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Kapitel 1

Wissenschaftliche Arbeit und ihre Organisation am Institut - ein Überblick

1.1 Institutsgeschichte und -entwicklung

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

ter der Leitung von *Dr. H. Kantz* ins Leben gerufen. Im gleichen Jahr nahm *Dr. M. Bär* als Leiter der Nachwuchsgruppe *Strukturbildung* seine Arbeit auf. Im Januar 1996 begann *Dr. K. Richter* mit dem Aufbau einer Gruppe auf dem Gebiet *Mesoskopische Systeme*. Dem folgte die Gruppe *Quantenchemie* unter der Leitung von *Dr. M. Dolg*.

1995-1998 • Als Sieger eines eingeladenen Architekturwettbewerbes für den Institutsneubau mit Gästehäusern ging das Architekturbüro Brenner und Partner (J. Wittfoht, Stuttgart) hervor, dessen Entwurf ab September 1995 am Standort Nöthnitzer Straße realisiert wurde. Nach knapp zweijähriger Bauzeit wurden das neue Institutsgebäude und die drei Gästehäuser am 23./24.9.1997 im Zusammenhang mit dem gleichzeitig stattfindenden Symposium *Complexity in Physics* feierlich eingeweiht. Zu dieser Zeit war das Seminar- und Gästeprogramm bereits auf gutem Weg, seine vorgesehene Größe zu erreichen und mehrere hundert Wissenschaftler waren bis dahin bereits am Institut zu Gast.

1999-2001 • *Dr. J. M. Rost* (Freiburg) wurde im Dezember 1998 zum Direktor der zweiten Abteilung des Instituts berufen und begann im Mai 1999 mit dem Aufbau seiner Abteilung *Endliche Systeme*. *Dr. A. Buchleitner* (Garching) konnte als Leiter der Arbeitsgruppe *Nichtlineare Dynamik in Quantensystemen* gewonnen werden. Nachdem *Dr. Dolg* im Jahr 2000 an die Universität Bonn berufen wurde, nahm *Dr. U. Birkenheuer* (TU München) als Nachfolger im März 2000 die Arbeit auf. *Dr. K. Richter* nahm einen Ruf an die Universität Regensburg an, woraufhin die Arbeit der Nachwuchsgruppe *Mesoskopische Systeme* endete. Dieses Fachgebiet wird in modifizierter Form von *Dr. H. Schomerus* (Leiden) weiter gepflegt, der im November 2000 mit dem Aufbau einer Nachwuchsgruppe *Wellen in komplexen Medien* begann.

2001-2003 • Um am Institut den immer wichtiger werdenden Bereich zwischen Physik und Biologie anzusiedeln, wurde im Jahr 2001 *Dr. F. Jülicher* (Paris) an das Institut berufen, so dass im Dezember 2001 mit dem Aufbau der dritten Abteilung *Biologische Physik* begonnen wurde. In der zweiten Jahreshälfte 2002 erfuhr die Abteilung *Biologische Physik* mit den neuen Arbeitsgruppen *Physik biologischer und weicher Materie* unter Leitung von *Dr. R. Everaers* (Mainz) sowie *Biologische Physik des Geruchsinns*, geleitet von *Dr. M. Zapotocky* (New York), eine weitere inhaltliche wie organisatorische Akzentuierung. Auch die Abteilung *Endliche Systeme* gewann mit *Dr. A. Becker* (Bielefeld) einen weiteren Gruppenleiter, dessen Gruppe auf dem Gebiet *Nichtlineare Prozesse in starken Laserfeldern* forscht.

2003-2004 • Im darauffolgenden Jahr 2003 begann *Dr. S. Kümmel* (New Orleans) mit dem Aufbau einer Emmy Noether-Gruppe auf dem Gebiet der *Elektronischen Struktur endlicher Systeme*. Im Oktober 2004 gründete *Dr. K. Kruse* eine Nachwuchsgruppe *Physik der Zellteilung* im Rahmen eines Forschungsprogramms *Physik biologischer Systeme*, das gemeinsam mit dem Max-Planck-Institut für molekulare Zellbiologie und Genetik initiiert wurde. Seit 2004 wird an einer Erweiterung des Institutsgebäudes gearbeitet. Die 35 neuen Arbeitsplätze sowie Seminar- und Besprechungsräume und Kommunikationsbereiche werden die in den letzten Jahren zunehmende Raumknappheit, der übergangsweise mit der Umwandlung von Fläche im Gästewohnhaus in Büros begegnet wurde, im Frühjahr 2006 beenden.

Ständig forschen etwa 50-100 Langzeitgäste am Institut, neben jährlich 1200-1500 Gästen, die an verschiedenen Seminaren und Workshops teilnehmen.

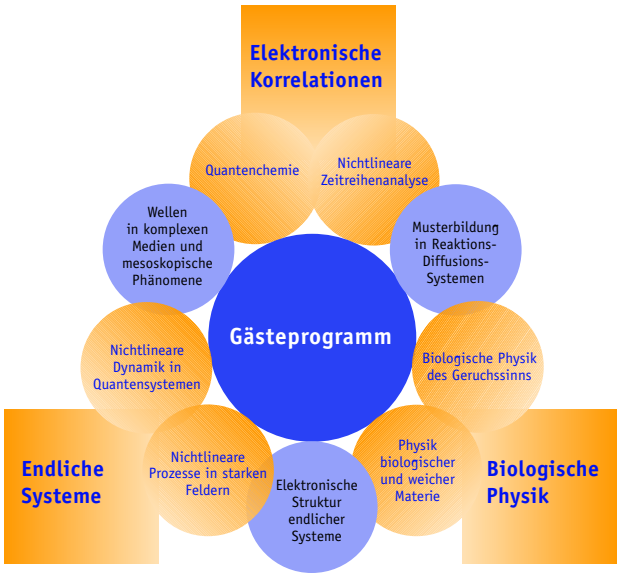
Ein seit 1995 bestehendes Kuratorium pflegt die Beziehungen zum Land Sachsen, zur Stadt Dresden und zahlreichen wissenschaftlichen Einrichtungen. Die Entwicklung des

Instituts wird seit Juni 1996 von einem wissenschaftlichen Beirat begleitet.

1.2 Forschungsschwerpunkte und Organisation

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

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



Darüber hinaus verstärken von den gegenwärtig neun Arbeitsgruppen sechs die jeweilige Arbeit an den Schwerpunkten.
Drei Gruppen, darunter zwei Nachwuchsgruppen, interpolieren und ergänzen die Schwerpunkte.

- Die Nachwuchsgruppe von *Dr. Schomerus* schlägt mit ihrem Forschungsinteresse *Wellen in komplexen Medien und mesoskopische Phänomene* inhaltlich eine Brücke zwischen den Abteilungen *Korrelierte Elektronen* und *Endliche Systeme*.

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

Im Jahr 2004 wurde die Gründung eines gemeinsamen Programms der Max-Planck-Institute für Physik komplexer Systeme und für molekulare Zellbiologie und Genetik zum Thema *Physik biologischer Systeme* beschlossen. In enger Zusammenarbeit werden drei Nachwuchsgruppen verschiedene Aspekte zellulärer Systeme untersuchen und dabei die Kompetenzen beider Institute zusammenführen. Als erste hat die von *Dr. Kruse* geleitete Nachwuchsgruppe *Physik der Zellteilung* im Oktober 2004 ihre Arbeit aufgenommen. Dabei werden die Prinzipien der räumlichen und zeitlichen Organisation von Zellen im Zusammenhang mit ihrer Teilung untersucht.

1.3 Workshop- und Gästeprogramm

Eine zentrale Aufgabe des Instituts ist die Durchführung von internationalen *Workshops und Seminaren* (S. 134). Hinsichtlich dieser Funktion nimmt das mpi**pks** eine Sonderstellung innerhalb der MPG ein. Ein kleiner, aber effizienter Mitarbeiterstab unter der Leitung von *Dr. S. Flach* übernimmt die logistische Organisation der Veranstaltungen und berät die in der Regel externen wissenschaftlichen Organisatoren bei der Planung und Durchführung ihrer Veranstaltung.
Das *Gästeprogramm* (S. 128) bietet Forschungsaufenthalte am Institut, die von wenigen Wochen bis zu zwei Jahren reichen können. Die Wissenschaftler haben mannigfache Möglichkeiten der Zusammenarbeit, indem sie sich einer der bestehenden Gruppen am Institut anschließen, mit anderen Gästen gemeinsam forschen, oder Forschungspartner bei einem der zahlreichen Workshops/Seminare finden. Darüber hinaus besteht auch die Möglichkeit, mit Partnern lokal an der TU Dresden oder einer der vielen anderen Forschungseinrichtungen in Dresden zu kooperieren. Von dieser Möglichkeit wird auch rege Gebrauch gemacht, wie die Veröffentlichungen dokumentieren (S. 177).
Vorschläge für Workshops/Seminare sowie die Bewerbungen für Gastaufenthalte werden von je einem Komitee evaluiert. Beide Komitees sind mit externen Wissenschaftlern und Vertretern des Instituts besetzt.
Zur weiteren Strukturierung des Gästeprogramms vergibt das mpi**pks** seit 2000 das *Martin-Gutzwiller-Fellowship* jährlich an einen international angesehenen erfahrenen Wissenschaftler. Mit ihm forschten *Prof. R. Kapral* (Toronto) 2003 und *Prof. A. Politi* (Firenze) 2004 jeweils bis zu einem akademischen Jahr am Institut (S. 131).
Ferner schreibt das mpi**pks** jedes Jahr ein *PKS-Distinguished Postdoctoral-Fellowship* aus. Hiermit sollen hervorragende Nachwuchswissenschaftler mit einiger Forschungserfahrung angesprochen werden (S. 129).

1.4 Lehre und Ausbildung

Das Institut strebt eine umfassende Weiterbildung junger Wissenschaftler an. Dies gilt selbstverständlich für die Forschung, aber auch für Lehre und Forschungsorganisation.
Lehre • Hierbei handelt es sich nicht nur um traditionelle Vorlesungen, die sowohl an der TU Dresden als auch an anderen Universitäten von Institutsmitarbeitern gehalten werden (S. 163). Vielmehr bietet sich im Rahmen der Öffentlichkeitsarbeit die Möglichkeit, Lehrerfahrung in Veranstaltungen für Lehrer und Schüler, sowohl am Institut als auch an den Schulen (S. 166), zu sammeln.
Forschungsorganisation • Durch unser großes Workshop-/Seminarprogramm haben wir die einmalige Chance, auch Training im Organisieren von Tagungen bieten zu können. Von 32 Veranstaltungen in den Jahren 2003-2004 (S. 134) waren bei einem Drittel (10) junge Wissenschaftler des mpi**pks** Mitorganisatoren. Das hat für unsere Nachwuchswissenschaftler einen Ausbildungs- und Profilierungseffekt und erleichtert den externen Organisatoren die Arbeit, da sie einen Wissenschaftler als direkten Ansprechpartner am Institut haben.

1.5 Öffentlichkeitsarbeit

Das Institut versteht seinen Auftrag im weitesten Sinn als eine Plattform für das Entstehen, den Austausch und die Weiterentwicklung kreativer Ideen in der Forschung. Dies betrifft in erster Linie die Wissenschaftler, schließt aber auch insbesondere potentielle zukünftige Wissenschaftler, also Schüler, sowie die wissenschaftlich interessierte Bevölkerung mit ein. Im Rahmen unseres Schul-Kontakt-Programms bieten wir von Workshops für Lehrer über mehrtägige Winterschulen für Schüler bis hin zu Vorträgen an den Schulen vielfältige Möglichkeiten, die Faszination aktueller Forschung hautnah zu erleben. Für die interessierte Bevölkerung organisiert das Institut seit 1999 im Dresdner Rathaus zusammen mit der Universität und der Stadt die Reihe *Wissenschaft im Rathaus*, in der prominente Wissenschaftler aktuelle Forschung bürgernah erläutern (S. 166). Außerdem ermutigen wir die Organisatoren von Workshops, einen öffentlichen Abendvortrag im mpi**pks** anzubieten.

1.6 Vernetzung der Forschung

Lokal • Das mpi**pks** befindet sich inmitten vielfältiger Forschungsaktivitäten, die von der Technischen Universität Dresden und zahlreichen außeruniversitären Forschungseinrichtungen getragen werden. Mit der Fachrichtung Physik der TU Dresden gibt es einen wissenschaftlichen Dialog, der sich in zwei gemeinsamen Seminaren (*Quantum Dynamics* mit Prof. Schmidt und *Complex Systems* mit Prof. Ketzmerick) niederschlägt. Außerdem sind Wissenschaftler des Instituts an mehreren Sonderforschungsbereichen und einer Forschergruppe beteiligt (S. 162). Eine Zusammenarbeit besteht weiterhin durch die Abteilung *Elektronische Korrelationen* mit dem IFW und dem benachbarten MPI für Chemische Physik fester Stoffe, sowie mit dem MPI für Zellbiologie durch die Abteilung *Biologische Physik*.
National und International • Die Auflistung der vielfachen internationalen und nationalen Kontakte findet sich in den folgenden Darstellungen der Arbeitsgruppen. Weiterhin

verfügt das Institut über ein kleines Budget, aus dem Zusammenarbeit mit experimentellen Gruppen gefördert wird (S. 133).

1.7 Kurzdarstellung der Arbeitsgruppen

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

Die Arbeiten in der Abteilung befassen sich mit elektronischen Korrelationen in Festkörpern und Molekülen im weitesten Sinn sowie u.a. mit dem Einfluss äußerer Magnetfelder auf die Eigenschaften ultrakalter Gläser.
Die Arbeiten über elektronische Korrelationen teilen sich auf in solche, welche auf *ab initio* Verfahren basieren und andere, die von Modellsystemen bzw. von vereinfachten Hamiltonoperatoren ausgehen. Bei den ab initio Verfahren wurden die Methoden zur Berechnung von Energiebändern vorangetrieben. Dies geschah in Zusammenarbeit mit der Arbeitsgruppe *Quantenchemie*. Zum einen wurde das ADC (algebraic diagrammatic construction) Verfahren von Molekülen auf Festkörper erweitert und exemplarisch auf die Berechnung der Energiebänder von LiF angewendet. Im Unterschied zu unseren bisherigen Verfahren basiert diese Methode auf der Berechnung der Selbstenergie der Green'schen Funktion. Zum anderen wurde ein vereinfachtes Verfahren zur Berechnung von Energiebändern von kovalenten Halbleitern entwickelt. Das geschah in Zusammenarbeit mit Prof. H. Stoll (Univ. Stuttgart). Außerdem wurde ein Weg gefunden, auch Grundzustandseigenschaften von Metallen mit Hilfe der Inkrementenmethode zu berechnen. Es wurden auch eine Reihe von Rechnungen im Rahmen der Dichtefunktionalstheorie (hier: LDA+U) durchgeführt. Besonders interessant war der Befund, dass in Magnetit Fe_3O_4 im Tieftemperaturzustand eine Gitterverzerrung auftritt, die mit der gemessenen und bisher unverstandenen Verzerrung übereinstimmt.
Bei der Verwendung von Modellhamiltonoperatoren wurden folgende Resultate erhalten. Es konnte gezeigt werden, dass eine Reihe von Verfahren, die insbesondere auf den Hubbard Hamiltonoperator angewendet wurden, identisch sind (Kakehashi: Adv. Phys.). Es sind dies die Many-Body Coherent Potential Approximation (MB-CPA), die Dynamical CPA, die Dynamical Mean Field Näherung (DMFA) sowie die Projection Operator Method (POM). Das war bisher nicht bekannt und wegen der verschiedenen Formulierungen der Theorien auch nicht unmittelbar ersichtlich. Außerdem wurde die POM auf nichtlokale Prozesse erweitert. Als unmittelbare Anwendung gelang es zu zeigen, dass ein Hubbard Modell auf dem Quadratgitter für einen spezifizierten Bereich der doping Konzentration und bei starken Korrelationen ein Marginal Fermi Liquid Verhalten zeigt, wie es experimentell in den Kupraten beobachtet wird.
Weiterhin wurde das duale Modell für $5f$ Elektronen ausgebaut. Für UPd_2Al_3 konnte die experimentelle Fermifläche und die großen, stark anisotropen Massenverhältnisse *parameterfrei* berechnet werden. Außerdem konnte überzeugend gezeigt werden, dass die Supraleitung bzw. Cooper-Paarbildung im selben Material nicht durch die Elektron-Phononwechselwirkung, sondern durch intra-atomare Anregungen zustande kommt. Das duale Modell hat inzwischen eine sehr starke Basis und hat unsere Vorstellungen über $5f$ Elektronen deutlich verändert.
Das neue Arbeitsgebiet über Ladungsfreiheitsgrade in frustrierten Gittern hat starke Impulse erfahren. Mit Hilfe exakter Diagonalisierung konnte für das Checkerboard

Gitter gezeigt werden, dass spinlose Fermionen bei halber Füllung einen flüssigkeitsähnlichen Grundzustand haben, wenn die Korrelationen stark sind. Dieser Grundzustand ist zwei- oder vierfach entartet. Das Bild von fractional charges im 3-dimensionalen Pyrochlore Gitter konnte erhärtet werden. Gegenwärtig arbeiten wir an der Statistik solcher Systeme und an der Verbindung zu Eichtheorien.
Schließlich wurde zusammen mit Dr. Kettemann (Univ. Hamburg) und einer experimentellen Gruppe um Mohanty von der Boston University ein Verfahren vorgeschlagen zur Messung von Drehmomenten an der Schnittstelle eines Ferromagneten mit einem Paramagneten, wenn durch diese ein Strom fließt. An der experimentellen Realisation wird kräftig gearbeitet. Eine Messung des Drehmoments würde eine Aussage darüber erlauben, wie groß jeweils der s-Elektronen- und d-Elektronenanteil am Strom ist. Diese Information ist anders nicht zu erhalten.

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

Wie schon in den Jahren zuvor, beschäftigt sich die Quantenchemiegruppe hauptsächlich mit der wellenfunktionsbasierten Bestimmung der elektronischen Struktur von Festkörpern und Polymeren. Wir verwenden lokalisierte Orbitale, und gelangen so zu einer *lokalen* Darstellung des Hamilton-Operators und der Wellenfunktionsbeiträge. Dadurch kann der vornehmlich kurzreichweitige Charakter der elektronischen Korrelationen voll ausgenutzt werden, um quantenchemische Vielteilchenmethoden zu entwickeln, die selbst auf unendliche periodische Systeme anwendbar sind. Meistens wird das Inkrementenschema herangezogen, um die einzelnen Korrelationsbeiträge zu erfassen.
Mit der Entwicklung eines leistungsstarken Schemas für quantenchemische Korrelationsrechnungen in unendlichen Wirtskristallen mit eingebetteten Clustern sind wir nun in der Lage, kationische (N-1)- und anionische (N+1)-Teilchenzustände periodischer Systeme einheitlich mit demselben Verfahren zu untersuchen. Die Valenz- und Leitungsbänder von Diamant, die bereits im vorher gehenden Bericht beschrieben wurden, sind ein Beispiel für eine solche Rechnung; die korrelierte Bandstruktur von *trans*-Polyazetylen (tPA), welche das Thema der Doktorarbeit von Viktor Bezugly war (beendet im Feb. 2004), oder von Zickzackketten aus Fluorwasserstoff (HF) sind andere Beispiele.
Mehrere Unzulänglichkeiten des ursprünglichen Ansatzes mussten dazu beseitigt werden. Das wichtigste war die Entwicklung einer speziellen Größenkonsistenzkorrektur für die offenschaligen Multireferenz-CI(SD) Rechnungen, die wir zur Bestimmung der angeregten (N-1)- und (N+1)-Teilchenzustände von tPA verwendet haben. Nur durch diese Technik konnte der Effekt der fehlenden Größenkonsistenz, die jeder verkürzten CI Methode (Konfigurationswechselwirkung) zu eigen ist, auf die einzelnen inkrementellen Beiträge so stark verringert werden, daß die inkrementelle Reihenentwicklung gut konvergiert.
Ein weiterer Aspekt in diesem Zusammenhang ist die Konstruktion geeigneter lokalisierter *virtueller* Orbitale. Hier konnte ein Bandentflechtungsverfahren (sehr ähnlich der von Marzari und Mitarbeitern für maximal lokalisierte Wannier-Funktionen vorgeschlagenen Methode) entwickelt werden speziell für den Wannier-Boys Lokalisierungsalgorithmus im Gauß-orbitalbasierten CRYSTAL-Programm, mit dem wir die

Hartree-Fock-Wellenfunktion des Wirtskristalls berechnen. Perfekte lehrbuchartige antibindende Orbitale für Silizium (und andere Substanzen) konnten so erzeugt werden, die energetisch genügend dicht an der Leitungsbandunterkante bleiben, um für die anschließenden MR-CI Rechnungen in Frage zu kommen.
In den letzten zwei Jahren haben wir begonnen, das Inkrementenschema (Grundzustandseigenschaften) und den lokalen Hamilton-Operator-Ansatz (Bandstrukturen) auszubauen, um auch andere Eigenschaften mit diesen Verfahren untersuchen zu können. So konnten wir inzwischen Paarenergien und Dichtematrizen der halbleitenden bzw. ionischen Materialen SiC und LiH mit Hilfe von Inkrementrechnungen bestimmen.
Erfolgreich waren wir auch in der Entwicklung eines lokalen Hamilton-Operator-Verfahrens für Exzitonen. Es wurde in enger Analogie zum lokalen Hamilton-Operator-Ansatz für Ein-Teilchenanregungen (Löcher oder Elektronen) entworfen und liefert für ausreichend stark gebundene Elektronen-Lochpaare (Frenkel-Exzitonen) gute Ergebnisse, wie unsere Rechnungen an einem prototypischen periodischen System, einer unendlichen strickleiterartigen H_2-Kette zeigen.
Die eigentliche Neuerung in der Quantenchemiegruppe ist jedoch die Verwendung von fortschrittlichen feldtheoretischen Greens-Funktionsmethoden als Alternative zum traditionellen lokalen Hamilton-Operator-Ansatz. Dieser Schritt wurde ausgelöst durch die Doktorarbeit von Christian Buth (angefangen im Dez. 2002). Solche Greens-Funktionsmethoden sind wesentlich besser geeignet, der steten Gefahr eines Zusammenbruchs des Ein-Teilchenbildes durch Auftreten von Satellitenzuständen in Bandstrukturberechnungen zu begegnen. Wir haben eine *lokale* Variante der wohl-etablierten auf der Dyson-Gleichung basierenden Technik der algebraisch-diagramatischen Konstruktion (ADC) entwickelt und implementiert, indem wir zu lokalen besetzen und virtuellen Wannier-Orbitalen übergegangen sind und die Translationssymmetrie des betrachteten Systems voll ausnutzen. Studien an den Valenz- und Leitungsbändern von HF-Ketten und kristallinem LiF belegen die Leistungsfähigkeit des neuen Ansatzes.
Derzeit in Arbeit ist auch eine ganz ähnliche Erweiterung für den nicht-Dyson ADC-Formalismus (der weit weniger rechnerintensiv ist als der Dyson-artige Ansatz). Eine unter Transformationen der besetzten und virtuellen Orbitale komplett invariante Formulierung ist möglich, was es uns erlaubt, selbst extrem lokalisierte nicht-orthogonale Orbitale als Basisfunktionen in Betracht zu ziehen. Dies gestattet die Verwendung noch stringenterer Abschneide- und Integralselektionskriterien und sollte schlußendlich zu hoch effizienten linear skalierenden Greens-Funktionsmethoden für periodische (oder andere ausgedehnte) Systeme führen.
Eine Zusammenarbeit mit der Gruppe für Theoretische Chemie an der Universität in Turin (Prof. C. Pisani) ist vereinbart worden, um die neuen Greens-Funktionsmethoden in das CRYSCOR-Programm für lokale MP2 (Møller-Plesset Störungstheorie 2-ter Ordnung) zu integrieren, das ganz ähnliche Erfordernisse hat wie unser CO-ADC-Ansatz für Kristallorbitale (COs). Dadurch kann die reiche Infrastruktur, die über das backend des CRYSTAL-Programms zur Verfügung steht, voll ausgenutzt werden.

Kooperationen

- Prof. C. Pisani, Dipart. di Chimica IFM, Università degli Studi di Torino, Italy: Integrierung des CO-ADC-Ansatzes in das CRYSCOR-Programm
- Prof. H. Stoll, Institut für Theoretische Chemie, Universität Stuttgart: Entwick-

lung vereinfachter Korrelationsrechnungen für Bandstrukturen

- Prof. V. Staemmler, Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum: Direkte Bestimmung lokaler korrelierter Loch-Wellenfunktionen
- Prof. M. Albrecht, Theoretische Chemie, Universität Siegen: Benchmark-Rechnungen zu korrelierten Bandstrukturen periodischer Systeme
- Prof. J. Schirmer, Theoretische Chemie, Universität Heidelberg: Molekulare lokale Dyson- und nicht-Dyson-artige ADC-Formalismen

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

Komplexe Dynamik bleibt eine Herausforderung sowohl an die Theorie wie auch die Praxis. Unsere Arbeitsgruppe konzentriert sich auf Aspekte von Komplexität in klassischen (d.h., nicht-quantenmechanischen) Systemen, wobei wir uns sowohl für grundlegende Eigenschaften wie auch für spezifische Phänomene interessieren. Größere und längerfristige Projekte der letzten zwei Jahre sind: Elimination von schnellen chaotischen Freiheitsgraden in Hamiltonschen Systemen und ihre Ersetzung durch weißes Rauschen, die Verallgemeinerung der Zeitversatzeinbettung für deterministische Systeme zu Markovketten für stochastische Systeme und das Studium von langreichweitigen Korrelationen und Vorhersagbarkeit in Oberflächenwind. Im Bereich der Anwendungen laufen die Aktivitäten zur Rauschunterdrückung für Sprache, wobei wir neuerdings den Erfolg mit kommerziellen Spracherkennungssystemen testen, und die Vorhersagen von Windböen, weiter.
Eine neue Aktivität unserer Gruppe bezieht sich auf extreme Ereignisse. Extreme Ereignisse sind kurzzeitige große Abweichungen eines Systems von seinem mittleren Verhalten. Es gibt Hinweise, dass die Fähigkeit eines Systems, Extremereignisse zu generieren, direkt mit der Komplexität seiner Dynamik gekoppelt ist. Wir studieren dynamische Mechanismen zur Erzeugung von Extremereignissen, wir versuchen die Rolle von Vorläuferstrukturen zu verstehen, und wir betrachten statistische Aspekte der Detektion und Charakterisierung von Extremereignissen.
Auf der Zeitskala der nächsten zwei Jahre ist unsere Arbeit durch die gegenwärtigen Projekte weitgehend vorgegeben. Insbesondere werden wir prototypische Modelle für die Erzeugung von Extremereignissen aufgreifen und verstehen und in einem neuen Netzwerk die Eigenschaften von Bodenwind auch unter dem Aspekt der Turbulenz intensiv studieren.

Kooperationen

- W. Just, London University; G. Radons, TU Chemnitz: Modellierung schneller Freiheitsgrade durch stochastische Prozesse.
- W. Just, London University: Eigenwerte von Fokker-Planck-Operatoren
- J. Peinke, Universität Oldenburg; im Konsortium mit R. Friedrich, Uni. Münster, A. Schaffarczyk, FH Kiel, C. Wagner, DLR Göttingen: Bodenwind, Turbulenz und Windkraftanlagen.

- S. Albeverio, Uni. Bonn: zeitabhängige Fokker-Planck-Gleichungen zur Modellierung von Autobahnverkehr.
- Prof. C. Grebogi, Univ. Sao Paolo, Brasilien: Einfluß von Rauschen auf deterministische Dynamik.
- N. Vitanov, IMB Sofia: Datenanalyse von Windgeschwindigkeiten, Turbulenz.

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

Unsere Gruppe interessiert sich für die nichtlineare Dynamik angeregter Systeme, die eine endliche Anzahl von Teilchen haben, insbesondere für Atome und Cluster. Innerhalb der letzten beiden Jahre haben wir unsere Arbeit an ultrakalten Gasen intensiviert, mit besonderem Augenmerk auf ultrakalte Plasmen. Das entsprechende Projekt, geleitet von *Dr. Thomas Pattard*, wurde von der DFG finanziert. Dies gilt auch für das Projekt *Theoretische Studien zu Energie- und Ladungstransfer in einzelnen Clustern und angeordneten Clustern auf Oberflächen* geleitet von *Dr. Ulf Saalmann* zusammen mit Prof. Garcia (Kassel). Dieses Projekt wird innerhalb des DFG-Schwerpunktes SPP 1153 gefördert.
Die Energie zur Anregung solcher Systeme kommt entweder vom Stoß mit geladenen Teilchen oder durch Wechselwirkung mit Licht. Insbesondere letztere spielt eine wichtige Rolle für die Forschung in der Gruppe und bildet auch den thematischen Überlapp mit der *Buchleitner* Gruppe. Mit der *Becker* Gruppe teilen wir das Interesse an der Dynamik von Molekülen in exterenen Feldern sowie im allgemeinen an Materie, die dem Licht von Freien Elektronen Lasern im VUV und Röntgenbereich ausgesetzt wird. Unsere Techniken reichen von quantenmechanischen Zugängen und Dichtefunktional theorie (TDLDA) über semiklassische Näherungen bis hin zur vollständig klassischen Behandlung mikroskopischer Phänomene. Dies schließt Techniken wie *Tree Codes* oder *Particle in a Cell* Formulierungen ein.
Bei Systemen mit einer kleinen Anzahl von Freiheitsgraden haben wir uns für quasiklassische Formulierungen grundlegender Streuprozesse interessiert, wie etwa Mehrfachphotoionisation und Elektronstoßionisation. Zum ersten Mal haben wir drei aktive Elektronen voll dynamisch im Photoionisationsprozess untersucht. Konkret für Lithium hat dies zu einem Verständnis der Elektronendynamik nach Dreifachionisation geführt, das sich auf die Analyse der Abfolge binärer Elektronenstöße stützt.
Themen, die sich auf Systeme mit vielen Freiheitsgraden beziehen, waren die Photoanregung dipolverbotener kollektiver Moden in Systemen mit delokalisierten Elektronen, Edelgascluster in intensiven Laserfeldern, insbesondere auch solcher Lichtpulse, wie sie die erste Phase des FEL in Hamburg geliefert hat (S. 77), und die Bildung und Relaxation ultrakalter Plasmen, wobei wir speziellen Wert auf Korrelationseffekte gelegt haben (S. 79).
Schließlich haben wir intensiv mit *Dr. Lein*, einem der mpi**pks** distinguished postdoctoral fellows, zusammengearbeitet, zur Erzeugung höherer Harmonischer in Molekülen und in Laser unterstützten Ion-Atom Stößen. Ebenfalls eine fruchtbare Zusammenarbeit ergab sich mit *Dr. Brand*, auch mpi**pks** distinguished postdoctoral fellow, zur schwellennahen Streuung an Bose Einstein Kondensaten.

Zukunftsperspektiven

Unsere Arbeit zur Dynamik von Wenig-Elektronensystemen werden wir fortsetzen. Die Resultate zur Dreifach-Photoionisation haben einen neuen Weg zum Verständnis von Viel-Elektronendynamik aufgezeigt, den wir, zusammen mit Dr. Emmanouilidou (Georgia Tech, Atlanta, USA), weiterverfolgen werden.
Langreichweitige Wechselwirkungsphänomene in ultrakalten Gasen sind jetzt experimentell zugänglich und stellen eine Herausforderung für die Theorie dar. Während wir für den Fall der Coulomb Wechselwirkung in ultrakalten Plasmen die theoretischen Werkzeuge für ein gutes Verständnis entwickelt haben, sind die Phänomene der dipolaren und van der Waals Wechselwirkung noch weitgehend unverstanden. Hier werden wir grundlegende quantenmechanische Elemente (wie Bloch Dynamik und Interefenzphänomene) mit der klassischen Bewegung der Atome im Gas auf sinnvolle Weise zusammenführen müssen.
Die nächste Phase des XFEL in Hamburg wird 2005 realisiert mit neuen Experimenten, welche die kurzen Pulse mit Photonenenergie um die 30 eV nützen werden. Wir werden zu den geplanten Clusterexperimenten Rechnungen durchführen, wobei wir uns nicht auf das Parameterregime des FEL in Hamburg beschränken werden. Vielmehr versprechen wir uns vom Abtasten des Parameterraumes, speziell in der Lichtfrequenz, ein besseres Verständnis der physikalischen Phänomene.

Kooperationen

mit experimentellen Gruppen
Wir haben mit den Gruppen von Prof. Müller (Uni Giessen) und Prof. Phaneuf (Univ. of Nevada, Reno, USA) über kollektive Anregung von Elektronen in komplexen Systemen zusammengearbeitet. Messdaten der C_{60} Vielfach-Photoionisation wurden aufgenommen, ausgewertet, interpretiert und gemeinsam publiziert.
Desweiteren existiert eine Zusammenarbeit mit Horst Schmidt-Böckings und Reinhard Dörners Gruppe (Universität Frankfurt), um die experimentellen Signaturen des Übergangs von der Regularität in das Chaos an doppelt angeregten Zwei-Elektronen Atomen zu erforschen. Eine erste Serie der sehr schwierigen Experimente ist inzwischen ausgeführt und hat neue Information über hochangeregte Coulombsysteme geliefert mit Wirkungsquerschnitten, bei denen der angeregte Zustand des Ions mitvermessen wurde.
Wir haben auch mit der Gruppe von Prof. Kaindl (TU Berlin) zusammengearbeitet, zu hochauflösender Photoabsorption an Helium. Publizierte Resultate thematisieren Isotopenverschiebungen in Heliumresonanzen und partielle Photoionisationswirkungsquerschnitte.

Mit theoretischen Gruppen (einige Beispiele):

- zu semiklassischer Theorie mit A. Ozorio de Almeida (Rio, Brazil)
- zur Photoionisation in komplexen Systemen mit H. Chakraborty (Manhattan, USA)
- zur Rolle der Zeit in der Quantenmechanik mit J. S. Briggs (Freiburg)
- zu Transport durch Cluster mit M. Garcia (Kassel)

Lokale Kooperationen
Der Austausch mit Prof. Rüdiger Schmidts Gruppe von der TU Dresden wurde fortgesetzt - Basis ist das gemeinsame Seminar *Quantum Dynamics*. Gemeinsame Forschungsaktivitäten umfassen *Adiabatische Quantenmolekulardynamik* direkt mit R. Schmidt, sowie *Semiklassische Propagationstechniken* mit F. Großmann von der TU Dresden. Zusätzlich gab es ein monatliches Seminar *Complex Dynamics* das den neu besetzten Lehrstuhl an der TU unter der Leitung von Prof. Ketzmerick miteinschließt, sowie von unserem Institut die *Buchleitner, Kantz, Rost* und *Schomerus* Gruppe.

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

Die Gruppe existiert seit Oktober 2002 und besteht zur Zeit aus zwei Postdoktoranden und einem Doktoranden. Unser Interesse ist auf die Wechselwirkung zwischen ultrakurzen intensiven Laserpulsen und Materie ausgerichtet. Die Arbeit hat dabei zwei Schwerpunkte, die Dynamik von einzelnen Atomen, Molekülen und Clustern in starken Feldern und die Selbsttransformation von Femtosekunden-Laserpulsen während ihrer Propagation durch ein optisches Medium. Techniken sind analytische Ansätze, S-Matrix Rechungen und numerische Simulationen.

Die Kopplung zwischen Elektronen und einem intensiven elektromagnetischen Feld, die von vergleichbarer Stärke wie die Wechselwirkungen zwischen den geladenen Teilchen in einem Atom oder Molekül ist, führt zu einer Reihe von interessanten nichtlinearen Effekten. Insbesondere ergibt sich die Möglichkeit durch Variation der Parameter des Feldes, wie Frequenz, Intensität oder Pulslänge, Materie kontrolliert zu verändern. In den letzten Jahren standen verschiedene Themen im Mittelpunkt unserer Arbeiten, dazu gehören die korrelierte Emission von zwei Elektronen aus einem Atom (siehe Report *Electron-electron momentum exchange in intense field double ionization*, Seite 81), der Einfluß der Symmetrie eines Orbitals und der Ausrichtung der internuklearen Achse auf die Ionisationswahrscheinlichkeit eines Moleküls, die Erzeugung von Hoch-Harmonischer Strahlung und von Attosekundenpulsen in einer Umgebung von Ionen und der Einfluß von linearen und nichtlinearen Effekten bei der Fokussierung eines Laserpulses auf die Fragmentation eines Moleküls.

Die Propagation eines intensiven Femtosekundenpulses in einem optischen Medium führt zu starken Veränderungen seines zeitlichen und räumlichen Profils, darüberhinaus kann es zu einer Kanalisierung des Laserpulses über große Strecken kommen. Die Kombination dieser Effekte eröffnet eine Reihe von möglichen Anwendungen von der Pulskompression bis zur Untersuchung der Atmosphäre mit der Lidar-Methode. In den letzten beiden Jahren haben wir uns auf zwei Aspekte dieser Forschungsrichtung konzentriert. Wir haben einen analytischen Ansatz zur Beschreibung der Selbstfokussierung entwickelt, in dem der Effekt des schwächeren äußeren Teils des Pulses als Störung berücksichtigt wird. Desweiteren haben wir numerisch die Erzeugung und Kanalisierung der Dritten Harmonischen untersucht (siehe Report *Propagation of femtosecond laser pulses in air*, Seite 83)

Zukunftsperspektiven

Wir werden unsere Arbeit zur Wechselwirkung von Atomen und Molekülen mit intensiven Laserpulsen fortsetzen. Es ist dabei eine Ausrichtung im Hinblick auf Atto-

sekundenpulse, Pulse mit wenigen Schwingungen als auch zeitlich geformte Laserpulse geplant. Wir entwickeln zur Zeit Programme zur numerischen Simulation der Wechselwirkung von kleinen (Ein- und Zwei-Elektronen) Systemen mit solchen Pulsen. Die Möglichkeit der Kontrolle der Dynamik steht dabei im Vordergrund.
Der Bau des Freie-Elektronen-Lasers in Hamburg und die Entwicklungen von Quellen zur Erzeugung intensiver Hoch-Harmonischer-Strahlung eröffnen einen bisher unerforschten Parameterbereich. Die hohen Photonenenergien bei gleichzeitig hohen Intensitäten ermöglichen z.B. Viel-Photonen-Prozesse aus inneren Schalen von Atomen und Molekülen. Mit Hilfe unserer Ansätze aus der S-Matrix-Theorie und der numerischen Simulation wollen wir diese und andere nichtlineare Prozesse, wie die Mehrfachionisation, in diesem Parameterbereich analysieren.
Im Bereich der Moleküle werden wir uns verstärkt mit größeren Systemen, z.B. Kohlenwasserstoffen oder C_{60}, beschäftigen. Uns interessieren dabei insbesondere die Mechanismen, die zur Ionisation und Fragmentation dieser Moleküle im Laserfeld führen.
Unsere Arbeiten zur Propagation von Laserpulsen wollen wir fortsetzen, wobei es uns in den nächsten Jahren um ein Verständnis geht, wie sich die Selbstfokussierung und Kanalisierung z.B. durch zeitlich oder räumlich geformte Pulse kontrollieren läßt. Darüberhinaus stellt uns die Progagation von ultrakurzen Pulsen mit wenigen Schwingungen vor eine neue Herausforderung. Dazu müssen theoretische und numerische Lösungen entwickelt werden, bei denen auf die Näherung einer Einhüllenden, die sich nur langsam verändert, verzichtet wird.
Das Seminar *Intense Laser-Matter Interaction and Pulse Propagation*, an deren Organisation am Institut im August 2005 wir beteiligt sind, wird uns die Gelegenheit geben, Forschungsrichtungen und -perspektiven auf diesen Feldern mit anderen Experten intensiv zu diskutieren.

Kooperationen

Wir sind an zwei internationalen Kooperationen beteiligt, die im Jahr 2004 iniitiert wurden, einem Center of Advanced Science and Technology (COAST) *Ultrafast Intense Laser Science* (Koordination: K. Yamanouchi, Tokio, Japan) und einem Special Research Opportunity Programm *Controlled electron rescattering: sub-A, sub-fs imaging of single molecules* (Koordination: M.Yu. Ivanov, Ottawa, Kanada).

Experimentelle Gruppen:

- mit S.L. Chin (Québec, Kanada) zur Propagation von Femtosekunden-Pulsen und, zusammen mit P. Agostini (Saclay, Frankreich), zur Fragmentation von Molekülen in intensiven Laserfeldern (siehe z.B. Report *Propagation of femtosecond laser pulses in air*). Wir betreuen auch die Doktorarbeit von Weiwei Liu (Québec, Kanada), der unsere Gruppe im letzten Sommer für zwei Monate besucht hat, gemeinsam.

- mit R. Dörner (Frankfurt) und P.B. Corkum (Ottawa, Kanada) zu Korrelationseffekten während der Doppelionisation in intensiven Feldern (siehe Report *Electron-electron momentum exchange in intense field double ionization*). Zukünftig wollen wir den Effekt der Phase zwischen oszillierendem Feld und Einhüllender auf den Prozess unter Einbeziehung der experimentellen Gruppe von U. Keller und J. Biegert (ETH Zürich, Schweiz) untersuchen.

- mit C.P. Schulz und I. Hertel (Berlin) zur Ionisation von C_{60} in intensiven Laserpulsen.

