part of the quantum spectrum of this system as a function of the deformation parameter X.

The spectrum of Fig. 2 can be divided into several regions. First, for very small values of X, the slopes $\partial E_\alpha/\partial X$ of all levels are zero. Second, as the value of X is increased, the levels acquire dispersion. While the majority of levels evolves slowly as a function of X, certain levels exhibit a strong parameter-dependence. These structures are due to wave functions localized in the vicinity of stable periodic orbits. In the range of X governed by stable classical motion ($X \lesssim 0.3$), we observe a large number of rather narrow avoided crossings. Third, as the value of X is increased beyond this region, the classical dynamics becomes chaotic. Correspondingly, the level repulsion increases and the spectrum exhibits highly irregular structures and universal behaviour — the numerical quantum data shown in Fig. 1 were obtained in this region.

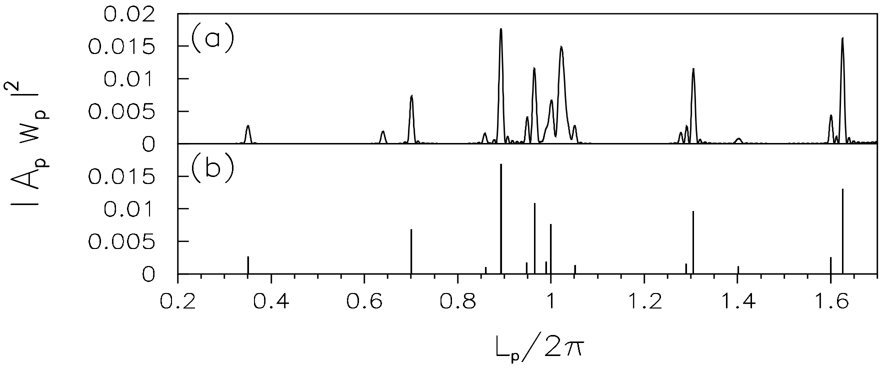

Figure 3: (a) Fourier transformation of $d(E, X)$ for $X = 0.5$. (b) Corresponding semi-classical spectrum.

In order to analyze the parametric derivatives $\partial E_\alpha/\partial X$ semi-classically, we define a density of parametric derivatives

$$d(E, X) = \sum_\alpha \frac{\partial E_\alpha}{\partial X}\, \delta(E - E_\alpha(X)). \tag{6}$$

Making use of the identity $\partial E_\alpha/\partial X = \langle \psi_\alpha(X)|\partial \widehat{H}_1/\partial X|\psi_\alpha(X)\rangle$, Eq. (6) can be written as a density of diagonal matrix elements of the quantum-mechanical operator $\widehat{A} = \partial \widehat{H}_1/\partial X$. Following[3,4], we use the semi-classical approximation

$$\begin{aligned} d(E, X) &= \sum_\alpha \langle \psi_\alpha(X)|\widehat{A}|\psi_\alpha(X)\rangle\, \delta(E - E_\alpha(X)) \qquad (7)\\ &= \langle d(E, X)\rangle + \mathrm{Re}\frac{1}{\pi\hbar}\sum_p A_p w_p \exp\Big[\frac{i}{\hbar}(S_p - \mu_p \frac{\pi}{2})\Big], \end{aligned}$$

where $w_p = T_p|\det(M_p - 1)|^{-1/2}$ denote the semi-classical (Gutzwiller) amplitudes. The sum in Eq. (7) is over the periodic orbits with action S_p. The actions S_p are related to the lengths L_p of the periodic orbits by $S_p = \sqrt{E} L_p$. μ_p denote the Maslov indices and M_p the monodromy matrices. The $A_p = T_p^{-1} \oint_p dt\, A(\boldsymbol{p}(t), \boldsymbol{q}(t))$ are averages of the observable $A(\boldsymbol{p}, \boldsymbol{q})$ around the periodic orbits p. In order to simplify the notation, the dependence of the semi-classical amplitudes $A_p w_p$ and the actions S_p on the energy E and the parameter X were omitted. Now according to Eq. (7), the Fourier transform of $d(E, X)$ with respect to $\sqrt{E}$ should exhibit peaks at the lengths L_p of the classical periodic orbits. This implies that parametric derivatives at different levels E_α and E_β (at the same value of X) are strongly correlated. Correlations at large energy separations are governed by short periodic orbits, whose actions and amplitudes depend on the system in question. Thus short periodic orbits give rise to non-universal correlations in the parametric spectrum of Fig. 2.

An example is given in Fig. 3, which shows the Fourier transform of $d(E, X)$ with respect to $\sqrt{E}$ at $X = 0.5$, together with the expected semi-classical amplitudes. The agreement between the quantum data and the semi-classical amplitudes is satisfactory, except for periodic orbits with lengths close to the circumference $L_p \sim 2\pi$, where one has to go beyond the lowest-order semi-classical approximation. Amplitudes corresponding to stable periodic orbits are not shown in Fig. 3(b) but can be treated accordingly.

Summary. The semi-classical theory of diagonal matrix elements can be successfully applied to evaluate parametric correlations in a complex spectrum, such as the one shown in Fig. 2. A semi-classical approach is particularly suited to assess non-universal long-range correlations in the spectrum. A study of parametric correlations involving non-diagonal matrix elements is underway.

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Localization in a Random Network of Coupled Quantum Wires: Model for Metal-Insulator Transition and Transport in Highly Conducting Polymers

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Recently, conjugated polymers such as polyacetylene, polyaniline and polypyrrole have attracted considerable interest in applied and fundamental research. Their common exciting feature is that the conductivity can be increased by a few orders of magnitude upon doping. In heavily doped Tsukamoto polyacetylene the room-temperature conductivity (σ_{RT}) has already reached that of Cu. However, in spite of the large σ_{RT}, the experimental study indicates that transport of the conducting polymers are still far from being traditional metallic: the conductivity decreases with lowering temperature. At the same part time their thermoelectric power and Pauli susceptibility suggest a metallic density of states at the Fermi level.

On the basis of these observations it was suggested, that the highly conducting polymers are close to a metal-insulator (MI) transition driven by disorder. Since their σ_{RT} much exceed those of all known systems near the MI boundary, one can conclude also that the highly conducting polymers exhibit a new type of localization-delocalization transition. For a physical explanation of the unusual transport properties of the polymers their chain nature seems to be very important. The most well-known polymer, polyacetylene, has a so-called fibril structure: single chains are coupled into fibrils which form an irregular cross-linked network. In the case of conducting polyaniline and polypyrrole there are crystalline regions where the chains are parallel and strongly interacting. These metallic islands are coupled into the network with the twisted and tangled chains.

As a result, we have a network of randomly coupled metallic wires. In the absence of the junctions all the electronic states of the quantum wires are localized by any weak disorder. The states become extended over the whole network only for strong enough interwire electron-transfers. For the present model within the supersymmetry method we determine the position of the MI transition and the critical behavior as a function of the intrinsic disorder and of the interwire coupling. It should be stressed that the existence of the delocalized phase in the network is a nontrivial phenomenon. Indeed, due to its irregularity, the random network should be considered as strongly disordered, and therefore all the electronic states might remain localized. However, it is not so and we prove the existence of the MI transition in the network, Fig. 1.

Whether the electronic states are localized or extended show up only in the low-temperature conductivity. At high temperatures, due to inelastic scattering electrons are delocalized, and the network has always a metallic conductivity even in the absence of cross-links. This property of our model can, in principle, reconcile the observable controversy between the high- and low- temperature conductivities of the polymers. One can also note that the thermodynamic characteristics of the network corresponds always to a metallic density of states at the Fermi level in both, the metallic and dielectric phases.

A MI transition in the intrafibril disorder produced by aging is observed in heavily doped polyacetylene and polypyrrole. In our model such a disorder is incorporated

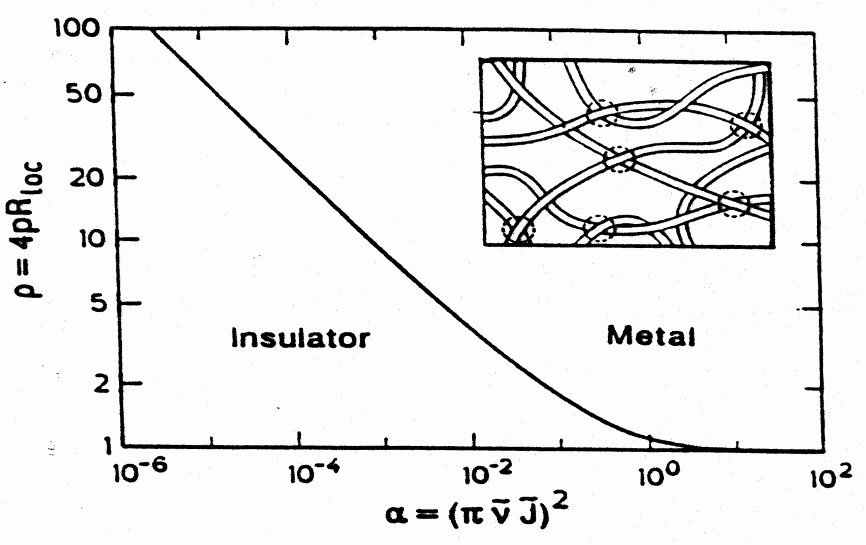

Figure 1: Diagram of states of the random quantum network. Here R_{loc} is the localization radius for a single wire, p is the linear concentration of interwire junctions and α is the parameter of coupling at a junction. Inset shows a schematic structure of the network.

into R_{loc}. Being inversely proportional to the concentration of the internal defects, R_{loc} decreases with disorder, and at the critical disorder the system becomes macroscopically dielectric. Note that according to the phase diagram in Fig. 1 the conducting state is more sensitive to the value pR_{loc} than to the strength of the interwire coupling α and, therefore, can be easier induced by an increase of pR_{loc}. Experimentally this tendency is seen in the appreciable enhancement of the low-temperature conductivity without signs of a saturation under application of the magnetic field, pressure and stretching. The fact that the conductivity is controlled by the cross-linkings was most explicitly demonstrated for polyaniline.

The temperature-dependent conductivity of the present model demonstrates a number of very specific dependencies. We note some of them. In the localized phase there is the temperature interval where the hopping transport over the nearest states is realized. The length of hops is of order or smaller than the localization radius and similar a regime is due to weak quantum localization. It is absent in amorphous semiconductors and in dirty metal. Its characteristic feature is power dependence of the conductivity on temperature, with a large exponent.

In contrast to the 3d Anderson localization that occurs due to strong disorder, the 1d interference localization due to weak disorder can be easily broken at room temperatures by phonon scattering. this explains the crossover from high-temperature metallic behavior to a low-temperature dielectric one, which is observed in the temperature dependence of the conductivity and dielectric response for the highly conducting polymers. A high anisotropy of phonon and impurity scattering in a quasi–1d system should be taken into account in order to obtain agreement between theoretical and experimental dependencies.

Thus, we suggested a new model for the description of transport properties in fibril-form polymers with a completely irregular structure. The MI transition studied within this model enables us to understand peculiarities of transport in the novel highly conducting polymers.

Unbiased determination of the dynamics underlying a noisy chaotic time series

H. Kantz

Modeling, prediction and controlling of chaotic systems requires the reconstruction of equations of motion from observed data. In many experimental situations only scalar time series are available. By Takens's time delay embedding one can reconstruct a space which is equivalent to the state space restricted to the attractor of a dynamical system. In this space the map from the actual state vector onto the next scalar observation is unique, if the underlying dynamics in fact is predominantly deterministic, i.e., if the observations represent a deterministic process only contaminated by observational noise. The minimization of the one step prediction error yields a map which within a certain class is the optimal predictor and simultaneously is assumed to represent the underlying dynamics in an optimal way. However, in the presence of high noise levels, when the determination of the dynamics is the only possibility to evidence the otherwise deterministic character of the process, there exists a systematic difference between the best predictor and the true underlying dynamics. Two modifications of the minimization problem are necessary to obtain the latter.

Let our time series $\{s_n\}$ be a set of observations, $n = 1, \ldots, N$, obtained by the application of an unknown measurement function $h(\vec{x})$ to state vectors $\vec{x}(t = n\delta t) \in \Gamma$ with a sampling rate δt. We assume that the dynamics in Γ is deterministic, i.e. $\dot{\vec{x}} = \vec{f}(\vec{x}) + \vec{d}(t)$, where $\vec{d}(t)$ is constant or periodic in time. Takens's delay embedding theorem states that a *delay vector* $\vec{s}_n = (s_n, s_{n-1}, \ldots, s_{n-m+1})$ can be considered as a state vector, if its dimension m is sufficiently large. For data on an D_f dimensional attractor $m > 2D_f$ yields a unique representation. A vector $\vec{s} \in \mathbf{R}^m$ thus unambiguously defines a state on the attractor and its time evolution is completely determined. There exists a map $g : \mathbf{R}^m \to \mathbf{R}$ which maps the current state vector onto the next scalar observation, $s_{n+1} = g(\vec{s}_n) + \eta_n$, apart from some noise η_n which is related to inaccurate observations $s_n = h(\vec{x}(n\delta t)) + \xi_n$.

The usual way to determine g from a series of experimental data is to choose a suitable ansatz $\tilde{g}_{p_i}$ and to minimize the one step prediction error with respect to the parameters p_i:

$$\sum (s_{n+1} - \tilde{g}_{p_i}(\vec{s}_n))^2 = \min. \tag{8}$$

In use are local linear fits and global nonlinear ansatzes like higher order multivariate polynomials, superpositions of radial basis functions, or neural nets. It is numerically convenient if the parameters p_i appear only linearly in $\tilde{g}$, since this allows to compute the minimum by a single matrix inversion.

Eq.(1) divides the variables into independent ones, the $\vec{s}_n$, and dependent ones, the s_{n+1}. Only if all measurement errors are only contained in the dependent variables, Eq.(1) leads to an unbiased result. Since in our problem both the $\vec{s}_n$ and s_{n+1} are contaminated by the same amount of noise, this assumption is violated and consequently the result g can be considerably wrong, i.e. $\tilde{g} \neq g$ due to systematic effects. This is demonstrated in Fig.1 for a simple model, the Hénon map.