Theoretische Gruppen:

- mit F.H.M. Faisal (Bielefeld) zur Ionisation von Molekülen in Laserfeldern,
- mit N. Aközbek und C.M. Bowden (Huntsville, USA) zur Erzeugung und Kanalisierung von Harmonischen,
- mit O. Kosareva und V.P. Kandidov (Moskau, Russland) zu nichtlinearen Effekten in der Fragmentation von Molekülen,
- mit L. Roso (Salamanca, Spanien) zur numerischen Simulation der Doppelionisation in intensiven Laserpulsen.

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

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

- die Anregungs- und Ionisationsdynamik von Helium unter dem Einfluß starker elektromagnetischer Felder, insbesondere im Spektralbereich doppelt angeregter Zweielektronenzustände (J. Madroñero);
- der Energiezuwachs der Schwerpunktsbewegung kalter, auf einem elektronischen Übergang spontan emittierender Atome in einem periodisch geschalteten (optischen) Stehwellenfeld (S. Wimberger);
- die resonante Überhöhung von Quantentransport entlang "Netzzuständen" im Phasenraum des periodisch gekickten harmonischen Oszillators (s. "Web-Assisted Tunneling in the Kicked Harmonic Oscillator", A.R. Ribeiro de Carvalho);
- die quantitative Charakterisierung von Zwei- und Vielteilchenverschränkung in Quantensystemen beliebiger endlicher Dimension (s. "Concurrence of Mixed Bipartite Quantum States in Arbitrary Dimensions", F. Mintert);
- die Dynamik quantenmechanischer Verschränkung unter dem Einfluß von Rauschen (F. Mintert & A.R. Ribeiro de Carvalho);
- das Anregungsspektrum des durch Bose-Einstein-Kondensate in optischen Gittern realisierten Bose-Hubbard-Hamiltonian (A. Ponomarev & A. Kolovsky & J. Madroñero) –

mit sehr engem Bezug zu aktuellen Experimenten in Quantenoptik und Atomphysik. Neben tiefliegenden mathematischen Methoden aus Operatoranalysis und Quantenwahrscheinlichkeitstheorie kommen hier auch modernste Methoden der rechnergestützten Physik auf einem der derzeit weltweit leistungsfähigsten Parallelgroßrechner, der IBM p690 des Rechenzentrums Garching der Max-Planck-Gesellschaft, zum Einsatz.
Zwischen Januar und Mai 2004 schlossen drei Doktoranden, Sandro Wimberger, Florian Mintert und Javier Madroñero, ihre Promotion erfolgreich ab. S. Wimberger und F. Mintert sind inzwischen als PostDocs im Ausland tätig; J. Madroñero tritt demnächst eine PostDoc-Stelle an der TU München an. Zwei PostDocs, Vyacheslav Shatokhin und Boris Fine, haben die Gruppe nach Ablauf ihrer (zweijährigen) Gaststipendien ebenfalls verlassen (nach Minsk bzw. Knoxville, Tennessee), dagegen konnten wir Alexey Ponomarev als neuen Doktoranden (seit Januar 2004) und Carlos Viviescas (seit Juli 2004) als neuen PostDoc gewinnen. Die engen Kontakte zu Arbeitsgruppen in Frankreich, Italien, Israel und Polen werden im Rahmen konkreter bilateraler Projekte durch die Studenten bzw. PostDocs der Gruppe getragen. Sämtliche Promotionen gehen daher mit längeren Gastaufenthalten bei den jeweiligen Partnern einher, was 2004 zum Abschluß einer binationalen Promotion zwischen den Universitäten Como und München führte (S. Wimberger). Das Gästeprogramm des Instituts ermöglichte erneut Gastaufenthalte renommierter Kollegen (K. Dietz, S. Fishman, I. Guarneri, M. Kuś, G. Summy). Drei internationale Workshops zu den Themen "Chaos and Quantum Transport" (Bad Honnef, März 2003), "Resonances, from Physics to Mathematics and back" (Dresden, Januar 2004) und "Entanglement, Information and Noise" (Krzyżowa, Juni 2004) kamen auf Initiative der Gruppe zustande und erfreuten sich regen Interesses verschiedener wissenschaftlicher Communities. Die Tagung in Krzyżowa führte außerdem zur Gründung der "Krzyżowa Initiative for Quantum Information", einem europaweiten Verbund auf dem Gebiet der Quanteninformation tätiger Forschungsgruppen. Vorlesungen über Theoretische Quantenoptik und Quantenchaos wurden von A. Buchleitner an der Universität München sowie im Rahmen der „Mitteldeutschen Physik-Kombo" (Halle, Jena, Leipzig) gehalten.
Die Forschungsaktivitäten der nächsten Jahre werden durch folgende Schwerpunkte unserer aktuellen Arbeit definiert:

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

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

III der Transport von Photonen oder Materiewellen in ungeordneten Streumedien bzw. in optischen Potentialen unter dem Einfluß zusätzlicher deterministischer und/oder zufälliger bzw. dissipativer Kräfte.

Während wir unter (I) die näherungsfreie Beschreibung der Fragmentationsdynamik des periodisch getriebenen Dreikörper-Coulombproblems – realisiert in aktuellen Experimenten zur Laserionisation von Helium – ins Auge fassen, zielt (II) auf auch experimentell handhabbare Größen zur quantitativen Beschreibung nichtklassischer Korrelationen – mit besonderem Augenmerk auf deren Robustheit gegenüber Rauschquellen,

bei gleichzeitiger Skalierbarkeit mit der Systemgröße. Dank eines von der Volkswagen-Stiftung bis Ende 2005 bewilligten Kooperationsprojektes mit der Polnischen Akademie der Wissenschaften (K. Życzkowski, M. Kuś) verfolgen wir letzteres Projekt im Rahmen einer intensiven bilateralen Zusammenarbeit. Last but not least widmet sich (III) grundlegenden Szenarien des kohärenten Quantentransports (schwache und starke Lokalisierung, kohärente Rückstreuung, Bloch-Oszillationen, Zufallslaser) in ungeordneten oder deterministisch chaotischen Systemen, die dank spektakulärer Fortschritte in der experimentellen Quantenoptik nun mit ungekannter Genauigkeit untersucht werden können.

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

Kernthemen unserer Forschungsprojekte sind aktive und dynamische Phänomene der Zellbiophysik und Zellbiologie. Dabei werden vorwiegend Methoden und Konzepte der Statistischen-, Vielteilchen- und Nichtgleichgewichtsphysik verwendet und weiterentwickelt. Ein wesentliches Ziel ist es, ausgehend von dem physikalischen Verständnis molekularer Prozesse (z.B. Motorproteine) elementare Mechanismen und Funktionsprinzipien komplexer zellulärer Systeme (z.B. Zellbewegung, Zellteilung, Stimulierung durch äußere Sinnesreize) zu charakterisieren. Dabei wird eine grundlegende theoretische und quantitative Beschreibung zellulärer Prozesse in biologischen Systemen angestrebt. Beispiele unserer Forschungsaktivitäten sind:

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

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

Aktive weiche Materialien: Das Zytoskelett ist ein polymerisches Material, das inhärent

aktiv ist und durch molekulare Prozesse ins Nichtgleichgewicht getrieben wird. Als Konsequenz besitzt es ungewöhnliche Materialeigenschaften. Es kann spontane Bewegungen und komplexe Dynamik hervorrufen. Ausgehend von mikroskopischen Beschreibungen auf der Ebene von Filamenten, entwickeln wir eine allgemeingültige hydrodynamische Beschreibung aktiver weicher Materialien, die die Physik viskoelastischer Fluide ins Nichtgleichgewicht verallgemeinert. Ausgehend von aktiven Materialgleichungen kann, unter Verwendung geeigneter Randbedingungen die Adhäsion und die Polymerisation von Filamenten berücksichtigen, z.B. die Physik der Bewegung von Zellen auf Unterlagen beschrieben werden.

Transport von Signalmolekülen in Zellen und zwischen Zellen: Zelluläre Prozesse werden von Signalmolekülen kontrolliert, die Informationen verarbeiten. Diese Signalsysteme sind selber Teil der aktiven dynamischen Prozesse der Zelle. Signalmoleküle werden von der Zelle hergestellt, transportiert und an Nachbarzellen weitergereicht. Während der Embryonalentwicklung eines Organismus spielen diese Prozesse eine wesentliche Rolle, um die genetische Information so zu verwenden, dass räumliche Muster und Morphologien von Zellverbänden entstehen. Ein einfaches Beispiel sind räumliche Gradienten von sogenannten Morphogenen, die Ortsinformationen an Zellen vermitteln können. Die entsprechenden molekularbiologischen Grundlagen werden insbesondere in der Fruchtfliege untersucht. Unsere Gruppe entwickelt theoretische Ansätze, mit deren Hilfe z.B. allgemeine nichtlineare Transportgleichungen hergeleitet werden können. Dies erlaubt uns in Zusmmenarbeit mit Zellbiologen die Rolle unterschiedlicher Transportmechanismen für die Entstehung von Morphogengradienten zu untersuchen und Fragen der Robustheit und Präzision des Gesamtsystems zu diskutieren.

Physik von Sinnezellen und des Gehörs: Haarzellen sind mechanisch empfindliche Sinneszellen, die in unserem Innenohr Schallsignale aufnehmen und in Nervensignale umsetzen. Unser Gehör ist mithilfe dieser Zellen in der Lage, über einen dynamischen Bereich von 12 Größenordnungen der Schallintensität zu arbeiten und extrem schwache Schallsignale wahrzunehmen. Dabei werden aktive und nichtlineare Verstärkungsmechanismen verwendet. Nichtlineare Oszillatoren und universelle Eigenschaften solcher Systeme in der Nähe eines kritischen Punktes bilden eine wichtige konzeptuelle Grundlage zum Verständnis aktiver Prozesse des Gehörs. Unsere Gruppe untersucht aktive molekulare Prozesse die im Haarbündel zu Oszillationen führen sowie die Rolle von Fluktuationen, die aufgrund aktiver und passiver molekularer Prozesse entstehen. Das universelle Verhalten kritischer Oszillatoren wird mithilfe feldtheoretischer und Renormierungsgruppenmethoden untersucht. Als weiteres Besipiel ist die Physik nichtlinearer Wellen zu nennen die, von aktiven zellulären Prozessen angetrieben, sich auf der Basilarmembran in der Schnecke des Innenohrs ausbreiten.

Diese Arbeiten erfolgen in enger Zusammenarbeit mit experimentellen Gruppen. Hervorzuheben ist dabei die Zusammenarbeit mit dem Institut Curie in Paris im Rahmen eines European Associate Laboratory sowie die Vernetzung mit dem MPI für molekulare Zellbiologie und Genetik (MPI-CBG) in Dresden. Unsere Gruppe unterhält auch einen Laborraum mit Mikroskopieaustattung im Gebäude des MPI-CBG. In enger Anbindung an theoretische Arbeiten werden dort insbesondere oszillierende Verteilungen von Min-Proteinen in Bakterien untersucht (Karsten Kruse), sowie physikalische Ei-

genschaften von Zellbewegung auf festen Substraten. Im Rahmen eines gemeinsamen Programms unseres Instituts mit dem MPI-CBG wurden drei gemeinsame Nachwuchsgruppen gegründet, zwei davon haben Ihre Arbeit im Herbst 2004 aufgenommen. Unsere Gruppe ist auch an das internationale PhD Programm "Cell Biology, Bioengineering, Biophysics" angeschlossen, welches vom MPI-CBG initiert wurde.

Zukunftsperspektiven

Biologische Systeme sind außerordentlich komplex und vielschichtig strukturiert. Die großen Fortschritte der Molekular- und Zellbiologie der vergangenen Jahrzehnte haben viele neue Fragen aufgeworfen und dabei die Komplexität zellulärer Prozesse und die Bedeutung aktiver Vorgänge in Zellen sehr deutlich gemacht. Aus der Sicht der theoretischen Physik gilt es grundlegende Konzepte zu vertiefen und weiterzuentwickeln, die z.B. zur Beschreibung fluktuierender Nichtgleichgewichtsprozesse, nichtlinearerer Systeme oder für das Verständnis komplexer Materialien geeignet sind. Dies ermöglicht es mithilfe physikalischer Ansätze theoretische und quantitative Beschreibungen von dynamischen Prozessen, die im Rahmen der Zellbiologie untersucht werden, zu entwickeln und grundlegende Prinzipien zu charakterisieren. Die Abteilung biologische Physik deckt gemeinsam mit den neu eingerichteten Nachwuchsgruppen Themenbereiche ab, die von den Eigenschaften biologischer Materialien, bis hin zur Physik komplexer zellulärer Vorgänge reichen. Seit der Arbeitsaufnahme in Dresden wurden im Zusammenarbeit mit dem MPI-CBG theoretische Arbeiten zur Beschreibung entwicklungsbiologischer Vorgänge begonnen. Eine Vielzahl verwandter Prozesse, die insbesondere Signalwege in der Zelle und die Regulierung zellulärer Prozesse durch Genexpression einschließen, werden in Zukunft in den Blickpunkt einer physikalischen Beschreibung treten. Dabei wird es von besonderer Bedeutung sein, zu verstehen, wie Materialeigenschaften und bewegungserzeugende Prozesse in der Zelle von signal- und informationsverarbeitenden Systemen reguliert werden.

Das Max-Planck-Institut für Physik komplexer Systeme bietet ein besonderes Umfeld für theoretische Arbeiten in biologischer Physik. Das breite Spektrum an Forschungskompetenz im Bereich komplexer Phänomene erlaubt den Austausch und die Zusammenarbeit mit anderen Gruppen, die sich z.B. mit nichtlinearer Dynamik beschäftigen. Die Nähe zum Max-Planck-Institut für molekulare Zellbiologie und Genetik (MPI-CBG), dem Biotechnologiezentrum, sowie der TU, ermöglichen eine Vernetzung mit vielfältigen verwandten Forschungsaktivitäten. Von besonderer Bedeutung ist die enge Zusammenarbeit mit dem MPI-CBG. Seit Ende 2004 ist im Rahmen eines gemeinsamen Programms beider Institute die Einrichtung von drei Nachwuchsgruppen begonnen worden. Diese Gruppen werden eine Brücke zwischen den Instituten bilden und zu einer noch engeren Verzahnung von Theorie und Experiment führen. Schwerpunkt dieses Programms sind integrierte zelluläre Prozesse deren Funktion aus dem Wechselspiel vieler verschiedener Komponenten hervorgeht. Derartige komplexe Systeme treten im Rahmen der sich schnell entwickelnden Systembiologie zunehmend ins Zentrum des Interesses. Physikalische Konzepte und Methoden werden in Zukunft in diesem Forschungsfeld eine besondere Rolle spielen.

Kooperationen

- Max-Planck-Institut für molekulare Zellbiologie und Genetik, Dresden
  - Zusammenarbeit mit den Gruppen von Jonathon Howard und Anthony Hyman zur Dynamik des Zytoskeletts, der Zellteilung und der Physik molekularer Motoren
  - Zusammenarbeit mit Marcos González-Gaitán zur Entstehung von Gradienten von Morphogenen in der Fruchtfliege Drosophila
  - Zusammenarbeit mit Andy Oates zur Segmentierung von Wirbeltieren durch oszillierende und raumzeitliche Genexpressionsmuster
- Universität Bayreuth
  - Zusammenarbeit mit Albrecht Ott zur Physik von DNA-chips
- Universität Regensburg
  - Zusammenarbeit mit Gianaurelio Cuniberti zur Physik von Motorproteinen
- Cavendish Laboratory, Cambridge, UK
  - Zusammenarbeit mit Thomas Duke zur Physik des Gehörs und aktiven Wellenphänomenen in der Schnecke
- Institute Curie, Paris
  Zusammenarbeiten im Rahmen eines European Associate Laboratory
  - Zusammenarbeit mit Jean-Francois Joanny und Jacques Prost (ESPCI, Paris) zur Physik aktiver Gele, der Dynamik des Zytoskeletts sowie zur Zellbewegung.
  - Zusammenarbeit mit Pascal Martin zur Physik von mechanosensiblen Sinneszellen (Haarzellen).
  - Zusammenarbeit mit Michel Bornens zur Orientierung der mitotischen Spindel sowie zur Zytokinese (dem Trennen der Tochterzellen nach der Zellteilung)
- AMOLF, Amsterdam
  - Zusammenarbeit mit Marileen Dogterom und Bela Mulder zur Entstehung kontraktiler Ringe und zur Dynamik des Zytoskeletts in Pflanzenzellen
- Ben-Gurion University, Beer-Sheva
  - Zusammenarbeit mit Anne Bernheim-Groswasser zur Physik aktiver Gele

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

Die Arbeitsgruppe wurde im November 2002 gegründet und besteht zur Zeit aus einem Doktoranden und zwei Postdocs. Wir benutzen Methoden der statistischen Physik, der nichtlinearen Dynamik und der Physik weicher kondensierter Materie um biologische Sinnessysteme zu untersuchen. Der Schwerpunkt liegt dabei auf dem olfaktorischen Sinn, dem Geruchssinn. Unser Interesse gilt in einem weiteren Sinne auch der Entwicklungsbiologie sowie der Theorie biochemischer Netzwerke.

Die Entdeckung der grossen Gruppe der Geruchsrezeptorproteine 1991 veränderte das Gebiet der Geruchsforschung und führte zum Verständnis des Aufbaus dieses Sinnessystems. Ergänzend liefern gegenwärtig funktionelle bildgebende Verfahren ein Übersichtsbild der neuronalen Aktivität in den ersten beiden Stufen des Systems (Riechepithel bzw. olfaktorischer Bulbus). Trotz dieser Fortschritte sind die Vorgänge im Geruchssinn bei Weitem noch nicht so gut verstanden wie z.B. im Sehsinn oder im Gehörsinn. Um die experimentellen Arbeiten zu ergänzen, werden theoretische Zugänge benötigt. Unsere Arbeit über den Geruchssinn beinhaltet einen weiten Bereich biologischer Ebenen: Genexpression, Signaltransduktion, Entwicklung sowie die Dynamik neuronaler Netzwerke. Zur Verdeutlichung stellen wir im Folgenden kurz drei unserer aktuellen Forschungsgebiete vor:

1. Signaltransduktion in den Geruchszilien: In den Zilien der Geruchszellen wird das äußere chemische (Eingangs-)Signal (die Art und Konzentration des Geruschsstoffs) in ein elektrisches Signal umgewandelt. Der entsprechende Signaltransduktionsweg ist biochemisch gut beschrieben und es ist bekannt, dass er einige durch intrazelluläres Kalzium vermittelte Rückkopplungsschleifen beinhaltet. In Projekt 3.1.16 (S. 101) entwickelten wir ein Minimalmodell der Signalleitung, das zwei wichtige Eigenschaften der olfaktorischen Zilien beschreibt: Die Adaption der Antwort auf wiederholte kurze Reizung sowie die oszillatorische Antwort auf einen anhaltenden Reiz. Uns gelang es zu zeigen, dass beide diese Effekte auf dem gleichen molekularen Mechanismus basieren. Dabei ist ein Punkt von generellem Interesse, dass die die Oszillationen erzeugende Hopf-Bifurkation in unserem Modell ausschließlich durch eine negative Rückkopplung entsteht und nicht wie im üblichen Fall der Ca^{2+} Oszillationen durch Kalzium-induzierte Kalziumabgabe. In einem zweiten Projekt untersuchen wir die Antwort der Zilien auf sehr geringe Geruchsstoffkonzentrationen mit dem Ziel, die physikalischen Grenzen der Genauigkeit der olfaktorischen Signalübertragung zu charakterisieren.
Die Signalleitung in den Geruchszilien besitzt eine grosse Ähnlichkeit zu der in Säugetierspermien. Unsere Ergebnisse sind deshalb auch für aktuelle Forschungsarbeiten in Dresden über Spermabeweglichkeit relevant (F. Jülicher und J. Howard).

2. Kollektiveffekte in der axonalen Zielfindung im olfaktorischen System: Während der Entwicklung werden Verbindungen zwischen Hirnbereichen durch wachsende neuronale Fortsätze, die Axone, gebildet. In den derzeit vorherrschenden Erklärungsmodellen wird jedes wachsende Axon unabhängig voneinander zum richtigen Ziel geleitet, indem es einen räumlich verteilten chemischen Signalstoff detektiert. Wir entwickeln Modelle in denen Axon-Axon Wechselwirkungen eine dominante Rolle spielen, wodurch die richtige Zielfindung ein Kollektiveffekt wird. Man vermutet, dass ein solcher Mechanismus wichtig ist für das 'Sortieren' der Axone der Geruchszellen auf ihrem Weg vom Riechepithel zu den Glomeruli im olfaktorischen Bulbus. Um diesen Prozess zu beschreiben,

verwenden wir statistische Physik aus dem Bereich der wechselwirkenden gerichteten Polymere.

3. Neuronale Netzwerkdynamik im olfaktorischen Bulbus: Das neuronale Netzwerk des olfaktorischen Bulbus verarbeitet Informationen des Riechepithels bevor es sie zum olfaktorischen Kortex weiterleitet. Wir untersuchen die zugrundeliegende Dynamik mit Hilfe vereinfachter neuronaler Netzwerke auf dem Computer. Im Besonderen interessiert uns, wie der olfaktorische Bulbus sehr schwache Geruchsreize verarbeitet und wie er die Komponenten eines Geruchsgemisches segmentiert. Im Projekt 3.1.17 (S. 103) untersuchen wir die Bedingungen unter welchen neuronale Netzwerke bei der Klassifikation schwacher, räumlich kodierter Reize von Rauschen profitieren. Für ein rekurrentes zweilagiges Netzwerk finden wir einen der stochastischen Resonanz ähnlichen Effekt. In einer verwandten Arbeit analysieren wir elektrophysiologische Messungen spontaner Aktivität im olfaktorischen Bulbus von Zebrafischen zur Charakterisierung der durch schwache Geruchsreize beeinflussten intrinsischen Netzwerkdynamik.

Unsere Forschung beschränkt sich nicht auf den Geruchssinn. Im Besonderen haben wir einige Kollaborationen mit Biologengruppen am MPI für Zellbiologie und Genetik (MPICBG) in Dresden gestartet. Zwei aktuelle Projekte werden im Folgenden beschrieben:

4. Dynamik der Gastrulation im Zebrafischembryo: Während der Zebrafisch-Gastrulation differenziert das Blastoderm in Ektoderm und Mesoderm, und die entstehenden Gewebeschichten bewegen sich in entgegengesetzten Richtungen auf dem darunterliegenden Dottersack. Das Hauptziel dieses Projektes ist es, die Kräfte welche die relative Bewegung bewirken zu identifizieren. Jüngste Ergebnisse der Heisenberg-Gruppe am MPICBG suggerieren, dass die beobachteten morphologischen Prozesse der Gewebeorganisation durch differentielle Adhäsion bedingt sein könnten. Wir verfolgen eine Beschreibung dieser Prozesse als komplexe Flüssigkeiten und zelluläre Automaten um in der Lage zu sein, quantitative Vorhersagen zu treffen, die auf obiger Annahme beruhen. Diese Vorhersagen werden wir mit detaillierten Messungen der Zellgeschwindigkeiten in den beiden Gewebeschichten vergleichen. Das Projekt beinhaltet die gemeinsame Betreuung einer Doktorandin mit dem MPICBG.

5. Verarbeitung mechanosensitiver Information beim Insektenflug: In jedem Flügel haben Fliegen ungefähr 100 mechanosensitive Rezeptoren. Das Ziel dieses Projektes ist es, die Rolle dieser Sensoren (und deren zugrundeliegenden neuronalen Schaltkreise) beim Insektenflug zu verstehen. Zur Zeit stattfindende Experimente geben Informationen darüber, wie der Flügel während des Fluges deformiert wird, wie jeder Mechanorezeptor auf diese Verformung reagiert und wie die Axone der mechanosensitiven Neuronen an die Motorneuronen knüpfen, die die Flugmuskeln kontrollieren. Die Ergebnisse werden es uns erlauben, ein neuronales Netzwerkmodell des Flugkontrollschaltkreises zu entwickeln. Das Computermodell kann dann gestestet werden, indem der Effekt selektiver Unterbrechung des mechanosensitiven Pfades auf das Flugverhalten ermittelt wird. Ein Antrag auf Förderung durch die VW Stiftung (zusammen mit J.Howard und S.Frey) wird zur Zeit geprüft.

Kooperationen

mit Biologen:
P. Feinstein und P. Mombaerts, Rockefeller University, New York
(Kollektiveffekte in der axonalen Zielfindung; Regulierung der Expression der Geruchsrezeptoren)
C.-P. Heisenberg, MPI für Zellbiologie und Genetik, Dresden
(Dynamik der Gastrulation im Zebrafischembryo)
T. Kuner, MPI für medizinische Forschung, Heidelberg
(Signaltransduktion in genetisch veränderten Geruchszilien)
R. Friedrich, MPI für medizinische Forschung, Heidelberg
(Rolle spontaner neuronaler Aktivität im olfaktorischen Bulbus)
J. Howard, MPI für Zellbiologie und Genetik, Dresden und S. Frey, ETH Zürich
(Verarbeitung mechanosensitiver Information während des Insektenfluges)

mit Theoretikern:
F. Jülicher, P.K. Mohanty, MPIPKS
J. Starke und J. Reidl, Universität Heidelberg
M. Eiswirth, Fritz-Haber-Institut, Berlin

Arbeitsgruppe: Physik biologischer und weicher Materie
(Leiter: Dr. Ralf Everaers)

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

Verhakungseffekte bei Polymeren: Polymere haben einzigartige viskoelastische Eigenschaften und bilden das Grundgerüst von so unterschiedlichen Systemen wie Autoreifen und dem Zytoskelett. Charakteristisch für lange Kettenmolekle ist das Auftreten topologischer Verhakungen auf molekularen Skalen. Ähnlich zu verknoteten Schnüren können sich Polymerketten aneinander vorbeibewegen, aber nicht durchkreuzen. Das Standardmodell der Polymerdynamik, das Röhrenmodell, basiert auf der Vorstellung, dass die Verhakungen mit anderen Ketten die Fluktuationen jedes Polymers

auf ein röhrenartiges Volumen um einen "primitiven Pfad" beschränken, der wiederum der geglätteten Kettenkonformation folgt. Es ist uns gelungen, die mikroskopischen Grundlagen dieses erfolgreichen phänomenologischen Modells durch die Einführung einer "primitiven-Pfad-Analyse" (PPA) des mikroskopischen topologischen Zustands zu etablieren (S. 106). Dies eröffnet die Möglichkeit eines systematischen Studiums der Dynamik und Deformationsabhängigkeit der primitiven Pfade in Polymerschmelzen und -netzwerken. Desweiteren arbeiten wir an einer vereinheitlichten Beschreibung von "locker verhakten" Schmelzen synthetischer Polymere und von "eng verhakten" Lösungen semiflexibler Biopolymere wie Aktin.

Polyelektrolyte: Polyelektrolyte sind Polymere mit ionisierbaren Seitengruppen. Beispiele sind Amino- und Nukleinsäuren ebenso wie Polyacrylsäure, das Material aus dem Babywindeln hergestellt werden. Daß viele Biopolymere in diese Klasse fallen, ist kein Zufall: irdisches Leben beruht auf einem Wechselspiel Kohlenstoff-basierter Makromoleküle in Wasser. Die Löslichkeit dieser typischerweise wenig polaren, organischen Moleküle beruht gerade auf dem Entropiegewinn der in wässriger Lösung dissoziierten Gegenionen. Die Behandlung der langreichweitigen elektrostatischen Wechselwirkungen ist besonders schwierig in der Umgebung unpolarer, hydrophober Elemente. Wir haben mit Unterstützung der Volkswagenstiftung begonnen, diese Effekte mit Hilfe eines Simulationsalgorithmus zu untersuchen, der die Berechnung elektrostatischer Selbstenergien und -wechselwirkungen in dielektrisch inhomogenen Medien ermöglicht.

DNA und Chromatin: Genetische Information ist in der komplementären Basensequenz der beiden Einzelstränge der DNA Doppelhelix gespeichert. Replikation und Transkription erfolgen durch lokale Dissoziation der Doppelhelix and Synthese komplementärer DNA- oder RNA-Stränge entlang der Einzelstränge. In eukaryotischen Zellen ist die DNA mit Proteinen komplexiert und hierarchisch in Chromatinfasern und Chromosomen organisiert. Die relevanten Längenskalen reichen von 1 nm (dem Durchmesser einzelner Basen) bis zu Gesamtkonturlänge der DNA von 2m in jeder menschlichen Zelle. Wir arbeiten z.Z. an Theorien und Computersimulationen zur Beschreibung der Assoziation komplementärer Basenpaare, der linearen Elastizität helikaler Filamente, der DNA Struktur und nicht-linearen Elastizität auf der Skala der Basen(-paare), der mechanischen Eigenschaften der 30 nm Chromatinfaser (S. 109), geometrischer und topologischer Aspekte der Faltung von DNA in Modell-Chromatinfasern, der Packung von DNA in viralen Kapsiden und elektrostatischer Wechselwirkungen in DNA und Chromatin.

Zukunftsperspektiven

Eine Herausforderung für die Zukunft ist die Untersuchung aktiver Prozesse im Zytoskelett und im Genom in Zusammenarbeit mit den Gruppen von Prof. Jülicher und Dr. Kruse. Daneben entwickeln wir aktive Kollaborationen mit experimentellen Gruppen (z.B. mit Prof. Richter (FZ Jülich/SANS Experimente an Polymerschmelzen und -netzwerken) und Prof. Ott (U Bayreuth/DNA-Chips)). Ein Schwerpunkt wird auf der verbesserten Integration der Gruppe in die vielfältigen wissenschaftlichen Aktivitäten im Bereich der Materialwissenschaften, der Biophysik und der Biotechnology im Raum Dresden bilden. Erste Kontakte mit dem Max-Planck-Institut für Zellbiologie und Genetik sowie dem Leibnitz-Institut für Polymerforschung wurden bereits geknüpft.

Kooperationen

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

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

Mesoskopische Systeme sind von Menschenhand (mittels hochspezialisierter Apparaturen) hergestellte Strukturen mit Abmessungen weniger Mikrometer bis hinab in den Nanometerbereich. Auf diesen Skalen sind Quanteneffekte merklich, die zu ungewöhnlichen elektrischen und optischen Eigenschaften führen. Wir untersuchen die theoretischen Grundlagen dieser Systeme in einem Team aus 5-6 PostDocs mit wissenschaftlichem Hintergrund in mesoskopischer Festkörperphysik und Quantenoptik, sowie in einer Vielzahl an nationalen und internationalen Kooperationen.
Folgende Themenschwerpunkte wurden während des aktuellen Berichtszeitraums gesetzt:

- Saubere, ballistische Systeme, welche vom universellen Verhalten verunreinigter Strukturen abweichen und es erlauben, Quanteneffekte (wie das Schrotrauschen bei kleinen Temperaturen oder die Zustandsdichte in Hybridstrukturen mit supraleitenden Komponenten) gezielt einzustellen. Grenzen der Universalität in stark verunreinigten Quantendrähten. Leitfähigkeit in wechselwirkenden Systemen.

  H. Schomerus, M. Titov, V. Gopar, R. Molina; mit P. A. Mello (mpi**pks** und Univ. Mexiko), C. W. J. Beenakker (Leiden), J. Tworzydło (Warschau), Ph. Jacquod (Genf), P. Brouwer (Cornell), J.-L. Pichard (Saclay/CEA), D. Weinmann (Straßburg), G.-L. Ingold (Augsburg), P. Woelfle (Karlsruhe), S. Rotter (Wien).

- Erzeugung nichtklassischen Lichts in der elektromagnetischen Umgebung mesoskopischer Leiterstrukturen; Die Beschreibung intermittiernder Systeme mittels Quantensprüngen, mit Anwendung auf fluoreszierende Quantenpunkte; Optische Eigenschaften metallischer Nanopartikel; Ausstrahlungseigenschaften von Mikrolasern. Diese Themengebiete liegen an der Schnittstelle der mesoskopischen Physik zur Quantenoptik.

  H. Schomerus, A. Budini, R. Molina; mit J. Wiersig (Bremen), M. Hentschel (Regensburg), R. Jalabert (Straßburg), C. W. J. Beenakker (Leiden).

- Wechselwirkung von Atomen mit starken Laserfeldern; Photodissoziation; mittels Semiklassik, Streu- und Floquettheorie.

  H. Schomerus, Th. Gorin, D. Martinez. Mit T. H. Seligman (UNAM Mexico), T. Prosen (Ljubljana), M. Znidaric (Ulm), H.-J. Stoeckmann (Marburg), W. Becker (MBI Berlin), C. Faria (London).

Nachwuchsgruppe: Elektronische Struktur endlicher Systeme
(Leiter: Dr. S. Kümmel (seit 7/2003))

Das Arbeitsgebiet der seit August 2003 bestehenden Emmy Noether-Nachwuchsgruppe ist die Untersuchung der elektronischen Struktur und Dynamik von Atomen, Molekülen und Clustern. Dabei liegt der Schwerpunkt unserer Forschung im Bereich der Dichtefunktionaltheorie und ihrer zeitabhängigen Formulierung. Diese Theorie ermöglicht es, ein Vielteilchensystem alleine anhand der anschaulich zugänglichen Größe „Teilchendichte“ quantenmechanisch zu beschreiben, d.h. ohne dass die nur unter großem numerischen Aufwand zu bestimmende Vielteilchenwellenfunktion berechnet werden muss. Ein Vorteil dieser alternativen Formulierung der Quantenmechanik ist der deutlich reduzierte numerische Aufwand in praktischen Rechnungen. So kann z.B. die Struktur eines Systems mit vielen Elektronen oder seine – auch nichtperturbative – Dynamik unter Berücksichtigung der Elektron-Elektron Wechselwirkung berechnet werden. Darüberhinaus ist ein weiterer ebenso wichtiger Vorteil, dass die Dichtefunktionaltheorie häufig einen anschaulichen Zugang zum Verständnis quantenmechanischer Prozesse eröffnet. Als „first principles“ Theorie ermöglicht sie damit, in Bereiche vorzustoßen, in denen wellenfunktionsbasierte Methoden an ihre rechnerischen Grenzen stossen, aber unser Verständnis noch nicht weit genug entwickelt ist, um die wesentlichen physikalischen Effekte in einfachen Modellen zu erfassen.
In der Praxis hängen Genauigkeit und Vorhersagekraft von Dichtefunktionalrechnungen von der Qualität der Näherung ab, die man für das sogenannte Austausch-Korrelationsfunktional macht, über das die quantenmechanischen Vielteilcheneffekte berücksichtigt werden. Ein Aspekt unserer Forschung ist die Entwicklung von räumlich und zeitlich nichtlokalen Funktionalen, mit denen wir Effekte beschreiben wollen, die mit bisherigen lokalen Näherungen wie z.B. der „Local Density Approximation“ nicht erfasst werden. Dazu gehören z.B. Polarisationseffekte in molekularen Ketten, für die man sich im Zusammenhang mit der Entwicklung nichtlinearer optischer Bauelemente, z.B. zur Frequenzverdopplung von Lasern, interessiert. Die Verwendung von Orbitalfunktionalen, d.h. implizit von der Dichte aber explizit von den Kohn-Sham Orbitalen abhängigen Funktionalen, führt hier zu entscheidenden Verbesserungen.

Ein weiterer Schwerpunkt unserer Arbeit liegt auf der Entwicklung von Methoden, die im Rahmen der zeitabhängigen Dichtefunktionaltheorie die Berechnung nichtlinearer und nichtperturbativer Anregungen von Vielelektronensystemen ermöglichen. Ein Zugang, mit dem wir ein besseres Verständnis der dabei wichtigen Korrelationseffekte zu erreichen hoffen, besteht darin, für einfache Modellsysteme die zeitabhängige Schrödingergleichung numerisch exakt zu lösen. Aus den so gewonnenen zeitabhängigen Dichten kann durch Inversion der Kohn-Sham Gleichungen das exakte zeitabhängige Korrelationspotential berechnet werden. Durch Vergleich mit diesen exakten Potentialen können Schwächen bisheriger Näherungen analysiert werden und man erhält Richtlinien für die Entwicklung verbesserter Funktionale. Diese wollen wir in realistischen, d.h. nicht modellhaften dreidimensionalen Rechnungen zur Untersuchung der Licht-Materie Wechselwirkung einsetzen, z.B. zur Untersuchung von Edelgasatomen und Silberclustern in Laserpulsen.

Zukunftsperspektiven

Neben dem allgemeinen Ziel, die Genauigkeit und Vorhersagekraft von Dichtefunktionalrechnungen zu erhöhen, soll unsere Arbeit vor allem dazu dienen, auf Grundlage der Dichtefunktionaltheorie solche Fragen zu beantworten, die auf absehbare Zeit nicht mit Wellenfunktionsmethoden geklärt werden können. Dazu gehört generell die oben angesprochene Problematik der Vielelektronendynamik in starken Feldern und im Speziellen das Zusammenspiel zwischen der intrinsischen Struktur eines Systems und der durch externe Felder auslösbaren Dynamik. So wollen wir z.B. den Zusammenhang zwischen dem Aufbau von Molekülen und deren nichtlinearen optischen Eigenschaften verstehen und versuchen vorherzusagen, wie nichtlineare Eigenschaften durch gezielte strukturelle Änderungen im Molekül (Austausch von Atomen oder Nebengruppen) beeinflusst werden können. Dieser Arbeiten stellen Schritte auf dem Weg zum langfristigen Ziel unserer Forschung dar: Eine dichtefunktionalbasierte „first principles“ Beschreibung der Struktur und Dynamik endlicher Systeme, die es uns erlaubt, Observable sowohl genau zu berechnen als auch anschaulich zu verstehen.

Kooperationen

Unsere Kerngruppe aus zwei promovierten Mitarbeitern und einem Doktoranden ist innerhalb des Instituts vor allem mit der Abteilung „Endliche Systeme“ vernetzt. So ergab sich zum Beispiel mit Dr. Manfred Lein eine fruchtbare Zusammenarbeit.
Neben internationalen Kollaborationen mit der Gruppe von John Perdew am Physics Department der Tulane University, USA und der Gruppe von Leeor Kronik am Department of Materials and Interfaces des Weizmann Institute of Science in Israel arbeiten wir weiterhin mit Manfred Lein, nun am Max-Planck Institut für Kernphysik in Heidelberg, und Michael Moseler vom Frauenhofer Institut für Werkstoffmechanik in Freiburg zusammen. Außerdem bestehen regelmäßige Kontakte zu Matthias Brack, Fakultät für Physik, Universität Regensburg und Paul-Gerhard Reinhard, Fakultät für Physik, Universität Erlangen und ihren Gruppen.

Arbeitsgruppe: Musterbildung in Reaktions-Diffusionsprozessen
(Leiter: Dr. M. Bär (bis 10/2004))

Die Nachwuchsgruppe existierte von November 1995 bis Oktober 2004. In dieser Zeit waren ca. dreißig Gastwissenschaftler (davon fünfzehn international) für im Schnitt ein Jahr sowie acht Doktoranden und ein Diplomand (davon vier international) Mitglieder der Gruppe. Abgeschlossen wurden im Rahmen der Gruppe vier Habilitationen (M. Bär, H. Hinrichsen, G. Schliecker und U. Thiele) und fünf Promotionen (U. Börner, L. Brusch, K. John, E. Nicola und C. Utzny). Es erschienen ca. 125 Publikationen, davon 20 Artikel in Physical Review Letters. Von den deutschen Mitgliedern der Gruppe erhielten drei unbefristete Positionen als Arbeitsgruppenleiter oder Professoren (M. Bär, A. Deutsch, H. Hinrichsen), drei weitere sind heute Nachwuchsgruppenleiter, Juniorprofessoren bzw. Arbeitsgruppenleiter auf befristeten Stellen (M. Falcke, Th. Höfer, M. Or-Guil).
Die Forschung konzentrierte sich zunächst auf komplexe Strukturen und Raum-Zeit-Chaos in chemischen und physikalischen Reaktions-Diffusions-Systemen. Im Laufe der Zeit bildete sich die Modellierung biologischer Prozesse als zweiter gleichwertiger Schwerpunkt heraus. Weitere wichtige Themen waren die Modellierung von Nichtgleichgewichtsphasenbergängen, die Theorie quasikristalliner und ungeordneter Systeme sowie die Modellierung der Strukturbildung in dünnen Filmen. Diese Themen wurden durch Projekte der Deutschen Forschungsgemeinschaft (3×), der Deutsch-Israelischen Gesellschaft (1×) und der Europäischen Union (2×) unterstützt.

Komplexe Strukturen
Strukturbildung wird in vielen physikalischen, chemischen und biologischen Systemen beobachtet. Übergänge zwischen einfachen (Fronten, Pulse, periodische Muster, Spiralen) und komplexen Strukturen (Raum-Zeit-Chaos, modulierte Strukturen, Musterdomänen) wurden mit Hilfe von numerischen Simulationen, Störungstheorien sowie numerischer Bifurkations- und Stabilitätsanalyse untersucht. Dazu ist uns eine nichtlineare Analyse sekundärer Instabilitäten periodischer Wellen gelungen, die neue Erkenntnisse über raumzeitlich chaotische Muster und modulierte Wellen, z.B. sogenannte Superspiralen, liefert. Außerdem ist die numerische Analyse von konvektiven und absoluten Instabilitäten und ihre Rolle in der Destabilisierung von einfach rotierenden Spiralen abgeschlossen worden.
Weitere Themen sind die Strukturbildung in anisotropen und heterogenen Medien sowie die externe Steuerung von Mustern. Hier haben wir uns mit der Homogenisierung und Ableitung von effektiven Diffusionskonstanten und ihre Anwendung auf die Musterbildung in chemischen Reaktionen in Mikroemulsionen beschäftigt.
Untersuchte experimentelle Anwendungen schliessen chemische Reaktionen in Gelen und auf Oberflächen sowie hydrodynamische Systeme (dünne Filme, Oberflächenwellen und Ferrofluide) mit ein. Im Falle dünner Filme wurden in letzter Zeit auch komplexe Situationen, z.B. Zweischichtsysteme und chemisch aktive dünne Filme analysiert (siehe langer Bericht von U. Thiele *et al.* auf S. 123). Fr chemische Reaktionen waren die Analyse von dreidimensionalen Strukturen und ihren Wechselwirkungen sowie die Einbeziehung von physikalischen Wechselwirkungen aus dem Gebiet der weichen Materie in Reaktions-Diffusions-Prozesse neue Themen.

Insbesondere Modelle aus der Physiologie (intrazelluläre Dynamik, Kalziumwellen) und Morphogenese (Aggregation von Bakterien und Schleimpilzen) wurden hier betrachtet. Methodisch wurde dabei insbesondere der Übergang von kontinuierlichen, deterministischen auf diskrete, stochastische Modelle untersucht. Hervorzuheben sind stochastische Modelle für intrazelluläre Kalziumdynamik und Proteinoszillationen in Bakterien sowie Dichtewellen in Myxobakterienkolonien („Rippling"), die auf Migration und Kollision basieren und Modelle zur Ausbildung von Orientierungsordnung in selbstbewegten Stäbchensystemen. Neuere Projekte beschäftigen sich mit der Beschreibung biochemischer Netzwerke, z. B. bei metabolischen Prozessen wie der Glykolyse oder im Falle von Kalziumoszillationen. Schließlich wurde die Strukturbildung in Lipidmembranen ausführlich untersucht und verschiedene Mechanismen der Domänenbildung gefunden.

Veranstaltungen

Mitglieder der Gruppe waren entscheidend beteiligt an der Koordination von zwei längeren Workshops am mpi**pks** „Trends in Pattern Formation" (M. Bär, 2003) und „Pattern Formation through Instabilities in Thin Liquid Films" (U. Thiele, 2004).

Kooperationen

Wir verfügen über vielfältige nationale und internationale Kooperationsprojekte. Unter anderem waren wir beteiligt an der DFG-Forschergruppe „Nanostrukturierte Funktionselemente in makroskopischen Systemen" der TU Dresden. Die Kooperation mit Prof. Meron (Beer-Sheva) und Prof. Pismen (Technion Haifa) wurde durch die Deutsch-Israelische Gesellschaft bis Ende 2003 im Projekt „Strukturbildung in der Katalyse: Von der Mikro- zur Nanoskala" unterstützt. Auf Zusammenarbeiten mit experimentellen Gruppen legen wir besonderen Wert; hier sind Projekte zur chemischen Strukturbildung (Prof. Müller (Magdeburg), Prof. Engel (TU Berlin) und zur Oberflächenkatalyse (Prof. Imbihl (Hannover) und Prof. Rotermund (FHI Berlin) zu nennen. Auf dem Gebiet der biologischen Systeme existieren Projekte zu räumlichen Organisation von Bakterien (Dr. Deutsch (TU Dresden) und Prof. Sogaard-Andersen (MPI Marburg)) sowie zu Biotransformationen (Dr. Bertau (TU Dresden)) und Lipiddomänen (Prof. Käs (Leipzig)). Weitere theoretische Kooperationen finden u.a. statt mit Prof. Bestehorn (Cottbus), Dr. Chate (Saclay), Prof. Kapral (Toronto), Prof. Knobloch (Berkeley), Prof. Paczuski (London) Dr. Torcini (Florenz) und Prof. Vega (Madrid).

Fazit und Ausblick

Alles zusammengenommen lassen sich drei Hauptthemen identifizieren: 1. Komplexe Strukturen in Reaktions-Diffusions-Systeme, 2. Modellierung von Strukturbildung in biologischen Systemen sowie 3. strukturbildende Prozesse in Fluiden und dünnen Filmen. Das erste Thema war der Ausgangspunkt und Markenzeichen der Gruppe, die beiden anderen Themen haben Zukunftsperspektiven eröffnet und werden von den ehemaligen Mitgliedern der Gruppe weiterhin bearbeitet. Am MPIPKS wird insbesondere das zweite Thema mittlerweile durch die Aktivitten der Abteilung „Biologische Physik" und thematisch verwandter Nachwuchsgruppen bedient. Das dritte Thema wird durch das von November 2004 an laufende EU-Projekt von U. Thiele am mpi**pks** vertreten.

Chapter 2

Scientific Work and its Organisation at the Institute - an Overview

2.1 History and Development of the Institute

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

and Mesoscopic Systems in January 1996, and *Dr. M. Dolg* of the group *Quantum Chemistry* shortly afterwards.
1995-1998 • At the same time, plans for the new institute building began to materialize. The architecture firm Brenner und Partner (Stuttgart) with J. Wittfoth won the competitive bidding, and constructions started in September 1995. After less than two years the institute took over the newly constructed main building, together with the three guest houses. The inauguration of the buildings was held during a simultaneous symposium on *Complexity in Physics*, September 23-24, 1997. In the meantime the Seminar- and Guest-Program were gaining momentum, with hundreds of scientists already having visited the institute.
1999-2001 • The next important step was the appointment of *Dr. J. M. Rost* (Freiburg) as head of the second division of the institute in December 1998. *Dr. Rost* started the activities on May 1st, 1999 by setting up the division *Finite Systems*. He appointed *Dr. A. Buchleitner* as head of a research group *Nonlinear Dynamics in Quantum Systems*. After *Dr. Dolg* accepted an offer for a professor position at the University of Bonn in 2000, *Dr. U. Birkenheuer* was appointed as his successor in March 2000. *Dr. K. Richter* soon afterwards also accepted the offer of a chair for Theoretical Physics at the University of Regensburg. This concluded the Junior Research Group *Quantum Chaos and Mesoscopic Systems*. To continue the successful work in this research field with modified premises, *Dr. H. Schomerus* (Leiden) was appointed as head of a new Junior Research Group *Waves in Complex Media and Mesoscopic Phenomena* in November 2000.
2001-2003 • To account for the increasing demand for bridging the field between physics and biology, *Dr. F. Jülicher* (Paris) was appointed as head of the third division *Biological Physics* in 2001. Shortly afterwards, two research groups on *Physics of Biological and Soft Matter* headed by *Dr. R. Everaers* (Mainz), and *Biological Physics of Olfaction: From Genes to Networks* headed by *Dr. M. Zapotocky* (New York) started their activities within the third division in 2002. The division *Finite Systems* also continued to broaden its research spectrum by appointing *Dr. A. Becker* (Bielefeld) as head of the new research group *Nonlinear Processes in Strong Fields* in 2002.
2003-2004 • In 2003 *Dr. S. Kümmel* (New Orleans) started the activities of an Emmy Noether-Group *Electronic Structure of Finite Systems*. It was followed in 2004 by setting up a Junior Research Group *Physics of Cell Division* headed by *Dr. K. Kruse* as one of three research groups within a joint program *Physics of Biological Systems* initiated together with the Max Planck Institute for Cell Biology and Genetics. The construction of an extension to the institute building was started in the same year 2004. The additional office space, discussion and seminar rooms as well as various communication areas will help to accomodate the enormous number of guest scientists.

The institute hosts approximately 50-100 long-term guest scientists at a given time, together with 1200-1500 short-term guests who annually participate in the workshop and seminar program.

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

2.2 Research Areas and Structure of the Institute

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

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

Furthermore, six of the currently nine research groups are broadening and strengthening the work of the corresponding division. Three more groups, among them two junior research groups, interpolate between and add to the above listed research topics.

- The research of the junior research group *Waves in Complex Media and Mesoscopic Phenomena* headed by *Dr. Schomerus* bridges the work of the divisions *Electronic Correlations* and *Finite Systems*.
- The Emmy Noether Group *Electronic Structure of Finite Systems* is headed by *Dr. Kümmel* strengthens further ties between the divisions *Electronic Correlations* and *Finite Systems*.
- The only permanent research group, headed by *Dr. Kantz*, is working on *Nonlinear Time Series Analysis*. Here, methods are applied and developed, related to various aspects of classical chaos, which play an important role also for research on semiclassical topics.

A joint program *Physics of Biological Systems* of the Max Planck Institute for the Physics of complex Systems and the Max Planck Institute for Cell Biology and Genetics started its activities in the fall of 2004. Three actively interacting Junior Research Groups are going to conduct research on various aspects of cellular systems with benefit for the research work of both institutes. The first Junior Research Group *Physics of Cell Division* headed by *Dr. Kruse* started its activities in October 2004, focussing on the principles of spatial and temporal organization of cells during division processes.

2.3 Workshop and Visitors Program

A central task of the institute is to conduct international *Workshops and Seminars* (p. 134), which makes mpi**pks** an almost unique institute within the Max Planck Society, only comparable with the mathematics institute in Bonn. A small but efficient group of staff headed by *Dr. Flach* is responsible for the logistics and the preparation of meetings, and gives advise to the (usually external) scientific coordinators on the various aspects of planning and conducting the corresponding event.
The *Visitors Program* (p. 128) offers research visits ranging from a few weeks to two years in duration. Guest scientists are using various ways of collaboration by joining research groups at the institute, by doing joint research with other guest scientists, or by starting collaborations with workshop and seminar participants. Further possibilities of collaboration include contacts with the TU Dresden or other local research institutions, well documented, e.g., by common publications (see p. 177).
Proposals for workshops and seminars, as well as applications for guest scientist positions, are evaluated by two different committees. Members of each committee include external scientists and scientists of the institute.
In order to further strengthen and structure the Visitors Program, mpi**pks** started in 2000 to annually award the *Martin Gutzwiller Fellowship* to an internationally recognized and experienced scientist. The awardees *Prof. R. Kapral* (Toronto) 2003 and *Prof. A. Politi* (Firenze) 2004 have spent up to one academic year at mpi**pks** (p. 131). The mpi**pks** also offers one *Distinguished PKS Postdoctoral fellowship* annually. It aims at excellent young researchers, shortly before accepting a tenure track position (p. 129).

2.4 Teaching and Training

The institute aims at a broad and far reaching education of young scientists in research, teaching and the organization of research.
Teaching • Standard lecture series are conducted by institute members, both at the TU Dresden and at other universities (p. 163). In addition, the public relations sector of our institute offers institute members possibilities to teach and lecture for high school teachers and high school students, both at mpi**pks** as well as at high schools (p. 166).
Research Organization • The large-scale Workshop and Seminar Program at mpi**pks** offers the unique possibility for young scientists to take part in the organization of meetings. Out of the 32 events during 2003-2004, young scientists of the institute took part in the coordination of 10. This has a positive educational effect for young scientists, and helps the external coordinators through the permanent contact with a local scientific coordinator.

2.5 Public Relations

The institute understands its mission in the broadest sense to provide a platform for the emergence, exchange and development of creative ideas in research. While mainly focusing on scientists, this also includes potential future scientists, i.e., high school students, teachers, as well as the general public interested in science. Within our school-contact-program we offer workshops for high school teachers, winter schools for high school students, and lectures at schools in order to spread the fascination of science as it happens.
Since 1999, mpi**pks** coordinates, together with the TU Dresden and the City of Dresden, the lecture series *Science in the City Hall*, aiming at a public interested in science. Well-known scientists are invited to give lectures for the broad public, which are intended to popularize modern research (p. 166).
Furthermore, coordinators of workshops are encouraged to offer one public evening lecture at mpi**pks**, in the course of the workshop.

2.6 Research Networking

Local • The mpi**pks** finds itself in the midst of a rich research environment, formed by the TU Dresden and many other research institutes. An intensive scientific dialogue with the Physics Department of the TU Dresden is taking place, e.g., with regular joint seminars (*Quantum Dynamics* with Prof. Schmidt and *Complex Systems* with Prof. Ketzmerick). Institute members are involved in several Collaborative Research Programs of the DFG and one Forschergruppe (p. 162). The division *Electronic Correlations* is cooperating with the IFW (Institut für Festkörper- und Werkstoffforschung) and with the neighbouring Max Planck Institute for Chemical Physics of the Solid State. The division *Biological Physics* established close contact to the Max Planck Institute of Molecular Cell Biology and Genetics.
National and International • The many different national and international collaborations and contacts are listed in the research group reports below. Furthermore, the institute has a small budget for collaborations with experimental groups (p. 133).

2.7 Reports by the Research Groups

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

The scientific program of the Department is mainly focussed on electron correlations in molecules and solids. But also other topics like the behavior of glasses at ultralow temperatures or spin effects in nanostructures are investigated.
As regards the work on electronic correlations it can be divided into ab initio calculations and investigations of model Hamiltonians. Within the ab initio type of work, calculations of energy bands based on quantum chemical methods have been further developed in collaboration with the Quantum Chemistry group. The ADC (algebraic diagrammatic construction) approach was extended to solids and as a test case the energy bands of LiF were computed. In distinction to our previous work the ADC is based

on Green's function calculations where the self-energy can be calculated with high precision. We developed also in collaboration with Prof. H. Stoll (Univ. Stuttgart) a simplified quantum chemical scheme in order to calculate the energy bands of covalent semiconductors. It should be also mentioned that a way was found to calculate ground-state wavefunctions and properties for metals by means of the method of increments. Within the frame of density functional theory (here: LDA+U) a number of materials were treated. Noticeable is the result that magnetite Fe_3O_4 has at low temperatures a distorted spinel structure which agrees well with a recently observed one.
Starting from model Hamiltonians the following results were obtained:
It was demonstrated (Kakehashi: Adv. Phys.) that a number of different methods which have been applied to study model systems like the Hubbard one, are in fact equivalent. These are the Many-Body Coherent Potential Approximation (MB-CPA), the Dynamical CPA, the Dynamical Mean Field Approximation (DMFA) and the Projection Operator method (POM). This equivalency was previously not realized since the different methods are formulated in quite different contexts so that their relations are not obvious at all. Also the POM was extended to include nonlocal processes. An immediate application enabled us to show that a Hubbard Hamiltonian on a square lattice shows Marginal Fermi Liquid behavior for a considerable range of doping concentrations when the correlations are strong. This is what is observed in the cuprates.
We extended also the Dual Model of $5f$ electrons, which was introduced by us three years ago with Prof. G. Zwicknagl (TU Braunschweig). For UPd_2Al_3 the observed Fermi surface as well as the large anisotropic mass ratios could be explained *without* an adjustable parameter. We could also demonstrate convincingly that Cooper pairs are formed in that material, not by electron-phonon interactions but rather by intra-atomic excitations of strongly correlated $5f$ electrons. The Dual Model has obtain a very solid base in the meantime and has changed our views on $5f$ electrons considerably.
A new area of research which we started two years ago, i.e., charge degrees of freedom in frustrated lattice systems has obtained fresh momentum. With the help of exact diagonalizations we could show that the ground state of spinless fermions is liquid-like and two- or fourfold degenerate. The assertion could be further substantiated that in a 3 dimensional pyrochlore lattice excitations with fractional charges $\pm e/2$ exist. At present we try to work out the statistics of these objects in $d = 2$ (checkerboard lattice) and the related gauge theory.
Finally it should be mentioned that with Dr. S. Kettemann (Univ. Hamburg) and an experimental group at Boston University (Prof. P. Mohanty) we devised a method to measure the torque which exists at the interface when a current passes from a ferromagnetic wire to a nonmagnetic one. The realization of a corresponding experiment on a nanoscale is under way. Knowing the torque one would be able to determine the relative contributions of s and d electrons to the current. This information cannot be obtained otherwise.

Research Group: Quantum Chemistry
(Leader: Dr. U. Birkenheuer)

As in the years before, the quantum chemistry group is focusing on the wave-function-based determination of the electronic structure of solids and polymers. We use localized orbitals to arrive at *local* representations of the Hamiltonian and the wave function

contributions. This allows to fully exploit the predominantly short-range character of electron correlations and to establish quantum chemical many-body techniques which are even applicable to infinite periodic systems. In most of our methods, the incremental scheme is employed to assemble the individual correlation contributions.
Having developed a powerful embedding scheme for quantum chemical correlation calculations of clusters in infinite host crystals, the so-called CRYSTAL-MOLPRO interface, we are now able to study both, cationic (N-1)-particle states and anionic (N+1)-particle states of periodic systems on the same footing. The valence and conduction bands of diamond already described in the previous report is one example of such a calculation, the correlated band structure of *trans*-polyacetylene (tPA) which was the subject of the PhD thesis of Viktor Bezugly (finished in Feb 2004) or hydrogen fluoride (HF) zig-zag chains are other ones.
Several drawbacks of the original approach had to be removed to achieve this aim. The most important was the development of a special size-consistency correction for the open-shell multi-reference CI(SD) calculations we used to determine the excited (N-1)-particle and (N+1)-particle states of tPA. By this technique the influence of the missing size-consistence inherent to all truncated configuration interaction (CI) methods on the individual incremental contributions could be reduced substantially such that good convergence was obtained for the incremental series.
Another important issue in this context is the construction of suitable localized *virtual* orbitals. Here, a band disentanglement procedure (very similar to the one proposed by Marzari and co-worker for maximally localized Wannier functions) could be designed especially for the Wannier-Boys localization algorithm used in the Gaussian-orbital-based CRYSTAL program package with which we calculate the Hartree-Fock wave functions of the host crystals. It allows to setup perfectly text-book-like anti-bonding orbitals for silicon (and other compounds), which remain energetically close enough to the bottom of the conduction bands to be suited for the subsequent MR-CI calculations.
In the last two years, we have started to extent the incremental scheme for ground state properties and the local Hamiltonian approach for band structures to enlarge the range of properties which can be investigated by these methods. In the meantime, pair energies and density matrices can be extracted from incremental calculations as was demonstrated on the semiconducting and ionic bulk materials SiC and LiH, recently.
We were also successful, in setting up a local Hamiltonian scheme for excitons. It is designed in close analogy to the local Hamiltonian approach for one-particle excitations (holes or electrons), and operates well for reasonably strong bound electron-hole pairs (Frenkel excitons) as shown for our prototype periodic system, an infinite, rope-ladder-like H_2 chain.
The major new aspect in the quantum chemistry group, however, is the use of advanced field-theoretical Green's function methods as an alternative to the traditional local Hamiltonian approach. It was initiated by the PhD thesis of Christian Buth (started in Dec 2002). These Green's function methods are much better suited to tackle the always present problem of a possible break-down of the one-particle picture, i.e., the occurrence of satellite states, in band structure calculations. We have designed and implemented a *local* variant of the well-established Dyson equation-based algebraic diagrammatic construction (ADC) technique by switching to local occupied and virtual Wannier orbitals and fully exploiting the translational symmetry of the system under consideration. Investigations on the valence and conduction bands of HF chains and

bulk LiF demonstrate the power of the new approach.
Work is in progress to extend the non-Dyson ADC formalism (which is computationally far less demanding than the Dyson-type ADC ansatz) in a similar way. A fully invariant formulation under transformations of the occupied and virtual orbitals is possible which enables us to even consider extremely localized non-orthogonal orbitals as basis functions. This allows to exploit even more stringent cutoff and integral screening criteria and should ultimately lead to highly efficient linear-scaling Green's function methods for periodic (or other extended) systems.
A collaboration with the Theoretical Chemistry group at the Univerity of Torino (Prof. C. Pisani) has been agreed on to incorporate the new advanced Green's function approaches into the CRYSCOR program code for local MP2 (Møller-Plesset perturbation theory up to 2nd order) calculations which has quite similar prerequisites than our CO-ADC ansatz for crystal orbitals (COs). This would allow to take full advantage of the rich infra structure provided by the back-end of the CRYSTAL program package.

Cooperations

- Prof. C. Pisani, Dipart. di Chimica IFM, Università degli Studi di Torino, Italy: Incorporation of the CO-ADC approach in the CRYSCOR program
- Prof. H. Stoll, Institut für Theoretische Chemie, Universität Stuttgart: Development of simplified correlation calculations for band structures
- Prof. V. Staemmler, Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum: Direct determination of local correlated hole wave functions
- J.-Prof. M. Albrecht, Theoretische Chemie, Universität Siegen: Benchmark calculations on correlated band structures of periodic systems
- Prof. J. Schirmer, Theoretische Chemie, Universität Heidelberg: Molecular local Dyson and non-Dyson ADC formalisms

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

Complex dynamical behaviour remains to be a challenge to theory and to practice. Our group concentrates on aspects of complexity in classical (i.e., non-quantum) systems, where we are both interested in basic properties and in specific phenomena. Major and longer lasting projects of the past two years are: Elimination of fast chaotic degrees of freedom from Hamiltonian dynamics and their replacement by white noise, generalisation of the time delay embedding for deterministic systems to Markov chain modelling for stochastic systems, study of long range correlations and predictability of surface wind. In terms of applications, we have continued our efforts concerning noise reduction for speech signals, where we started to quantify the success of noise reduction through the improvement of the recognition rate of sentences by commercial speech recognition systems. There are also ongoing activities in the area of the prediction of turbulent wind gusts.
A new activity of our group concerns extreme events. Extreme events are large short-time deviations of a system from its mean behaviour. It seems that the ability of a

system to exhibit extreme events is closely related to the complexity of its dynamics. We are studying dynamical mechanisms which are able to create extreme events, we try to understand the rôle of precursors, and we consider statistical aspects for the detection and characerization of extreme events.
On the time scale of the next two years, our work is well determined by current projects. In particular, setting up and understanding prototypic models for the generation of extreme events, and the more intense study of properties of surface wind also in terms of turbulence within a newly formed German network, will be dominating.

Cooperations

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

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

The group is interested in the non-linear dynamics of excited systems which consist of a finite number of particles, focusing on atoms and clusters. Over the last two years, our work on ultracold gases has intensified with an emphasis on ultracold plasmas. The latter project, headed by *Dr. Thomas Pattard*, was funded by the DFG, the same holds true for the project *Theoretical study of energy and charge transfer in single clusters and cluster arrays at surfaces* lead by *Dr. Ulf Saalmann* together with Prof. Garcia (Kassel). This project is fundend within the DFG-Priority Program SPP 1153.
The energy to excite these systems can come either from charged particles or photon impact. Particularly, the interaction with laser light has been an important element in our research - this is also a common interest between the *Rost* and the *Buchleitner* group, with the first one concentrating on strong laser pulses in the near infrared, the latter one being interested in weak pulses in the microwave regime. With the *Becker* group we share the interest in the dynamics of molecules in external fields and in general on matter exposed to light from VUV and X-ray free electron laser sources.
Our techniques range from full quantum approaches and density functional theory (TDLDA) over semiclassical approximations to a full classical treatment of microscopic phenomena including advanced techniques such as *tree codes* and *particle in a cell* formulations.
For systems with a small number of degrees of freedom we have been interested in quasiclassical formulations of basic scattering processes such as multiple photoionization and electron impact ionization. For the first time we have investigated three active

electrons fully dynamically in the photo ionization process. This has lead specifically to an understanding of the electron dynamics following triple photoionization of Lithium, in terms of different sequences of binary electron collisions.
Topics which refer to systems with more than a few particles include the excitation of dipole forbidden collective modes in photo cross sections of systems with delocalized electrons, rare gas clusters in intense laser fields, including the new type of radiation which was delivered in the first operation phase by the FEL at DESY in Hamburg (p. 77), and the formation and relaxation of ultracold neutral plasmas with special emphasis on long range correlation phenomena (p. 79).
Finally, *Dr. Lein*, one of our mpi**pks** distinguished postdoctoral fellows, has collaborated intensively with our group, on high harmonic generation in molecules and in laser assisted ion-atom collisions. We also had a fruitful collaboration with *Dr. Brand*, also mpi**pks** distinguished postdoctoral fellow, on scattering from Bose Einstein condensates.

Perspectives for the future

Our work on the dynamics of few-electron systems will continue. The results on triple ionization of Lithium have opened a new perspective for the understanding of multi-electron dynamics in terms of binary electron collisions. This route will be followed in work together with Dr. Emmanouilidou (Georgia Tech, Atlanta, USA).
Long range interaction phenomena in ultracold gases have become experimentally accessible and are a challenge for the theoretical description. While for the case of (dominant) Coulomb interaction in ultracold plasmas we have developed the theoretical tools for a good understanding of the phenomena, dipolar and van der Waals interaction in neutral cold gases are not well understood. Conceptually, we will have to merge basic quantum mechanical elements (e.g. Bloch type of dynamics under a laser field and interference phenomena) with classical motion of the gas.
In 2005 the next stage of the X-ray free electron laser (XFEL) at DESY, Hamburg, will be realized with new experiments coming on line making use of short intense pulses with photon energies of about 30 eV. We plan to specifically address the new cluster experiments which will be carried out at DESY and explore the adjacent parameter regime of the light, not available at DESY, to gain a deeper understanding of the underlying mechanisms.

Cooperations

With experimental groups
We have collaborated with the groups headed by Prof. Müller (Uni Giessen) and Prof. Phaneuf (Univ. of Nevada, Reno, USA) on collective excitation of electrons in complex systems by photons. Data on C_{60} multiple photoionization have been taken, evaluated, and published jointly.
Furthermore, a collaboration with Horst Schmidt-Böcking's and Reinhard Dörner's group, (University of Frankfurt) exists, concerning experimental traces of the transition from regularity to chaos in the photoionization via highly doubly-excited atoms. The very difficult experiments were successful and provide through cross sections with fixed final excitation of the ion a new type of information on highly excited Coulomb systems.
We have also collaborated with the group of Prof. Kaindl (TU Berlin) on high resolution photoabsorption in Helium. Published results include isotope shifts in doubly

excited resonances of Helium and partial photoionization cross sections.

With theoretical groups (some examples):

- on semiclassical theory with A. Ozorio de Almeida (Rio, Brazil)
- on photoionization in complex systems with H. Chakraborty (Manhattan, USA)
- on time in quantum mechanics with J. S. Briggs (Freiburg)
- on transport through single clusters and cluster arrays with M. Garcia (Kassel)

Local cooperations
The interaction with Prof. Rüdiger Schmidt's group from the TU Dresden has continued - the basis is the weekly common seminar *Quantum Dynamics*. It takes place at the mpi**pks** with external speakers invited by both groups. Common research activities include *quantum adiabatic molecular dynamics* directly with R. Schmidt, as well as *semiclassical propagation techniques* with F. Großmann from the TU Dresden. In addition we have initiated a monthly seminar *Complex Dynamics* which includes the newly founded department headed by Prof. Ketzmerick at the TU Dresden and from our institute the *Buchleitner, Kantz, Rost* and *Schomerus* group.

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

The group has been established in October 2002 and hosts currently two Post-docs and one PhD student. Our interests are focused on the interaction between ultrashort laser pulses and matter. The research splits into two main lines, namely the dynamics of single atoms, molecules and clusters exposed to an intense (infrared) field and the self-transformation of a femtosecond laser pulse during its propagation in an optical medium. Our techniques range from analytical theories over S-matrix calculations to full numerical simulations.

The strong coupling of electrons to an intense electromagnetic field, which is of the similar strength as the Coulombic interactions between the charged particles in an atom or molecule, give rise to a number of interesting nonlinear effects. This leads to the possibility to induce changes in the target in a controlled way by variation of the parameters of the external laser pulse, e.g. its intensity, spectral content or duration. In the recent years we have studied a number of specific topics, including the analysis of the correlated emission of two electrons from an atom (see report *Electron-electron momentum exchange in intense field double ionization*), the influence of the symmetry of an orbital and of the orientation of the internuclear axis on the ionization of linear molecules, the generation of high harmonic and attosecond pulses in an environment of ions (e.g. an expanding cluster) and the influence of linear and nonlinear focusing effects on the fragmentation of molecules.

The propagation of an intense femtosecond laser pulse in an optical media results in strong modifications of its shape in the spatial as well as temporal domain, but can also lead to a filamentation of the pulse over long distances. It is the combination of these effects which has raised interest in view of a variety of possible applications ranging from pulse compression to remote sensing using a Lidar. In the past two years we have focused on two aspects, namely an analytical description of self-focusing of

a pulse including the effect of its weak background via perturbation theory and the numerical study of the generation and co-filamentation of an intense third-harmonic pulse (see report *Propagation of femtosecond laser pulses in air*).

Perspectives for the future

We will continue our work on the interaction of atoms, molecules and clusters with intense laser pulses. A focus will be set on the new laser sources, which are now available. The generation of few-cycle and attosecond pulses as well as a variety of possibilities to generate temporally shaped laser pulses have been demonstrated recently. Currently, we develop numerical methods to explore the dynamics of small (one- and two-electron) systems exposed to such pulses. We will focus on the possibilities how to achieve a control over the dynamics.

Further, the construction of the X-ray free electron laser in Hamburg as well as the development of intense high-harmonic sources will soon provide light sources in a previously unexplored parameter regime. The large photon energies together with the expected high intensities will make it possible, e.g. to study multiphoton processes in inner shells of atoms and molecules. New light will be also shed on nonlinear processes, which are already well understood in the low- and high-frequency limits.

Regarding our work on molecules we will concentrate on large hydrocarbons and fullerenes (e.g. C_{60}) and analyze the ionization and fragmentation pathways in these molecules, when subjected to an intense laser pulse.

The work on propagation of femtosecond pulses will continue, with an emphasis on the question, how self-focusing and filamentation can be controlled e.g. by temporally or spatially shaped laser pulses. Further, the propagation of few-cycle pulses gives a new challenge, since it requires the development of theoretical approaches beyond the slowly-varying envelope approximation.

The International Seminar and Workshop on *Intense Laser-Matter Interaction and Pulse Progagation*, which we co-organize in August 2005 at the institute, will give us the possibility to discuss the status and future perspectives of these research areas with other experts.

Collaborations

We are part of two international collaborations, which were established in 2004, namely a Center of Advanced Science and Technology (COAST) on *Ultrafast Intense Laser Science* (coordinated by K. Yamanouchi, Tokyo, Japan) and a Special Research Opportunity Program on *Controlled electron rescattering: sub-A, sub-fs imaging of single molecules* (coordinated by M.Yu. Ivanov, Ottawa, Canada).

Experimental groups:

- with S.L. Chin (Québec, Canada) on propagation of femtosecond pulses in air and, including P. Agostini (Saclay, France), on fragmentation of molecules by intense laser pulses (see e.g. report *Propagation of femtosecond laser pulses in air*). There is a joint supervision of the PhD work of Weiwei Liu (Québec, Canada), who has visited our group for two months in 2004.

- with R. Dörner (Frankfurt) and P.B. Corkum (Ottawa, Canada) on correlation effects in strong field double ionization (see report *Electron-electron momentum exchange in intense field double ionization*). In future, we plan to study the effect of the carrier-envelope phase by integrating the experimental group of U. Keller and J. Biegert (ETH Zürich, Switzerland).

- with C.P. Schulz and I. Hertel (Berlin) on ionization of C_{60} in intense laser pulses.

Theoretical groups:

- with F.H.M. Faisal (Bielefeld) on strong-field ionization of molecules,

- with N. Aközbek and C.M. Bowden (Huntsville, USA) on harmonic generation and channeling,

- with O. Kosareva and V.P. Kandidov (Moscow, Russia) on nonlinear effects in fragmentation of molecules,

- with L. Roso (Salamanca, Spain) on numerical simulation of double ionization in intense laser pulses.

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

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

- the excitation and ionization dynamics of helium under the action of strong electromagnetic fields, particularly in the spectral range of doubly excited two-electron states (J. Madroñero);

- the energy growth in the center of mass motion of cold atoms in a periodically switched optical lattice, amended by spontaneous transitions between electronic states of the atoms (S. Wimberger);

- the resonant enhancement of quantum transport along "web states" in the phase space of the periodically kicked harmonic oscillator (see "Web-Assisted Tunneling in the Kicked Harmonic Oscillator", A.R. Ribeiro de Carvalho);

- the quantitative characterization of two- and multiparticle entanglement in quantum systems of arbitrary finite dimension (see "Concurrence of Mixed Bipartite Quantum States in Arbitrary Dimensions", F. Mintert);

- the dynamics of quantum entanglement under the influence of noise (F. Mintert & A.R. Ribeiro de Carvalho);

- the excitation spectrum of the Bose-Hubbard Hamiltonian, probed in experiments on Bose-Einstein condensates loaded into optical lattices (A. Ponomarev & A. Kolovsky & J. Madroñero) –

in close contact to ongoing experiments in quantum optics or atomic physics. Besides profound mathematical methods from operator analysis and quantum probability theory, also most advanced techniques of computational physics are employed on one of the currently most powerful parallel supercomputers worldwide, the IBM p690 at the Rechenzentrum Garching of the Max Planck Society.
Between January and May 2004 three PhD students, Sandro Wimberger, Florian Mintert, and Javier Madroñero successfully defended their dissertations. S. Wimberger and F. Mintert are by now working as PostDocs abroad, J. Madroñero will soon commence a PostDoc position at the TU München. Two PostDocs, Vyacheslav Shatokhin and Boris Fine, left the group after termination of their (two years) visitors grants, towards Minsk and Knoxville, Tennessee, respectively. On the other hand, we could recruit Alexey Ponomarev as a new PhD student (since January 2004), and Carlos Viviescas as a new PostDoc (since July 2004). Close links with research groups in France, Italy, Israel, and Poland are maintained by bilateral research projects which are pushed ahead by the group's students and PostDocs. All PhD students therefore spend extended research periods abroad. In particular, this led to a binational PhD of S. Wimberger, between the Universities of Como and Munich, in 2004. In turn, the visitors program of the institute once more allowed us to host renowned colleagues (K. Dietz, S. Fishman, I. Guarneri, M. Kuś, G. Summy). Three international workshops on "Chaos and Quantum Transport" (Bad Honnef, March 2003), "Resonances, from Physics to Mathematics and back" (Dresden, January 2004) and "Entanglement, Information and Noise" (Krzyżowa, June 2004) were initiated by the group and attracted broad interest from different communities. The meeting in Krzyżowa also led to the creation of the "Krzyżowa Initiative for Quantum Information", a Europe-wide network of research groups active in the area of Quantum Information. Lecture courses on Theoretical Quantum Optics and on Quantum Chaos were delivered by A. Buchleitner at the University of Munich, and in the framework of the "Mitteldeutsche Physik-Kombo" (a joint PhD lecture program of the Universities Halle, Leipzig, Jena), respectively.
The research activities of the next years are defined by the following principle subjects of our current work:

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

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

III the transport properties of photons and of matter waves in disordered scattering media or in optical potentials under the additional action of deterministic and/or random and dissipative forces.

Whilst striving in (I) at the approximation-free description of the fragmentation dynamics of the periodically driven three body Coulomb problem – realized in current experiments on the laser ionization of helium – , we focus on experimentally accessible quantities for the quantitative description of nonclassical correlations in (II) – with particular emphasis on their robustness under the (detrimental) influence of noise and the requirement of scalability with system size. Thanks to a cooperation with the Polish Academy of Sciences (K. Życzkowski, M. Kuś), which will be funded by the VolkswagenStiftung until the end of 2005, we are realizing this project in the framework of an intense bilateral cooperation. Last but not least, (III) addresses fundamental scenarios of coherent quantum transport (weak and strong localization, coherent backscattering, Bloch oscillations, random lasers) in disordered or deterministically chaotic systems which – thanks to spectacular advances in experimental quantum optics – are now amenable to experimental tests of unprecedented accuracy.

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

Our research focuses on active and dynamic phenomena in cellular biophysics and cell biology. We use and further develop approaches and concepts from statistical physics, non-equilibrium and nonlinear physics for the description of active cellular processes. Our goal is, starting from the physical properties of molecular processes (e.g. motor proteins) to extract and characterize general mechanisms and underlying principles governing complex cellular systems (e.g. cell locomotion, cell division, sensory systems). We aim at a theoretical and quantitative description of dynamic processes in cells. Examples of our research activities are:

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

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

filaments. The physics of ciliar dynamics is a generalization of the dynamics of semi-flexible polymers to intrinsically active fulaments.

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

Transport of signaling molecules in cells and between cells: Cellular processes are regulated by signaling systems which process information. These signaling systems are themselves part of the intracellular dynamic processes. Signaling molecules are produced by the cell, transported and transferred to neighboring cells. During development, such processes play a key role to generate patterns and morphologies of tissues on the basis of the genetic information. A simple example are spatially graded concentration profiles of morphogens, which provide positional information to cells. Such morphogens and the molecules they interact with are currently being investigated for example in the fruit fly Drosophila. Our group develops theoretical approaches which allow us for example to derive effective nonlinear trsnaport equations, starting from cellular trafficking processes. In collaboration with developmental biologists, we characterize the role of different microscopic transport processes for the formation of morphogen gradients.

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

These research activities are carried out in close collaboration with experimental groups. Of particular importance is the collaboration with the Institut Curie in Paris in the context of a European Associate Laboratory and the joint research program with the MPI for Molecular Cell Biology and Genetics in Dresden (MPI-CBG). In the context of this program, three joint junior research groups were created two of which started work in fall 2004. Furthermore, our group operates a laboratory room with microscope facility which is located in the building of the MPI-CBG. There, experimental studies

of oscillations of Min-proteins in bacteria are performed in close contact with theory (Karsten Kruse). Furthermore we study physical properties of cell locomotion on solid substrates using Zebrafish Keratocyte cells which occur on fish scales. Our group is also linked to the international Max-Planck research school on Cell Biology, Bioengeneering, and Biophysics which was initiated by MPI-CBG.

Future Perspectives

Biological systems are of extraordinary complexity. The advances in molecular and cell biology in recent decades have opened new lines of research highlighting the importance of dynamic processes. From the point of view of theoretical physics, the aim is to adapt and to further develop general concepts to describe fluctuating systems, non-equilibrium phenomena, nonlinear systems or complex materials. Using such approaches from physics, theoretical and quantitative descriptions of dynamical processes relevant to cell biology can be developed. The division biological physics, together with the newly created joint research groups with the MPI-CBG, covers subjects ranging from the properties of biological materials to the complex dynamics in living cells. Furthermore, new research activities to describe developmental processes were started in collaboration with groups at the MPI-CBG. Many related phenomena, which involve in particular signaling pathways and the regulation of cellular processes by gene expression will in the future become accessible to theoretical analysis and physical approaches. Of particular importance will be the study of the regulation of material properties and motion generating processes in cells by signaling pathways and information processing systems.

The Max Planck Institute for the physics of complex systems provides a special environment for theoretical work in biological physics. The wide range of research in the area of complex systems allows for stimulating interactions and exchanges with other groups working e.g. on nonlinear systems. The vicinity to the MPI for molecular cell biology and genetics (MPICBG), the biotechnology center and the technical university provide a diverse network of related activities. Of particular importance is the collaboration with the MPI-CBG. Since fall 2004, both institutes created a joint research program consisting of three joint junior research groups which represent a strong link between the institutes and bring together theory and experiment. Focus of this joint research program is the study of integrated cellular processes, the function of which emerges from a large number of interacting cellular components. The study of such biological systems is rapidly attracting attention in the context of the new field of systems biology. Concepts of physics and theoretical approaches will play in the future a key role in this new field which is rapidly developing.

Cooperations

- Max Planck Institute for Molecular Cell Biology and Genetics, Dresden
  - Collaboration with the groups of Jonathon Howard und Anthony Hyman on the dynamics of the cytoskeleton, cell division and the physics of motor proteins

  - Collaboration with Marcos González-Gaitán on the formation of morphogen gradients in the fruit fly Drosophila
  - Collaboration with Andy Oates on the segmentation of vertebrates through oscillating and spatio-temporal gene expression patterns

- Universität Bayreuth
  - Collaboration with Albrecht Ott on the physics of DNA-chips

- Universität Regensburg
  - Collaboration with Gianaurelio Cuniberti on the physics of motorproteins

- Cavendish Laboratory, Cambridge, UK
  - Collaboration with Thomas Duke on the physics of hearing and active wave phenomena in the cochlea

- Institute Curie, Paris
  Collaboration within a European Associate Laboratory
  - Collaboration with Jean-Francois Joanny and Jacques Prost (ESPCI, Paris) on the physics of active gels, the dynamics of the cytoskeleton as well as cell locomotion.
  - Collaboration with Pascal Martin on the role of fluctuations in mechanosensory hair cells (hair bundles).
  - Collaboration with Michel Bornens on the orientation of the mitotic spindle as well as on cytokinesis (the separation of the daughter cells after cell division)

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

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

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

The group was initiated in November 2002 and currently includes one doctoral student and two postdoctoral researchers. We use techniques from statistical physics, nonlinear dynamics and soft condensed matter physics to study biological sensory systems, with emphasis on olfaction (the sense of smell). Our interests also extend more broadly into developmental biology and biochemical network theory.