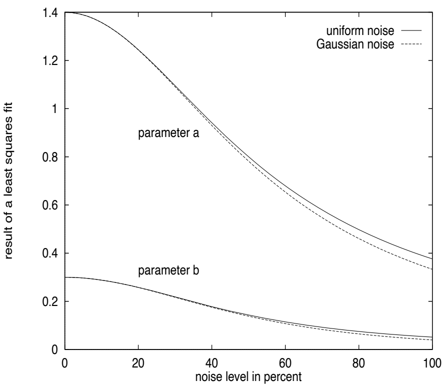

Figure 1: Biased results obtained by the minimization of Eq.(1): Fitting the map $\tilde{g} = 1 - as_n^2 + bs_{n-1}$ to infinitely long time series of the Hénon map $g = 1 - a_0 x_n^2 + b_0 x_{n-1}$ with $a_0 = 1.4$ and $b_0 = 0.3$ leads to systematically wrong results for a and b, if the noise level is high.

In a geometrical interpretation, the task is to determine a hypersurface in $\mathbf{R}^{m+1}$ which fits best a cloud of data points. If in fact only the s_{n+1} were noisy, the minimization of only the s_{n+1}-component of the vector between a noisy point $(s_{n+1}, s_n, \ldots, s_{n-m+1})$ and the hypersurface would be justified and Eq.(1) thus correct. In our case, instead, the orthogonal Euclidean distances between noisy points and hypersurface should be minimal, since the probability of a clean point to be shifted to the observed position has spherical symmetry. Thus the new cost function reads

$$\sum \min_{\vec{y}} \left((x_{n+1}, \vec{x}_n) - (\tilde{g}(p_i, \vec{y}), \vec{y})\right)^2 = \min, \tag{9}$$

where the summands are just the Euclidean distances between the observed points and the hypersurface described by the dynamics. In fact, one can show for linear g and $\tilde{g}$ that this minimization problem leads to $\tilde{g} = g$.

In general, however, there is an additional problem: A least squares problem yields an unbiased estimator of a statistical quantity (here: the coefficients of $\tilde{g}$) only if the distribution of the input data is Gaussian, since it is derived by the maximum likelihood principle exactly under this assumption. The invariant measure of data on an attractor usually is strongly non–Gaussian. The consequence is shown in Fig.2: Since the attractor has only a finite support, the continuation of the function $\tilde{g}$ outside is not determined by our data, but more importantly, close to the border of the support the lack of points outside leads to a bias in the "best graph".

From a geometrical point of view (fitting a hypersurface to a cloud of data points) the solution thus found is optimal and there is no geometrical information which can be used for an improvement. However, the points on the attractor stem from a scalar time series and thus are dynamically correlated. Without noise they should fulfill an exact image–preimage relation under the dynamics $\tilde{g}$. With noise, one cannot use this demand as a constraint, but the violation of such a relation should be minimal. Therefore a cost function which can suppress the bias is a mutual k–step error in the following sense: for each segment of length k of the experimental series, $\vec{s}_n$, $\vec{s}_{n+1}$, …, $\vec{s}_{n+k}$, one constructs a sequence $\vec{y}_n^{(1)}$, …, $\vec{y}_n^{(k)}$, which fulfills the dynamics $\tilde{g}$ exactly, i.e. $\vec{y}_n^{(l+1)} = (y_{n,l+1}, y_{n,l}, \ldots, y_{n,l-m+2})$ with $y_{n,l+1} = \tilde{g}(p_i, \vec{y}_n^{(l)})$, and simultaneously is as close as possible to the corresponding point $\vec{s}_{n+l}$. In the limit $k = 1$ the cost function

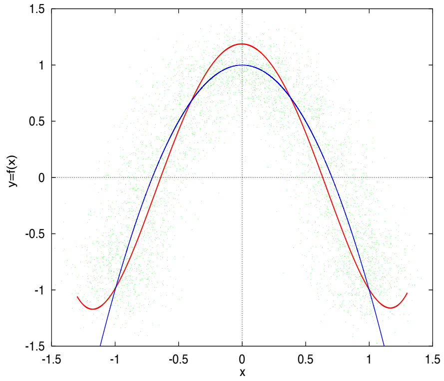

Figure 2: Noisy data of the logistic equation $x_{n+1} = g(x_n) = 1 - 1.8x_n^2$ together with the graph of g and of $\tilde{g}$, obtained by the minimization of Eq.(2), where $\tilde{g}$ is a polynomial of fourth order. Since the data have a finite support, at its borders the "wrong" graph $\tilde{g}$ creates less costs than the true graph g.

Eq.(2) should be found. Thus the new minimization problem reads:

$$\begin{aligned}
S^{(k)} \quad = \quad & \sum_{n=m}^{N-k} \min_{\vec{y}_n^{(1)}} \left((s_{n+1}, \vec{s}_n) - (\tilde{g}(p_i, \vec{y}_n^{(1)}), \vec{y}_n^{(1)}) \right)^2 \\
& + ((s_{n+2}, \vec{s}_{n+1}) - (\tilde{g}(p_i, \vec{y}_n^{(2)}), \vec{y}_n^{(2)}))^2 \\
& + \ldots \\
& + ((s_{n+k}, \vec{s}_{n+k-1}) - (\tilde{g}(p_i, \vec{y}_n^{(k)}), \vec{y}_n^{(k)}))^2 . \qquad (10)
\end{aligned}$$

The minimization has to be performed with respect to the "initial conditions" $\vec{y}_n^{(1)}$ for each segment of length k of the experimental data, and with respect to the parameters p_i in $\tilde{g}$. In comparison to Eq.(1) this increases the numerical effort tremendously, but can be done on workstations within a reasonable amount of CPU time.

Eq.(3) states that for noisy data the problem of finding the most probable deterministic dynamics cannot be separated from the problem of finding the most probable clean trajectory, which is the well known shadowing problem. For chaotic data, the construction of a shadowing trajectory is extremely difficult (although it can be assumed to exist also in nonhyperbolic systems, since we are speaking of measurement noise). Due to the sensitivity on initial conditions, there exists a theoretical bound for k which depends on the maximal Lyapunov exponent λ_+ of the dynamics and on the precision of the data representation on the computer, and which is of the order of $40/\lambda_+$. In practice, k=4 to 6 can be realized with reasonable effort.

We use two measures for the quality of the results. The first one is very strict but cannot be exploited easily in a quantitative way. It is the difference between the attractor of the true dynamics g and the one obtained from iteration of the fitted dynamics $\tilde{g}$. Since the shape of an attractor depends very sensitively on details of the dynamical equations, this comparison reveals whether from a dynamical point of view the fit contains all relevant features.

Alternatively, one can measure the difference $|g - \tilde{g}|$ on the relevant subset of the state space, which is the attractor $\mathcal{A}$ of the dynamics g. This leads to an error measure

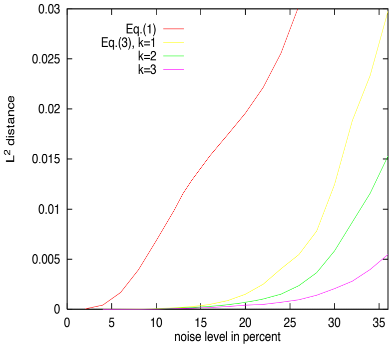

Figure 3: The error measure d_{L_2} for fits of the dynamics of the Ulam map $x_{n+1} = 1 - 2x_n^2$, obtained from noisy time series of length 1000 and a fourth order polynomial as ansatz for $\tilde{g}$.