The 1991 discovery of the large family of odorant receptor proteins transformed the field of olfaction and lead to the understanding of the architecture of the system. In addition, current functional imaging techniques provide a global picture of neural activity in the

first two stages of the system (the olfactory epithelium and the olfactory bulb). Despite these advances, the process of olfaction remains poorly understood in comparision to vision or hearing. Theoretical approaches are needed to complement the experimental advances. Our work on olfaction brings together a wide range of biological levels: gene expression, signal transduction, development, and neural network dynamics. To illustrate this, we briefly discuss three current research topics:

1. Signal transduction in olfactory cilia: In the cilia of olfactory sensory neurons, the initial external chemical signal (odorant identity and concentration) is transduced into an electrical signal. The corresponding signal transduction pathway is well characterized biochemically, and is known to include several feedback loops mediated by intra-ciliar calcium. In project 3.1.16 (page 101), we developed a minimal model of the pathway that captures two important properties of olfactory cilia: adaptation of response to repeated short stimuli, and oscillatory response to sustained stimuli. We were able to show that both these effects are due to the same underlying molecular mechanism. A point of general interest is that in contrast to the usual case of Ca^{2+} oscillations due to calcium-induced calcium release, the Hopf bifurcation in our model arises solely from negative feedback. In a second project, we study the response of the cilium to very low odorant concentrations, with the goal of characterizing the physical limits on the precision of olfactory signaling.
Strong similarities exist between signaling in olfactory cilia and in the cilia of mammalian sperm. Our results are therefore also relevant to current work in Dresden on sperm motility (F. Jülicher and J. Howard).

2. Collective effects in olfactory axon guidance: During development, connections among brain areas are formed by growing neural tubes (axons). In the prevalent picture of this process, each growing axon is independently guided to the proper target by sensing a spatially distributed chemical cue. We develop models in which axon-axon interactions play a dominant role, and proper targeting thus becomes a collective effect. Such a mechanism is thought to play an important role in the sorting of axons of olfactory sensory neurons on their way from the epithelium to glomeruli in the olfactory bulb. To describe this process, we use the statistical physics framework of interacting directed polymers.

3. Neural network dynamics in the olfactory bulb: The neural network of the olfactory bulb processes information from the olfactory epithelium before passing it to the olfactory cortex. We study the underlying dynamics using simplified computational neural networks. We are particularly interested in how the olfactory bulb processes very weak odor stimuli, as well as in how it segments the components of an odor mixture. In project 3.1.17 (page 103), we investigate the conditions under which neural networks benefit from noise during classification of weak, population-encoded stimuli. For a recurrent 2-layer network we obtain a marked effect reminiscent of stochastic resonance. In related work, we analyse electrophysiological recordings of spontaneous activity in the olfactory bulb of zebrafish to characterize the intrinsic network dynamics that is entrained by weak odor stimuli.

Research in our group is not limited to olfaction. In particular, we have developed several collaborations with biology groups at the MPI for Cell Biology and Genetics in Dresden. Two current projects are described below:

4. Dynamics of gastrulation of the zebrafish embryo: During gastrulation, the blas-

toderm tissue differentiates into ectoderm and mesendoderm, and the resulting two tissue layers move in opposite directions on the egg. The main goal of the project is to identify the forces driving the relative motion. Recent work from the Heisenberg group at MPI-CBG suggests that the tissue rearrangements are driven by differential cell adhesion. We are pursuing a continuum complex fluid description as well as a cellular automaton approach to generate quantitative predictions based on this hypothesis. The predictions will be compared with detailed measurements of the distribution of cell velocities in the two tissues. This project includes joint supervision of a doctoral student at MPI-CBG.

5. Processing of mechanosensory information during insect flight: Flies have approximately 100 mechanosensory receptors in each wing. The aim of this project is to understand the role of these sensors (and their underlying neuronal circuits) in flight control. Ongoing experiments give information on how the wing is deformed during flight, how each of the mechanoreceptors responds to these deformations, and how axons on the mechanosensory neurons project onto the motor neurons that control flight muscles. This will allow us to develop a neural network model of the flight control circuit. The computational model will be tested by determining the effect of selectively disrupting the mechanoreceptive pathways on the flight behavior. A grant application to VW Stiftung (with J. Howard and S. Frey) is currently under review.

Cooperations

With biology groups:
P. Feinstein and P. Mombaerts, Rockefeller University, New York
(collective effects in axon guidance; regulation of expression of odorant receptors)
C.-P. Heisenberg, MPI for Cell Biology and Genetics, Dresden
(dynamics of gastrulation of the zebrafish embryo)
T. Kuner, MPI for Medical Research, Heidelberg
(signal transduction in genetically modified olfactory cilia)
R. Friedrich, MPI for Medical Research, Heidelberg
(role of spontaneous neural activity in the olfactory bulb)
J. Howard, MPI for Cell Biology and Genetics, Dresden, and S. Frey, ETH Zurich
(processing of mechanosensory information during insect flight)

With theorists:
F. Jülicher, P. K. Mohanty, MPI-PKS
J. Starke and J. Reidl, University of Heidelberg
M. Eiswirth, Fritz Haber Institut, Berlin

Research Group: Physics of Biological and Soft Matter
(Leader: Dr. Ralf Everaers)

The group was founded in November 2002 and reached its current size of two PhD students and four post-doctoral guest scientist in January 2004. Regarding biological systems as "living soft matter," our research interest are at the interface between material science and biological physics. We use methods from statistical physics with a particular emphasis on the combination of computer simulations with analytical and scaling theories.

The theoretical description of the interplay of lipids, proteins and nucleic acids in living cells requires similar methods as the analysis of gels and solutions containing colloidal particles, polymers or surfactant molecules. "Soft" condensed matter is strongly affected by thermal fluctuations, owes its name to its large susceptibility to external stresses, electric or magnetic fields and often exhibits unusual flow properties. Typically the systems possess or self-assemble into structures which are much larger than atomic or molecular scales. We use methods from statistical physics to study the relation between microscopic interactions, structure and dynamics at mesoscopic scales, and macroscopic physical properties or biological function. Our research is focused on three topics:

Polymer entanglement: Polymers have unique visco-elastic properties and are the basic structural element of systems as different as tire rubber and the cytoskeleton. A characteristic feature is the presence of topological constraints on a molecular scale. Similar to entangled ropes, polymer chains can slide past but not through each other. The standard model of polymer dynamics, the tube model, assumes that entanglements confine chain fluctuations to a narrow tube-like region along the coarse-grained chain contour. We have established the microscopic foundation of this highly successful phenomenological model by introducing a "primitive path analysis" (PPA) of the microscopic topological state (see p. 106). Our ansatz opens the possibility of a systematic analysis of the dynamics and strain dependence of primitive paths in polymer melts and networks. Furthermore, we are working on a unified view of "loosely entangled" melts of synthetic polymers and "tightly entangled" solutions of semi-flexible biopolymers such as actin.

Polyelectrolytes: In aqueous solution polymers with ionizable side-groups dissociate into charged macroions and small counter ions. Macromolecules of this type are commonly referred to as polyelectrolytes. Most water-soluble polymers fall into this class which comprises proteins and nucleic acids as well as synthetic polymers such as sulfonated polystyrene and polyacrylic acid. The treatment of the long-range electrostatic interactions is particularly complicated in the presence of non-polar, hydrophobic elements which typically have a very low dielectric constant compared to water. With the support of the Volkswagenstiftung we have started to explore the consequences of this effect. For this purpose we employ a new simulation algorithm which allows the evaluation of electrostatic self-energies and charge-charge interactions in dielectrically inhomogeneous media.

DNA and chromatin: Genetic information is stored in the base sequence along two complementary strands of double-helical DNA molecules. In eucaryotic cells DNA is hierarchically compactified into chromatin fibers and chromosomes by association with proteins. The genetic information is replicated and transcribed by synthesizing complementary DNA or RNA strands along locally dissociated strands of the double helix. The relevant length scales range from 1 nm (the size of individual bases) to the total contour length of 2m of DNA in each human cell. We are currently working on theories and computer simulations describing the association of complementary sDNA strands, the linear elasticity of helical filaments, the DNA structure and non-linear elasticity at the base(pair) level, the mechanical properties of the 30 nm chromatin fiber

(see p. 109), a number of geometrical and topological aspects of the folding of DNA in chromatin fibers, the packing of DNA in viral capsids and electrostatic interactions in DNA and chromatin.

Future perspectives
A challenge for the future is the investigation of active processes in the cytoskeleton and the genome with our structure based approach in close collaboration with the groups of Prof. Jülicher and Dr. Kruse. Furthermore, we are developing active collaborations with a number of experimental groups (e.g. with the groups of Prof. Richter (FZ Jülich/SANS experiments with polymer melts and networks) and Prof. Ott (U Bayreuth/DNA chips)). A particular focus will be on the improved integration of the group into the numerous scientific activities related to material science, biophysics and biotechnology in the Dresden area. First contacts have been made with the Max-Planck-Insititute for Cell Biology and Genetics and the Insititute for Polymer Research in Dresden.

Collaborations

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

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

Mesoscopic systems are man-made structures (fabricated with the help of sophisticated equipment) with features of the order of a few microns and down to the nanometer range. On these scales quantum-mechanical effects bring about unconventional electrical and optical properties. We investigate the theoretical principles of these systems in a team of 5-6 PostDocs with background in mesoscopic condensed matter physics and quantum optics, as well as in national and international collaborations.
Our research focused on the following areas:

- Clean ballistic structures which depart from the universal behavior of dirty samples and allow to adjust quantum effects such as the low-temperature shot noise or the density of states of hybrid systems with superconducting components. Limits of universality in dirty quantum wires. Conductance of interacting systems.

  H. Schomerus, M. Titov, V. Gopar, R. Molina; in collaboration with P. A. Mello (mpipks and Univ. Mexiko), C. W. J. Beenakker (Leiden), J. Tworzydło (Warsaw), Ph. Jacquod (Geneva), P. Brouwer (Cornell), J.-L. Pichard (Saclay/CEA), D. Weinmann (Strasbourg), G.-L. Ingold (Augsburg), P. Woelfle (Karlsruhe), S. Rotter (Vienna).

- Generation of non-classical light in the electrodynamic environment of mesoscopic conductors; the description of intermittent systems by quantum jumps, with application to fluorescent quantum dots; optical properties of metallic nanoparticles; radiation characteristics of microlasers.

  These topic are at the interface of mesoscopic physics and quantum optics.

  H. Schomerus, A. Budini, R. Molina; with C. W. J. Beenakker (Leiden), R. Jalabert (Strasbourg), M. Hentschel (Regensburg), J. Wiersig (Bremen).

- Strong-field atom interaction; photodissociation. Here we apply methods (semiclassics, scattering theory and Floquet approach) which can be transferred from the other research areas.

  H. Schomerus, Th. Gorin, D. Martinez. With T. H. Seligman (UNAM Mexico), T. Prosen (Ljubljana), M. Znidaric (Ulm), H.-J. Stoeckmann (Marburg), W. Becker (MBI Berlin), C. Faria (London).

Junior Research Group: Electronic Structure of Finite Systems
(Leader: Dr. S. Kümmel (since 7/2003))

Our Emmy Noether-Group, founded at the MPI-PKS in August 2003, is investigating the structure and dynamics of finite electronic systems, e.g., atoms, clusters and molecules, with a particular focus on (time-dependent) density functional theory. The power and charm of density functional theory lie in the fact that it allows for a quantum-mechanical description of many-electron systems in terms of only the particle density, i.e., without having to calculate the many-body wavefunction. This leads to a tremendous reduction in computational effort and the density-based description in many instances also opens a route to an intuitive understanding of quantum mechanical processes.
There is a price to be paid for this gain in simplicity and transparency: The non-trivial many-body effects must be incorporated into the theory via an exchange-correlation functional. This functional is not known exactly and therefore has to be approximated. The quality and predictive power of density functional calculations depend sensitively on this approximation. Therefore, a central aspect of our work is the development of improved functionals that are nonlocal in space and time and go beyond the commonly used local approximations like the well-known "Local Density Approximation". Nonlocality can elegantly be incorporated by using orbital functionals, i.e., functionals that depend only implicitly on the density and explicitly on the Kohn-Sham orbitals. Such functionals allow, e.g., to accurately calculate the electrical response of molecular

chains which are of practical interest for building advanced non-linear optics devices. Due to the limitations of the local approximations, the response of these systems so far had been inaccessible to a density-functional based description. With our improved methods we can contribute to an understanding of the microscopic processes that govern their electronic response.
A second focus of our work has been on developing methods that allow to calculate the dynamics – in particular also in the non-linear and non-perturbative regime – of many electron systems accurately from time-dependent density functional theory. One particular way by which we gain insight into the correlation effects that are important there is the construction of the exact, time-dependent correlation potential for paradigm systems like the one-dimensional Helium model-atom. For such simple systems, the time-dependent Schrödinger equation can be solved numerically and from the thus obtained exact time-dependent density, the exact correlation potential can be calculated by inversion of the Kohn-Sham equations. Analyzing the exact potential allows to identify shortcomings of the approximations that have been used so far and lights the way for the development of improved functionals. The latter can then be used in realistic (i.e., not-model) three-dimensional calculations. In particular we are starting to investigate laser-induced electron dynamics in noble-gas atoms and silver clusters.

Perspectives
Besides working on the general task of improving the accuracy and predictive power of density functional theory, we are trying to answer questions which require to take electronic interactions into account but which cannot be accessed by wavefunction based methods due to their complexity. Generally speaking, the questions related to many-electron dynamics in strong fields (see above) fall into this realm. In particular we want to investigate the interplay between a system's electronic structure and the dynamics that can be induced by external fields. To give a practical example, we plan to investigate, understand, and (hopefully) be able to predict how changes in a molecule's structure (e.g., changing an atom or side-group) influence the molecule's response properties. Thus, our research is aimed at taking steps towards our long-term goal: a density-functional, first-principles description of a finite system's structure and dynamics which allows to calculate observables with reasonable accuracy, yet remains transparent enough to allow for an intuitive understanding of the microscopic processes.

Collaborations
Within the MPI-PKS our group of two postdoctoral researchers and one PhD student is associated with the Finite Systems department and a particularly fruitful collaboration developed with Dr. Manfred Lein.
International collaborations link us to the groups of John Perdew at the Physics Department of Tulane University, USA and Leeor Kronik at the Department of Materials and Interfaces at the Weizmann Institute of Science, Israel. On the national level we continue to collaborate with Manfred Lein, now at the Max-Planck-Institut für Kernphysik in Heidelberg, and with Michael Moseler at the Frauenhofer Institut für Werkstoffmechanik in Freiburg. In addition, we are in regular contact with Matthias Brack at the Physics Department of the Universität Regensburg and Paul-Gerhard Reinhard at the Physics Department of the Universität Erlangen.

Research Group: Pattern Formation in Reaction-Diffusion Processes
(Leader: Dr. M. Bär (until 10/2004))

The junior research group ,,Pattern formation" existed from November 1995 to October 2004. During this time around 30 guest scientists (15 from abroad) with an average residence of one year and 8 Ph. D. student as well as 1 Diploma student including 4 students from abroad have been members of the group. Four german scientist received their habilitation (M. Bär, H. Hinrichsen, G. Schliecker und U. Thiele) and five Ph. D. degrees (U. Börner, L. Brusch, K. John, E. Nicola und C. Utzny) as well as one Diploma degree (P. Kano) have been awarded. About 125 publications appeared in refereed journals (80%) and proceedings (20%) including 20 articles in Physical Review Letters. Three german group members (M. Bär, A. Deutsch, H. Hinrichsen) obtained permanent positions as group leaders or professors, three other members (M. Falcke, Th. Höfer, M. Or-Guil) moved on to positions as junior research group leader, junior professor or non-permanent group leader.
Research concentrated initially on complex patterns and spatiotemporal chaos in chemical and physical reaction-diffusion systems. In the course of time, modelling of biological systems became the second equally important topic. Further significant research dealt with nonequilibrium phase transition, theory of disordered and quasicrystalline systems as well as the modelling of structure formation in thin liquid films. The research has been supported by projects of the Deutsche Forschungsgemeinschaft (3×), the German-Israeli Foundation (1×) and the European Union (2×). Group members have launched the network MTBio (A. Deutsch) and the Initiative Biology (2000-2002) in mpi**pks**.

Complex Pattern Formation
Pattern formation occurs in a wide variety of physical, chemical and biological systems. Transitions between simple patterns (fronts, pulses, periodic patterns, spirals) and complex patterns (spatiotemporal chaos, modulated structures, pattern domains and bound states) are investigated by numerical simulations, numerical bifurcation and stability analysis and perturbation theoretical approaches in reaction-diffusion models. We have carried out a nonlinear analysis of secondary instabilities of periodic waves leading to spatiotemporal chaos and modulated waves, e.g. superspirals. Moreover, we have achieved a complete numerical analysis of absolute and convective instabilities of travelling waves and their role in the destabilization of simple rotating spirals. Other aspects include anisotropic pattern formation, impact of heterogeneities and spatiotemporal forcing as well as the control of pattern formation. Here, we dealt with issues of homogenization and the derivation of effective diffusion coefficients and their role in pattern formation in microemulsions.
Applications range from chemical reactions in gels and surface catalysis to hydrodynamical systems (thin films and ferrofluids). For thin films, the emphasis has been shifted to complex situations like two-layer systems or chemically active films (see longer report by U. Thiele *et al.* on p. 123). For chemical reactions we have dealt with three-dimensional structures like scroll waves and their interaction as well as the incorporation of physical interactions and their influence on reaction-diffusion processes in soft matter.

Here, mostly models from physiology (intracellular dynamics, calcium waves) and morphogenesis (bacterial growth, aggregation and pattern formation) have been considered. Emphasis has been put on the transition from continuous deterministic models (differential equations) to discrete stochastic models. A stochastic model has been developed to reproduce abortive calcium waves known as sparks and puffs. A project on stochastic modelling of protein oscillations has been started in collaboration with colleagues in the biological physics department. Stochastic simulations of myxobacterial aggregation and formation of standing waves (ripples) therein have yielded a quantitative agreement with recent experiments. Discrete and continuum models of swarming and aggregation of self-propelled rod-shaped particles have been studied to describe the early phase of myxobacterial aggregation. Other recent projects address biochemical networks, e. g. in metabolic processes like glycolysis and lipid domain formation in biomembranes, for which various mechanism have been studied and compared.

Cooperations

We maintain numerous national and international collaborations. A collaborative project on ,,Pattern Formation in Catalysis" with Profs. Meron (Ben-Gurion) and Pismen (Technion) had been supported by the German-Israeli Foundation until the end of 2003. Other collaborations with experimentalists cover chemical pattern formation (Profs. Müller (Magdeburg) and Engel (TU Berlin)) and surface catalysis (Profs. Imbihl (Hannover) and Rotermund (FHI Berlin)) as well as myxobacteria (Dr. Deutsch (TU Dresden) and Prof. Sogaard-Andersen (MPI Marburg)), biotransformations (Dr. Bertau (TU Dresden)) and lipid domains (Prof. Käs (Leipzig)). Theoretical collaborations exist with the groups of Prof. Bestehorn (Cottbus), Dr. Chate (Saclay), Prof. Kapral (Toronto), Prof. Knobloch (Berkeley), Prof. Paczuski (London) Dr. Torcini (Firenze) und Prof. Vega (Madrid).

Final Remarks

Altogether we can identify three major areas of activity: 1. Complex pattern formation in reaction-diffusion systems, 2. modelling of pattern formation in a large variety of biological systems and 3. pattern forming processes in complex fluids and thin films. The first of these topics has been the origin and trademark of the group, while the other two subjects opened perspectives and are still quite actively pursuit by former members of the group in their new affiliations. At mpi**pks** the topic of biological pattern formation now plays also a role in research projects of the department ,,Biological Physics" and topically related junior research groups. The third area is currently pursued in the framework of a larger EU project directed by Dr. U. Thiele.

Chapter 3

Details and Data

3.1 Selection of Research Results

3.1.1 Superconductivity through intra-atomic excitations

Peter McHale, Peter Thalmeier, Peter Fulde and Gertrud Zwicknagl

Since the work of Fröhlich on electron-phonon interactions and the discovery of the isotope effect, this particular interaction has been considered the main source of electron-electron attraction and Cooper pair formation. It is known that an effective electron attraction is not necessarily required for superconductivity to occur. Instead, what is required is that the BCS ground state has a lower energy than the normal state, i.e., a state without pair formation. As discussed, e.g., by Bogoliubov et al. [1], Cooper pairs may form even when the electron interactions are purely repulsive. They may lead to an energy gain, provided the variation of the repulsive interaction in momentum space is appropriate. Despite all these considerations the general belief has been, at least until the discovery of heavy-fermion and high-temperature superconductivity, that electron-pair formation is caused by the exchange of phonons. The high superconducting transition temperatures observed in some of the cuprate perovskites have called that belief into question and have led to a number of suggestions as regards non-phononic pairing interactions. But they have been mainly qualitative and not quantitative and therefore remained inconclusive.

Here we want to draw attention to a particular non-phononic interaction which has led to quantitative and experimentally confirmed predictions as regards its influence on the formation of a superconducting state. It concerns intra-atomic or crystal field excitations of strongly correlated $4f$ or $5f$ electrons and applies in particular to systems with rare-earth or U ions. When those ions are put as impurities into a superconductor, the inelastic intra-atomic excitations caused by conduction electrons can be either pair-breaking or pair-forming, depending on the relative size of the respective matrix elements. When the latter involves time reversal invariant interactions between the conduction electrons and localized f electrons they act as pair formers [2]. But they act as pair breakers when the interactions break time-reversal symmetry [3]. This may change when, e.g., the U ions form a lattice. In that case the intra-atomic excitations form a band of magnetic excitations, i.e., magnetic excitons. When the interactions of the conduction electrons with the magnetic excitations are largest near the zone

boundary (implying antiferromagnetic correlations) Cooper pairs can form even when the local interactions break time-reversal symmetry. But in this case the resulting superconducting order parameter has necessarily to have nodal lines, i.e., it must be of an anisotropic form. We shall show that UPd_2Al_3 belongs into that category. The superconducting transition temperature as well the enhanced quasiparticle mass can be well explained this way [4]. The same holds true for the observed node structure of the order parameter [5].

There is growing evidence that actinide ions may have itinerant as well as localized $5f$ electrons. Model calculations show that the dual nature of the U 5f states ultimately arises from intra-atomic correlations as described by Hund's rules. The underlying physics can be understood as follows: The U compound under consideration is in the mixed-valent regime with $n_f \simeq 2.5$. Therefore the low-energy states will be formed by the $5f^2$ and $5f^3$-configurations. As there are either two or three $5f$ electrons at a site there will be only one of them hopping from site to site. Which of the $5f$ orbitals will delocalize is determined by intra-atomic correlations. To see how this happens it is important to note that the energy gain due to multiplet formation must exceed the one obtained from the kinetic energy. As a consequence, a coherent $5f$ band will form only if the local intra-atomic correlations are preserved. This constraint selects the symmetry of the delocalized $5f$ orbital in an anisotropic crystal.

The localized and delocalized $5f$ subsystems interact mutually leading to a mass enhancement of the delocalized quasiparticles. The situation resembles that in Pr metal where a mass enhancement of the conduction electrons by a factor of 5 results from virtual crystal field (CEF) excitations of localized $4f^2$ electrons [6]. The underlying hypothesis of two kinds of $5f$ electrons is supported by a number of experiments including susceptibility measurements, photoemission and neutron inelastic scattering experiments on UPd_2Al_3. The presence of localized $5f^2$ configurations is also suggested by the antiferromagnetic order which develops below T_N=14.3 K and which is characterized by an almost atomic size ordered moment μ=0.85μ_B. At T_c=1.8 K, the normal heavy Fermi liquid becomes unstable and a superconducting phase forms with Cooper pairs of the heavy quasiparticles. The two ordering phenomena, i. e., superconductivity and antiferromagnetic order coexist down to lowest temperatures.

A direct confirmation of this dual nature of 5f- electrons in UPd_2Al_3 was obtained from neutron inelastic scattering [7]. The data exhibit a resonance like structure in the dynamical structure function of localised moments which appears below T_c and is linked to the superconducting quasiparticles. The coupling between the heavy quasiparticles and the excitations of localized $5f$ electrons give rise to structures in the tunneling density of states [8].

As shown before [9], the dual model explains the shape of the Fermi surface of UPd_2Al_3 as well as the strong anisotropies of the heavy quasiparticle mass. Both are measured in de Haas-van Alphen experiments. There is no adjustable parameter in the theory.

Here we are interested in the superconducting properties which follow from virtual excitations of the internal degrees of freedom of the localized $5f^2$ system. The latter can be described in good approximation by a $|\Gamma_4\rangle = (1/\sqrt{2})(|J_z = 3\rangle - |J_z = -3\rangle)$ ground state and $|\Gamma_3\rangle = (1/\sqrt{2})(|J_z = 3\rangle + |J_z = -3\rangle)$ excited state. Neutron experiments give an energy splitting of $\delta \simeq$7 meV [10].

For a consistent description of superconductivity and the enhanced effective mass a model calculation has been performed in Ref. [4] which uses a fit of the three-

dimensional magnetic exciton dispersion derived from inelastic neutron scattering. The dispersion is most pronounced in the c-direction and we shall approximate it by

$$\omega\left(q_z\right) = \omega_{\rm ex}\left[1 + \beta\ cos\left(cq_z\right)\right] \tag{1}$$

with $\omega_{\rm ex}$=5 meV, β=0.8 and c denoting the lattice constant perpendicular to the hexagonal planes. The form (1) of the magnetic exciton spectrum simplifies solving Eliashberg's equations for the conduction electron self-energy $\sum(p_z, \omega_n)$ and order parameter $\Delta(p_z, \omega_n)$. They are of the form

$$\begin{aligned}
\Sigma\left(p_z, \omega_n\right) &= \frac{T}{N_z}\sum_{p'_z, m} K\left(p_z - p'_z; \omega_n - \omega_m\right)\int \frac{dp'_\perp}{(2\pi)^2} G\left(p'_\perp, p'_z, \omega_m\right) \\
\Delta\left(p_z, \omega_n\right) &= -\frac{T}{N_z}\sum_{p'_z, m} K\left(p_z - p'_z; \omega_n - \omega_m\right)\Delta(p'_z, \omega_m) \\
&\quad \int \frac{dp'_\perp}{(2\pi)^2}\left|G\left(p'_\perp, p'_z, \omega_m\right)\right|^2
\end{aligned} \tag{2}$$

and the integration over $dp'_\perp$ can be done first. Note that N_z is the number of lattice sites along the c-axis. Equations (2) assume that the order parameter has even parity (singlet channel). The self-energy enters Green's function in the well-known way

$$G^{-1}(\vec{p}, \omega_n) = i\omega_n - \epsilon_p + \mu - \Sigma(p_z, \omega_n) \quad . \tag{3}$$

The boson propagator $K(p_z, \omega_\nu)(\omega_\nu = 2\pi T_\nu,\ \nu = \text{integer})$ describes the magnetic-exciton exchange between the quasiparticles which form Cooper pairs. It is of the form

$$K\left(q_z, \omega_\nu\right) = g\frac{\omega_{\rm ex}^2}{\left(\omega(q_z)\right)^2 + \omega_\nu^2} \tag{4}$$

with a coupling constant g given by

$$g = \frac{I^2}{4}\left(\frac{1}{c}\ \frac{p_0^2}{2\pi}\right)\frac{1}{\omega_{\rm ex}} \quad . \tag{5}$$

Here the coupling constant I refers to the interaction between the conduction electrons having partially $5f$ character and the localized $5f^2$ electrons. The two levels $|\Gamma_3\rangle_i$ and $|\Gamma_4\rangle_i$ at a uranium site i are described by a pseudospin τ_{iz} so that $\tau_{iz}|\Gamma_{3(4)}\rangle_i = \pm\frac{\delta}{2}|\Gamma_{3(4)}\rangle_i$. For the interaction Hamiltonian we assume a simple Ising-like form

$$H_{c-f} = I\sum_i \sigma_{iz}\tau_{ix} \quad . \tag{6}$$

After the $dp'_\perp$ integrations are done, solving the Eliashberg equations reduces to a one-dimensional problem. The following point is essential and should be stressed: the kernel K(q, ω_ν) is strongly peaked at $q_z = \pi/c$ and ω_ν=0. Therefore, roughly speaking, for the singlet channel the gap equation is of the type [4]

$$\Delta\left(p_z, \pi T\right) = -C\left(p_z\right)\Delta\left(p_z - \frac{\pi}{c}, \pi T\right) \quad . \tag{7}$$

This suggests the form

$$\Delta\left(p_z\right) \sim cos\left(cp_z\right) \tag{8}$$

with a line of nodes perpendicular to the c-axis. Note that they are situated at the AF Brillouin zone boundary. Such a node structure was recently found in experiments on the directional dependence of the thermal conductivity in an applied magnetic field [5]. When actual numbers are used for the various quantities one finds not only that the strong anisotropy of the semi-heavy quasiparticle mass can be explained without adjustable parameter, but also the size of the superconducting transition temperature is obtained approximately. Therefore, the indications are strong that UPd_2Al_3 is indeed a superconductor with a non-phononic interaction leading to pair formation. A more detailed summary of the features described above is found in [11].

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3.1.2 Marginal Fermi liquid in the Hubbard model

Yoshiro Kakehashi and Peter Fulde

After the discovery of high-temperature superconductivity in layered Cu based perovskites it was found that those materials exhibit quite unusual properties in the normal state. For example, in underdoped materials, i.e., for hole concentrations less than the one leading to the highest superconducting transition temperature, the temperature dependent resistivity is found to be ρ(T)$\sim$T in the normal state. Also the nuclear relaxation rate, e.g., of $YBa_2Cu_3O_7$ has an unusual temperature independent contribution.

Aiming for an explanation of these strong deviations from a normal metal behavior Varma et al. [1] developed the Marginal Fermi Liquid (MFL) theory. This theory assumes that the frequency ω and temperature T dependent self-energy $\Sigma(\omega$,T) of the electrons behaves for $\omega >$T like Re$\Sigma(\omega, T) \sim \omega \ln|\omega|$ and Im$\Sigma(\omega$,T)$\sim |\omega|$ in contrast to ordinary Fermi liquid theory where Re$\Sigma(\omega$,T)$\sim \omega$ and Im$\Sigma(\omega$,T)$\sim \omega^2$ holds. Note that at zero temperature the MFL form of the self-energy implies a diverging effective mass at the Fermi energy. With these assumptions most of the observed strong deviations from normal metal behavior could be explained surprisingly well. However, the microscopic origin of MFL behavior of the self-energy has remained an open problem. There have been detailed studies of the two-dimensional (2D) Hubbard model as a simple model for the high-T_c cuprates [2] mainly by using advanced numerical techniques. We mention in particular the Lanczos method [2], the Quantum Monte-Carlo (QMC) [3] method or calculations based on the Dynamical Cluster Approximation (DCA).

A perturbation analysis of the half-filled case at $T = 0$ has shown that in the weak Coulomb interaction limit a MFL type of self-energy is obtained [4]. It is due to the van Hove singularities which one is dealing with in this particular case. But we know that electron correlations are strong in the superconducting cuprates and that at $T = 0$ the system is an antiferromagnet [2,3]. It is also known that by hole doping the antiferromagnetic correlations are rapidly suppressed [2,3]. Nevertheless MFL behavior continues to exist in the underdoped regime and the question is whether or not it can be explained within the 2D Hubbard model with fairly strong interactions. We have shown that MFL behavior can indeed be derived from a doped 2D Hubbard model on a square lattice at T=0 and large on-site interaction [5]. This is done by applying a self-consistent projection operator method when calculating the retarded Green function. It is an extension of a projection operator coherent potential approximation [6] to the nonlocal case. With it one can perform high resolution calculations of the self-energy as regards momentum and energy and avoid certain problems previous numerical calculations have had to face. We could calculate with it the zero-temperature self-energy $\sum(\mathbf{k}, \omega)$ for the 2D Hubbard model on a square lattice and found a marginal Fermi liquid like behavior for quite a large range of hole doping concentration and Hubbard parameter U. In that regime the effective mass shows considerable momentum dependence. In cases where a comparison with finite temperature results [3] can be made the agreement is good. When U>6.5 a discontinuous change takes place with increasing hole concentration from more localized electrons in the lower Hubbard band to fully itinerant ones. For small hole concentrations the spectral weight of the lower Hubbard band is reduced. It is precisely the transfer of spectral density from the lower Hubbard band to higher energies which results in MFL behavior at low hole concentrations. In that regime Luttinger's theorem is not applicable. Very close to half-filling, long-ranged antiferromagnetic correlations are expected to modify the present results. Those correlations have been neglected here. The calculated Fermi surface is hole-like in the underdoped region and electron-like in the overdoped region. A 'kink' structure appears in the quasiparticle dispersion curves in the underdoped region due to a mixing between the quasiparticle states and the short-range antiferromagnetic excitations. It strongly depends on the doping concentration. Our results justify the phenomenological maginal Fermi liquid theory and explain features of cuprates in the normal state.

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3.1.3 Degenerate Fermi liquid in a checkerboard lattice

Erich Runge, Frank Pollmann, Peter Fulde

It has been suggested earlier [1] that charge degrees of freedom of fermions (as well as boson) in a geometrically frustrated lattice can give raise to excitations with fractional charges. This is possible even in a three-dimensional lattice like the pyrochlore lattice. In order to shed further light on this interesting feature we have studied numerically a system of spinless fermions with strong nearest-neighbor repulsions V on a checkerboard lattice. This lattice type can be obtained by projecting a pyrochlore lattice onto a plane. Exact diagonalization of up to 8×6 sites have yielded the following results for the half-filled case [2]:
The ground state is liquid like but two- or four-fold degenerate. The different configurations contributing to the ground-state wavefunctions can be characterized by two topological quantum numbers. Configurations are connected by ring hopping processes involving at least six sites. They are proportional to t^3/V^2 where t is a nearest-neighbor hopping matrix element. Ring processes conserve the topological quantum numbers. There are many low energy excitations when the exponentially large number of degenerate configurations is lifted by ring hopping. The corresponding specific heat is almost linear in temperature T, like in a metal. It is large since the high degeneracy associated with the frustrated lattice structure is lifted on a scale t^3/V^2. In the case of doping, the system supports excitations with fractional charges $\pm e/2$. At present we are studying the statistics of those excitations.

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3.1.4 Local Hamiltonian approach to excited-state wave functions in solids

Viktor Bezugly, Dmitry Izotov, Uwe Birkenheuer

The independent particle picture of electrons in solids only provides a rough insight into the electronic structure of condensed matter. Inclusion of electron correlation, i.e. the explicit consideration of the electron-electron interaction beyond a mean-field approximation, is crucial for a proper determination of material properties. Density functional theory [1, 2] is the common tool in solid state physics to account for electron correlation in ground state properties; for the description of band structures the GW approximation [3] has become quite popular. Yet, both methods rely on strong assumptions, and it is hard to control the accuracy of these approaches in a systematic way.

Wave-function-based techniques offer an appealing alternative here. They have been used very successfully in quantum chemistry for many decades, and it has been shown in the meantime [4–9] that these methods can even be applied to infinite systems such as solids and polymers, despite the, in principle, infinite number of electrons which enter the wave functions. A strict use of *local descriptions* in terms of local orbitals and basis functions together with suitable cut-off criteria is the major idea beyond all these ansatzes.

The local Hamiltonian approach is one of these tools. It allows to perform quantum chemical post-Hartree-Fock correlation calculations such as MRCI (multi-reference configuration interaction) to determine the 'correlated' band structure of periodic systems, that is, to calculate the various excitation energies of the (N–1)- and (N+1)-particle states of an extended system including electron correlation.

It sets out from the observation that in many cases there is a close correspondence between these correlated states and their counterparts on the Hartree-Fock (or independent particle) level of theory. This mapping is used to setup in a mathematically strict and sound way a local description of the many-body Hamiltonian $\hat{H}$ of the infinite system in the subspace of a pre-selected set of relevant (N–1)- and (N+1)-particle states Ψ_n (with excitation energies $E_n - E_0^N$):

$$\hat{H}^{\text{eff}} = \sum_n |\Psi_n\rangle (E_n - E_0^N) \langle \Psi_n| = \sum_{ij} |\Lambda_i\rangle H_{ij}^{\text{eff}} \langle \Lambda_j| \tag{1}$$

where the localized correlated wave functions $|\Lambda_i\rangle = \sum_n |\Psi_n\rangle U_{ni}$ are determined such that the leading determinants in the CI expansion of the new wave functions Λ_i become one-hole (or one-particle) configurations

$$\Phi_a = \hat{c}_{\psi_a} \Phi_{\text{HF}} \quad \text{and} \quad \Phi_r = \hat{c}^\dagger_{\psi_r} \Phi_{\text{HF}} \tag{2}$$

with *maximally localized* orbitals ψ_a and ψ_r being removed from (or added to) the Hartree-Fock reference determinant Φ_{HF}. Due to the pre-dominantly local character of electron correlation, the local matrix elements H_{ij}^{eff} turn out to be highly transferable from one cluster of the solid to another. This allows to assemble the local Hamiltonian element-by-element from a series of highly sophisticated quantum chemical correlation calculations on finite cluster models. The incremental scheme [5] is usually applied to reduce the computational effort for these calculations further.

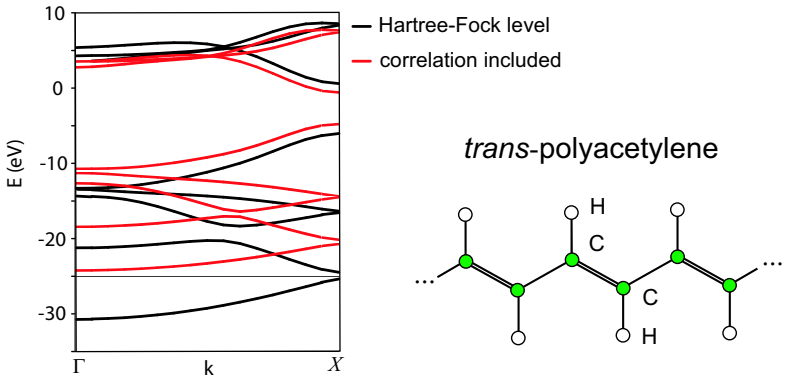

Figure 1: *Band structure of an infinite tPA chain.*

The correlated band structure of several periodic systems could be determined this way. One of the most recent applications is the band structure of *trans*-polyacetylene (tPA), a conjugated hydrocarbon with a relatively small band gap [9]. In Fig. 1 the valence and conduction bands of an isolated tPA chain are shown as calculated with a flexible cc-pVTZ basis set employing the MRCI method. The standard quantum chemical program package MOLPRO [10] was used for that purpose. As can be seen from Fig. 1 the valence and conduction bands exhibit quite substantial shifts upon inclusion of electron correlation and the band gap closes from 6.42 eV on the Hartree-Fock level down to 4.11 eV for the correlated band structure.
Similar calculations were performed for isolated hydrogen fluoride (HF) chains, with the HF molecules arranged like in solid HF crystals (for details see separate report on Green's function approaches). The cluster-in-solid embedding tool developed by the quantum chemistry group at the **mpipks** has been used for that purpose to ensure that the molecular clusters used to extract the local Hamiltonian matrix elements experience the proper crystalline environment during the spatially restricted correlation calculations.

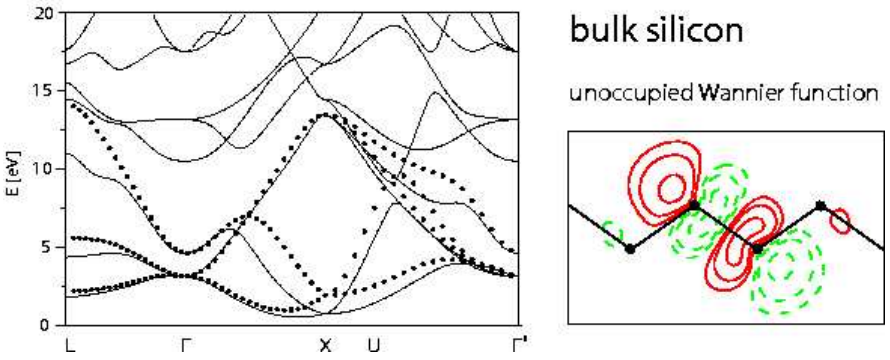

Figure 2: *Disentangled (dotted) and original (solid) conduction bands of silicon and the resulting Wannier function (±0.022, ±0.046, ±0.10 bohr$^{-3/2}$).*

To be able to generate well-localized unoccupied Wannier functions even in the case of highly interwoven unoccupied energy bands (which is usually the case in real matter)

we had to develop a suitable band disentanglement procedure [11] which automatically constructs linear combinations of Bloch functions such that the resulting hybrid energy bands decompose into non-interfering band complexes. In Fig. 2 an example for such hybrid energy bands is shown for bulk silicon together with the resulting localized unoccupied Wannier function. It is a reasonably compact, typical Si-Si antibonding orbital with an orbital energy well in the middle of the four lowest conduction bands of silicon.

The local Hamiltonian approach outlined so far is not only able to provide the wave functions of correlated (N–1)- and (N+1)-particle states in solids. In a perfect analogue way, it can also be used to determine the many-body(!) wave functions (and energies) of a system with bound excitons. From a quantum chemical point of view these wave functions are just the excited-state wave functions of the neutral N-particle system which are easily accessible in post-Hartree-Fock correlation methods such as MRCI.