$d_{L_2} = \int_{\mathcal{A}} (g - \tilde{g})^2 d\mu \approx \frac{1}{N} \sum (x_{n+1} - \tilde{g}(\vec{x}_n))^2$, where the $\{x_n\}$ form a clean trajectory of g. Note that a small value of d_{L_2} does not imply that the trajectory $\{x_n\}$ is stable under the dynamics $\tilde{g}$, such that the attractor of $\tilde{g}$ could be very different from the one of g. In Fig.(4) we present this error measure as a function of the noise level for different k.

Many more examples, including experimental data with unknown dynamical equations show that the cost function Eq.(3) in fact leads to a much better fit of the dynamics than the one step prediction error Eq.(1), and that it allows for a faithful determination of the dynamics for noise levels up to 30 and more percent. The relevance lies in the fact that for noise levels beyond 2% the standard methods like correlation dimension and Lyapunov exponent cannot be used any more to evidence the deterministic nature of data. Nonlinear noise reduction allows to suppress noise by only a factor of about 5, so that data with more than 10% noise can only be shown to possess a predominantly deterministic source, if one is able to construct a model which reproduces the main features of the data.

Konferenzen, Workshops und Symposien 1994-1995

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“Elektronisch hochkorrelierte metallische Materialien”
Schellerhau (Sachsen), 7. - 11. März 1994, 95 Teilnehmer.
Leitung: W. Aßmus (J.W. Goethe-Universität Frankfurt a.M.), B. Lüthi (J.W. Goethe-Universität Frankfurt a.M.), G. Zwicknagl (MPI für Physik komplexer Systeme)

“International Symposium on Chaos and Mesoscopic Systems”
Freital (Sachsen), 7. - 10. Juni 1994, 55 Teilnehmer.
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Vorlesungen an der TU Dresden

Lectures at TU Dresden

“Semiclassical Quantization of Chaotic Billiards”
U. Smilansky (Rehovot); Februar 1994; Vortragsreihe

“Non Fermi Liquid Effects in Low Dimensional and Constrained Systems”
A. Finkelstein (Rehovot); Juni 1994; Vortragsreihe

“Lecture Series on Turbulence and Pattern Formation”
I. Procaccia (Rehovot), G. Falkovich (Rehovot), V. L’vov (Rehovot), V. Steinberg (Rehovot), A. Nepomnyashchy (Haifa), L. Pismen (Haifa); April - Juli 1995; Vorlesungsreihe veranstaltet vom Minerva Center for Nonlinear Physics of Complex Systems und vom MPI für Physik komplexer Systeme.

“Elektronische Korrelationen in Molekülen und Festkörpern”
P. Fulde; Wintersemester 1995/96

“Ausgewählte Themen der Festkörperphysik”
P. Fulde; Sommersemester 1996

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Bücher

Fulde, P.:
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Habilitationen

Habilitations

Kantz, Holger: Time series analysis from the viewpoint of nonlinear dynamics
Dresden, 1995

Dissertationen

Dissertations

Mehlig, Bernhard: Grundzustand und Anregungsspektrum des Hubbardmodells
Stuttgart, 1994

Mödl, Martin U.: Ab initio-Rechnungen an den Alkalithioferraten (III) Na_5FeS_4 und $Na_6Fe_2S_6$
Dresden, 1995

Paulus, Beate: Elektronische Korrelationen in Halbleitern
Dresden, 1995

Auszeichnungen

Awards

Dolg, Michael: Heinz-Maier-Leibnitz-Preis, 1994

Mehlig, Bernhard: Otto-Hahn-Medaille der Max-Planck-Gesellschaft, 1995

Vorträge und Seminare in Dresden 1994–1995

Seminar talks given in Dresden 1994-1995

Termin	Thema	Vortragender
22.02.94	A Magnetic Impurity in a Strongly Correlated Electronic System	Dr. K. Hallberg, Stuttgart
21.04.94	Electronic Correlations in the Karpov Institute	Dr. A. Tchougreev, Dresden
27.04.94	The Integer Quantum Hall Effect: a Special Exactly Solvable Model	Dr. R. Gade, Dresden
05.05.94	Numerical Evidence on the Existence of Self Trapping State for 3-D Acoustic Polarons	Dr. X. Wang, Dresden
11.05.94	Diffusion Models and Quantum Problems	Prof. I. Peschel, Berlin
19.05.94	Kosterlitz-Thouless Transition in Layered High Temperature Superconductors	Prof. K.H. Fischer, Jülich
26.05.94	Statistical Physics of Analog Neurons	Dr. R. Kühn, Heidelberg
31.05.94	Electron Tunneling in a Double Well Potential	Dr. E. Heiner, Chemnitz
02.06.94	Cluster Calculations for Hartree Fock Energies of Solids	B. Paulus, Dresden
06.06.94	Chaos in Mechanical and Aerospace Systems	Prof. E. Dowell, N. Carolina
09.06.94	The One Dimensional Electronic Properties of the Bechgaard Salts	Dr. F. Mila, Toulouse
15.06.94	Ein Verfahren zur Berechnung von Korrelationsfunktionen in Fermi und Bose Systemen	Prof. P. Schuck, Grenoble
21.06.94	Ein Phänomenologisches Wechselwirkungsmodell für die Kuprat-Supraleiter	Prof. R. Ferrell, Maryland
23.06.94	Monte Carlo Methoden in der Festkörperphysik: von Flußliniengittern zu Hubbardmodellen	R. Hetzel, Würzburg
30.06.94	Valence State of the Samarium (Sm) Metal	Dr. Y. Jang, Korea
14.07.94	Quantum Mechanical Models and Many Electron Wave Functions for Catalysis	Dr. A. Tchougreev, Dresden

Termin	Thema	Vortragender
19.07.94	Ultrafast Dephasing of Coherent Optical Phonons in Semiconductors	Dr. U. Wenschuh, Stuttgart
21.07.94	Berechnung dynamischer Eigenschaften korrelierter Elektronensysteme in der Lokalen Näherung	Dr. T. Pruschke, Regensburg
26.07.94	Perturbation Theory for Strongly Correlated Electron Systems Around the Atomic Limit	Dr. Q. Qin, Bremen
28.07.94	Zur Feldtheorie des Quanten Hall Effekts	Prof. W. Weller, Leipzig
04.08.94	Berechnung dynamischer Eigenschaften stark korrelierter Elektronensysteme mit der Renormierungsgruppentheorie	Dr. R. Bulla, Regensburg
18.08.94	Structural Stability of a Substitutional Binary Alloy	Dr. G. Martinez, Sao Paulo
23.08.94	Spectral Density of Nickel	Dr. J. Igarashi, Gunma
25.08.94	Metal-Insulator Transitions and the Renormalization of Magnetic Coupling Constants in the Three-Band Hubbard Model	Prof. H. Kaga, Niigata
06.09.94	The Fermi Liquid in Quasi-One Dimensional Metals	Prof. I.E. Dzyaloshinskii, Irvine
15.09.94	Lanczos Calculations for Small Carbon Atom Clusters	Dr. C. Rosciszewski, Krakow
04.10.94	Tunneling in a Breathing Double Well Potential	Dr. V. Fleurov, Tel Aviv
13.10.94	Rayleigh-Benard Convection in a Gas near the Gas-Liquid Critical Point	Dr. V. Steinberg, Rehovot
14.10.94	Orbital Magnetic Response and Transport in the Anderson Localized Phase	Prof. J. Imry, Rehovot
17.10.94	Quantum Echo and Spatial Structure of Wavefunctions in a Random System	Dr. V. Prigodin, Stuttgart
20.10.94	Quantum Transport in Ballistic Microstructures in the Semiclassical Limit	Dr. K. Richter, Augsburg
03.11.94	Lattice Vibrational Localization due to Anhamonicity	Dr. S. Flach, Dresden
04.11.94	Exact Results for Quantum Spin-Chains	Prof. J. Zittartz, Köln

Termin	**Thema**	**Vortragender**
17.11.94	Quasi-Particle Spectrum Around a Vortex Line in a d-Wave Superconductor	Prof. N. Schopohl, Bochum
24.11.94	Electrons and Phonons in doped C_{60}	Prof. O. Gunnarsson, Stuttgart
29.11.94	Kondo Impurity in a Correlated Band	Dr. G.G. Khaliullin, Dresden
06.12.94	Electronic Structure, Magnetism and Large Mass Enhancement in U_2T_2X Intermetallics	Dr. M. Divis, Dresden
07.12.94	Greens Functions of Strongly Correlated Electrons with Magnetic Coupling	Prof. Nguyen Van Hieu, Hanoi
08.12.94	Interaction between Conduction and f-Electrons in the Anderson Impurity Model	Prof. J. Keller, Regensburg
13.12.94	Theory of Instabilities in Nonlinear Dynamical Systems with Retardation	Dr. A. Pelster, Stuttgart
15.12.94	Roughening Interfaces in Deterministic Dynamics	Dr. J. Kurths, Potsdam
20.12.94	Semiclassical Analysis of Matrix Elements for a Chaotic Billard	Dr. B. Mehlig, Dresden
05.01.95	Thermodynamics at Filling Factor One: Itinerant Ferromagnetism in Two Dimensions	Dr. M. Kasner, Bloomington
12.01.95	Flow Equations for Hamiltonians	Prof. F. Wegner, Heidelberg
19.01.95	Pattern Formation in Fluids and Biomembranes	Dr. W. Zimmermann, Jülich
26.01.95	Froths and Biological Cellular Structures: Theory and Simulation	Dr. J.R. Iglesias, Orsay
31.01.95	Impurity Effects on Anisotropic s-Wave Superconductors with Inter-Layer Pair Tunneling Mechanism	Dr. Y. Bang, Trieste
02.02.95	Hubbard and Jain Scheme for Highly Correlated Electron Systems	Dr. T. Domanski, Lublin
07.02.95	Complex Dynamics of Spiral Waves in Excitable Media	Dr. Michailov, Berlin

Termin	Thema	Vortragender
14.02.95	Scaling Theory of the Quantum Hall Effect	Prof. M. Zirnbauer, Köln
16.02.95	The Integral Quantum Hall Effect: Lattice and Network Models	Dr. K. Ziegler, Karlsruhe
21.02.95	Localization without Randomness	Prof. R. MacKay, Dijon
24.02.95	Long Range Order selected by Quantum Fluctuations	Prof. H. Shiba, Tokyo
02.03.95	Anderson Localization in a Chaotic Model System: The Quantum Kicked Rotator	Dr. A. Altland, Köln
03.03.95	Scaling Approach to Correlations in the Anderson Model	Dr. Y. Li, Dresden
09.03.95	Morphological Phase Transitions of Growth Structures	Prof. U. Bahr, Dresden
10.03.95	Slow Dynamics in Spin Glasses - Cluster Dynamics, Critical Dynamics and Ageing Phenomena	Prof. H. Takayama, Tsukuba
14.03.95	Superconducting Phase of a 2-Chain Hubbard Model	Dr. T. Yanagisawa, Tsukuba
17.03.95	d-d Excitations in Transition Metal Oxides by the Effective Crystal Field Method	Dr. A. Tchougreeff, Dresden
22.03.95	Spin-Phonon Kopplung in Anomalen f-Elektronen Systemen	M. Eikerling, Aachen
24.03.95	Classical and Semiclassical Fluctuations in Chaotic Systems	Prof. B. Eckhard, Oldenburg
29.03.95	Electron-Lattice Induced Pairing Interactions in Cuprates: Concepts and Properties	Prof. E. Sigmund, Cottbus
30.03.95	Ferromagnetism of Insulating Cu(II) Compounds	Prof. W. Weber, Dortmund
31.03.95	The Exact Statistics of Wave Functions in Disordered Conductors	Dr. V. Fal'ko, Stuttgart
04.04.95	Collective Phenomena in Unstable Quantum Systems	Prof. V.V. Sokolov, Novosibirsk
05.04.95	Magnetic Properties of Cuprate Materials	Dr. T. Chattopadhyay, Grenoble
18.04.95	Low Temperature Properties of Kondo Insulators	Dr. A. Mishchenko, Moscow

Termin	Thema	Vortragender
25.04.95	Chaos and Quantum Transport in Antidot Lattices	Dr. F. von Oppen, Heidelberg
27.04.95	The Role of Chemistry in the GALLEX Experiment	Prof. K. Ebert, Heidelb./Karlsruhe
02.05.95	Chiral Hamiltonians in Heisenberg Spin Systems: Coupled Spin Chains and Frustrated Lattices	Dr. Subrahmanyam, Trieste
04.05.95	Antiintegrability in Dynamical and Variational Problems	Prof. S. Aubry, Saclay
09.05.95	Quantum Chaos in Three Dimensions	Prof. U. Smilansky, Rehovot
11.05.95	Properties of an Open Quantum System	Dr. M. Müller, Rossendorf
15.05.95	Quantum Monte Carlo a Useful Tool in Quantum Chemistry	Dr. H. J. Flad, Stuttgart
16.05.95	Tangential Bifurcation of Plane Waves	Dr. S. Flach, Dresden
18.05.95	Dynamical Entropy and Predictability of Nonlinear Processes	Prof. W. Ebeling, Berlin
19.05.95	Quantum Monte Carlo Calculations for Transition Metal Atoms and Molecules	Dr. H. J. Flad, Stuttgart
30.05.95	Bosonization in 1+1/2 Dimension	Dr. A. Lopez, Oxford
01.06.95	Fractal Relaxation in Glassforming Liquids	Prof. W. Götze, München
12.06.95	Coupled Image Lattices as Models for Fully Developed Turbulence	Dr. C. Beck, London
13.06.95	QMC Simulations of Real Materials	Prof. R. Martin, Stuttgart
14.06.95	Magnetic Anisotropies in Copper Oxide-Planes	Dr. J. Stein, Tel Aviv
15.06.95	Spin and Charge Dynamics in Doped Hubbard Models	Dr. W. Brenig, Köln
22.06.95	Quantum Phase Slip in SDW and CDW	Prof. K. Maki, Los Angeles
04.07.95	Domains without Frustration in +-J Ising Lattices	Dr. E. Vogel, Temuco
12.07.95	Superconducting Ground State in a Model with Bond-Charge Interaction	Dr. M. Airoldi, Trieste