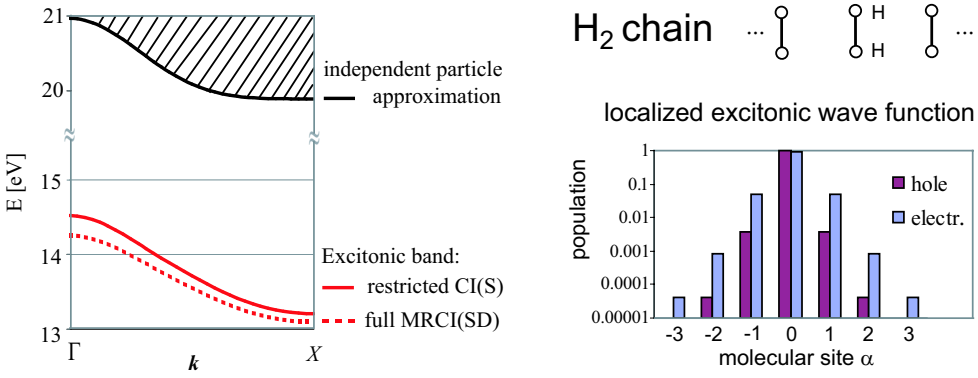

Figure 3: *Excitonic band of an infinite H_2 chain together with the site populations of the localized excitonic wave function Λ_0 (for details see text).*

We have applied this idea to an "ab initio" model system consisting of an infinite chain of parallel oriented H_2 molecules. The lowest excitonic band, i.e., the energy of the exciton as a function of its total crystal momentum, is shown in Fig. 3 exhibiting an energy stabilization of more than 6 eV upon formation of the exciton. Also shown are the site populations $q_h(\alpha) = \sum_\beta q_\alpha^\beta$ and $q_e(\beta) = \sum_\alpha q_\alpha^\beta$ of the *localized* excitonic wave function Λ_0 from the reference unit cell of an H_2 chain with α and β labeling the individual H_2 units. Here $q_\alpha^\beta = \sum_{a\in\alpha, r\in\beta} |t_a^r|^2$ are the site populations of the 1h-1e-configurations $\Phi_a^r = \hat{c}_a \hat{c}_r^\dagger \Phi_{\mathrm{HF}}$ in the CI expansion $\Lambda_0 = \sum_{a,r} t_a^r \Phi_a^r + \ldots$ of the localized excitonic many-body wave function. The local character of this wave function is evident, but also discernible is the significantly higher compactness of Λ_0 along the hole 'coordinate' as compared to the electron 'coordinate'.

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3.1.5 Quantum chemical Green's function approach to correlation in solids

Christian Buth, Viktor Bezugly, Uwe Birkenheuer

One-particle excitations, which describe the energetics of an infinite system after removal or adding of a single electron, are the most fundamental excitations in solids. They provide the band structure of periodic compounds and also the fundamental band gap of crystalline materials.
The one-particle excitations are given by the many-body wave functions of the excited (N–1)- and (N+1)-particle eigenstates of a system under consideration. Usually there is a close relation between these correlated wave functions and the single-determinant one-particle configurations

$$\Phi_a(-k) = \hat{c}_{\psi_{ak}}\Phi_{\mathrm{HF}} \quad \text{and} \quad \Phi_r(k) = \hat{c}^{\dagger}_{\psi_{rk}}\Phi_{\mathrm{HF}} \tag{1}$$

where ψ_{ak} and ψ_{rk} are occupied and unoccupied Bloch orbitals, respectively, and Φ_{HF} is the Hartree-Fock reference determinant of the neutral N-particle system. This way it is possible to assign band (and spin) indices a and r to the correlated (N–1)- and (N+1)-particle states of a periodic system and to arrive at a 'correlated' band structure. The local Hamiltonian approach is an efficient way to calculated such a band structure by means of quantum chemical post-Hartree-Fock correlation methods (for details see separate report). Yet, often, there also exist (N–1)- and (N+1)-particle eigenstates in condensed matter which are dominated by three-particle (or more) configurations such as the (2h,1p)-configurations $\hat{c}^{\dagger}_{\psi_{rk}}\hat{c}_{\psi_{ak'}}\hat{c}_{\psi_{bk''}}\Phi_{\mathrm{HF}}$. They give rise to so-called satellite peaks in photoemission spectra. Preferentially, they occur in small band gap systems, where the energy to create an additional electron-hole pair is relatively small. They also show up quite frequently in conjunction with inner-valence hole states or highly excited (N+1)-particle states. No band indices can be assigned to such states, and as soon as these satellites states start to interfere heavily with the band structure generating 'one-particle' states describes above, the one-particle (or band structure) picture of a solid breaks down.
The local Hamiltonian approach is not able to describe satellite states. Therefore we have developed, as an alternative, a quantum chemical *ab initio* Green's function formalism for infinite periodic systems. It is based on the algebraic diagrammatic

construction (ADC) which is well-established for molecular systems [1–3]. It sets out from the following analytical ansatz

$$\Sigma(\omega) = \Sigma^{\infty} + M^{+}(\omega) + M^{-}(\omega) \quad (2)$$

with

$$M^{\pm}(\omega) = U^{\pm\dagger}\,(\omega\mathbb{1} - C^{\pm})^{-1}\,U^{\pm} \quad (3)$$

for the self-energy $\Sigma(\omega)$ and determines the unknown quantities Σ^{∞}, $U^{\pm}$, and $C^{\pm}$ by expanding them in powers of the residual interaction V from $\hat{H} = \hat{H}_0 + V$ and comparing the various contributions with the corresponding Feynman diagrams for the self-energy. The resulting scheme is termed ADC(n), where n is the order in V up to which the ADC ansatz recovers the diagrammatic series for $\Sigma(\omega)$ completely. Yet, in fact, the above ansatzes for $M^{\pm}(\omega)$ go much further because they effectively establish an infinite summation of proper Feynman diagrams in addition to the infinite summation of Feynman diagrams already provided by the Dyson equation. Another important point about the ADC formalism is, that it allows to replace the numerically cumbersome pole search in the Green's function $G(\omega) = \left[G_0^{-1}(\omega) - \Sigma(\omega)\right]^{-1}$ (which gives the excitation energies) by an eigenvalue problem $Bx = \omega x$ with

$$B = \begin{pmatrix} H_0 + \Sigma^{\infty} & U^{+\dagger} & U^{-\dagger} \\ U^{+} & C^{+} & 0 \\ U^{-} & 0 & C^{-} \end{pmatrix} \quad (4)$$

which can be solved very robustly by block-Lanczos diagonalization [4, 5].

We have developed a new variant of the ADC formalism which allows to perform such ADC calculations for infinite periodic systems. This cannot be done by simply switching from canonical Hartree-Fock orbitals to Bloch orbitals, because the resulting matrices are simply too large. Localized orbitals had to be introduced together with suitable configuration selection schemes which take fully into account the translational symmetry of the compounds, the compactness of the localized orbitals and the predominantly short-range character of electron correlation [6]. We have implemented this scheme starting from the WANNIER code (which has been developed at the mpi**pks** some years ago [7]) in a strictly quantum chemical way, using flexible Gaussian-type basis functions and being *ab initio* in the sense that we use the full non-relativistic many-body Hamiltonian of our system.

The program is operating, and one of the first applications was a comparison of the valence band structure of infinite hydrogen fluoride (HF) chains in zig-zag arrangement (like in crystalline HF) with the results obtained by the local Hamiltonian approach [8]. The outer-most three F 2p-like valence bands have been chosen for that purpose and a standard cc-pVDZ basis set is employed. The local Hamiltonian matrix elements are extracted from MRCI (multi-reference configuration interaction) calculations with *all* (1h)-, (2h,1p)- and (3h,2p)-configurations being included in the CI space (like in previous studies [9]). The result of these comparison is shown in Fig. 1. The correlated energy bands coincide within 0.0-0.2 eV which impressively demonstrates the ability of the new crystal-orbital-ADC(2) formalism. In particular it shows that the perturbative treatment of the off-diagonal matrix elements of $\hat{H}_0$ which is inherent to our new CO-ADC technique is well justified.

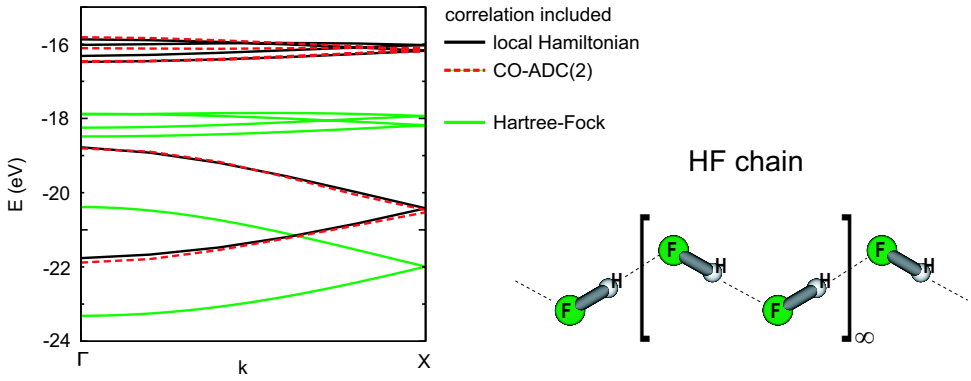

Figure 1: *Band structure of infinite HF zig-zag chains.*

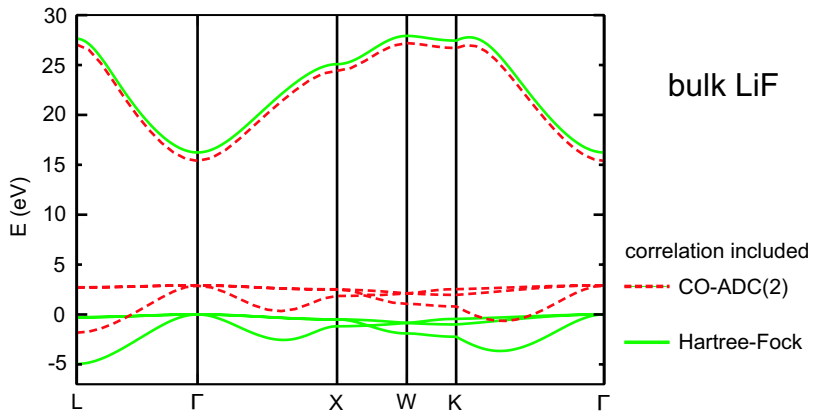

Figure 2: *Band structure of bulk LiF using 19 unit cells as support for the local three-particle configurations.*

Bulk systems can be describes by our CO-ADC program as well, as can be seen from our study on LiF, a rock-salt-like ionic crystal. It mainly served to check the required extent of the *local* three-particle configurations entering the auxiliary matrices $U^{\pm}$ and $C^{\pm}$. Inclusion of all configurations with localized orbitals from up to the 2^{nd} nearest-neighbor unit cell (19 cells all together) were necessary to produce the sound upward shift of about 3 eV of the valence bands discernible in the correlated band structure of LiF (see Fig. 2). Of course, conduction bands can be handled by our Green's function approach as well, as is corroborated by the unoccupied band occurring at 15-30 eV.
The new CO-ADC formalism is a very promising scheme, and we are currently working on improving both, the formalism itself and its implementation. In particular, we plan to link the CO-ADC code to a more advanced periodic quantum chemical program package such as the CRYSTAL code [10].

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3.1.6 Hamiltonian chaos acts like a finite energy reservoir: Accuracy of the Fokker–Planck approximation

Anja Riegert, Nilüfer Baba, Katrin Gelfert, Wolfram Just, Holger Kantz

Introduction – While fluctuations and damping in thermodynamic systems, i.e. in many–particle systems close to equilibrium, are fairly well understood the corresponding features in low–dimensional Hamiltonian dynamics are still under debate. Although it might be conjectured that, on the basis of general arguments, fast chaotic Hamiltonian degrees of freedom can be modelled by suitable stochastic forces the question is far from being settled. In fact, the just mentioned problem has several facets. Firstly, it is relevant for principal aspects of physics like damping and fluctuations on atomic scales (cf. e.g. [1]) or in nuclear physics. Secondly, modelling of systems with different time scales as they appear, e.g., in such diverse fields like molecular dynamics and climate research [2] is important from the practical point of view as the implementation of numerical schemes requires step sizes which can cope with the smallest time scale of the effective dynamical model. Whereas our previous work was concerned with the general (dissipative) case, we address here the problem how to deal with *Hamiltonian dynamics* where two kinds of degrees of freedom enter, fast chaotic and slow variables. We will demonstrate that suitable stochastic models are capable to describe the motion of the slow degrees of freedom accurately. The difficulty as compared to the general case has two sources: The existence of additional structure which has to be conserved by the derivation of the stochastic model (energy conservation) and the fact that the Hamiltonian nature of the equations of motion introduce a mixing of the time scales.
In the past two years we were able to fundamentally clarify many issues of principal and practical relevance related to the stochastic modelling of Hamiltonian dynamics. In our derivation of a Fokker Planck equation for the phase space density in the slow subspace we trace explicitly the time scale separation through an expansion parameter ϵ. For consistency, the total energy of the full system has to scale like $1/\epsilon$, which affects the Einstein–like relation between the viscous damping and diffusion term of the effective stochastic model. We find a damping which is one order ϵ smaller than the diffusion. The energy conservation of the full system translates into a multiplicative

noise term which guarantees that the invariant density of the Fokker–Planck equation has a bounded support. Being intimately linked to the Hamiltonian structure of the full system, these features are captured by a proper fluctuation–dissipation relation. Finally, we demonstrate by suitable examples that the system specific damping and diffusion terms of the stochastic model can be obtained with reasonable effort by a (numerical) analysis of the fast dynamics alone, and that the stochastic model yields very good approximations of the full dynamics on all time scales beyond $t \sim \mathcal{O}(\epsilon)$.

Reduced equation – To set up the notation we consider a Hamiltonian of the form

$$H(q,p,Q,P) = \frac{1}{\epsilon} H_f(q,p) + H_s(Q,P) + V_c(q,Q)\ . \tag{1}$$

We assume an *a priori* separation of slow variables Q, P and fast variables q, p, mediated by the small parameter $\epsilon \ll 1$. The variables may be vector valued, but to keep the notation simple we refrain from labelling the different components. We intend to approximate the Hamiltonian equations of motion of the slow variables by a suitable stochastic model. Whereas the effective equation of motion for Q is identical to the exact equation, the time evolution of P will be governed by a suitable stochastic equation. To determine the parameters of the latter on a merely empirical level, one has to compute [4] the first two moments

$$\tau D_P^{(1)}(Q,P) + \mathcal{O}(\tau^2) = \langle \widetilde{P}(\tau) \rangle_{q,p} - P \tag{2a}$$

$$\tau D_{PP}^{(2)}(Q,P) + \mathcal{O}(\tau^2) = \left\langle (\widetilde{P}(\tau) - P)^2 \right\rangle_{q,p}\ . \tag{2b}$$

Here, $\widetilde{P}(\tau) = \widetilde{P}(\tau; q,p,Q,P)$ is the solution of the initial value problem $(Q,P,q,p)(0) = (Q,P,q,p)$ of the equations of motion derived from Eq. (1). $\langle \ldots \rangle_{q,p}$ denotes the average over q and p on the energy shell $H(q,p,Q,P) = E/\epsilon$ where the scaling of the total energy with $1/\epsilon$ is suggested by the time scale separation of the Hamiltonian (1). If a stochastic description is appropriate and if higher order moments are neglected then, following the spirit of the Kramers–Moyal expansion [5], the stochastic differential equation

$$dP = D_P^{(1)}(Q,P)dt + \sqrt{D_{PP}^{(2)}(Q,P)}dW \tag{3}$$

yields an approximation of the statistical properties of the slow degrees of freedom. Here, dW denotes as usual the differential of the Wiener process, i.e. a Gaussian white noise. This approximation becomes meaningful if $\epsilon \ll \tau$. It guarantees that on the time scale τ the correlations of the fast motion decay by assumption and a description in terms of a Langevin equation or the corresponding Fokker–Planck equation becomes feasible.

Until here we have not proven that a stochastic model (3) is justified, nor does the above method supply an analytical determination of the drift and diffusion terms. Such a theoretical derivation may be obtained by applying a formal second order perturbation expansion with respect to the time scale separation parameter ϵ to the Liouville equation governing the dynamics of the full phase space density $\rho_t(q,p,Q,P)$. Under suitable projection we obtain the following effective Fokker–Planck equation for the reduced density $\bar{\rho}_t(Q,P) = \int \rho_t \, dp \, dq$ describing the properties of the slow degrees of freedom in a probabilistic way (see also e.g. [6] for related concepts in the context of

dissipative dynamical systems)

$$\partial_t \bar{\rho}_t = -i\langle \mathcal{L} \rangle_{ad} \bar{\rho}_t + \epsilon^2 \partial_P \frac{\partial H_s}{\partial P} \gamma \bar{\rho}_t + \epsilon \partial_P^2 \hat{D}^{(2)}_{PP} \bar{\rho}_t \tag{4}$$

where the diffusion coefficient $\hat{D}^{(2)}_{PP}(Q,P)$ and the damping γ are given by

$$\hat{D}^{(2)}_{PP}(Q,P) = (1 - \epsilon H_s \partial_E) d_0 + \mathcal{O}(\epsilon^2) \tag{5a}$$

$$\gamma = Z_0^{-1} \partial_E \left(d_0 Z_0 \right) + \mathcal{O}(\epsilon) \tag{5b}$$

Here $d_0 = \kappa^2 \int_0^\infty \langle \delta_{ad} q \; \delta_{ad} q_f(t) \rangle_{ad} dt$ denotes the integral over the autocorrelation function of the fast fluctuations of the fast chaotic variables. $\langle \dots \rangle_{ad}$ abbreviates the average over the adiabatic density in lowest order $\rho^{(0)}_{ad} = \delta(H_f - E)/Z_0$ with $Z_0 = \int \delta(H_f - E) dq \; dp$, $\delta_{ad} q = q - \langle q \rangle_{ad}$ and $q_f(t)$ denotes the time dependent solution of the fast system with $q_f(0) = q$. For simplicity, we have considered a harmonic coupling $V_c(q,Q) = -\kappa q Q$. We want to stress that Eq. (4) and the expressions (5) are based solely on the smallness of the parameter ϵ and on the assumption of an exponential decay of the fast auto-correlations due to chaos. In particular, no assumptions on the size of the coupling V_c are needed. Since Z_0 and d_0 do not depend on P and Q, their numerical values can be determined by integrating the fast subsystem alone.

In Eq. (4) the first term contains the adiabatically averaged Liouvillian $\mathcal{L}$. The second contribution yields a viscous damping term of order ϵ^2 if $H_s(Q,P) = P^2/2 + U(Q)$, since in lowest order the damping coefficient (5b) does not depend on the slow variables. The diffusion coefficient (5a) depends in such a way on the slow variables that it vanishes when the slow subsystem contains the total energy. Eqs. (5) linking the damping constant with the diffusion coefficient express a fluctuation–dissipation relation for our system.

Accuracy – By the help of examples we have explored the accuracy of the effective model Eq. (4) in two ways: we compared the drift and diffusion terms of Eq.(5) to those computed empirically by Eq.(2), assuming the validity of a stochastic model, and we verified the ability of our Fokker–Planck equation with drift and diffusion terms of Eqs.(5) to reproduce the dynamics of the full system. The latter was done in view of both asymptotic and dynamical aspects: The invariant densities of the full systems were compared to densities of the Fokker Planck model, and different correlation functions were studied. Also the relaxation towards equilibrium was investigated in detail. In all cases, we found that the approximation started to be good for time scale separations of more than one order of magnitude. Known violations of the Markov approximation on very short time scales of the slow motion introduce deviations between the Fokker–Planck model and the full system on exactly these time scales, but do not propagate to intermediate time scales. Another source of non-Markovian properties are stable islands inside the chaotic component of a Hamiltonian system. Due to effects summarised as stickiness such systems often have slower than exponential decay of auto-correlation functions. It turns out that in the studied examples stickiness does not lead to any order ϵ-effects which are not already contained in our Fokker–Planck model.

Comparing the results of the effective dynamics with the exact one, the approximation by a Fokker Planck equation works surprisingly well on all time scales larger $\mathcal{O}(\epsilon)$. Non–Gaussian and non–Markovian features of the fast chaotic motion are negligible, but the correct form of the diffusion and the size of the damping are crucial for respecting the

conservation of energy. Thus fast chaos acts like a reservoir with a finite heat capacity, generating a stochastic slow motion with a finite support. Altogether this opens the possibility of efficient long time simulations with high accuracy.

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3.1.7 Recurrence time statistics of long range correlated data

Eduardo G. Altmann and Holger Kantz

Introduction – Recurrence time analysis is a powerful tool to characterise temporal correlations in the occurrence of well defined events. It has been recently extensively performed in a rich variety of experimental time series: records of the climate [1, 2], seismic activities [3], solar flares [4], spikes in neurons [5], turbulence in magnetic confined plasma [6] and stock market [7]. Calculated essentially in the same way, these analyses receive different names: waiting time distribution, inter-occurrence time statistics, distribution of inter-spike intervals, distribution of laminar phases, etc. Of particular interest are systems with long range correlations. An estimate of recurrence time statistics (RTS) is usually statistically much more robust than an estimate of the auto-correlation function at large time lags. Whereas on the level of the latter long range correlations imply generally the existence of power law tails, its translation into RTS contrarily to what one might conclude from studying the literature, is not unique: In many phenomena one would expect power law distributions for recurrence times, whereas recently it has been shown that stretched exponentials can be found as well. The other interesting issue is the dependence of the RTS on the observable. There are clear indications that the observable has a strong influence on the nature of the correlations found: e.g., in [1] precipitation data did not show any long range correlations, whereas maximum daily temperatures taken at the same continental stations do show long range correlations and a stretched exponential RTS with $\gamma \approx 0.7$. Both types of data characterise the dynamics of the weather at these places.

Recurrence time statistics – Given a time series $\{x_n\}, n = 1, \ldots, N$, and having defined a recurrence interval I as a subset of the data range, then the ith *recurrence time* T_i is the time interval Δn between the ith and the $i + 1$st visit of a time series point in I. The RTS characterises the statistical properties of these T_i. The sequence of recurrence times generated this way depends sensitively on the choice of I. A potential

dependence of the RTS on I is a still poorly studied but relevant issue. While for the recurrence of extreme events the recurrence interval is defined by the points above a threshold [8] $I_{ext}(q) = [q, \infty[$ in a more general way it may be defined around a position X_c with a semi-width δ [6,9] $I(X_c, \delta) = [X_c - \delta, X_c + \delta]$.

In dynamical systems' theory the concept of Poincaré recurrences, observed in the phase space of the Hamiltonian system, plays a central role. The relation between time series recurrences and Poincaré recurrences can be established by an observable $x = x(\vec{\gamma})$, when $\vec{\gamma}(t) \in \Gamma$ is the trajectory in phase space of the Hamiltonian system. The recurrence volume $\mathcal{V}$ is mapped to an interval $I_{\mathcal{V}}$ on the real axis by the observation function $x(\vec{\gamma})$. However, the sequence of recurrence times of the series $x_n := x(\vec{\gamma}(t = n\Delta t))$ with respect to $I_{\mathcal{V}}$ is generally *not* identical to the sequence of Poincaré recurrences of $\vec{\gamma}(t)$ with respect of $\mathcal{V}$, since there is usually a large set $\bar{\mathcal{V}}$ which also maps to $I_{\mathcal{V}}$ due to the non-invertibility of $x(\vec{\gamma})$.

Long-term correlations and recurrence times – If time series data $\{x_n\}$ are exponentially (short range) correlated, the RTS is well known to be Poissonian, independent of the choice of I (in the limit of small interval $\mu(I) \to 0$) [9]. The same result applies to Poincaré recurrences (independently of $\mathcal{V}$) if the underlying dynamics is hyperbolic [10]. Hence, for systems with an exponential decay of correlations, details of defining recurrence times and further details of the system are irrelevant; instead there exists a unique RTS.

Many time series data have been found to be long-term correlated, i.e., their mean autocorrelation time diverges [1,2,13]. Typically, their auto-correlation function follows a power law decay, $c(\tau) = \langle x(t)x(t+\tau)\rangle \propto \tau^{-\gamma_c}$ with $0 < \gamma_c < 1$. In a recent paper [8], Bunde et al. analysed the effect of long-term correlations on the return periods of extreme events. The main result of Ref. [8], verified in Refs. [1, 2] for experimental data, is that the statistics of T follows a stretched exponential $\ln P(T) \propto -(T/\langle T\rangle)^{\gamma}$, where γ is identical to the correlation exponent γ_c;

Even if one might argue that the findings of Ref. [8] are restricted to the class of the model data chosen there, the reproduction of these findings for empirical data suggests some generality of the stretched exponential distribution. However, the temporal properties of typical data are *not* fully specified by the autocorrelation function, what explains why there cannot be a unique RTS for long-term correlated data. Connections between the long-term correlation exponent γ_c and the RTS have to be established independently in every class of long-term correlated dynamical systems, as was done for Hamiltonian systems with mixed phase space [11] and fractal renewal point processes [12]. We argue that the stretched exponential is valid for long-term correlated *linear* time series. Assuming the validity of the stretched exponential distribution for *all* possible recurrence times $T \in [0, \infty[$, we can make use of normalisation and of the mean value to compute the full analytic expression of a stretched exponential, depending on the sole parameter γ in $P_\gamma(T) = ae^{-(bT)^\gamma}$. Further simplification is obtained performing the following transformation of variables $\tau = \frac{T}{<T>} = \mu(I)T$, i.e., counting the time in units of the mean recurrence time (where $\mu(I)T$ is the measure of the recurrence interval). The complete stretched exponential distribution for recurrence times is then written as

$$p_\gamma(\tau) = a_\gamma e^{-(b_\gamma\,\tau)^\gamma},\ \text{with}\ \begin{cases} a_\gamma = & b_\gamma\,\frac{\gamma}{\Gamma(1/\gamma)}, \\ b_\gamma = & \frac{(2^{1/\gamma})^2\Gamma(\frac{2+\gamma}{2\gamma})}{2\sqrt{\pi}}, \end{cases} . \tag{1}$$

For experimental or numerical data, where neither a nor γ are known a priori, the relation between both is indispensable to correctly visualise and fit the RTS. We note that in practice the numerical fitting of the exponent γ is very sensitive and typically depends on the choice of the pre-factor a. In fact, the stretched exponential could be verified to hold with very high accuracy for numerically generated data with long range correlations and known correlation exponent γ_c with $\gamma = \gamma_c$, if the recurrence times are measured with respect to extreme events. We want to stress that in this comparison there is no free fitting parameter.

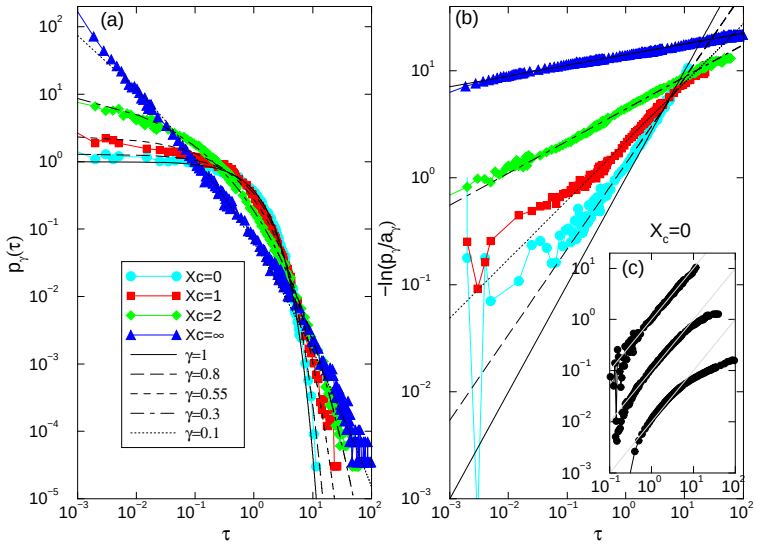

Figure 1: *RTS of long-term correlated time series with $\gamma_c = 0.1$ and different recurrence intervals (centred in X_c with measure $\mu(I) = 10^{-3}$). The lines are stretched exponentials distributions and the symbols connected by lines are the numerical simulations. From (a) to (b) we use the values given by a_γ of the best fitting of Eq. (1) in (a). In (c) we analyse the case $X_c = 0$ for different values of $\mu(I)$, from bottom to top: $\mu = 10^{-1}$ (shifted down by 10^2), $\mu = 10^{-2}$ (shifted by 10) and $\mu = 10^{-3}$. The gray lines are the Poissonian distribution ($\gamma = 1$ in Eq. (1)). $a_{\gamma=1} = 1$ was used for all three cases.*

Interestingly, if we define the "events" by a finite recurrence interval $I(X_c, \delta)$ centred around some value $X_c < \infty$, the RTS is still accurately described by stretched exponentials, however, we find $\gamma > \gamma_c$. Decreasing the value of X_c from ∞ to 0 ($\langle x \rangle = 0$) results in an transition from $\gamma = \gamma_c$ to $\gamma = 1$, i.e., the stretched exponential passes over into the Poissonian statistics (see Fig. 1)

Change of observables – The link between recurrence times on time series data and Poincaré recurrences motivates the issue of the change of observables. All of the empirical data exhibiting long-term correlations mentioned before represent systems which involve a huge number of degrees of freedom. Hence, there is a similarly huge arbitrariness in choosing a given observation function $x(\vec{\gamma})$, and the natural question is what to expect when we change this observation function. In fact, such considerations will also

explain the observed transition from $\gamma = \gamma_c$ to $\gamma = 1$ discussed above. Generally, two different observables x and y are functions of the $d-$dimensional phase space vectors $\vec{\gamma}$, and no simple function connecting x and y exists. For simplification, we consider here the special case that the observable y is a unique and even invertible function of x. In particular, we study the family of transformations $y_n = \frac{1}{x_n - (X_c - \delta)}$. This transformation implies that recurrence events of the x-series obtained for an "extreme" recurrence interval I_{ext} correspond to recurrence events in series y for an centred finite interval $I(X_c, \delta)$ and *vice versa*. Hence, the recurrence statistics of the transformed series for a given interval I_0 is identical to the statistics of the original series for a transformed interval I_0'. The above results hence confirm that the RTS of, e.g., extreme events indeed does change dramatically by such a transformation. Of course, also the auto-correlation function is not invariant under such a transform.

A multi-fractal detrended fluctuation analysis [13] applied to the transformed time series gives a much more complete characterisation of the temporal correlations than the auto-correlation function. Whereas the original data x are mono-fractal with a single generalised Hurst exponent $h(s) = 1 - \gamma_c/2$, the y-series are multi-fractal, i.e., show a nontrivial dependence of $h(s)$ on s. In this sense, the original representation of the data in terms of x is distinguished, and one might consider to find a back-transformation for empirical data, thereby making them mono-fractal, in order to calibrate correlations in data. How to find such a transformation is part of future work. The current state of this analysis definitely shows that the statistical properties of extreme events in the first place are not invariant under the change of variables, so that they do not characterise the underlying dynamics, but the joint effect of dynamics and observations. This is of high relevance for the correct interpretation of results in the study of extreme events.

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3.1.8 Collective electron motion in rare gas clusters induced and probed by intense laser pulses

Ulf Saalmann, Christian Siedschlag and Jan M. Rost

Collective electron motion is well known in the condensed phase and also in metal clusters. The finite cluster size and geometry (roughly spherical) make the surface plasmon with a frequency of $\omega_p/\sqrt{3}$ the dominant collective excitation mode, where the plasma frequency ω_p depends only on the density of the electrons. While single photon excitation of the dipole plasmon is well established in many metallic systems, it was shown more recently experimentally and theoretically that metal clusters in intense laser fields can also be collectively excited [1]. The behavior is more complicated since the cluster ions Coulomb explode after substantial ionization due to the strong laser pulse and therefore ω_p decreases as a function of the cluster size which is in turn time dependent. We have also predicted a resonant energy absorption behavior for small rare gas clusters [3], however, not due to collective electron excitation, but due to enhanced ionization, an effect which also occurs in diatomic molecules [2]. It is due to a cooperative behavior of an atom interacting with its next neighbors in a strong field. The question arises if collective electron motion occurs and leads to a resonance effect in larger rare gas clusters which develop sufficient space charge to hold back a substantial number of electrons even in an intense laser field. To answer this question we have investigated microscopically the dynamics of ions and electrons motion in Xenon clusters with 150 to 1500 atoms [4]. While the charging of the cluster shows clear indication for a resonant absorption mechanism the amplitude of the electronic center of mass (CM) motion does not increase at the resonance. This could point to a strongly damped dynamics and the only reliable indication of resonant driving is the phase lag ϕ between the driving field and the CM motion which should pass through $\pi/2$ at resonance. This is indeed the case as Fig.1 reveals confirming resonant energy absorption by a collective motion of the electrons inside the cluster.
Surprisingly, the collective electron dynamics, more specifically its CM motion, can be described quite well by a driven damped oscillator,

$$\ddot{X}(t) + 2\Gamma_t \dot{X}(t) + \Omega_t^2 X(t) = F_0(t)\cos(\omega t) \tag{1}$$

with the solution $X(t) = A_t \cos(\omega t - \phi_t)$. The amplitude A_t, phase ϕ_t, damping Γ_t, and eigenfrequency Ω_t are quasistationary variables whose change in time is much slower than the laser period $2\pi/\omega$. The four variables are not independent, one can express Γ and Ω in terms of A and ϕ [4]. This allows us to extract the physically interesting eigenfrequency and damping from the CM-velocity, provided it really obeys the dynamics $X(t)$ of a driven damped harmonic oscillator. The result, along with the determination of the eigenfrequency directly from the density of ions in the expanding cluster, is shown in Fig.2. Hence, rare gas cluster under intense laser pulses exhibit collective electron motion which leads to an efficient and resonant coupling of energy from the laser pulse to the cluster if the eigenfrequency of the electrons matches the laser frequency, $\Omega_t = \omega$. Moreover, the collective electron behavior can be well described by a driven damped harmonic oscillator. The damping comes from the gain (through inner ionization of bound electrons from the ions) and loss (electrons leave the cluster) of collectively moving electrons in time.

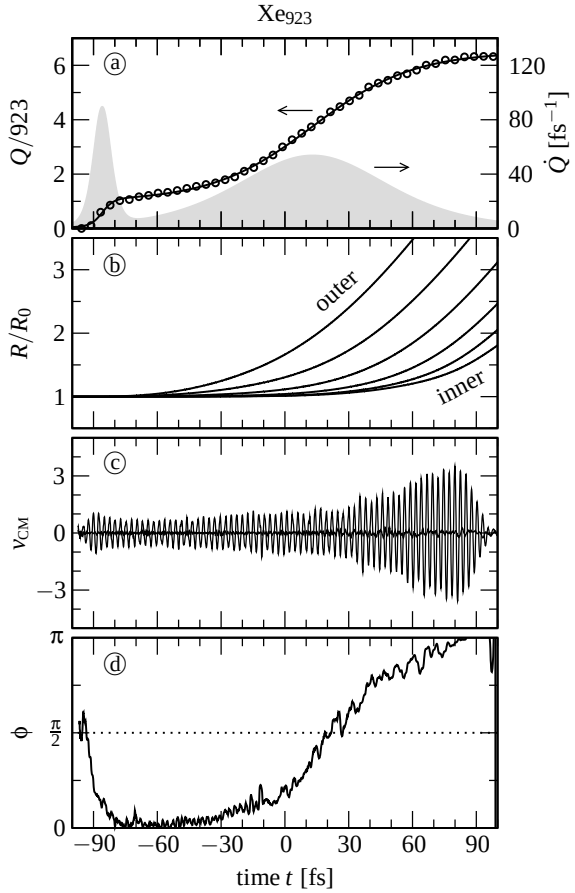

Figure 1: *Time dependent dynamics of Xe_{923} in a strong laser pulse ($\lambda = 780\,nm$, $I = 9 \cdot 10^{14}\,W/cm^2$, rise and fall time 20 fs, plateau for $|t| < 80\,fs$).a: Average charge Q per atom (left axis, circles and fit through circles) and rate dQ/dt (gray, right axis).b: Radii R of all cluster shells in units of their initial radii R_0.c: Center-of-mass velocity $v_{\rm CM} = \dot{X}$ of the electronic cloud inside the cluster volume. Note, that the oscillations are spatially along the linear polarization of the laser, whereas the electron velocity perpendicular to the laser polarization is very small and hardly to see in the figure.d: Phase shift ϕ_t of the collective oscillation in laser direction with respect to the driving laser, see text.*

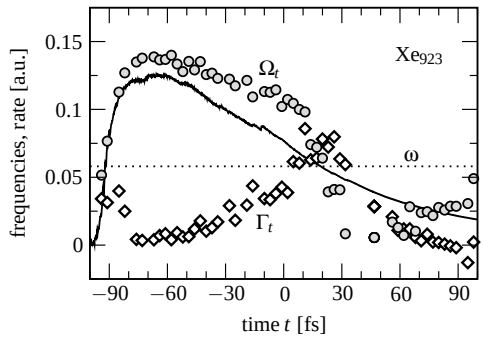

Figure 2: *Eigenfrequency Ω_t (circles) and damping rate Γ_t (diamonds) extracted from A_t and ϕ_t as calculated in Fig. 1. For comparison the eigenfrequency $\omega_p/\sqrt{3} = \sqrt{Q_{\rm ion}(t)/R(t)^3}$ for a spherical, uniformly charged cluster (solid line) is shown. The laser frequency ω is indicated by a dotted line.*

Soft VUV pulses as produced by the Free Electron Laser at DESY [5] can also induce a fast relaxing electron plasma in quite small rare gas clusters of only a few tens atoms [6]. Here, the electrons are excited from their bound states but not completely ionized due to the small quiver amplitude at these laser frequencies. We have proposed the combination of infrared and VUV pulses in a pump-probe scheme to obtain a detailed insight into the collective electron dynamics of the cluster [7].

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3.1.9 Coulomb crystallization of a freely expanding laser-cooled neutral plasma

Thomas Pohl, Thomas Pattard and Jan M. Rost

Ultracold gases as created in magneto-optical traps (MOT) offer a completely new parameter regime to study the dynamics of particles interacting via long-range forces. One attractive feature is the prospect to create, by photoionization of the atoms, strongly coupled neutral plasmas with a Coulomb coupling parameter $\Gamma \gg 1$ where $\Gamma = e^2/akT$ measures the ratio of potential energy e^2/a ($a \propto \rho^{-1/3}$ is the average distance of the charged particles in terms of their density ρ) to kinetic energy kT expressed via the temperature T [1]. Traditionally, the strong-coupling regime is only realized in exotic plasmas like the interior of stars where enormous temperatures lead to high kinetic energy which is nevertheless dominated by the potential energy due to the huge density of the plasma. An ultracold plasma, on the other hand, is extremely dilute with very low potential energy, yet the kinetic energy is even lower at ultra-low temperatures. Formally, such a trapped gas can reach $\Gamma \sim 10^4$; in reality, however, only $\Gamma \sim 10^0$ has been achieved. The reason is the heating of the plasma upon its creation from the ultracold gas. The latter is in a disordered state and the ionized atoms have higher potential energy than in equilibrium which is quickly approached by converting potential into kinetic energy, thereby heating the plasma and lowering Γ drastically.

The question arises if one could reach the strongly coupled regime nevertheless. Theoretically feasible would be to start with an "overcorrelated" state, i.e., the cold atoms arranged in an optical lattice. This could even lead to "correlation cooling", because now the potential energy is lower than in equilibrium. However, firstly the cooling achievable is marginal [2] and, secondly, even a very small number (less than 1%) of defects destroys the cooling effect, rendering this way practically impossible with present means where the lattice arrangement of cold atoms can be achieved with about 10-15% defects. Another possibility would be to cool the ions while the neutral plasma expands. This requires atoms with two optically active electrons (one is ionized forming the neutral plasma, the second one is available for the laser cooling transition). However, it is a priori not clear at all if $\Gamma \gg 1$ can be achieved in this way, eventually leading to crystallization of the plasma. Among many questions to answer one needs to know (i) Is the cooling, necessary to reach $\Gamma > 174$ which is the known crystallization limit for infinite homogeneous systems, achievable in a realistic experimental situation? (ii) Does a freely expanding plasma which is most of the time in a non-equilibrium state crystallize at all? (iii) How do recombination and other loss processes influence the build-up of strong correlations in the plasma?

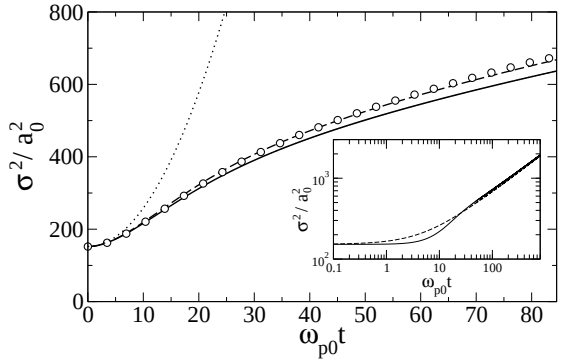

Figure 1: *Expansion of a neutral plasma with and without (dotted) laser cooling. The solution of the quasi-analytical kinetic equations (dashed) matches the mean-field numerical treatment (circles), demonstrating that the difference to the hybrid-MD simulation (solid) is due to ionic correlations. The inset shows a comparison of the numerical solution with the analytical approximation Eq. (1).*

In order to realistically answer these questions we had to develop a hybrid molecular dynamics code (H-MD) which can describe the time evolution of the neutral plasma over a sufficiently long time (which is of the order of 100μ s, or 100 and more ionic plasma cycles ω_p^{-1}) [3]. It is numerically impossible to fully resolve the dynamics of the electrons over such a long time. Rather, we treat them as a fluid, while the ions with all their interactions are fully propagated using tree code techniques. This allows us to evolve a neutral plasma with up to 10^5 ions. In parallel, we have developed a semi-analytical description based on kinetic equations [4] in order to assess the dependence of the plasma dynamics on external parameters such as the initial width σ_0 of the spherical Gaussian plasma (the geometry of the MOT leads to an approximate radial Gaussian shape of the cold atom cloud), the ion mass m_i, the initial electronic temperature T_e, and the Doppler cooling rate β.