Termin	**Thema**	**Vortragender**
21.07.95	Transport in Quantum Dot Systems	Dr. D. Pfannkuche, Stuttgart
03.08.95	Charge Ordering and Heavy Fermions in the Semimetal Yb_4As_3	B. Schmidt, Dresden
08.08.95	Mixed, Coherent, Squeezed and Number State in Bosonic Systems	Dr. E. Heiner, Chemnitz
10.08.95	An Alternative Density Functional Theory	Dr. R.K. Nesbet, Almaden
16.08.95	Spin and Antiferromagnetic Correlations in Strongly Correlated Electron Systems	Dr. S.Q. Shen, Dresden
17.08.95	Magnetic Impurity Coupled to a Strongly-Correlated Electron System in Two Dimensions	Prof. J. Igarashi, Gunma
22.08.95	Dynamical Susceptibility of Highly Correlated Electron Systems	Prof. A. Loidl, Darmstadt
23.08.95	Raman- and Infrared Spectroscopy in High-Tc Superconductors	Dr. C. Thomsen, Berlin
31.08.95	Wavelet Correlations in Hierarchical Cascade Processes	Dr. M. Greiner, Giessen
05.09.95	Spatial Organization in Bi- and Multimolecular Diffusion Limited Reactions	Dr. H. Wio, Bariloche
14.09.95	Flux Lines, DNA, and all that: The Statistical Mechanics of Polymers	Dr. M. Lässig, Berlin
19.09.95	Self-Induced Criticality and Forest Fire Models	Prof. I. Peschel, Berlin
21.09.95	New Tools for Optimization on Rugged Landscapes	Dr. F.M. Dittes, Rossendorf
06.10.95	Ab-Initio Simulation of Structural and Electronic Properties of Liquid Magnesium, Bismuth and Mg_3Bi_2	Prof. G. Pastore, Trieste
10.10.95	Manifestation of Periodic Orbit Bifurcations in Quantum Systems	Dr. S. Flach, Dresden
11.10.95	The Jahn-Teller Effect in VC_{14}	Prof. R. Pitzer, Ohio
12.10.95	Ab-Initio Calculations with Relativistic Energy-Adjusted Pseudo-potentials on Compounds with Heavy and Ultraheavy Elements	Dr. M. Dolg, Stuttgart

Termin	**Thema**	**Vortragender**
26.10.95	Propagating S=1/2 Particles in S=1 Haldane Systems	Dr. K. Penc, Dresden
01.11.95	New Methods and Products for Measuring Pressure	Dr. S. Strässler, Würenlos
23.11.95	Back Scattering from a Random Amplifying Medium	Dr. A. Zyuzin, St. Petersburg
30.11.95	Modelling High Temperature Superconductivity	Prof. M. Peter, Genf
01.12.95	The Density Matrix Renormalization Group Technique for 1 D Fermions: Interaction vs. Disorder	P. Schmitteckert, Augsburg
05.12.95	A Common Framework for Transport Theories and Renormalization	Dr. J. Rau, Trento
07.12.95	Theory of Superconductivity in the Hubbard Model and a Comparison with Experiments	Prof. L. Tewordt, Hamburg
08.12.95	Ultrasonic Investigation of the Low Carrier 4f-Systems	Prof. T. Goto, Sendai
14.12.95	Gap Solitons, Resonant Kinks and Intrinsic Localized Modes in Paramagnetically Excited Diatomic Lattices	Prof. G. Huang, Madrid
19.12.95	Phase Diagram of a Three-Legs Fermionic Ladder: A Renormalization-Group Study	Dr. E. Arrigoni, Würzburg
20.12.95	The Hubbard Model within Projection Technique	S. Mallwitz, Dresden

Vorträge und Seminare in Stuttgart 1994–1995

Seminar talks given in Stuttgart 1994-1995

Termin	**Thema**	**Vortragender**
10.05.94	Supraleitung und schwere Fermionen in dotierten Nd_2CuO_4: akustische Eigenschaften	S. Röschenthaler, Stuttgart
11.05.94	Einführung in die nichtlineare Dynamik	Prof. W. John, Stuttgart
20.05.94	Can AuF be synthesized? An ab initio and plasma modelling study	Prof. Schwerdtfeger, Auckland
06.06.94	Algebraic Bethe Ansatz and its application to teh $1D$ Hubbard Model	Prof. H. Barentzen, Stuttgart
10.06.94	Flussgleichungen für das Andersonmodell	Dr. A. Mielke, Heidelberg
14.06.94	Electronic Excitations in Transition Metals	Dr. P. Unger, Stuttgart
17.06.94	Spectral Properties of the Hubbard Bands	Dr. H. Eskes, Stuttgart
24.06.94	Band Structure of Diamond by Means of Local Increments	Dr. J. Gräfenstein, Stuttgart
01.07.94	Correlation Energy of MgO	K. Doll, Stuttgart
26.07.94	Electronic Structure of $C28$ and U at $C28$	Prof. M.R. Pitzer, Columbus
29.07.94	Spin Gap and Magnetic Excitations in the Copper-Oxide Superconductors	Dr. G. Stemmann, Stuttgart
19.08.94	Vibrational-rotational Correction to Molecular Poperties - are they important?	M. Seth, Auckland
07.10.94	Relativistic Effects in Solids	Dr. N. Geipel, Bonn
04.11.94	Analysis of Electron Densitites in Molecules and Solids	Prof. W.H.E. Schwarz, Siegen
22.11.94	Quantum Monte Carlo for Atoms, Molecules and Solids	Prof. M. Caffarel, Paris
20.12.94	Theory for Magnetic Excitations of Hich-T_c Superconductors	Dr. J. Schmalian, Berlin

Termin	Thema	Vortragender
21.02.95	Renormalization Group Study of Growth Processes	Dr. M. Marsili, Manchester
10.03.95	Enhanced Eelectron Pairing in a Lattice of Berry Phase Molecules	N. Manini, Trento
07.04.95	Universality in Quantum Chaos: Theory and Application	Prof. B. Simons, London
18.04.95	Quark-like Objects in Fractionally Quantized Hall Liquids	Dr. M. Greiter, Geneva
25.04.95	Truncated Configuration Interaction and Size-Extensitivity Problems	Prof. J.-P. Daudey, Toulouse
28.04.95	Decay of the Vacuum and Creation of δ -Electrons in Heavy-Ion Collisions	M. Massoth, Stuttgart
05.05.95	Multifractional Properties of Electronic States in the Anderson Model of Localization	Prof. M. Schreiber, Chemnitz
09.05.95	Level Correlation near the Anderson Transition	Prof. J. Lerner, Birmingham
12.05.95	Universal Fluctuations in Metals and Superconductors	Prof. C. Beenakker, Leiden
19.05.95	Logarithmically-normal Distributions in the Problem of Anderson Localizaiton	Prof. V. Kravtsov, Trieste
02.06.95	Ab-initio Rechnungen zur Austausch-Wechselwirkung in sauerstoffüberbrückten zweikernigen Übergangsmetall-Komplexen	V. Staemmler, Bochum
16.06.95	Accurate Calculations for Atoms and Small Molecules using the CC-SDT-R 12 Method	Prof. W. Kutzelnigg, Bochum
19.06.95	Effect of the Interaction in Disordered Mesoscopic Rings	Dr. G. Bouzerar, Toulouse
27.06.95	Ab initio Calculation of the Heisenberg Exchange Interaction in Antiferromagnetic Cuprates	Prof. W.C. Nieuwpoort, Groningen
10.07.95	Coherent Propagation of two Interacting Particles in a Random Potential	Prof. Y. Imry, Rehovot
21.07.95	Energy Level Statistics in One-Dimensional Disordered System	Prof. W. John, Stuttgart
27.07.95	Making Use of Quantum Chaos in Electronic Microstructures	Prof. C. Marcus, Stanfort

Termin	**Thema**	**Vortragender**
08.08.95	One-Particle Dynamics of the Hubbard Model	Dr. G. Polatsek, Dresden
18.08.95	Parity and Time Reversal Violation in Atoms	Dr. A. Shukla, Stuttgart
07.09.95	Interactions, Localization and Quantum Hall Effect	Dr. B. Huckestein, Köln
08.09.95	Anderson Impurity Model for Correlated	S. Tornow, Stuttgart
15.09.95	Electrons and Phonons in Quasiperiodic Systems	Prof. M. Janssen, Köln
22.09.95	Statistics and Scaling in Quantum Hall Systems	Prof. M. Janssen, Köln
25.09.95	Semiclassical Approach to Transport and Magnetism in the Mesoscopic Regime	Prof. R. Jalabert, Strasbourg
06.10.95	Phase Coherent Transport in Mesoscopic Superconductors	Dr. C.J. Lambert, Lancaster
11.10.95	From Anderson Localization to Quantum Chaos	Prof. B. Altshuler, Princeton
27.10.95	Density of States Driven Anisotropies induced by Momentum Decoupling in HighT_c Superconductors	Dr. G. Varalogiannis, Rom
07.11.95	Photoemission from Underdoped Cuprates	Prof. P. Lee, Nordita
21.11.95	μ Studies in Heavy-Fermion Superconductors	Dr. R. Feyerhern, Zürich
30.11.95	Level Statistics of N x N Random Matrices	Dr. M. Letz, Stuttgart
01.12.95	Microscopic Oscillation in the Quantum Nucleation Vortices in Thin Superconducting Films: A Quantum Field Theory Approach	Prof. G. Jug, Milano
07.12.95	Level Statistics of N x N Random Matrices II	S. Tornow, Stuttgart
14.12.95	Brownian Motion and Random Matrices	C. Grimaldi, Stuttgart
18.12.95	Spin and Charge Fluctuations in $NiO : Li$	S. Marini, Pavia

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Eschrig, Helmut Professor Dr.	AG "Theorie komplexer und korrelierter Elektronensysteme" der MPG an der Technischen Universität Mommsenstraße 13 01069 Dresden
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Schrieffer, J. Robert Professor Dr.	Department of Theoretical Physics National High Magnetic Field Labor 1800 E. Paul Dirac Drive Tallahassee, FL 32306-4005 USA

Smilansky, Uzy Professor Dr.	Department of Nuclear Physics Weizmann Institute of Science Rehovot 76100 ISRAEL
Tosatti, Erio Professor Dr.	SISSA International School for Advanced Studies Via Beirut n. 2-4 34013 Trieste ITALY
Weidenmüller, Hans A. Professor Dr.	Max-Planck-Institut für Kernphysik Saupfercheckweg 1 69117 Heidelberg

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Amtszeit bis 31.12.2000

Eggers, Harald	Geschäftsführer Siemens Microelectronics Center GmbH & Co. OHG Scharfenberger Straße 66, 01139 Dresden
Eschelbacher, Hans C. Dr.-Ing.	Ministerialdirigent im Bundesministerium für Bildung Wissenschaft, Forschung u. Technologie Heinemannstraße 2, 53175 Bonn
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Meyer, Hans-Joachim Professor Dr.	Staatsminister im Sächsischen Staatsministerium für Wissenschaft und Kunst Archivstraße 1, 01097 Dresden
Schmidt, Joachim, MdB Dr.	Vorsitzender der CDU-Landesgruppe Sachsen Lessingstraße 46, 09599 Freiberg
Wagner, Herbert Dr.	Oberbürgermeister der Landeshauptstadt Dresden Dr.-Külz-Ring 19, 01067 Dresden
Walter, Bernhard	Mitglied des Vorstands Dresdner Bank AG 60301 Frankfurt/M.

Mitarbeiter am Max-Planck-Institut für Physik komplexer Systeme

<u>Stand:</u> 1. Juni 1996

1. Planstelleninhaber	**22**
1.1 Wissenschaftliches Personal	
Wissenschaftliche Mitglieder	1
Wissenschaftliche Mitarbeiter (einschließlich vier Nachwuchsgruppen)	13
1.2 Mitarbeiter in technischen Berufen	1
1.3 Verwaltungs- und Infrastrukturmitarbeiter	7
2. Wissenschaftliche Mitarbeiter, finanziert aus Drittmitteln	**1**
3. Doktoranden	**16**
3.1 Deutsche Doktoranden (MPG Mittel)	11
3.2 Ausländische Doktoranden (MPG Mittel)	4
3.3 Doktoranden (Drittmittel)	1
4. Gastwissenschaftler	**38**
4.1 Deutsche Wissenschaftler	15
4.2 Ausländische Wissenschaftler (MPG Mittel)	22
4.3 Ausländische Wissenschaftler (Drittmittel)	1

Deutsche wissenschaftliche Mitarbeiter 1994–1995 (inkl. Gastwissenschaftler und Doktoranden)

W = Wissenschaftler
D = Doktorand

Name	**Zeitraum**	**W/D**	**Arbeitsthema**
Allekotte, Ingomar	seit 8/93	W	Gästeprogramm
Blawid, Stefan	seit 3/94	D	Transporttheorie in stark korrelierten Elektronensystemen
Dolg, Michael	seit 2/94	W	Korrelierte und relativistische quantenchemische Untersuchungen an Atomen, Molekülen und Festkörpern
Doll, Klaus	seit 1/95	D/W	Elektr. Korrelationen in Ionenkristallen
Fischer, Kurt	seit 10/91	D	Energieskalen von Störstellensystemen
Flach, Sergej	seit 9/94	W	Dynamische Lokalisierung in nichtlinearen diskreten Systemen
Flad, Heinz-Jürgen	seit 7/94	W	Monte-Carlo-Verfahren in der Quantenchemie
Gade, Renate	seit 10/94	W	Ungeordnete Systeme in 2 Dimensionen und Turbulenzen
Gräfenstein, Jürgen	7/93 – 1/96	W	Korrelationen in Halbleitern
Hegger, Rainer	seit 8/95	W	Nichtlineare Zeitreihenanalyse
Jäger, Lars	seit 2/95	D	Nichtlineare Zeitreihenanalyse
John, Walter	2/95 – 8/95	W	Ungeordnete Systeme
Kalvoda, Simon	seit 7/95	D	Grundzustand von 4-f Systemen
Kantz, Holger	seit 1/95	W	Nichtlineare Zeitreihenanalyse
Klemm, Thomas	seit 10/93	D	Spektrale Dichten hoch korrelierter elektronischer Systeme
Küchle, Wolfgang	seit 1/95	D	Moleküle mit Aktinidatomen