It is clear that the expansion must be as slow as possible to have a long time available for the Doppler cooling. For asymptotically long times the cooling changes the expansion $\sigma(t)$ of the plasma not only quantitatively but also qualitatively from $\sigma^2 \propto t^2$ to

$$\sigma^2(t) \approx \sigma^2(0)(1 + 2t/\tau_{\rm exp})^{1/2}\,, \quad \tau_{\rm exp} = \beta m_i \sigma^2(0)/2kT_e. \tag{1}$$

This analytical result is confirmed by the full H-MD calculations, see Fig. 1. The dependence on the relevant parameters enters in the expansion time constant $\tau_{\rm exp}$. Longer exposure to the cooling laser tends to make the ions colder, hence a slow expansion and a large $\tau_{\rm exp}$ is desirable. It is reasonable that slower expansion can be achieved by heavier ions, a big atom cloud (large $\sigma(0)$), a large cooling rate β itself and a low electronic temperature T_e reducing the hydrodynamic pressure on the ions. Yet, one has to be cautious taking into account side effects. Three-body recombination (i.e. forming atoms out of the plasma) will heat the plasma and should be avoided. Since low T_e favors recombination one should rather increase $\sigma(0)$, i.e., at constant ion density simply increase the number of ions, than decrease T_e in order to make $\tau_{\rm exp}$ larger. The cooling rate $\beta \propto m_i^{-1}$ must be of the order of $\omega_{p0}/10 \propto m_i^{-1/2}$ to achieve sufficient cooling. Since β decreases faster with m_i than ω_{p0}, lighter ions should be preferred for which sufficient cooling can be achieved experimentally. For our simulation, we therefore chose Be ions (which can be laser cooled [5]). We have found crystallization of the plasma in spherical shells [6], growing from the center of the plasma (in contrast to ions confined by an external potential), for 50000 Be ions with an initial density of 1.1×10^8 cm^{-3} and $T_e = 8.6$K (Fig. 2).

Coming back to the questions raised above, we can say that an expanding neutral plasma can crystallize although it is not in equilibrium. The scenario under which

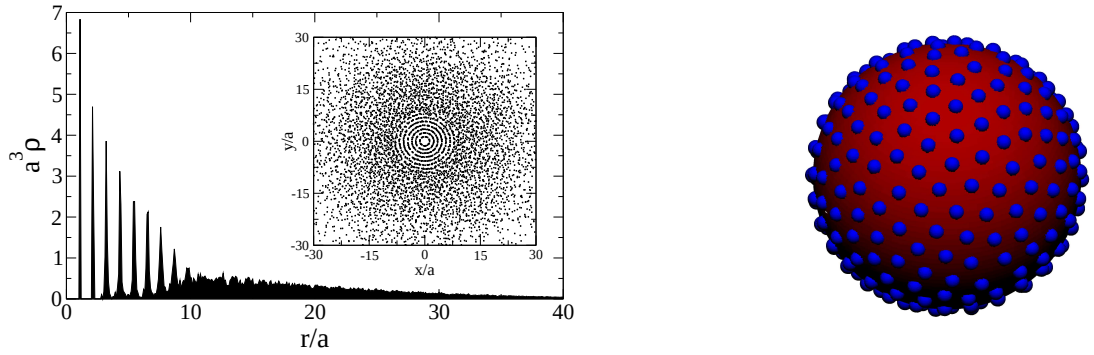

Figure 2: *Radial density after a time of $t = 24\,\mu s$ ($\omega_{p0}t = 110$). The inset shows a two-dimensional cut through the plasma cloud, clearly revealing the formation of concentric shells. (For better contrast, cuts with $x = 0$, $y = 0$ and $z = 0$, respectively, have been overlayed.) The picture on the right visualizes the ions on the fifth shell.*

this happens is experimentally feasible and experiments to find the crystallization are under way. In general, neutral ultracold plasmas pave the way to novel cold atomic physics phenomena as well as to experimentally measurable non-equilibrium plasma effects which are largely unknown presently.

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3.1.10 Electron-electron momentum exchange in intense field double ionization

Andreas Becker

Double ionization of atoms in an intense laser field is one of the key processes to study the correlated electron motion in a three-body Coulomb system. The three-body problem is here closely interrelated with the highly nonlinear electron-field interaction. The result are unexpected large probabilities for a joint emission of the two electrons, which exceed the theoretical predictions for a step-wise or sequential ionization of one electron after the other by many orders of magnitude [1]. It is widely accepted nowadays that the rescattering process [2, 3] is the basic mechanism for the double electron ejection at infrared wavelengths. In this picture, one electron gets ionized first by the intense field, accumulates energy during about one half of a field cycle, is driven back to the parent ion and assists to set the second electron free in a scattering process.

The process corresponds to the leading Feynman diagram of a systematic intense-field many-body S-matrix analysis of strong field double ionization in the semiclassical limit (for a review, see [4]).
The first step of the process is of single-active electron nature and relatively well understood, but the physics of the electron impact ionization in the presence of the strong field in the second step is still under active debate. How does the first active electron exchange its energy and its momentum with the ion and the second electron? Recently, we have shown [5] that additional field energy is transfered from the field to the two electrons during the inelastic (re-)scattering process.
The apparent importance of the inter-electron correlation in the double ionization raises further the question whether its acts predominantly during the collisional ionization or the two electrons are coupled together in the laser field through their Coulomb interaction even after their escape from the atom. In a joint experimental and theoretical study we have addressed this question by investigating the momentum balance between the electrons in the direction perpendicular to the direction of a Ti:sapphire laser field [6]. In this kinematical geometry the subteleties of the Coulombic interactions can be tested, since the perpendicular momentum components are not affected by the field (e.g. [7]).

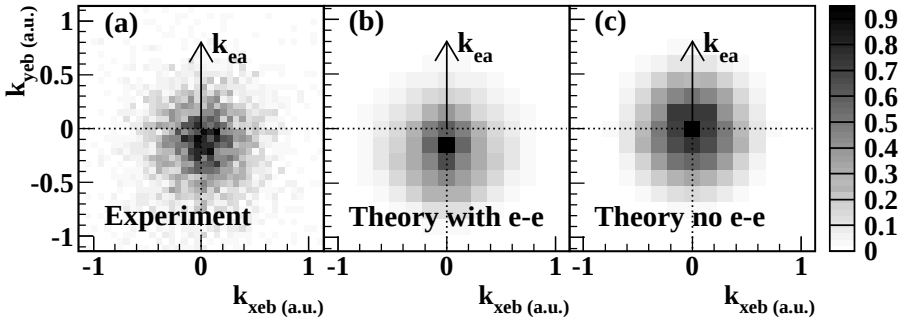

Figure 1: *Momentum distribution of electron b in the plane perpendicular to the field polarization, $\hat{\epsilon}$, in double ionization of Ar at 780 nm and 1.9×10^{14} W/cm^2. The perpendicular component of the momentum of electron a is shown by the arrow. The data are integrated over all momentum components along $\hat{\epsilon}$ and the magnitude of the momentum of electron a. A comparision is shown between (a) the experimental data, (b) theoretical results, including electron-electron interaction in the final state, and (c) theoretical results, neglecting electron-electron interaction (from [6]).*

In Fig. 1 the distribution of the momentum components perpendicular to the polarization axis of one of the electrons, b, is plotted. The momentum component of the other electron in the same plane is shown by the arrow, the parallel components of both momenta as well as the magnitude of the momentum of electron a are not resolved in the experiment (integrated in the theory). The experimental data (panel a) show clearly that the two electrons are emitted to opposite sides. This back-to-back emission is found to be due to the strong interaction between the two electrons after their double escape, as can be seen from the results of S-matrix calculations displayed in the other panels.

Theoretical predictions and experimental data are in good agreement with each other (panel b), when the full Coulomb interaction between the two emerging electrons is taken into account. This can be done by using the exact solution of the Schrödinger equation of two Coulomb-interacting electrons subjected to the laser field in the final state of the S-matrix calculations [8]. The results neglecting the final-state electron-electron interaction (panel c) do not show the back-to-back charateristics found in the experiment. This reveals the importance of the full electron-electron repulsion after the instant of scattering for the nonsequential double ionization process.
This work has been done in collaboration with the experimental groups of R. Dörner (Frankfurt) and P.B. Corkum (Ottawa, Canada).

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3.1.11 Propagation of femtosecond laser pulses in air

Edward Arevalo and Andreas Becker

The propagation of a high peak-power femtosecond laser pulse in optical media has attracted considerable attention recently [1]. Fundamentally, the physics of filamentation is based on the phenomenon of Kerr self-focusing, which is known from the 1960's. Filamentation and spectral broadening of the pulse were also observed already about 30 years ago for the first time. So, what is new that makes the phenomenon so interesting today? With the 'long' pulses in the nano- and picosecond regime laser induced breakdown masked many interesting filamentation phenomena. Nowadays, powerful femtosecond laser pulses, which are short enough to avoid the effect of avalanche ionization, can propagate over long distances in air (up to several kilometers) in a filament. The filaments are mainly formed due to a balance of the Kerr self-focusing and the plasma defocusing effects. This phenomenon is encompassed by a self-transformation of the pulse into a chirped white light laser (for a review, see e.g. [2]) and opens up possibilities for a wide variety of potential applications, such as compression into energetic few-cycle pulses [3] or atmospheric remote sensing [1]. Besides these applications the phenomenon of filament formation is also interesting from a fundamental nonlinear dynamical point of view. We have investigated different aspects of the process

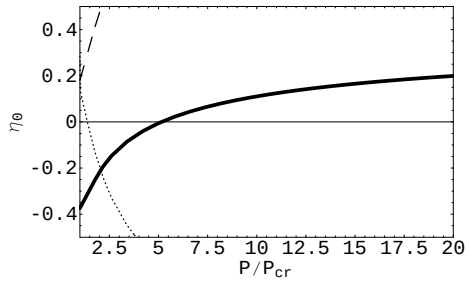

Figure 1: *Relative error of the predictions of a variational analysis for the self-focusing distance, including the background effect (solid line), with respect to exact numerical solutions as a function of the input power (scaled in units of the critical power for self-focusing). Also shown are the relative errors for earlier models, in which the background effect is neglected.*

using numerical solution methods as well as approximate theories, two examples are discussed below.

Variational analysis of self-focusing

The analysis of optical pulse propagation is usually based on the description of the pulse in terms of its complex field envelope, neglecting the underlying rapid oscillations at its carrier frequency. The resulting higher dimensional nonlinear Schrödinger equations are not integrable, however they can be analyzed using numerical solution methods. In order to get deeper insight into a physical process it is often useful to develop approximate theories, even if full numerical solutions are available. We have derived a quasianalytical approximation of the self-focusing phenomenon using a variational approach [4].

From numerical simulations one can observe that during self-focusing the pulse $u(\xi, r)$ seperates into two components (scaled coordinates are used):

$$u(\xi, r) = \Psi_0(\xi, r) + \epsilon\Psi_1(\xi, r), \tag{1}$$

where Ψ_0 is the high intensity inner core of the pulse, which self-focuses, and $\epsilon\Psi_1$ is the low intensity outer part, which propagates forward following the linear propagation mode. Recently, it has been found [5] that this weak background plays a decisive role during the propagation of femtosecond pulses.

We have performed a variational analysis of the self-focusing process using a trial solution:

$$u(\xi, r) = \Psi_0(\xi, r) \exp(iS_1(\xi, r)), \tag{2}$$

in which the perturbation of the inner core by the background is taken into account as a correction in the phase ($\Psi_1(\xi, r) = |\Psi_1(\xi, r)| \exp(iS_1(\xi, r))$). The phase correction can be obtained for any shape of the inner core by taking its derivative and seperating the phase.

Quasianalytical solutions for the width, intensity and self-focusing distance are derived. The relative error of the predictions of the present theory for the self-focusing distance with respect to the results of numerical solutions is less than 20% as soon as the input power exceeds twice the critical power for self-focusing, as shown in Fig. 1 (solid line). It is clearly seen from the Figure that a much closer quantitative agreement with the

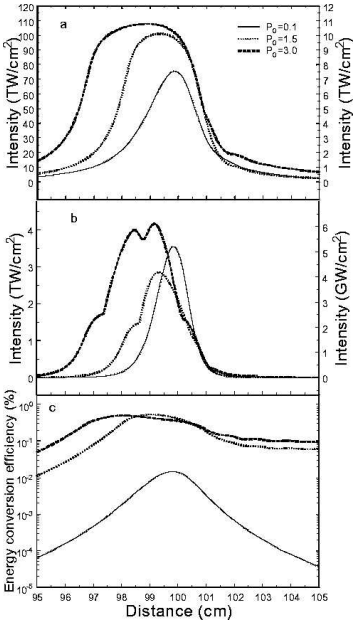

Figure 2: *Numerical results for the on-axis peak intensity of (a) the fundamental pulse and (b) the third-harmonic pulse for different input powers (scaled in units of the critical power) as a function of the propagation distance. In panel (c) the total conversion efficiency is shown. The beam was focused with a lens of f = 100 cm.*

exact results is obtained than in earlier models (dotted and dashed lines) [6,7], in which the effect of the background has not been taken into account.

Third-harmonic generation and filamentation

The intensity in the long filaments generated in air is about mid of 10^{13} W/cm^2 and is sufficient to generate higher harmonics. We have shown both theoretically and experimentally [8] that indeed an intense ultrashort third-harmonic pulse is generated inside the filament. Results of numerical simulations show that the on-axis peak intensity of the pump (Fig. 2a) and the third-harmonic pulses (Fig. 2b) remain unchanged over a distance of several centimeters as soon as the input power exceeds the critical power for self-focusing, i.e. both pulses undergo filamentation. The co-filamentation becomes also obvious from the third harmonic conversion efficiency (Fig. 2c). There is no apparent temporal walk-off between the two pulses, which means that they travel inside the filament with nearly the same group velocity. This is found to be due to a nonlinear locking of the envelope phases of the two pulses. The results of numerical calculations for this phenomenon are confirmed by experimental data.

The generation of an intense third harmonic pulse in the filaments has important implications for potential applications. During its propagation the third-harmonic pulse itself generates a broad continuum, which can overlap with the continuum of the fundamental pulse and extends the spectral region of the white light laser into the UV [9]. This potentially opens the possibility to simulataneously monitor chemical pollutants and biological species at remote distances using femtosecond laser pulses.

The work on third-harmonic channeling has been done in collaboration with the group of C.M. Bowden (Huntsville, USA) and the experimental group of S.L. Chin (Quebec, Canada).

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3.1.12 Concurrence of mixed bipartite quantum states in arbitrary dimensions

Florian Mintert, Marek Kuś, and Andreas Buchleitner

In classical physics, one can always divide a system into subsystems, such that complete information on the entity implies a complete description of its individual parts, and vice versa. In quantum physics, this no longer holds true: whilst one can still divide a system into subsystems, a complete description of the system state in terms of a pure state does not necessarily assign a pure state to each subsystem. The subsystems of generic pure states are correlated in a way without classical analog – they are *entangled*. A pure state entanglement measure for bipartite systems, which expresses entanglement in terms of the information loss upon trace over one subsystem is *concurrence*, defined [1] as $c(\psi) = \sqrt{|\langle\psi|\psi\rangle|^2 - \mathrm{Tr}\varrho_r^2}$, where the reduced density matrix ϱ_r is obtained by tracing over one subsystem. The concurrence of mixed states ϱ is then given as the convex roof

$$c(\varrho) = \inf \sum_i p_i c(\Psi_i), \quad \varrho = \sum_i p_i |\Psi_i\rangle\langle\Psi_i|, \quad p_i \geq 0, \tag{1}$$

of all possible decompositions into pure states Consequently, $c(\varrho)$ vanishes if and only if ϱ exhibits purely classical correlations, i.e. if the state is *separable* and hence can be represented as a convex sum over product states, $\varrho = \sum_i p_i \varrho_i^{(1)} \otimes \varrho_i^{(2)}$, with $p_i \geq 0$, and $\varrho_i^{(1)}$ and $\varrho_i^{(2)}$ states on the subcomponents $\mathcal{H}_1$ and $\mathcal{H}_2$ of the total Hilbert space $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2$. Given the dimensions n_1 and n_2 of $\mathcal{H}_1$ and $\mathcal{H}_2$, respectively, eq. (1) defines a high dimensional optimisation problem which is rather cumbersome to solve. Furthermore, such optimisation can only yield an upper bound for $c(\rho)$, by virtue of the definition of the infimum.

Here, we derive the first estimate of $c(\rho)$ from below, in arbitrary finite dimensions. To do so, we first replace, for convenience, the $|\Psi_i\rangle$ by the subnormalized states $|\psi_i\rangle = \sqrt{p_i}|\Psi_i\rangle$ in eq. (1). Given a valid decomposition $\{|\phi_i\rangle\}$ of ϱ into subnormalized states, any other suitable set $\{|\psi_i\rangle\}$ is obtained by transformations $V \in \mathbf{C}^{N\times r}$, with r and N

the lengths of the sets $\{|\phi_i\rangle\}$ and $\{|\psi_i\rangle\}$, respectively,

$$|\psi_i\rangle = \sum_{j=1}^{r} V_{ij}|\phi_j\rangle \ , \ \sum_{i=1}^{N} V_{ki}^\dagger V_{ij} = \delta_{j,k} \ . \tag{2}$$

It is now crucial to realize that the concurrence of a pure state $|\psi\rangle$ can be expressed as the square root of the function

$$\begin{aligned} f(\psi_1,\psi_2,\psi_3,\psi_4) = \langle\psi_2|\psi_1\rangle\langle\psi_4|\psi_3\rangle - \\ \mathrm{Tr}_1\left((\mathrm{Tr}_2|\psi_1\rangle\langle\psi_2|)\,(\mathrm{Tr}_2|\psi_3\rangle\langle\psi_4|)\right) \ , \end{aligned} \tag{3}$$

evaluated at $\psi = \psi_1 = \psi_2 = \psi_3 = \psi_4$, where Tr_1 and Tr_2 denote the traces over the first and the second subsystem. f is linear in its first and third, and anti-linear in the second and fourth argument. Due to these properties the definition (1) can be reformulated as an infimum over transformations V:

$$c(\varrho) = \inf_V \mathcal{C}, \quad \text{with} \quad \mathcal{C} = \sum_{i=1}^{N} \left(\left[V \otimes V A\, V^\dagger \otimes V^\dagger \right]_{ii}^{ii} \right)^{\frac{1}{2}} \ . \tag{4}$$

Herein, the tensor A, defined by $A_{jk}^{lm} = f(\phi_j,\phi_l,\phi_k,\phi_m)$ [2] is hermitian, $A_{jk}^{lm} = (A_{lm}^{jk})^*$, and symmetric with respect to a simultaneous exchange of both its co- and contravariant indices $A_{jk}^{lm} = A_{kj}^{ml}$. Due to the symmetry of the transformation $V \otimes V$ under exchange of the subsystems of A, we can replace A_{jk}^{lm} in eq. (4) by the symmetrised elements

$$\mathcal{A}_{jk}^{lm} = \frac{1}{2}\left(A_{jk}^{lm} + A_{kj}^{lm}\right) \ , \tag{5}$$

which is equivalent to a symmetrisation over both subsystems in eq. (3). It can be shown that $\mathcal{A}$ is positive semidefinite and that its support lies in an antisymmetric subspace, *i.e.*, all elements of $\mathcal{A}$ with respect to fully symmetric linear combinations of product states vanish. Since the antisymmetric subspace has dimension $m = n_1(n_1-1)n_2(n_2-1)/4$, $\mathcal{A}$ has at most m non-vanishing eigenvalues.
Due to the discussed symmetries $\mathcal{A}$ can be expanded in a basis of real symmetric matrices $\Lambda^\alpha \in \mathbf{R}^{r\times r}$

$$\mathcal{A}_{jk}^{lm} = \sum_{\alpha,\beta} B_{\alpha\beta}\, \Lambda_{jk}^{\alpha}\Lambda_{lm}^{\beta}, \tag{6}$$

with B hermitian and positive semi definite. With the eigenvalues and associated eigenvectors of B ($B\vec{x}^\alpha = \mu_\alpha \vec{x}^\alpha$ and $\vec{x}^\alpha = [x_1^\alpha,\ldots,x_i^\alpha,\ldots]^T$) we can construct a properly normalised eigensystem T^α of $\mathcal{A}$

$$T_\alpha = \sqrt{\mu_\alpha}\sum_\beta x_\beta^\alpha e^{i\phi_\alpha}\Lambda^\beta = \mathcal{T}_\alpha e^{i\phi_\alpha} \ , \ \alpha = 1,\ldots,m. \tag{7}$$

We explicitly take into account the free phase factors $\exp(i\phi_\alpha)$, as they will be crucial in the following. Consequently,

$$\mathcal{A}_{jk}^{lm} = \sum_\alpha T_{jk}^\alpha\,(T_{lm}^\alpha)^* = \sum_\alpha \mathcal{T}_{jk}^\alpha\,(\mathcal{T}_{lm}^\alpha)^* \ . \tag{8}$$

Hence, eq. (4) can now be rewritten as

$$\mathcal{C} = \sum_{i=1}^{N} \Big(\sum_{\alpha} \Big| \Big[V T^{\alpha} V^{T} \Big]_{ii} \Big|^{2} \Big)^{\frac{1}{2}} \ , \tag{9}$$

the infimum of which gives the concurrence of the mixed state ϱ.
With the Cauchy-Schwarz inequality we obtain an estimate from below,

$$c(\varrho) \geq \inf_{V} \sum_{i=1}^{N} \Big| \Big[V \Big(\sum_{\alpha} z_{\alpha} \mathcal{T}^{\alpha} \Big) V^{T} \Big]_{ii} \Big|, \tag{10}$$

for any set $z_{\alpha} = y_{\alpha} \exp(i\phi_{\alpha})$, with $y_{\alpha} \geq 0$, $\sum_{\alpha} y_{\alpha}^{2} = 1$. The infimum on the rhs is given by $\lambda_1 - \sum_{i>1} \lambda_i$, where λ_j are the singular values of $\mathcal{T} = \sum_{\alpha} z_{\alpha} \mathcal{T}_{\alpha}$, i.e., the square roots of the eigenvalues of the positive hermitian matrix $\mathcal{T}\mathcal{T}^{\dagger}$ in decreasing order [3]. Hence, we arrive at the desired lower bound,

$$c(\varrho) \geq \lambda_1 - \sum_{i>1} \lambda_i, \tag{11}$$

with the λ_j dependent on the choice of the y_{α} and ϕ_{α}.
Note that each set $\{y_{\alpha}, \phi_{\alpha}\}$ provides a lower bound of $c(\varrho)$, which can be tightened by numerical optimization. However, all the examples we have considered so far suggest that there is one matrix $\mathcal{T}^{\alpha}$ that gives the main contribution to the rhs of eq. (10). Hence, the singular values of this matrix provide a purely algebraic lower bound for c, which often leads to satisfactory results even without further numerical refinement. Indeed, we could show [4] that such purely algebraic lower bounds even detect entangled states with positive partial transpose [5] – where the standard criterium [6] identifying a mixed state as nonseparable via negativity of its partial transpose is inoperational.
In conclusion, a suitable representation of the concurrence of bipartite mixed quantum states in terms of the eigensystem of a tensorial quantity allows for the derivation of a lower bound of $c(\varrho)$, for arbitrary ρ. Not only can this bound be tightened by an optimisation under the comparatively simple constraint $\sum_{\alpha} |z_{\alpha}|^{2} = 1$, over a *complex* vector space of dimension $n_1(n_1-1)n_2(n_2-1)/4$ – at least a factor $4n_1n_2$ smaller than dimensions of optimisation procedures hitherto available. It also can be reduced to a purely algebraic bound which provides good estimates.

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3.1.13 Web-assisted tunneling in the kicked harmonic oscillator

André R. Ribeiro de Carvalho and Andreas Buchleitner

Controlling the state and the time evolution of quantum systems is one of the central themes of current research in experimental and theoretical atomic physics, quantum optics, and mesoscopics. During the last decade, it has become clear that generic features of strongly coupled ("complex") quantum systems allow for novel and often extremely robust strategies of quantum control. In such systems, studied in much detail in the area of quantum chaos, peculiar eigenstates emerge which exhibit unexpected (and unexpectedly robust) localization properties and dynamics. Most prominent examples thereof are nondispersive wave packets in periodically driven quantum systems [1], quantum resonances [2], and quantum accelerator modes [3]. Recently, peculiar transport properties of non-KAM systems have attracted particular interest in electron transport in superlattices [4], where enhanced transport accross the lattice was observed, due to the sudden (non-KAM) appearence and disappearence of unbounded stochastic web-structures in classical phase space.

Here we expose a different pathway for the controlled enhancement of transport in another non-KAM system, the kicked harmonic oscillator [5], at *fixed* phase space structure, by simply tuning the effective value of $\hbar$. The classical Hamiltonian of the kicked harmonic oscillator describes a harmonically trapped (in 1D, with trap frequency ν) particle of mass m, subject to a one dimensional, spatially periodic potential (wave vector $k = 2\pi/\lambda$, modulation depth A) which is periodically switched on and off at integer multiples of the kicking period τ:

$$H = \frac{p^2}{2m} + \frac{m\nu^2 x^2}{2} + A\,\cos(kx)\sum_n \delta(t - n\tau)\,. \tag{1}$$

The classical phase space structure is completely determined by the parameters

$$K = \frac{Ak^2}{m\nu} \qquad \text{and} \qquad \alpha = \nu\tau \equiv \frac{2\pi}{q}\,, \tag{2}$$

which, respectively, define the stochasticity parameter and the ratio between kicking and oscillator period. A specific property of the kicked harmonic oscillator is that it exhibits peculiar symmetry properties determined by the ratio $q = (2\pi/\nu)/\tau$ of oscillator and kicking period: For integer q, in addition to confined regular islands, it displays a stochastic web (reaching out to infinity in phase space) with crystal ($q \in q_c \equiv \{3,\,4,\,6\}$) or quasi-crystal symmetry ($q \notin q_c$), along which the system diffuses for suitable initial conditions.

With the harmonic oscillator annihilation operator $\hat{a}$ and its hermitean conjugate $\hat{a}^\dagger$ derived from the suitably scaled center of mass coordinates of the trapped particle, the quantum version of (1) reads

$$\hat{H} = \hbar\nu\hat{a}^\dagger\hat{a} + \hbar\tilde{K}\left\{\cos\left[\eta(\hat{a} + \hat{a}^\dagger)\right]\right\}\sum_{n=0}^{\infty}\delta(t - n\tau), \tag{3}$$

with $\tilde{K} = K/2\eta^2$, and the Lamb-Dicke parameter $\eta = k\sqrt{\hbar/2m\nu}$. Note that the latter measures the ratio of the width of the harmonic oscillator ground state in units of

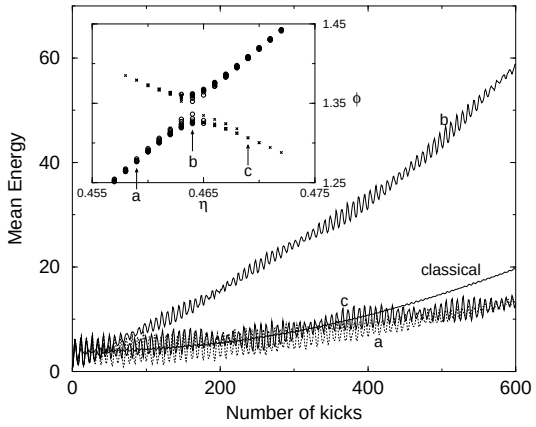

Figure 1: *Mean energy as a function of the number of kicks, for $q = 6$, $K = 2.0$, $|\psi_0\rangle = |0\rangle$, and Lamb-Dicke parameter $\eta = 0.459$ (a), 0.464 (b), 0.469 (c), at fixed classical phase space structure (eq. (2)). Also the classical time evolution is shown, for comparison. The inset zooms into the energy level dynamics as a function of η. Circles and crosses indicate eigenstates with an overlap larger or smaller than 10^{-2} with the initial state $|\psi_0\rangle$. Dramatic enhancement of the energy absorption by the trapped particle from the kicking field is observed exactly at the center b of the avoided crossing.*

the wave length of the kicking potential, and that its squared value plays the rôle of an effective Planck constant – which can be tuned easily in state of the art ion trap experiments.

Since (3) is periodic in time, the time evolution of any initial state $|\psi_0\rangle$ is given by the action of the one-cycle Floquet propagator

$$\hat{U}|\varepsilon_j\rangle = e^{-i\alpha\hat{a}^\dagger\hat{a}}e^{-i\tilde{K}\cos\left[\eta(\hat{a}+\hat{a}^\dagger)\right]}|\varepsilon_j\rangle = e^{i\phi_j}|\varepsilon_j\rangle, \tag{4}$$

with ϕ_j the quasi-energies and $|\varepsilon_j\rangle$ the associated Floquet eigenstates. Due to the δ-term in (3), the Floquet propagator factorizes into a free evolution and a kicking part, and inspection of the former shows that the above classical condition for the emergence of a web structure in classical phase space is also quantum mechanically distinguished, since integer q is equivalent to a (fractional) revival condition for the free evolution right upon the subsequent kick. One therefore expects quantum signatures of web-sustained transport in classical phase space – which we shall now establish by combining dynamical and spectral information.

In Fig. 1 we plot the mean energy of the kicked (quantum) particle, initially prepared in the harmonic oscillator ground state, as a function of the number of kicks imparted on it by the external field, for slightly different values of the Lamb-Dicke parameter η, and for crystal symmetry $q = 6$. We see that a change of η by merely one percent dramatically affects the energy absorption by the particle from the field, eventually leading to quantum transport which is much more efficient than the classical excitation process. Note that the latter is unaffected by such tiny changes of η, since the results displayed in the figure are obtained for fixed K and q, hence for fixed phase space structure!

Whilst this latter observation appears puzzling on a first glance, it is readily resolved by inspection of the evolution of the quasienergy spectrum of (4) as a function of η. The inset in Fig. 1 zooms into the level structure around an isolated avoided crossing

at ($\eta = 0.464; \phi = 1.35$). Here, two quasienergies undergo an isolated avoided crossing, with maximal tunneling coupling between the associated eigenstates at its center at $\eta = 0.464$. Note from Fig. 1 that enhanced quantum transport is observed *precisely* at this value (marked by the label b in the inset of Fig. 1). In contrast, for only slightly smaller or larger values of the Lamb-Dicke parameter, labeled by a and c in the inset, i.e. slightly shifted with respect to the center of the avoided crossing, the trapped particle absorbs energy with a much smaller rate, rather similar to the classical energy absorption. Hence, the width of isolated avoided crossings induces the sharp reponse of the system to tiny changes in η, opening a narrow parameter window in which the system can efficiently tunnel from its initial state $|\psi_0\rangle$ into another eigenstate which mediates rapid transport. Indeed, further inspection of the spectrum [6] reveals this latter eigenstate as a "web-state", localized on the stochastic web in classical phase space, reaching out to the effective boundary of the phase space which is defined by the finite size of the basis which we use for the diagonalization of U.
In conclusion, the web eigenstates of the kicked harmonic oscillator lend support for enhanced quantum transport as observed in Fig. 1, at sharply defined values of the effective Planck constant (parametrized by the Lamb-Dicke parameter), where near-resonant tunneling from the ionic initial state onto the web becomes possible. Since the Lamb-Dicke parameter is tuned easily by variation of the trap frequency ν or of the kicking lattice's wavelength $2\pi/k$, such web-enhanced tunneling from the harmonic oscillator ground state allows for *efficient experimental control* of the diffusion properties of the complex quantum system under study.

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3.1.14 Nonlinear transport processes during patterning of developing organisms

Tobias Bollenbach, Karsten Kruse, and Frank Jülicher

During development of an organism, cellular processes ensure the reliable and precise formation of cellular patterns and morphologies in a concerted way. This regulation involves information exchange between cells and signaling molecules which provide positional information [1]. An important role in this process is played by a particular class of signaling molecules called morphogens. These are produced in specific source cells and subsequently spread into the tissue adjacent to the source where they establish a graded concentration profile. The future properties and function of cells in this adjacent tissue is determined by the local morphogen concentration. Cells respond

to morphogens via receptor molecules on the cell surface to which the morphogens bind specifically. There are certain threshold levels of the morphogen concentration at which the induced cell fate changes. This way, positional information is encoded in the gradient. An important system where the cell biological components which govern these processes are studied is the fruit fly Drosophila. As an example, the experimentally observed gradient of the morphogen Dpp is displayed in Fig. 1.
A key question is by which mechanisms morphogens are transported in the target tissue. Transport mechanisms determine the dynamics of morphogen spreading and are important for robustness and precision of the process. First of all, free diffusion of morphogen molecules in the extracellular space is relevant to morphogen transport [2]. Furthermore, recent experimental data for spreading of Dpp in the wing-disc of Drosophila larvae suggest that active transport of morphogens via the cell interior plays an important role for gradient formation. This so-called transcytosis involves the internalization of bound Dpp-receptor pairs into the cell and the later possibility of the pair to resurface at a different location on the cell surface, see Fig. 2. The fact that the cell is able to control intracellular trafficking suggests that active cellular transport mechanisms are important to achieve robustness and precision of gradient formation.
We investigate transport mechanisms and their role in gradient formation in collaboration with the experimental group of M. González-Gaitán at the Max Planck Institute for Molecular Cell Biology and Genetics in Dresden. To this end, we developed theoretical descriptions of morphogen transport in a two dimensional geometry corresponding to the situation in the wing disc, see Fig. 1. In experiments, the spreading Dpp profile is confronted with small regions of cloned cells which are mutant to specific genes affecting the internalization of receptors by endocytosis. The effect of the clone region

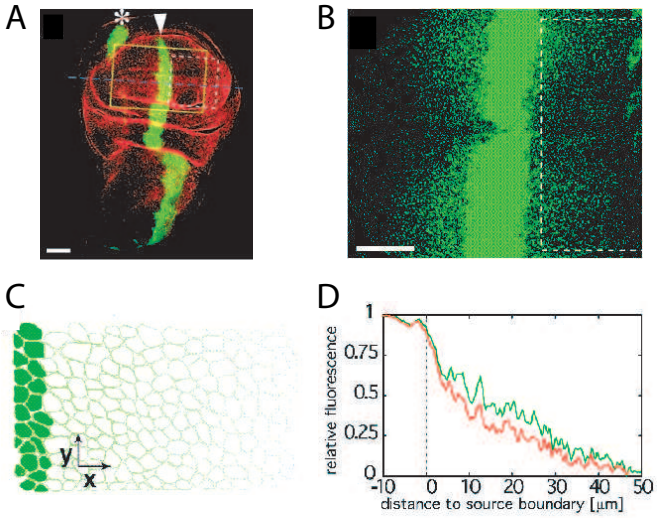

Figure 1: *Gradient of the morphogen Dpp in the Drosophila wing disc. (A) View of the wing disc. Dpp-expressing cells are labeled in green. (B) Magnified view of the Dpp gradient in the region indicated by the yellow box in A. (C) Schematic representation of the wing disc tissue indicated by the dashed white box in B. (D) Fluorescence intensity profile of the Dpp gradient shown in B. Dpp was labeled by a green fluorescent protein (GFP) to be visualized. Scale bars* 50μm. *Image courtesy P. Pantazis and M. González-Gaitán.*

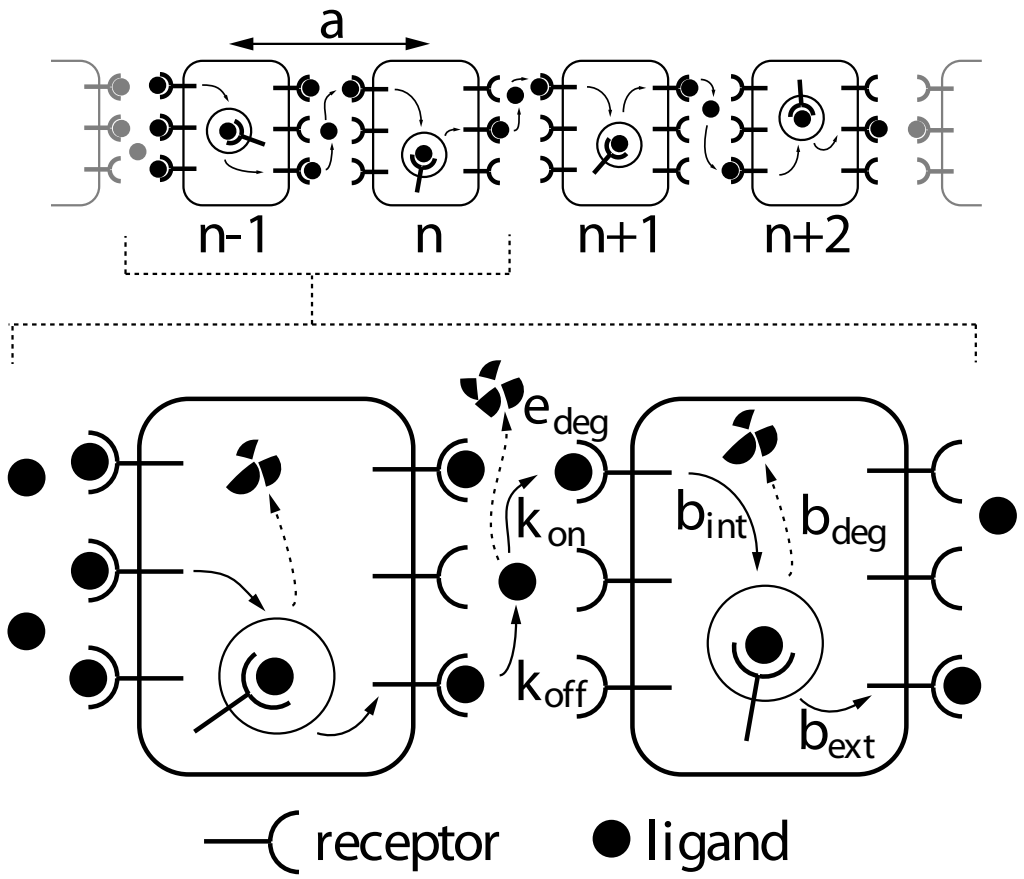

Figure 2: *Schematic representation of transport by transcytosis in a chain of cells of diameter a indexed by n. The rates of morphogen-receptor binding and un-binding, internalization and externalization of morphogen-receptor pairs are denoted $k_{\rm on}$, $k_{\rm off}$, $b_{\rm int}$ and $b_{\rm ext}$. Degradation of morphogen occurs inside the cells with rate $b_{\rm deg}$ and in the extracellular space with rate $e_{\rm deg}$.*

is to generate transient or permanent "shadows" of morphogen profiles behind it [3]. Following the dynamics of spreading of fluorescently labeled morphogen, the effects of the clone on morphogen distributions can be measured and compared to theory, see Fig. 3 [4]. We find that transport purely by extracellular diffusion does neither reproduce the observed concentrations of the morphogens nor those of the cell surface receptors in two different experiments. However, taking into account transport via the cell interior by transcytosis, the experimental observations can be consistently described within a single framework. We thus conclude that transcytosis is an essential transport mechanism for Dpp spreading in the wing disc.

The experimentally observed spreading dynamics can be captured by effective transport equations valid in a continuum limit on scales larger than the cell size [5]. We derive these nonlinear transport equations starting from a discrete array of cells in one or two dimensions, see Fig. 2. Local rates of incorporation of receptors, resurfacing of ligand-receptor pairs, the degradation of ligands as well as diffusion in the space between cells are expressed by a set of coupled differential equations. An adiabatic elimination of fast variables permits us to derive effective transport equations. In the most simple case of

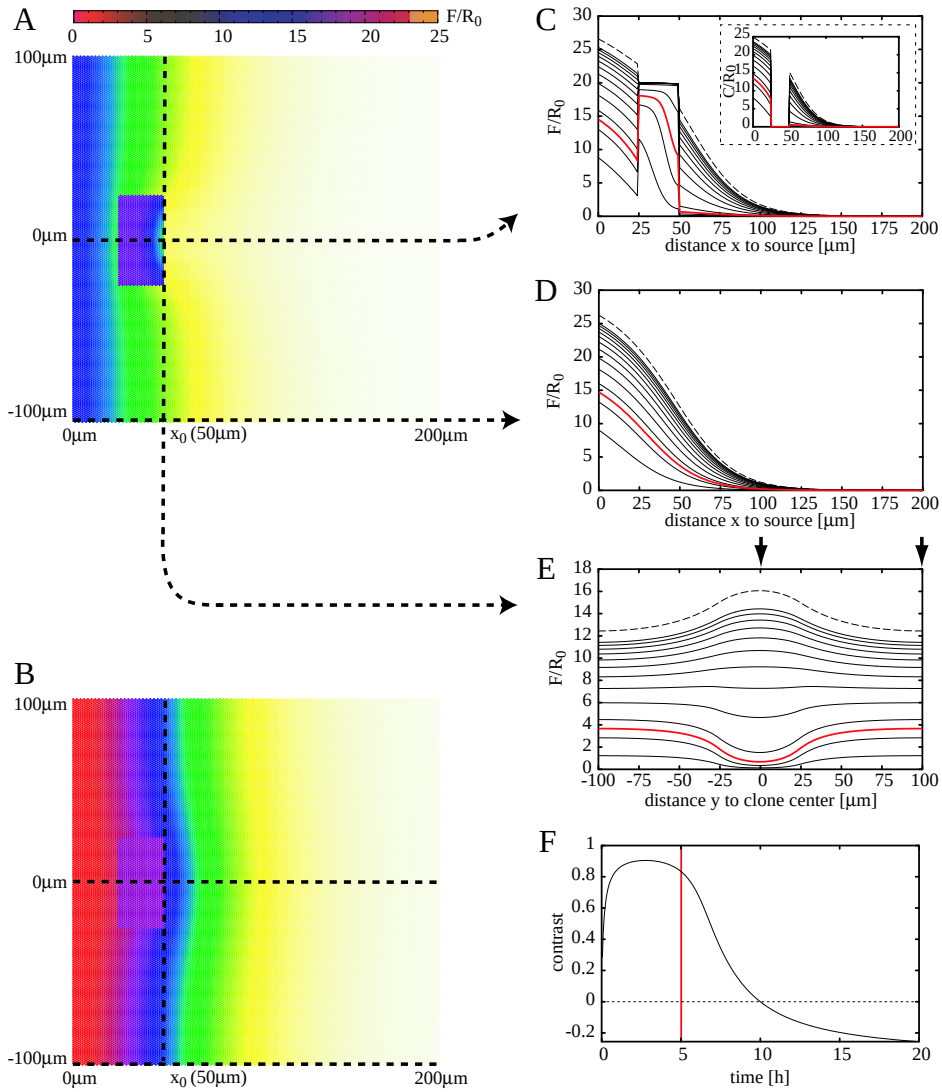

Figure 3: *Evolution of the total morphogen distribution in the extracellular diffusion model with vanishing internalization rates in a rectangular region describing the clone. (A,B) Color coded distribution of the total morphogen concentration F at 5 hours (A) and 24 hours (B) after blocking internalization in the clone region. (C-E) Total morphogen concentration along the dashed lines indicated in (A). Solid black lines are separated by 2h. The dashed lines represent the steady state distributions, the red line the distributions after 5h, the time when the observations were made in the experiments discussed in [3]. The inset in (C) shows the concentration of internal bound morphogen, which vanishes inside the clone. The profile of the morphogen concentration behind the clone is shown in (E). At 5h, a clear shadow is present which vanishes and turns into a persistent anti-shadow. (F) Contrast of the shadow.*

constant receptor number on the cell surface, the total morphogen concentration as a function of position in a one-dimensional description $\lambda(x,t)$ obeys the equation

$$\partial_t \lambda = \partial_x (D(\lambda)\partial_x \lambda) - k(\lambda)\lambda \quad . \tag{1}$$

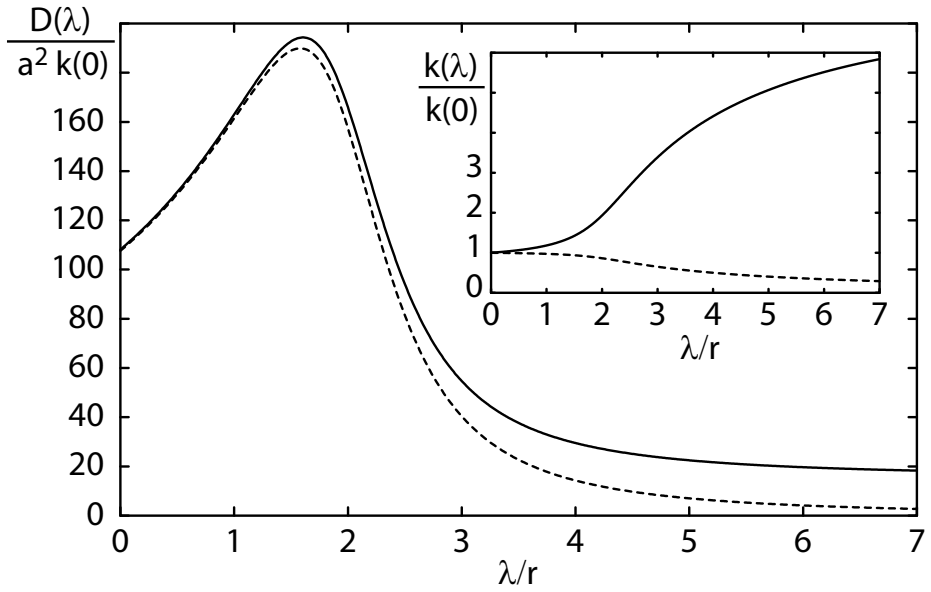

Figure 4: *Effective diffusion coefficient $D(\lambda)$ as a function of morphogen concentration λ in the presence (solid line) and absence of extracellular diffusion (dashed line). Inset: effective degradation rate $k(\lambda)$ as a function of λ in the presence (dashed line) and absence of extracellular degradation (solid line).*

The concentration dependence of the effective diffusion coefficient $D(\lambda)$ and the effective degradation rate $k(\lambda)$ is shown in Fig. 4 for a typical parameter choice.
Using Eq. (1), we can calculate the steady state profile for a given secretion rate of morphogens at the source determined by the morphogen current $j = j_0$ at $x = 0$ as a boundary condition, where $j = -D(\lambda)\partial_x\lambda$. The steady state solution can be expressed as

$$x = -\int_{\lambda(0)}^{\lambda(x)} d\lambda'\; D(\lambda')/j(\lambda') \quad , \tag{2}$$

where the morphogen current j in the steady state is given by

$$j(\lambda) = \left[2\int_0^{\lambda} d\lambda'\; k(\lambda')D(\lambda')\lambda'\right]^{1/2} \quad . \tag{3}$$

The steady state profile behaves for large x as $\lambda \sim e^{-x/\xi}$, with $\xi = (D(0)/k(0))^{1/2}$ being a characteristic length. For small x, extracellular diffusion is relevant and $\lambda \sim e^{-x/\xi_d}$ where $\xi_d = (D_0/e_{\rm deg})^{1/2}$, D_0 denotes the extracellular diffusion coefficient and $e_{\rm deg}$ the extracellular degradation rate. If for simplicity we assume that extracellular diffusion is absent, the steady state profile exhibits formally a singularity at $x = x^* < 0$ where λ diverges as

$$\lambda \sim (x - x^*)^{-1}(-\ln(x - x^*))^{-1/2}. \tag{4}$$

This singularity has a remarkable consequence for these steady state gradients. If the singularity moves closer to $x = 0$, morphogen gradients become robust with respect to variations in the secretion rate j_0. The robustness characterizes how sensitively the position $x(\lambda)$ at which a given concentration λ of the morphogen is present, depends on the secretion rate j_0. We define the robustness as the dimensionless quantity $\mathcal{R}(j_0) :=$

$a(j_0\partial_{j_0}x(\lambda))^{-1}$. Using the steady state solution, we show that the robustness increases rapidly for large currents j_0 as $\mathcal{R} \sim j_0^{-1}e^{j_0^2/j_c^2}$, if extracellular diffusion is absent [5]. The presence of extracellular diffusion limits robustness at large j_0 which is then given by $\mathcal{R}_{\max} = a/\xi_d$, where a denotes the cell diameter and ξ_d the extracellular diffusion length.

In summary, our analysis demonstrates that transcytosis leads to robust morphogen gradients with respect to variation in the morphogen production rate while extracellular diffusion does not. Indications for the robustness of the Dpp gradient in the wing disc have been found [6]. Together, these points again suggest that active transport processes are relevant for gradient formation. In particular, the regulation of transport by the cells through the control of the number of receptor molecules on the cell surface might be important for robust patterning of organisms. Related mechanisms of robust gradient formation have been discussed in Refs. [7, 8]

An important step towards the ultimate identification of the transport mechanism for Dpp will be to quantitatively measure the relevant rates like those of internalization, externalization, degradation, and extracellular diffusion. These rates enter our theoretical description and define the relative contributions of the two transport mechanisms. An important step in this direction is the measurement of apparent diffusion coefficients for Dpp in different mutant backgrounds which are currently performed using fluorescence recovery after photo-bleaching.

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3.1.15 Dynamics of the cytoskeleton: bundles, rings and active gels

Karsten Kruse and Frank Jülicher

The prototype system for the study of active cellular processes is the cell cytoskeleton. It is a complex three dimensional network of protein filaments which plays an essential role in many dynamic cellular processes such as cell locomotion, cell division and intracellular transport. The network of cytoskeletal filaments forms a gel-like material. The cell regulates the structure and the material properties of this network. Furthermore, processes on the molecular scale driven by the energy of a chemical fuel, such as force generation by motor molecules but also the growth and shrinkage of filaments at their ends by polymerization and depolymerization, turn this system into an inherently active material. As a consequence, cytoskeletal networks can exhibit spontaneous dynamic behaviors and active material properties. Examples are complex filament patterns formed by self-organization phenomena. Such patterns can be dynamic and exhibit oscillations. Furthermore, active filament networks are able to generate mechanical stresses and contractile behaviors. On the molecular scale, forces are generated for example by motor aggregates which form mobile cross-links and generate internal stresses in the gel.

A number of simple situations which are biologically relevant motivate our work. Force generating structures in cells occur in the form of so-called stress fibers where actin filaments form bundles which are active and contractile. Such contractile bundles form also during cell division, when a ring of bundled actin filaments assembles around the cell. This ring subsequently contracts and cleaves the two daughter cells. Different but related ring-structures formed by microtubules occur in plant cells. The mechanisms which lead to ring formation in cells and the contractile and dynamic properties of such rings and bundles are still unknown.

We have studied the properties of fluid active filament systems using a microscopic description of filament dynamics on small scales as well as an effective hydrodynamic description of the active gel on large scales [1–6]. Both descriptions can be related which provides insights in how active molecular processes can generate new physical behaviors and effective material properties in the hydrodynamic limits [4]. Within the microscopic framework, we could demonstrate, that polymerization and depolymerization processes together with static cross-linkers can generate active behaviors similar to ones induced by aggregates of motor proteins, see Fig. 1a,b. Thus, very different active microscopic processes can lead to the same effective behaviors on large scales.

In our hydrodynamic description, the filament dynamics is described by two field variables, the filament density ρ and the polarization $\mathbf{p}$, see Fig. 1c. The polarization of the gel is a consequence of the structural polarity of cytoskeletal filaments and characterizes the average orientation of filaments in a small volume. In general, the dynamic equations have the form

$$\partial_t \rho = -\partial_\alpha j_\alpha + s \tag{1}$$

$$\partial_t p_\alpha = w_\alpha \quad . \tag{2}$$

The filament current

$$j_\alpha = \eta \partial_\beta \sigma_{\alpha\beta} \tag{3}$$

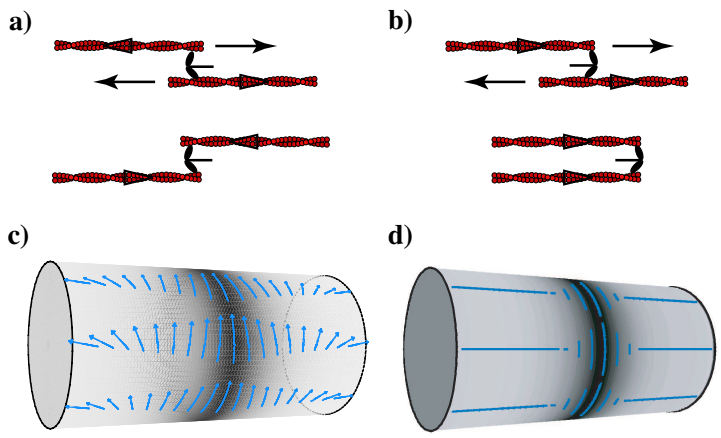

Figure 1: *Active phenomena in cytoskeletal dynamics.* ***a)*** *Relative sliding of two anti-parallel filaments induced by a mobile cross-link formed by molecular motors. On a filament, a motor moves into the direction indicated by the open arrow-head.* ***b)*** *Relative sliding between two parallel filaments typically leads to filament alignment.* ***c,d)*** *Filament patterns on a cylindrical surface. The filament density is indicated by gray levels. (c) Polar ring, the gel polarization is indicated by arrows. (d) Nematic ring, the nematic order is indicated by rods.*

results from the stresses which are locally generated in the gel by active processes and characterized by the stress tensor $\sigma_{\alpha\beta}$. Here, we have assumed that the gel moves with respect to an immobile solvent as is the case in the vicinity of a surface. The stress tensor $\sigma_{\alpha\beta}$, the source terms s related to polymerization and depolymerization of filaments and the rate of change of the polarization $\mathbf{w}$ can be expressed in a generic systematic expansion in powers of the fields which includes all terms allowed by symmetry. In situations where filaments orient in an non-polar way, a nematic order parameter $q_{\alpha\beta}$ is used to characterize the filament pattern, see Fig. 1d.
The power of this approach can be discussed for a cylindrical geometry which is motivated by contractile rings and ring formation in plant cells. The cylinder represents the cell shape, the density ρ and the polarization $\mathbf{p}$ characterizes the filament patterns that form on the cell membrane [5,6]. Fig. 1c,d show examples of stable ring patterns which occur as steady state solutions to our dynamic equations. Such rings can become unstable with respect to oscillatory dynamics. In this case, the ring periodically moves from one end of the cell to the other. Our description also provides information on the stresses which are generated by the filament patterns on the cell surface. We can thus discuss the contractile stresses which for a soft cell leads to invaginations and division.
So far we have discussed active fluids where elastic properties of the gel have been ignored. In many situations, the intracellular material has elastic properties which are important for cellular processes. An important example is cell locomotion where a gel is polymerized at the leading edge of the cell and subsequent contraction of this gel in the cell gives rise to forces which the cell exerts on a substrate and which are relevant

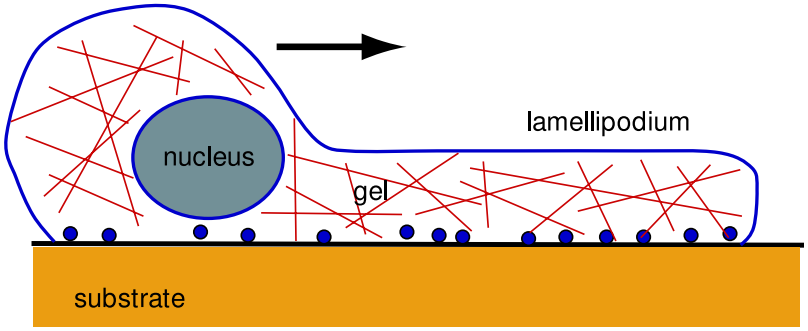

Figure 2: *Schematic representation of a moving cell on a substrate. The cell extents a thin sheet, the lamellipodium, filled by the cytoskeleton that polymerizes at the leading edge. Contraction of the gel in the lamellipodium drags the cell body containing the nucleus. The cell adheres to the substrate by adhesion molecules represented as black dots.*

for the motility of the cell with respect to the substrate, see Fig. 2. This process can be discussed most clearly for sperm of nematode worms. In this case, the cytoskeleton is made of filaments called major sperm protein (MSP) for which no motor molecules exist. This allows for a simpler description without active stresses. During nematode sperm locomotion, the cell body is dragged forward by polymerization of the gel in the front and graded swelling which is induced by a pH-gradient. We have calculated the stress distribution in the MSP-gel using a purely elastic description of the gel including swelling. Cell locomotion emerges if in addition to gel swelling and polymerization we also include the dynamics of the adhesion molecules and their rupture from the substrate if a threshold force is exceeded [7].
In general, the intracellular material combines the aspects discussed above. The cytoskeletal gel is inherently active and stresses and flows are induced in the material. On short times and if active processes are switched off, the material is elastic. We have developed a general hydrodynamic theory of active visco-elastic and polar gels which combines all these limits in a common framework [8]. The theory is based on three conjugate pairs of fluxes and forces which are the basis of a systematic expansion in the viscinity of thermodynamic equilibrium: The strain rate tensor $u_{\alpha\beta}$ is conjugate to the stress tensor $\sigma_{\alpha\beta}$, the rate of change $\dot{\mathbf{p}}$ of the polarization is conjugate to a field h_α and finally, the rate r at which the chemical fuel ATP is consumed is conjugate to the chemical potential difference $\Delta\mu$ of fuel and reaction products. To linear order, we write Onsager relations which couple all processes as symmetry allows. Furthermore, we construct the theory in such a way that it includes the Maxwell model of visco-elastic gels as a special limit if active processes are absent. The resulting constitutive equations of the material are quite rich [9]. For the simple case where the filament orientation is imposed, we find for the relation between stress and strain rate

$$2\eta u_{\alpha\beta} = (1 + \tau\frac{D}{Dt})\{\sigma_{\alpha\beta} + \Delta\mu\zeta\delta_{\alpha\beta} + \Delta\mu\bar{\zeta}p_\alpha p_\beta\} \tag{4}$$

where τ is a relaxation time and D/Dt denotes the co-rotational convected derivative of a tensor.

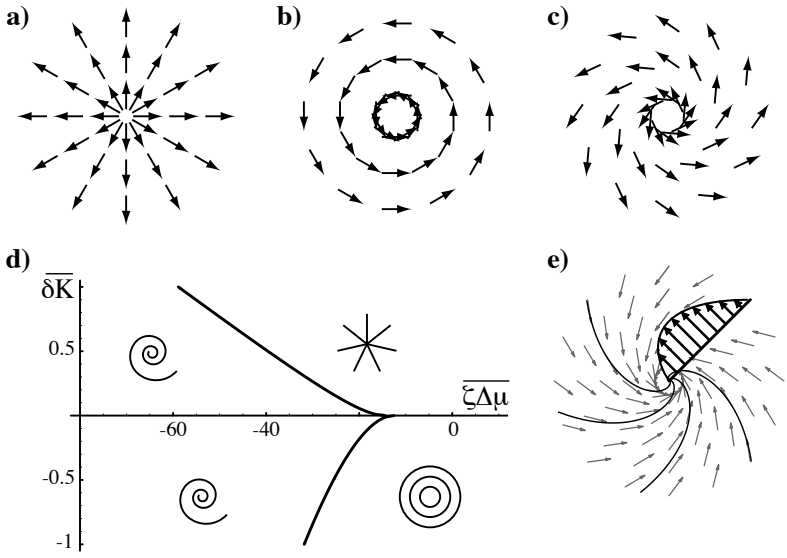

Figure 3: *Topological point defects of the polarization in an active gel,* ***a)*** *aster,* ***b)*** *vortex, and* ***c)*** *spiral.* ***d)*** *Stability diagram of asters and vortices as a function of $\zeta\Delta\mu$ which characterizes the distance to equilibrium. The parameter δK characterizes the elasticity of the orientation field. At thermodynamic equilibrium, $\zeta\Delta\mu = 0$, asters and vortices are stable. Beyond a threshold value of the active stresses, these states become unstable and rotating spirals appear.* ***e)*** *Velocity profile and filament orientation of a rotating spiral defect.*

As a first example for the resulting physical behaviors, we have studied the dynamics of a point defect in the filament orientation field in two dimensions. This is motivated by in vitro experiments of motor-microtubule mixtures where various types of patterns were observed. The theoretical analysis reveals that three types of stable defects exist: asters, vortices and spirals, see Fig. 3a-c. Asters and vortices are the solutions for the particular case where the system is passive, $\Delta\mu = 0$. In an active system these solutions still exist but can become unstable beyond a critical contractile stress generated by active processes, see Fig. 3d. Beyond this instability, the symmetry is broken and spiral patterns appear. Because of their symmetry and the fact that they correspond to a non-equilibrium steady state, they rotate. For a simple choice of elastic properties of the filament orientation, the angular velocity profile as a function of the distance form the singularity r is given by

$$v_\theta(r) = \omega_0 r \log(\frac{r}{r_0}) \quad , \tag{5}$$

where r_0 is the size of the system with $v_\theta(r_0) = 0$, see Fig. 3e. The angular frequency ω_0 can be calculated as a function of the phenomenological parameters and is proportional to $\Delta\mu$.
Thus, these rotating defects provide examples for spontaneous motion and patters generated far from equilibrium. They can be compared to observed rotating spiral patterns in motor filament mixtures.

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3.1.16 Sensory transduction in olfactory cilia

Peter Borowski and Martin Zapotocky

Olfactory cilia are cylindrical dendritic extensions of olfactory sensory neurons. They are located at the surface of the nasal epithelium and serve as the detection units of the olfactory system. Odorant molecules interact with specialized receptor proteins embedded in the membrane of the cilia. This interaction initiates an intra-ciliar transduction cascade shown schematically in Fig. 1. The initial external signal is transduced first into an intracellular chemical signal (production of "second messenger" cAMP) and then into an electrical signal (flux of Ca^{2+}, Na^{+} and Cl^{-} ions, resulting in a change of transmembrane voltage). Calcium ions play a central role in this transduction process: they both amplify the electrical response, and mediate negative feedback on it through several feedback loops.

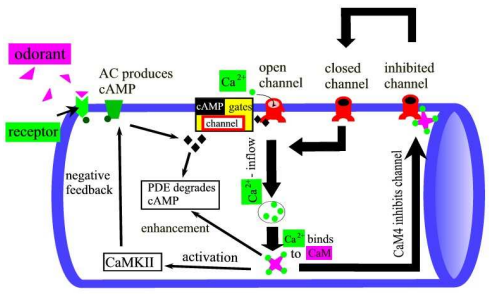

Figure 1: *Scheme of the signal transduction pathway. The binding of odorants to the receptor results in the production of cAMP, which in turn activates* Ca^{2+}*–permeable ion channels. Calmodulin (CaM) reacts with the inflowing* Ca^{2+} *to CaM4 which inhibits the channels, resulting in negative feedback (thick arrows).*

Olfactory cilia exhibit sensory adaptation: following the presentation of a brief odorant stimulus, a repeated presentation of the same stimulus results in a response of reduced magnitude. Fig. 2 shows superimposed experimental recordings of the electrical response of olfactory cilia to two stimuli separated by an increasing time interval. The adaptation effect is seen to persist for a time scale of seconds.
When the cilium is presented instead with a sustained stimulus, the response is oscillatory (Fig. 3), with oscillation period that only weakly depends on the stimulus

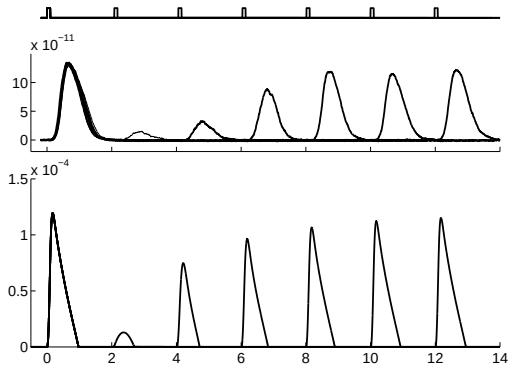

Figure 2: *Adaptation of response to repeated short stimuli.Top row: stimulus trace; middle row: experimental data of Ref. [1]; bottom row: prediction of the model.The horizontal time scale is in seconds.*

strength. We asked the question whether both of these effects — sensory adaptation and oscillatory response — arise from the same molecular mechanism.

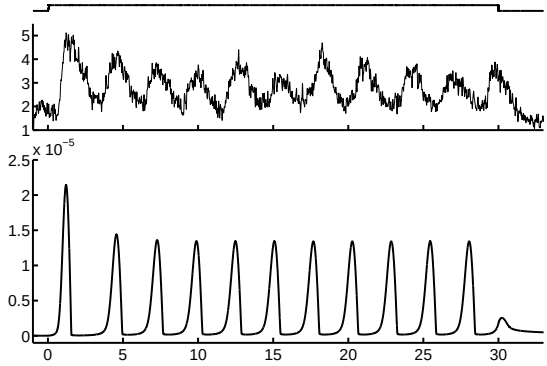

Figure 3: *Oscillatory response to a sustained stimulus. Top row: stimulus trace; middle row: experimental data of Ref. [2]; bottom row: prediction of the model.*

Biochemical data suggest that the adaptation effect is primarily due to the negative feedback mechanism in which Ca^{2+} reacts with calmodulin and inhibits the Ca^{2+}–permeable ion channel (Fig. 1). Chemical oscilations, however, typically depend on the presence of positive feedback (autocatalysis). [This the case in the most common mechanism for Ca^{2+} oscillations, calcium-induced calcium release from intracellular stores]. We therefore first asked if in principle, the negative feedback loop defined above can give raise to a Hopf bifurcation. To answer this question we used the powerful framework of stoichiometric network analysis [3]. This method uses the decomposition of the network dynamics into "elementary currents" to formulate general criteria for when a steady state becomes unstable. We found that a Hopf bifurcation is possible provided that Ca^{2+} extrusion from the cilium operates near saturation.
To obtain quantitative results, we formulated a detailed kinetic model for the concentrations of intra-ciliar calcium Y, activated channels X_a, calmodulin loaded with calcium Z, and channels inhibited by calmodulin X_i. The resulting rate equations

$$\frac{d}{dt}X_a = k_{\rm act}(X_{\rm tot} - X_a - X_i) - k_1 X_a - k_2 X_a Z \quad (1)$$

$$\frac{d}{dt}Y = \frac{1}{\sigma} i_Y X_a - k_3 \frac{Y}{Y+K_Y} - 4k_4 Y^2 (Z_{\rm max} - Z - \frac{1}{\sigma}X_i) + 4k_5 Z \quad (2)$$

$$\frac{d}{dt}Z = k_6 Y^2 (Z_{\rm max} - Z - \frac{1}{\sigma}X_i) - k_7 Z - \frac{1}{\sigma}k_8 Z(X_{\rm tot} - X_i) + \frac{1}{\sigma}k_9 X_i \quad (3)$$

$$\frac{d}{dt}X_i \;=\; k_{10}Z(X_{\rm tot}-X_i)-k_{11}X_i \qquad (4)$$

depend on a number of kinetic constants, almost all of which we were able to deduce from published biochemical and electrophysiological data. Fig. 2 shows the time course of $[Ca^{2+}]$ obtained by numerically solving the system under the conditions of the adaptation experiment (here k_{act}, the parameter representing the stimulus strength, was fitted to obtain good agreement with experiment). Fig. 3 shows the Ca^{2+} oscillations predicted by our model (here k_{act} was appropriately scaled to take into account the difference in concentration of the odorant cineole used in the two experiments, and there are no remaining free parameters). The model produces oscillations with approximately correct frequency, as well as the ratio of the height of first and second peaks. We also obtain a reasonable agreement with the experimentally determined upper boundary of the oscillatory region in terms of stimulus strength, and capture the observed effect of increase in oscillation period upon decreasing extraciliar sodium concentration.

In the regime where the odorant concentration is very low, the deterministic description of Eqs. (1)–(4) becomes inadequate. In collaboration with F. Jülicher and M. Gopalakrishnan, we are studying this regime to characterize the limits on the precision of olfactory signaling. We have developed a model in which we explicitly treat the stochastic gating kinetics of ion channels, as well as spatial and temporal fluctuations in calcium concentration. The presence of feedback leads to non-Markovian kinetics of the channels, which we treat analytically in a perturbative framework.

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3.1.17 Noise-enhanced categorization in recurrent neural networks

Christopher Monterola and Martin Zapotocky

The role of noise in neural information processing is a topic of much current interest. It has received significant attention particularly in the context of stochastic resonance [1] — a mechanism in which noise is used to enhance the detection of weak signals of a particular frequency. In the case of stochastic resonance, information is encoded in the temporal structure of the stimulus. This is in contrast to "spatial" encoding, in which the stimulus is mapped into the pattern of activity across a set of neurons at a specific time. As opposed to the case of frequency-encoding systems, the beneficial role of noise in spatially encoding systems has not been investigated extensively.

In this project, we contrast the cases of feed-forward and recurrent networks performing categorization of transient, spatially-encoded stimuli. We first train a feed-forward

network to recognize a set of Gaussian-distributed profiles of unit strength. We then evaluate the performance of the network for stimuli of arbitrary strength and in the presence of noise. For stimuli below a certain strength, the feed-forward network fails to classify correctly, independently of the magnitude of noise. To obtain enhancement of performance by noise, we reconnect the feed-forward network into a recurrent network (Fig. 3.1.1). We present the stimulus at the initial time step, and let the network evolve to its attractor state before the performance is evaluated. The recurrently-reconnected network (RNN) has a high success rate of classification of subthreshold stimuli provided that noise of suitable magnitude is added during the network dynamics.

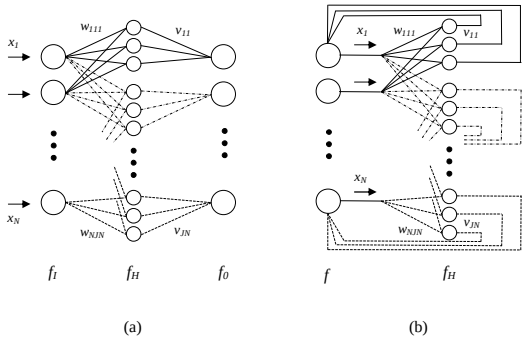

Figure 1: *Network architecture.* (*a*) *Three-layer fully connected feed-forward network with* $f_I(x) = x$. (*b*) *The collapsed two-layer recurrent network, now with each node acting as a thresholding neuron.*

The standard three-layer feed-forward neural network (NN) of Fig. 3.1.1a has the following dynamics. The mapping of the N inputs $\{x_i; i = 1, 2, ...N\}$ to the N outputs $\{\Phi_k; k = 1, 2, ...N\}$ as mediated by J hidden nodes per input is defined by the expression :

$$\Phi_k = f_0(\sum_{j=1}^{J} Y_{jk} v_{jk}); \qquad Y_{jk} = f_H(\sum_{i=1}^{N} f_I(x_i) w_{ijk}) \tag{1}$$

where $\{w_{ijk}\}$ and $\{v_{jk}\}$ are the synaptic weights that are fixed during training. The hidden (f_H) and the output (f_0) nodes have thresholded activation functions while the input (f_I) nodes have linear activation functions. (The results shown below were obtained for N=25 and J=3.)

During training, we feed inputs of form: $x_k = S \exp(\frac{-[k-X]^2}{2\sigma})/(\pi\sigma)^{1/2}$, i.e. Gaussian profiles with strength (S), mean (X) and variance (σ). Learning was achieved by updating the weights so that these inputs are mapped into one of the 3 desired memory states ($\boldsymbol{\psi}^1, \boldsymbol{\psi}^2, \boldsymbol{\psi}^3$). These were chosen to be Gaussian profiles with identical strength and variance ($S = 1$, $\sigma = 2$) but varying mean ($X^1 = 7$, $X^2 = 13$, $X^3 = 19$). Following 10^5 epochs of training, the non-recurrent network can categorize perfectly the Gaussian inputs with unit strength.

To evaluate the performance of the network in the presence of noise, uniform white noise of width α and zero mean was added to the state $\boldsymbol{x}^t$ at each time step, starting at $t = 0$. In a biological neural network such noise can correspond e.g. to spontaneous activity or to synaptic noise. We define the success rate, S_{rate}, as the fraction of runs starting with a given stimulus that resulted in convergence to the correct memory state. For the feed-forward network, S_{rate} decays with increasing α, and reaches nearly 0 at $\alpha = 0.4$ for $S^{t=0} < 0.5$ (Fig. 3.1.1a). The non-recurrent network thus does not benefit from noise.

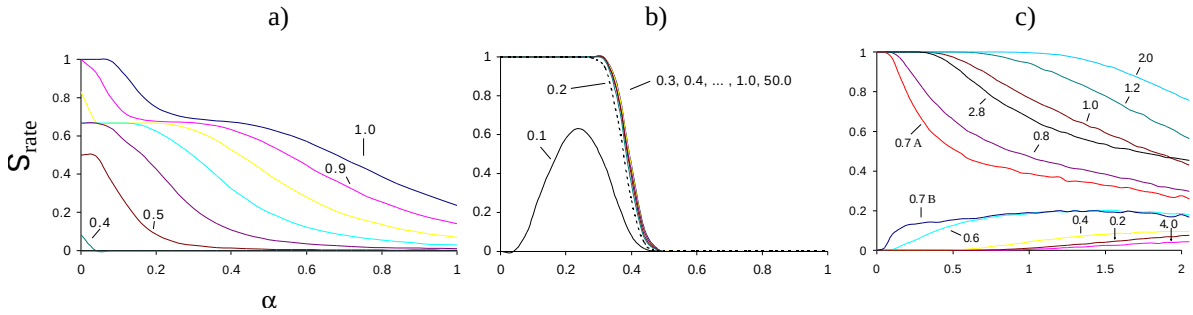

Figure 2: *Success rate of a) non-recurrent, b) recurrently-reconnected, and c) Hopfield networks in the presence of noise. Average S_{rate} is shown as a function of noise strength α at the indicated stimuli strengths $S^{t=0}$.*

A different result is obtained for the recurrently reconnected network (RNN). In the absence of noise, the RNN fails to respond to stimuli of strength $S^{t=0} < 0.12$ (i.e., it evolves as if no stimulus were presented). When noise is added, however, such subthreshold stimuli can be classified correctly (Fig. 3.1.1b). The shape of the $S_{rate}(\alpha)$ curves is reminiscent of stochastic resonance: the highest S_{rate} is obtained at a non-zero optimal noise strength, α_{opt}. The average S_{rate} for signals of strength $S^{t=0} = 0.1$ reaches 60% at $\alpha_{opt} \approx 0.24$ — thus the optimal noise strength exceeds the stimulus strength.

The origin of the optimal noise strength can be understood by examining the attractors of the dynamics of the system. The trajectories $\boldsymbol{x}^t$ for the noiseless case are visualized in Fig. 3.1.1, where the three axes (d_1, d_2, d_3) are the vector projections of $\boldsymbol{x}^t$ on the three target states $\boldsymbol{\psi}^i$ (in the units of $|\boldsymbol{\psi}^i|$). By construction, the target states are stable fixed points of the dynamics. The trajectories form four clusters, three of which converge to one of $\boldsymbol{\psi}^i$, and the fourth cluster consists of a thin region (with thickness $\Delta d \approx 0.24$) oriented along the diagonal directions (see Fig. 6*b*). In the latter region, $\boldsymbol{x}^t$ asymptotically alternates between ($d1$, $d2$, $d3$) $\simeq$ (0, 0, 0) and (0.68, 0.69, 0.68). The attractor of this region, which includes the zero stimulus trajectory, is thus a limit cycle of period two. In the presence of noise, the trajectory can switch in between the basins of attraction of the zero-noise system. When the noise strength α becomes comparable to the thickness $\Delta d \approx 0.24$, the trajectories starting in the subthreshold basin are likely to escape from it. If noise is too strong ($\alpha > 0.29$), the trajectory is unlikely to become permanently trapped in the vicinity of one of the target states, and instead hops randomly among their basins of attraction. The existence of the optimal value of noise strength α_{opt}, is then seen to be a compromise maximizing the chance of escaping the basin of subthreshold stimuli and subsequently not escaping the basin of attraction of the desired memory state.

Can these arguments be generalized to arbitrary recurrent neural networks? To answer this question, we constructed a Hopfield network (a one-layer recurrent network with symmetric weights), with three memory states ${}^{\mathbf{H}}\boldsymbol{\psi}^q$ similar to those in the RNN case. The success rate S_{rate} of the Hopfield network in the presence of noise is shown in Fig. 3.1.1c. S_{rate} never exceeds 1/3, i.e. the success rate that corresponds to classification performed at random. Therefore the implemented Hopfield network does not show noise-mediated categorization. This illustrates that the conditions necessary for noise-mediated detection of subthreshold stimuli will not always be met in

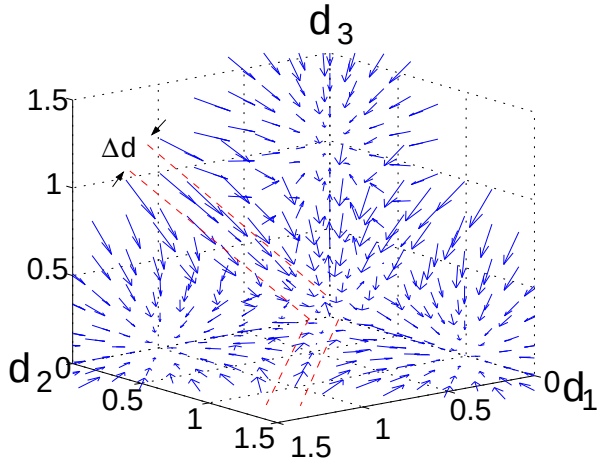

Figure 3: *Flow diagram of the RNN. Shown are the projections d_i of the state $\boldsymbol{x}^t$ on the memory states $\boldsymbol{\psi}^i$. Included are trajectories for stimuli from the set $0 \leq S^{t=0} \leq 2$; $1 \leq X^{t=0} \leq 25$; $1 \leq \sigma^{t=0} \leq 25$.*

recurrent neural networks. Compared to the RNN case, the size of the basin of attraction in the Hopfield network for the zero-stimulus fixed point $\{x_k = -1\}$ is larger, both in absolute terms and relative to the size of basins of attraction for the memory states ${}^{\mathbf{H}}\boldsymbol{\psi}^q$. In addition, the dynamics is strongly influenced by the spurious fixed points $\mathrm{sgn}(\pm{}^{\mathbf{H}}\boldsymbol{\psi}^1 \pm {}^{\mathbf{H}}\boldsymbol{\psi}^2 \pm {}^{\mathbf{H}}\boldsymbol{\psi}^3)$. When designing a neural network capable of noise-mediated categorization, particular care should be given to the minimization of the basins of attraction of unwanted attractors.

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3.1.18 Rheology and microscopic topology of entangled polymeric liquids

Carsten Svaneborg and Ralf Everaers

The relation between the complex viscoelastic properties of polymer liquids and their microscopic structure and dynamics is a key issue in modern materials science and biophysics [1]. A prototypical example is natural rubber. Strictly speaking, natural rubber is a (highly viscous) liquid, even though over a large frequency range it presents the same rubber-elastic response to oscillatory mechanical deformations as vulcanized rubber [2]. This response can be characterized by a temperature and concentration dependent material constant, the plateau shear modulus G_N^0, which is of the order of 10^6 Pa, or five orders of magnitude smaller than the shear moduli of ordinary solids. The origin of this behavior can be traced back to the molecular scale where flexible polymers act as *entropic* springs where the relaxation of tension is due to (topologically constrained) Brownian motion: Similar to entangled ropes, polymer chains can slide past but not through each other. Tube models [1,3] of polymer dynamics and rheology are based on the idea that entanglements confine chain fluctuations to a narrow region along the coarse-grained chain contour.

What has been lacking, however, is a good understanding of the microscopic foundations of the tube model. Entanglements impose topological constraints on polymer conformations [4] similar to those one experiences in manipulating a knotted string. So far theoretical and computational efforts to introduce elements from mathematical knot theory into polymer statistical mechanics have not led to a systematic derivation of the tube model or its parameters.

In Refs. [6, 7] we followed a different strategy and introduced a physically motivated analysis of the melt topology. Our method is based on the concept of primitive paths introduced by Edwards [5] to complement his tube model [3]. Edwards considered a test chain embedded in an array of rigid, infinitely thin, spatially fixed line obstacles representing the constraints imposed by the other polymers on thermal fluctuations of the test chain. He identified the random walk-like axis of the tube with what he called the "primitive" path: the shortest path between the endpoints of the original chain into which its contour can be contracted without crossing any obstacle. Similar to the tube, the primitive path is usually discussed without specifying the relation between the obstacles and the melt structure. In Refs. [6, 7] we argued that the obstacles encountered by a test chain are themselves polymers with identical properties. As a consequence we proposed to simultaneously apply the primitive path analysis to all polymers in the system.

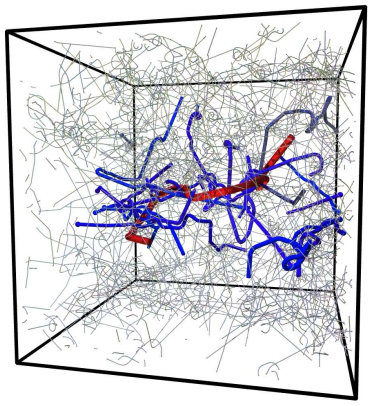

Figure 1: *Result of the primitive path analysis of a melt of 200 chains of* 350 *beads. The figure shows the primitive path of one chain (red) together with all of those it is entangled with (blue). The primitive paths of all other chains in the system are shown as thin lines.*

The implementation of this idea into a simulation code for bead-spring chains is straightforward. Figure 3.1.1 shows that resulting primitive paths consist of straight segments of strongly fluctuating length and more or less sharp turns at entanglement points between two paths. Being both random walks, the orginal chains and the primitive paths can be characterized by a Kuhn length (l_K and a_{pp} respectively) and a contour length, (L and L_{pp} respectively) which are related by $L_{pp}a_{pp} \equiv Ll_K$. Due to their shorter contour length, the primitive paths have a correspondingly larger Kuhn length in order to reach the same spatial extension as the original chains [1]. (In contrast, the packing length $p \equiv (\rho_{chain} l_K L)^{-1}$ which characterizes the length scale where different chains start to spatially interpenetrate is invariant under the primitive path analysis.) To establish the microscopic foundation of the tube model, we used the standard expression [1]

$$G_N^0 = \frac{4}{5}\frac{k_B T}{p\, a_{pp}^2}, \tag{1}$$

which relates the plateau modulus to the Kuhn length of the primitive path. The parameter-free mapping of our results to the available experimental data from all major classes of synthetic polymers in Figure 2 suggests that our topological analysis enables the tube model to predict plateau moduli from first principles.