Name	**Zeitraum**	**W/D**	**Arbeitsthema**
Lehner, Christoph	seit 1/94	D	Spektrale Dichten in 4-f Systemen
Letz, Martin	seit 9/95	W	Supraleitung
Mallwitz, Steffen	seit 7/93	D	Korrelationen in niedrigdim. Sytemen
Massoth, Michael	seit 2/95	D	Quantenchemische ab initio Rechnungen am System Nd_2CuO_4
Mehlig, Bernhard	seit 3/94	W	Quantenchaos
Mödl, Martin	seit 4/95	D/W	Magnetische Eigenschaften von Molekülen
Müller, Kirsten	6/95 – 7/95	W	Quantenchaos
Olbrich, Eckehard	seit 1/95	D/W	Nichtlineare Zeitreihenanalyse
Pardon, Roland	7/93 – 12/94	D/W	Korrelationen in Halbleitern
Paulus, Beate	seit 9/93	D/W	Elektron. Korrelationen in Halbleitern
Peschel, Ingo	4/94 – 5/94	W	Reaktions-Diffusions-Modelle
	9/95	W	Nichtgleichgewichtsprobleme
Scherrer, Hubert	seit 7/93	D/W	EDV
Schmidt, Burkhard	seit 1/94	D	Theorie für Yb_4As_3
Schork, Thomas	seit 7/93	W	Schwere Fermionen
Schreiber, Thomas	4/95	W	Nichtlineare Dynamik
Schwerdtfeger, Peter	5/94	W	Relativistische Effekte in Molekülen
Stemmann, Guntram	5/94 – 10/94	W	Magnetische Eigenschaften von Supraleitern
Thalmeier, Peter	seit 9/94	W	starke elektronische Korrelationen, Magnetismus, Supraleitung
Tornow, Sabine	seit 7/93	D/W	Schwere Fermionen
Unger, Patrick	7/93 – 11/95	W	Korrelationen in Kupraten
Wenschuh, Ulrich	seit 7/95	D	Kurzzeitspektroskopie
Ziesche, Paul	seit 7/94	W	Elektronische Strukturen
Ziegler, Klaus	seit 7/95	W	Quantensysteme

Ausländische Gastwissenschaftler und Doktoranden 1994 - 1995

W = Gastwissenschaftler

D = Doktorand

Name	**Land**	**Zeitraum**	**W/D**	**Arbeitsthema**
Arrigoni, Enrico	Italien	2/94 – 1/95	W	Slave Bosons
Chattopadhay, Tapan	Indien	seit 8/95	G	Spinanregungen
Christiansen, Freddy	Dänemark	8/95 – 9/95	G	Nichtlin. Dynamik
Domanski, Tadeusz	Polen	2/95 – 3/95	W	Elektr. Korrelationen
Dzyaloshinskii, Igor	Rußland	8/94 – 9/94	W	Vielteilchentheorie
Efetov, Konstantin	Rußland	seit 1/95	W	Mesoskopische Systeme
Fleurov, Victor	Israel	2/95 – 3/95	W	Lokalisierung in nichtlinearen diskreten Systemen
Ganduglia-Pirovano, V.	Argentinien	2/95 – 9/95	W	ab inito Rechnungen für metallische Oberflächen
Grimaldi, Claudio	Italien	seit 2/94	D	Supraleitende Tunnel
Hallberg, Karen	Argentinien	seit 8/93	W	Niedrigdimensionale korrelierte Elektronensysteme
Hoang, Anh Tuan	Vietnam	seit 4/95	W	Metall-Isolator-Übergänge
Huang, Guo Xiang	China	11/95 – 2/96	W	Nichtlineare Anregungen in Systemen kondensierter Materie
Igarashi, Junichi	Japan	8/94 – 9/94 7/95 – 8/95	W W	Schwere Fermionen in $Nd_{2-x}Ce_xCuO_4$
Jang, Youngrok	Korea	4/94 – 7/94	W	Elektronische Korrelationen
Kaga, Hiroyuki	Japan	7/94 – 9/94	W	Slave Bosons
Kashinje, Stanislaus P.	Tanzania	11/93 – 12/93	W	Schwere Fermionen
Khaliullin, Guiniatoulla	Rußland	10/94 – 12/94	W	Kondo Systeme

Name	**Land**	**Zeitraum**	**W/D**	**Arbeitsthema**
Kladko, Konstantin	Ukraine	seit 3/95	D	Projektionstechnik
Kravtsov, Vladimir	Rußland	5/95	W	Mesoskopische Systeme
Lepri, Stefano	Italien	4/95 – 5/95	W	Nichtlineare Dynamik
Li, Yanmin	China	3/94 – 3/95	W	Luttinger Flüssigkeiten
Liu, Wenjian	China	seit 5/95	W	Quantenchemische Untersuchungen an Lanthanoiden und Aktinoiden
L'Vov, Victor	Rußland	5/95	W	Turbulenz
Maki, Kazumi	Japan	6/95	W	Supraleitung mit unkonventioneller Paarung
Martinez, Gerardo	Brasilien	6/94 – 8/94	W	Elektronische Korrelationen
Mila, Frederic	Frankreich	5/94 – 6/94	W	Kuprate
Naumkin, Fedor	Rußland	6/95 – 5/96	W	Elektronische Struktur in Molekülen
Nguyen, Toan Thang	Vietnam	8/94 – 10/94	W	Elektronische Korrelationen
Penc, Karlo	Ungarn	seit 9/95	W	Stark korrelierte Elektronensysteme
Peterson, Kirk	USA	6/95 – 9/95	W	Quantenchemie
Prigodin, Vladimir	Rußland	seit 1/95	W	Synthetische Materialien
Rosciszewski, K.	Polen	7/94 – 10/94	W	Korrelationen in Molekülen
Rosciszewski, K.	Polen	8/95 – 10/95	W	Korrelationen in Molekülen
Shen, Shun Qing	China	seit 5/95	W	Symmetrien von Grundzuständen
Shi, Fajian	China	seit 8/95	W	Halbleiter
Shukla, Alok	Indien	seit 6/95	W	Quantenchemische Verfahren
Seth, Michael	Australien	8/94 – 10/94	W	Quantenchemie
Smilansky, Uzy	Israel	1/94 – 2/94	W	Semiklassik
Steinberg, Victor	Israel	6/95	W	Strukturbildung
Tchougreev, Andrei	Rußland	4/94 – 3/95	W	Magn. Eigenschaften von Molekülen

Name	**Land**	**Zeitraum**	**W/D**	**Arbeitsthema**
Tien, Tran Minh	Vietnam	seit 1/94	D	Kondo Systeme
Vemuru, Subrahmanyam	Indien	seit 9/95	W	Spinsysteme
Wang, Xiao Qun	China	2/94 – 2/96	W	Exakte Diagonalisierungen
Yanagisawa, Takashi	Japan	2/95 – 1/96	W	Exakte Diagonalisierungen
Yu, Ming	China	seit 4/95	W	Elektronische Korrelationen in Molekülen
Zevin, Vilen	Israel	8/94 – 10/94	W	Schwere Fermionen
Zevin, Vilen	Israel	7/95 – 8/95	W	Schwere Fermionen