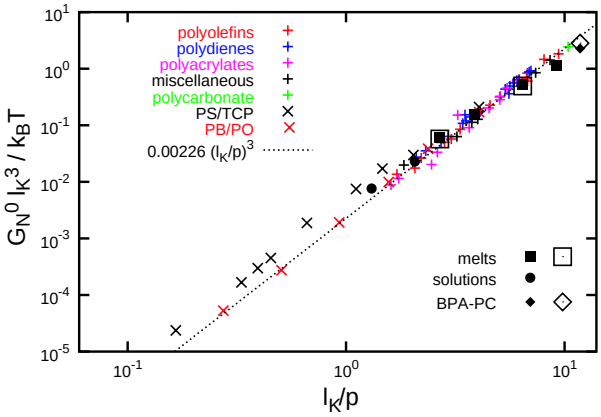

Figure 2: *Dimensionless plateau moduli Gl_K^3/k_BT as a function of the dimensionless ratio l_K/p of Kuhn length l_K and packing length p. The figure contains (i) experimentally measured plateau moduli for polymer melts (+, colors mark different groups of polymers as indicated) and semi-dilute solutions (×), (ii) plateau moduli inferred from the normal tensions measured in computer simulation of bead-spring melts (□) and a semi-atomistic polycarbonate melt (◇) under an elongational strain, and (iii) predictions of the tube model Eq. 1 based on the results of our primitive path analysis for bead-spring melts (■), bead-spring semi-dilute solutions (●) and the semi-atomistic polycarbonate melt (◆).*

In the near future, we plan to extend our analysis to isotropic solutions of semi-flexible polymers such as actin, to investigate the dynamics of the primitive paths, and to link the PPA to our recent results on of the relation between the macroscopic elastic properties of polymer networks and the length-scale dependent microscopic deformations [8–10]. Besides assisting in the systematic development of rheological theories the primitive path analysis also opens up new practical opportunities: While new algorithms allow the equilibration of the *static* structure of polymeric melts in (atomistic) simulations, the determination of the time-dependent viscoelastic properties from atomistic molecular dynamics simulations is still out of question. However, using our approach it should also be possible to systematically link the atomistic structure to dynamic simulations on primitive path level. Since these ideas are neither restricted to monodisperse samples, nor to linear chain architectures, small deformations or equilibrium systems, they may help pave the way to the computer assisted development of materials with customized rheological properties.

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3.1.19 Nucleosome core particle interactions in chromatin fibers: fiber stiffening and hairpin formation

Ralf Everaers

DNA of all eucaryotic organisms is wrapped around millions of cylindrical protein spools, so-called histone octamers. Each complex has a radius of 5 nm and a height of 6 nm and – together with the stretch of linker DNA connecting to the next such spool – is called nucleosome, the basic unit of the chromatin complex [1]. While the structure of the nucleosome core particle (the protein spool with the 2 turns of wrapped DNA) is known up to atomistic resolution [2] there is still considerable controversy about the details of the structure on larger scales. For low salt concentrations a 'beads-on-a-string' structure is observed, sometimes referred to as the 10-nm fiber. For higher salt concentrations (> 40 mM) the fiber appears to thicken into a condensed structure with a diameter of roughly 30 nm [3]. The degree of compaction also depends strongly on the presence of linker histones. They cause the in- and outcoming DNA to form a short stem-like structure [4]. In the absence of linker histones the entry-exit angle of the in- and outcoming DNA is larger, leading to more open structures. At present, it is not clear whether the 30 nm-fiber is more appropriatly described by the solenoid [5] or the crossed-linker model [6]. Even less is known about how chromatin folds into chromosomes on larger scales and about the role of chromatin in epigenetic gene regulation.

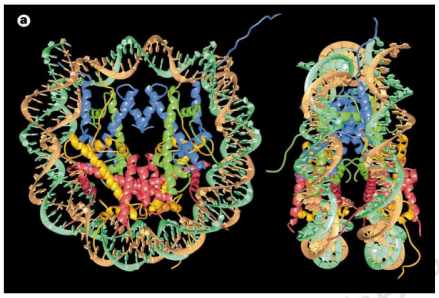

Figure 1: *Structure of the nucleosome core particle at atomistic resolution [2]: A DNA double helix consisting of 147 base pairs wrapped around a cylindrical complex of eight histone proteins.*

There is little hope that these questions could be addressed in brute-force atomistic simulations even though they could built on the experimentally known structure of the

core particles. Typical DNA simulations deal with 20 base pair oligomers compared to 200 base pairs contained in a single nucleosome. Problematic for all attempts to model chromatin are the soft parts of the nucleosome. The charges on the linker histones H1/H5 and the histone tails are under biochemical control, allowing the cell to regulate the stem formation and the attractive interactions between nucleosomes.

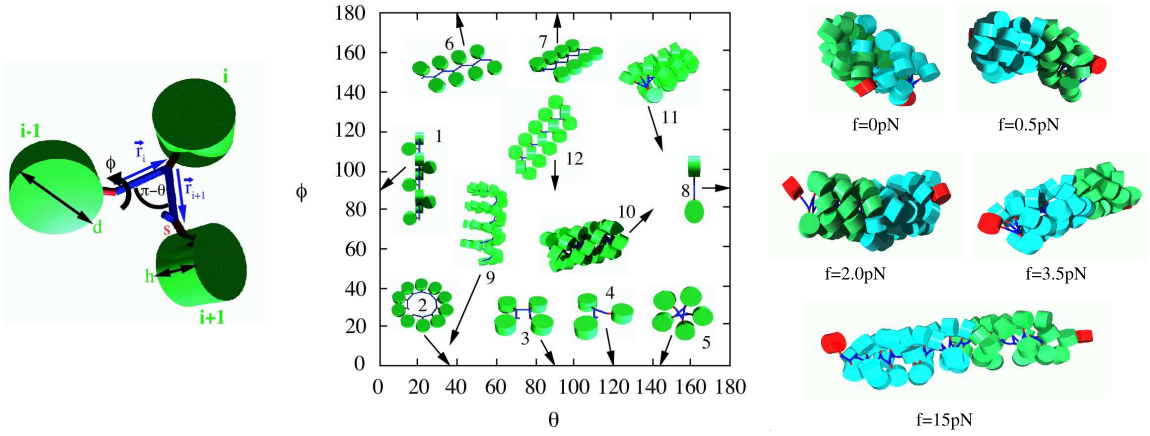

Figure 2: *Lhs: Portion of the model fiber including three nucleosomes connected via stems (red) to the DNA linkers (blue). Also indicated are the two underlying angles: the deflection angle θ and the rotational angle ϕ. Center: Examples of two-angle fibers with the arrows denoting their position in the (θ, ϕ)-plane. Rhs: Snapshots of fiber conformations in the presence of weak attractive interactions between the core particles ($4k_BT$ per pair at contact). An external stretching force of the order of 2 pN is required to open the hairpin conformation.*

An alternative are coarse-grained descriptions based on a two-angle model of the chromatin fiber [6]. While some of the geometrical aspects of chromatin folding and the mechanical properties of the linker-DNA backbone can be calculated analytically [7–9], computer simulations allow the inclusion of thermal fluctuations and (generic) internucleosome attractive and excluded volume interactions [10, 11]. In Ref. [12] we have extended our earlier work on the structure and elasticity of DNA [13] to shed new light on apparently contradictory findings on the mechanical properties of 30 nm chromatin fiber: While the mechanical theories [8, 9] suggest a bending persistence length of the order of 20 nm (compared to 50 nm for DNA and a fiber *diameter* of 30 nm!), Langowski and coworkers [11,14] have presented convincing evidence from experiments and simulations for much larger persistence length of the order of 300 nm. In spite of this large bending rigidity, there are indications that chromatin fibers curl up into chromonema fibers [15, 16] with diameters ranging between 60 to 130 nm. Furthermore, the quasi-plateau at 5 pN that Cui and Bustamante observed in their stretching experiments of chromatin fibers points to rather delicate features in the structure of the 30 nm fiber (for comparison, the B-S transition in DNA is observed at a critical force of 65 pN [18]).

Our results [12] clearly show that the stiffness of dense fibers is dominated by excluded volume interactions between nucleosomes. The observed persistence lengths of the order of 250 nm exceed estimates based on the linker backbone elasticity by one order of magnitude. Already for relative short (and therefore effectively stiff) fibers weak attractive interactions between the core particles (4 k_BT at contact) are sufficient to

induce the formation of hairpin defects, i.e. of a structural feature *beyond* the 30 nm fiber. In our simulations the hairpin opening led to a pseudo-plateau at 2 pN in the force-extension curve. Quite interestingly, the characteristic length scale associated with the observed hairpin defects coincides with the observed diameters of chromonema fibers.
Currently we are working on local structural transitions in chromatin fibers triggered by changes of the internucleosomal interactions, on an extensive comparison between solenoid and crossed-linker conformations of 30 nm-fibers and on topological aspects of the folding of DNA into chromatin fibers.

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3.1.20 Mesoscopic transport beyond universality

Henning Schomerus

One of the main goals in the theory of mesoscopic systems is to describe their equilibrium and non-equilibrium properties without resorting to microscopic details. Disordered mesoscopic systems indeed enjoy a large degree of universality, both in their spectral statistics (for closed systems) as well as in their transport properties (for open systems). Prominent examples are universal degrees of level repulsion, which follow

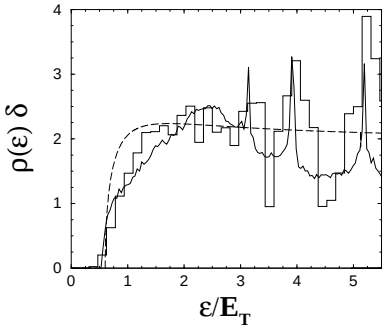

Figure 1: *The density of states $\rho(\varepsilon)$ (rescaled with the mean-level spacing $\delta = h/t_H$) for a model of a quantum dot next to a superconductor with $t_D/t_B = 5$ and $t_{\rm Ehr}/t_B \approx 4.4$ (solid line) is compared to SRMT (histogram) and the RMT prediction (dashed line).*

the Wigner surmise, and universal conductance fluctuations of the order of the conductance quantum e^2/h. An all-encompassing framework to describe these phenomena is random-matrix theory (RMT), which is applied either to the Hamiltonian or to the scattering matrix. RMT assumes that all modes are well mixed, hence, that the system displays well-developed wave-chaos. Impurities serve well for this purpose, since s-wave scattering couples into all directions with the same strength.

In clean ballistic systems, scattering is off the boundaries, which is not as diffractive as the scattering from an impurity, and hence wave chaos takes a longer time to establish itself. Does this imply deviations from universality, and to which extent? This question interests us for various reasons: i) it forces us to understand the limits and conditions of universality and RMT, ii) it forces us to extent both concepts, iii) the deviations themselves are interesting, since present-day experiments (and future device physics) aim at the accentuation and intensification of quantum effects, not at their leveling-out.

A good starting point to investigate the departure from universality is the setting of classically chaotic systems, for which limits are known in which RMT *does* apply. Classical ergodicity restricts the number of relevant parameters to four time scales: The mean time between encounters with the boundary t_B, the mean dwell time t_D, the inverse Lyapunov exponent λ^{-1}, and the Heisenberg time t_H. Wave chaos is established for times larger than the Ehrenfest time, which comes in three different variants depending on the quantity studied:

(a) $t_{\rm Ehr} = \lambda^{-1} \ln(t_B t_H/t_D^2)$ for transport properties,

(b) $t_{\rm Ehr} = \lambda^{-1} \ln(t_H/t_D)$ for escape out of the system, and

(c) $t_{\rm Ehr} = \lambda^{-1} \ln(t_H/t_B)$ for spectral properties of closed systems.

The differences originate in the number of passages through the openings of the system (two in the case of transport; one for escape; and none for closed systems). Cases (a) and (b) refer to open systems, with the dwell time t_D in the typical range $t_B \simeq \lambda^{-1} \ll t_D \ll t_H$. Universality breaks down when $t_{\rm Ehr}$ becomes of order t_D, which is achieved in the classical limit $t_H/t_B \to \infty$. Case (c) applies to closed systems and is less interesting since the relevant time scale is $t_H \gg t_{\rm Ehr}$.

We systematically studied transport- and escape properties in open quantum systems and identified the phenomenology of the deviations from universality. The results can be explained by an amended RMT which incorporates the short-time dynamics semiclassically (SRMT). Results are presented in Figures 1-4.

Figure 1 shows the density of states in a model of a quantum dot coupled to a superconductor [1], which falls into the class (a) because of Andreev particle-hole conversion at the interfaces. At the Fermi energy this process is accompanied by total destructive interference, which gives rise to a gap of order $E_T = h/t_D$. A finite Ehrenfest time

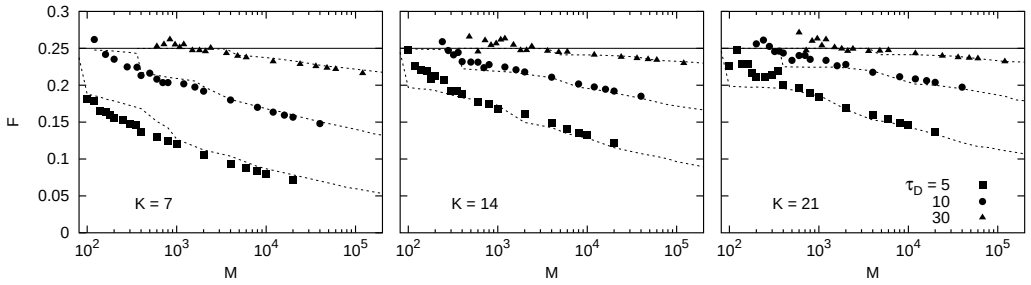

Figure 2: *Shot noise (normalized to the Poissonian value) as a function of $M = t_H/t_B$, for various degrees of chaos K and dwell times t_D (both in units of t_B). The curves are the prediction of SRMT.*

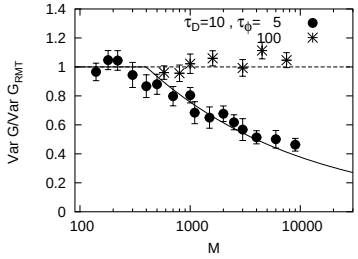

Figure 3: *Variance of the conductance fluctuations (normalized to the RMT value) as a function of $M = t_H/t_B$. Each data set is for a fixed value of t_D and dephasing time τ_ϕ (in units of t_B). The curves are the prediction of SRMT.*

weakens the destructive interference because it allows to form states along sufficiently short classical trajectories. Hence, if $t_{\rm Ehr} \gtrsim t_D$ the gap is reduced and the density of states develops system-specific fluctuations, which are amenable to SRMT.

Figure 2 shows the shot noise in the model of the quantum dot [2] as a function of $M = t_H/t_B$. This transport property [class (a)] is suppressed below the RMT value by a factor $\exp(-t_{\rm Ehr}/t_D)$ when the degree of wave chaos is reduced by either increasing $M = t_H/t_B$ or the Lyapunov exponent $\lambda \simeq \ln K/2$.

Universal conductance fluctuations and the weak-localization correction also fall into class (a), but turn out to be more robust than the mean density of states and the shot noise, since only a few wave-chaotic channels are needed in order to bring these quantum-interference effects into existence. We verified that departure from universality *does* occur when dephasing is taken into account [3]. Figure 3 exemplifies this for the case of universal conductance fluctuations, which are suppressed below the RMT value by a factor $\exp(-t_{\rm Ehr}/\tau_\phi)$, where τ_ϕ is the dephasing time.

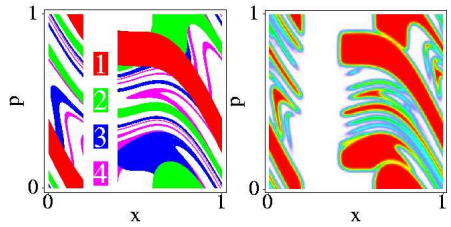

Figure 4: *Classical phase-space regions of escape after $n = t/t_B < t_{\rm Ehr}/t_B$ bounces off the boundary (left) are compared to the support of fast-decaying states.*

Deeper insight into the effect of the Ehrenfest time can be obtained by studying the quasi-bound states of an open system [4]. This concerns the escape out of the system and hence falls into class (b). We find that a large number of very short-lived states is formed in the part of the classical phase space where escape is quicker than $t_{\rm Ehr}$. The fraction of states with RMT characteristics shrinks to zero in the semiclassical

limit. This can be translated into a fractal Weyl law for the long-living states (which are associated to the universal fluctuations in the RMT regime). Such laws have been previously predicted by quantization of the classical repeller, based on the Gutzwiller trace formula for chaotic systems. We find that the effect can be explained on the mean-field level, which allows us to consider non-chaotic situations as well. Figure 4 demonstrates the mean-field correspondence of short-lived states with classical regions of fast escape for the case of a soft-chaotic system (the phase space is divided into stable and unstable regions).
Traditionally, semiclassics and random-matrix theory have been viewed as complimentary methods. It is good to see that they can be combined to open up new areas of applicability where each method by itself was at a failure.

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3.1.21 Multiscaling in Anderson localization

Mikhail Titov and Henning Schomerus

Anderson localization is one of the most remarkable phase-coherent phenomena. It reveals itself in an exponential decay of the wave function of a classically free particle. This phenomenon is a result of multiple phase-coherent backward scattering, which is especially pronounced for a particle restricted to a single spatial dimension (to a line). Small fluctuations in the potential landscape do not affect the classical motion of a particle, while quantum-mechanically they can act as an effective potential barrier.
Unlike many other phase-coherent phenomena, Anderson localization cannot be understood within the well-developed framework of quasi-classical theory and requires a thorough theoretical investigation. At present, the detailed theory is limited to a simple class of one-dimensional non-interacting systems, which have many specific features of their own. It remains to be a challenge to distinguish the universal properties of these systems from those which are model-dependent.
In a series of recent works [1–4] we expand the existing theory of localization to a broader class of models. In particular we study the effects of lattice symmetry on the universal properties of the conductance, density of states, time-delay etc. The analytical method developed in Ref. [1] appears to be very successful in the scaling analysis of the universal fluctuations of these quantities. The general arguments given by Anderson, Thouless, Abrahams, and Fisher as early as in 1980 on the basis of scaling theory provide us with the conjecture that the conductance fluctuations in disordered metals are universally characterized by a single parameter. Our analytical approach

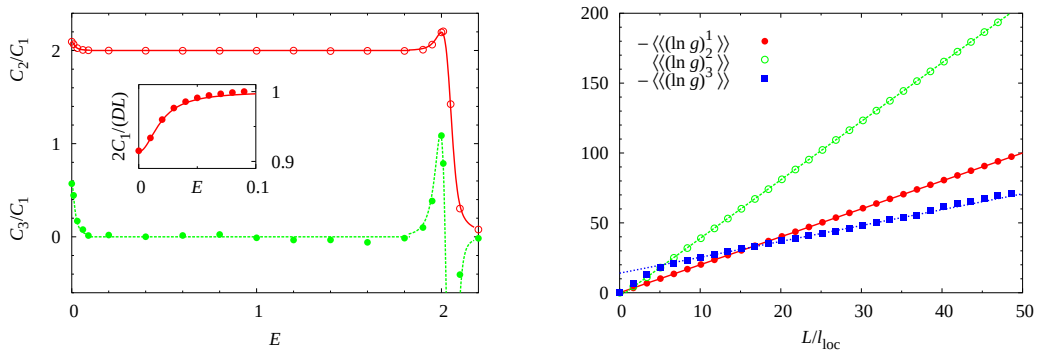

Figure 1: *Weak band-center and band-edge anomalies in the standard one-dimensional Anderson model with white-noise disordered potential. The left panel shows the coefficients C_n as the function of energy. The finite ratio C_3/C_1 indicates the violation of the single parameter scaling. The data points are the result of a numerical simulation of Ref. [2]. The curves are the analytical predictions of Ref. [1,2]. The right panel shows the first three cumulants of $\ln g$ at the band center as the function of system size L. The linear growth of the cumulants is the result of the central limit theorem. The slopes of the straight lines follow the predictions of Ref. [2].*

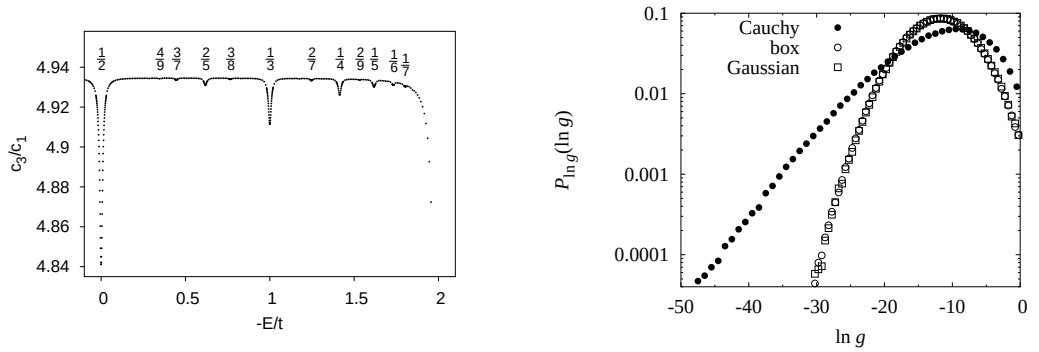

Figure 2: *The figure illustrates the multiscaling in the Anderson model with Cauchy disorder (Lloyd model). The left panel shows the ratio C_3/C_1 according to the analytical result of Ref. [4]. The ratio reveals anomalies at energies $E = -2t\cos(\pi p/q)$ with p and q integers. The corresponding rational number p/q is indicated in the figure. The right panel shows the distribution function of the logarithm of the conductance obtained numerically in Ref. [4] from the Anderson model with Cauchy disorder (full circles), box disorder (open circles), and Gaussian disorder (open squares). The deviation from the parabolic form for the case of Cauchy disorder is a signature of multiscaling.*

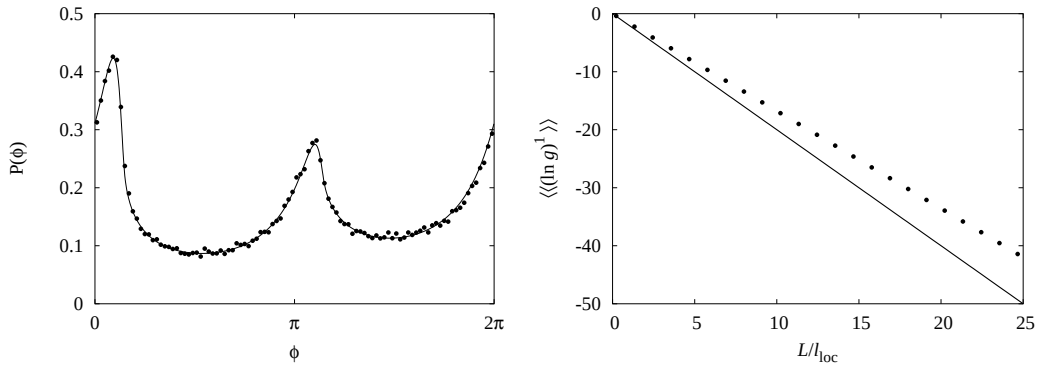

Figure 3: *This figure refers to an Anderson model with correlated disorder (correlation length: three lattice constants) at energy $E = 1$ (quarter band). The left panel shows the non-uniform distribution of the phase of the reflected wave, obtained from numerical simulations (filled circles) and our analytical theory (solid curve). The right panel show the mean of* $\ln g$ *from the numerical simulations (filled circles), which clearly deviate from the prediction of perturbation theory (solid line).*

allows to find and explain important situations where such single parameter scaling fails.

The violation of the single parameter scaling is shown to be related to the lattice symmetry of the model and can be essentially enhanced if disorder is short-range correlated. It turns out that a specific disordered potential can have different effects on the wave-functions at different energies. In one dimension this leads to a partial delocalization of certain states on the lattice. A well-known example is the Dyson singularity in the localization length (affecting also other quantities, such as the density of states) which is caused by the presence of a completely delocalized state at the band center. It emerges in systems where the potential disorder is absent and only hopping integrals fluctuate. The existence of similar effects in lattice models with potential disorder and the ensuing deviations from single-parameter scaling is an entirely new development [1–4].

We discuss these effects in terms of the self-averaging behavior of the logarithm of the conductance g. In one-dimension, $\ln g$ is an additive quantity in the sample length n (measured in units of the lattice constant). The fluctuations of $\ln g$ are shown to fulfill the central limit theorem, which predicts a linear growth of cumulants with the system size $\langle\langle(-\ln g)^j\rangle\rangle = C_j n + \mathcal{O}(1)$, where the coefficients C_j are proven to be universal. In the simplest model of white-noise potential disorder the single parameter scaling predicts $C_2 = 2C_1$ with all other coefficients vanishing, $C_j = 0$ for $j \geq 3$. However, small deviations from such behavior can be observed in the vicinity of the band center and of the band edge [2]. The ratios C_2/C_1 and C_3/C_1 are plotted at Fig. 1. The finite value of the ratio C_3/C_1 demonstrates the violation of single parameter scaling.

The possibility to observe Anderson localization of electrons is limited to low dimensional systems at low temperatures. However, a similar phenomena (dynamical localization) exists in optical lattices. In experiments on atoms driven by a regular train of laser pulses, the probability distribution function of atoms in momentum space is seen to relax from an initial Gaussian into an exponential profile, demonstrating the absence of diffusion in momentum direction.

The widely used model which captures many essential details of the experiments is the kicked rotator, which in turn has been mapped onto the Anderson model with an effectively random Cauchy-distributed potential (Lloyd model). The wave-function profile Ψ in the localized regime is again characterized by the coefficients C_j in the central limit theorem, $\left\langle\left\langle (\ln|\Psi|^2)^j \right\rangle\right\rangle = C_j n + \mathcal{O}(1)$, with the only difference that n counts the number of laser pulses (kicks). We demonstrate in Ref. [4] that the lattice model with Cauchy disorder gives rise to multiscaling behavior. Some of our results are presented in Fig. 2.
Work in progress indicates that the anomalies of the wave-function fluctuations are greatly enhanced if the disordered potential has finite-range correlations. As an example, we consider a model of disorder with correlations over three lattice sites. As shown in Fig. 3, at energy $E = 1$ the phase of the reflected wave is not uniformly distributed, and the localization length departs from the perturbative estimate. Both observations violate the basic assumptions of single-parameter scaling.

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3.1.22 Electrical response of molecular chains from density functional theory

Stephan Kümmel, Leeor Kronik, and John P. Perdew

Molecular chains are systems that consist of a linear sequence of molecular units. Such chains are important in different fields and contexts, ranging from biochemistry to plastics fabrication. Among the many classes of molecular chains, conjugated chains, i.e., chains with alternating single and double bonds, are of particular interest in the field of molecular electronics and nonlinear optics. The prototypical example of a conjugated chain is polyacetylene, the electronic structure of which is schematically depicted in Fig. 1. The valence electrons in such a chain show a very high mobility along the backbone of the chain, but very little perpendicular to it. This leads to a fast, large, and directional electrical response in the linear as well as in the nonlinear regime. Therefore, hopes are high that materials based on such chains can be used as alternatives to inorganic solids for non-linear optics tasks such as frequency doubling of lasers, and also to build advanced nonlinear optics devices.

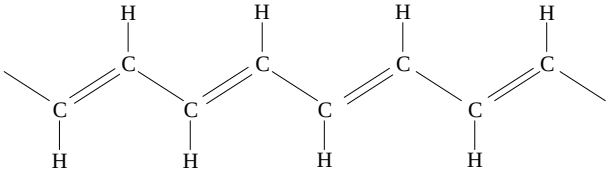

Figure 1: *Schematical sketch of the electronic structure of the conjugated chain trans-polyacetylene.*

Theory can guide the development of such new, nonlinear optics materials since it can lead to an increased understanding of the microscopic processes that govern the electronic response. Moreover, theoretical investigations ideally can be part of the search for improved materials directly by "testing" the response properties of newly designed molecules quickly and cheaply in the computer, i.e., by calculating them from first principles, instead of in the lab. In how far this possibility can be used in practice however hinges on whether the employed theory is accurate enough to reliably predict the properties of interest, computationally tractable enough to be applied to realistic systems containing many electrons, and transparent enough so that its results can be clearly interpreted. Density functional theory (DFT) has the potential to fulfill all of these requirements and thus appears particularly suitable for the task.

So far, however, this potential of DFT could hardly be exploited. The crucial quantity on which the accuracy of DFT calculations rests is the exchange-correlation functional. This functional has to be approximated and the most popular approximations to date are the local density approximation (LDA) and the semilocal generalized gradient approximations (GGAs). These functionals reliably predict ground-state properties of many solids and molecules [1], but unfortunately, they are of little use for the problem mentioned above: LDA and GGAs fail badly in predicting the response of molecular chains. Whereas typical GGA errors are of the order of a few percent, the hyperpolarizabilities that govern the nonlinear response of molecular chains are overestimated by orders of magnitude [2, 3].

Insight into the reasons for this dramatic failure can be gained from studying hydrogen chains [3], i.e., linear chains of H atoms with alternating H – H distances of 2 and 3 a_0. They are ideal test cases for several reasons. They mimic the electronic features of polymers like polyacetylene such as bond-length alternation, high and directional electron mobility, and large response coefficients, while at the same time their electronic structure is transparent enough to keep technical details (basis sets or grid parameters) well controlled; ab initio correlated wavefunction calculations are available for comparison [4]; and most importantly, current-DFT calculations [5] showed that among various molecular chains, hydrogen chains are the ones that are the most difficult to describe accurately within DFT. It can thus be expected that, if they are described correctly, then other chains will be described correctly too.

Previous studies of such chains [3] had shed some light onto why the semilocal approximations fail to predict the response correctly but also raised the serious question of a possible fundamental limitation of Kohn-Sham density functional theory. Ab initio wave-function methods showed that the response properties are dominantly determined by exchange effects, i.e., Hartree-Fock theory alone already leads to reasonable values for, e.g., the linear polarizability and the second hyperpolarizability. However, the response coefficients obtained from approaches that have usually been regarded as equivalent to Kohn-Sham DFT exact exchange turned out to be considerably less realistic than the ones from Hartree-Fock theory, i.e., wavefunction exact exchange [3]. This raised the question whether the Kohn-Sham approach with its local effective potential had some fundamental limitation that is avoided in the wave-function approach with its integral-operator potentials.

The answer to this question turns out to be *no* [6] and Fig. 2 allows to understand what is going on in a molecular chain when an external electrical field is applied. As the external field (straight dotted line) shifts some density from the right to the

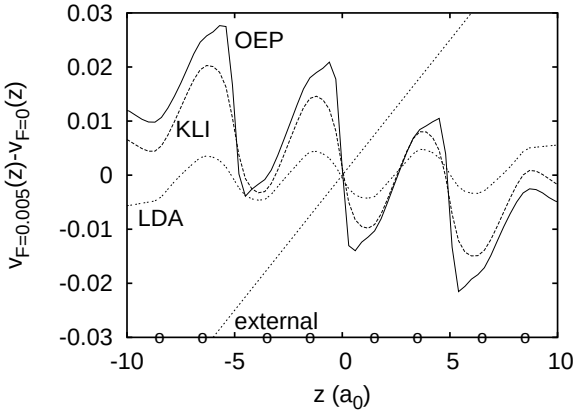

Figure 2: *In a molecular chain (here, a segment of eight hydrogen atoms is shown with the atomic positions denoted on the z-axis), the exact Kohn-Sham exchange potential (full line) builds up an internal field that counteracts an externally applied electrical field (straight dotted line). See text for further discussion.*

left part of the chain, the potential that describes the exchange-correlation effects in the local density approximation due to the very nature of the local approximation must follow the density, i.e., it goes down at that end of the chain where the density increases. In other words, the LDA potential works with the external field (as seen from the double-dotted line marked LDA). The exact Kohn-Sham exchange potential (calculated with a recently developed method [7], full line marked OEP), however, shows exactly the opposite behavior: It goes up at the end of the chain to which the density is shifted, i.e., works against the external field. It thus correctly leads to a much smaller polarization and the numerical values for the response coefficients closely agree with the ones from wavefunction calculations [6]. The reason why previous DFT calculations deviated considerably from the wavefunction results becomes clear from the dashed line marked KLI: The previous calculations used the exact exchange energy functional but did not calculate the corresponding self-consistent potential exactly. Instead, they used an approximation for the exchange potential which is usually referred to as the KLI-approximation (named after its developers Krieger, Li, and Iafrate) [8]. This approximation was considered to be quasi exact since it leads to very accurate ground-state energies. As seen in Fig. 2, however, this approximation does not correctly describe the dynamical rearrangement effects that are induced by the applied field and thus does not lead to a strong enough field-counteracting potential. So it turned out that DFT can in fact describe the electrical polarization in chains correctly, and we hope to apply these methods to realistic molecules soon.

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3.1.23 Exact time-dependent exchange-correlation potentials for strong-field electron dynamics

Manfred Lein and Stephan Kümmel

Time dependent density functional theory (TDDFT) [1, 2] has become a standard approach to calculate the excitations of electronic systems. A particular strength of the theory is that it allows to straightforwardly go beyond linear response theory, i.e., non-linear and non-perturbative excitations can readily be calculated. This is of great importance because calculating the correlated wavefunction is already computationally very demanding for stationary problems. Doing the same for the time-dependent case, i.e., solving the time-dependent many-body Schrödinger equation for realistic three-dimensional systems becomes computationally overwhelming. On the other hand, the availability and wide-spread use of pulsed-laser systems allows to experimentally probe the regime of strong-field electron dynamics and theoretical input is needed to understand the observed phenomena. TDDFT is one of the methods of choice for investigating situations where non-perturbative excitations are important and electron interaction effects cannot be neglected.

The accuracy of TDDFT depends on the approximation made for the exchange-correlation potential, i.e., the situation is similar to ground-state density functional theory: In principle the theory is exact, but in practice, the many body effects of exchange and correlation must be approximated. The favorite functional of TDDFT practitioners is the time-dependent local density approximation (TDLDA). TDLDA is based on using information from the ground state of the homogenous electron gas for systems that are inhomogenous in space and time. It therefore appears as a rather crude approximation at first sight, but it has met impressive successes [3, 4], e.g., in the linear response regime and in cluster physics when delocalized electrons that spread out over nearly the entire system are dominating the physical effects.

However, for one of the paradigm situations of strong-field dynamics, i.e., for the realm where, as stated above, TDDFT is most urgently needed, TDLDA and also all other standard functionals fail not only quantitatively but even qualitatively: In the laser-induced double ionization of noble-gas atoms, electron correlation substantially enhances the double-ionization yield in the region of low laser intensities due to "non-sequential ionization", leading to the famous "knee structure" [5, 6] in the intensity dependence of the double ionization probability – but this "knee" is not reproduced by any TDDFT calculation so far [7].

It is thus a challenge to understand why TDDFT fails for this problem and it is clear that problems with a density-based description of ionization can show up on two levels: First, in the approximations that are made for the time-dependent exchange correlation potential $v_{\mathrm{xc}}(\mathbf{r}, t)$ and second, in the approximations that are used to calculate the ionization probability from the density. It is clear from earlier studies that for a high-accuracy description, both issues must be addressed. But the qualitative feature of the missing "knee" is a failure of the approximations that so far were used for $v_{\mathrm{xc}}(\mathbf{r}, t)$ [7, 8]. For this reason, our first investigation focused on the time-dependent exchange-correlation potential.

The central idea of our approach is that we calculate the (within numerical limitations) *exact* $v_{\mathrm{xc}}(\mathbf{r}, t)$ from the exact time-dependent density $n(\mathbf{r}, t)$ by inverting the

Kohn-Sham (KS) equations. Since obtaining the exact time-dependent density requires solving the time-dependent Schrödinger equation, one might ask what is to be gained from this. The gist of our approach is that the time-dependent many-electron Schrödinger equation can easily be solved for model systems like the one-dimensional Helium atom described below. Although the model does not fully reproduce the experimental situation, it captures the most important physical effects. By calculating the exact $v_{\rm xc}(\mathbf{r},t)$ and comparing it to approximations used so far, we can understand what is missing in the approximations and develop improvements. These improvements are general, i.e., not specific to the model system, and can therefore be easily transferred to yield a density-functional description of the realistic situation (i.e., for the true Hamiltonian without the model's simplifications).
The He model atom in an electric field $E(t)$ is described by the Hamiltonian

$$H = \sum_{j=1,2} \left(\frac{p_j^2}{2m} + v_0(z_j,t) \right) + W(z_1 - z_2) \tag{1}$$

with electron coordinates z_1, z_2, momenta p_1, p_2, and the soft-core interaction $W(z) = e^2/\sqrt{z^2+1}$. The external potential is $v_0(z,t) = -2W(z) + ezE(t)$. This model has been demonstrated to capture the essential physics of the He double-ionization process [8]. The time-dependent Schrödinger equation $i\hbar\partial\Psi/\partial t = H\Psi$ is solved numerically for this model by means of the split-operator method on a grid that is chosen large enough to contain the entire wave function. From the two-electron wave function, we calculate the density and current

$$n(z,t) = 2\int |\Psi(z,z',t)|^2 \, dz', \tag{2}$$

$$j(z,t) = \frac{2\hbar}{m} \Re \int \Psi^*(z,z',t) \frac{\partial}{i\partial z} \Psi(z,z',t) \, dz', \tag{3}$$

and these quantities uniquely determine the KS orbital [9]. After the construction of the KS orbital, the KS potential is obtained by inversion of the split-operator time-propagator:

$$v_{\rm s}(z,t) = -\frac{\hbar}{2\delta t} \arcsin \Im \frac{e^{+iT\delta t/\hbar}\varphi(z,t+\delta t)}{e^{-iT\delta t/\hbar}\varphi(z,t-\delta t)} + \text{const}, \tag{4}$$

where T is the single-particle kinetic-energy operator and $v_{\rm s}(z,t)$ denotes the KS potential, i.e., the effective single-particle potential which yields the exact density. This potential is decomposed according to

$$v_{\rm s}(z,t) = v_0(z,t) + v_{\rm h}(z,t) + v_{\rm xc}(z,t) \tag{5}$$

where $v_{\rm h}(z,t) = \int n(z',t) W(z-z') dz'$ is the Hartree potential. The exchange-correlation potential $v_{\rm xc}(z,t)$ is defined by Eq. (5) and can be split into its exchange ($v_{\rm x}$) and correlation ($v_{\rm c}$) parts.
The first situation we investigate is the ionization of the correlated two-electron atom by an external DC electric field, because field-induced ionization is the first stage of the recollision mechanism which appears to be responsible for non-sequential double ionization [10]. In our model calculation, the direction of the field is chosen such that the

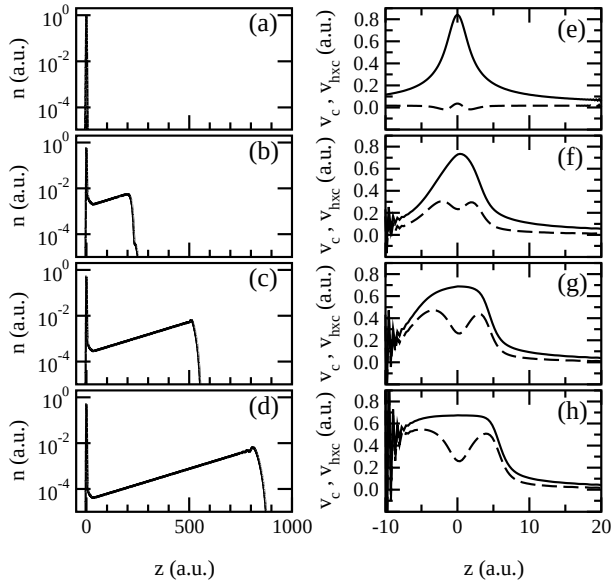

Figure 1: *Left column: The density of the Helium model atom after an ionizing static electrical field of strength* $E_0 = 0.141$ *a.u. has been applied. Time increases from top to bottom. Right column: The total electronic interaction potential* $v_{\rm hxc}(z,t)$ *(solid curves) and the correlation potential* $v_{\rm c}(z,t)$ *(dashed curves) for the same times. Note that the correlation potential increases dramatically with time.*

electrons can escape towards $z \to \infty$. The right column in Fig. 1 shows the total electronic interaction potential (sum of Hartree and exchange-correlation potentials, full line) and the correlation potential (dashed line), calculated according to the description given above. One clearly sees that the importance of the correlation contribution grows with time and that a feature similar to a plateau develops. This plateau-like feature can be shown [9] to be the time-dependent analogue of the derivative discontinuity with respect to particle number that is well known from ground-state density functional theory [11]. It is missing in all the functionals employed in TDDFT so far and Fig. 1 shows it to be a crucial feature. We therefore modeled this discontinuity in a straightforward way [9] and then used the obtained density functional to calculate the intensity dependence of the double ionization probability. The latter calculation shows the Helium knee in a qualitatively correct way [9]. Thus, the construction of the exact time-dependent correlation potential revealed a crucial aspect that must be taken into account in improved approximations for the exchange-correlation potential and opens a route to (hopefully) make TDDFT a useful tool for the description of correlated strong-field electron dynamics.

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3.1.24 Structure formation in thin liquid films: Beyond the case of a single evolution equation

U. Thiele, K. John and M. Bär

Introduction

The rupture of homogeneous films, self-propelled running drops, and transversal instabilities of liquid fronts are examples of structure formation in thin liquid films [1]. Related subjects are studied for centuries, however, especially ultrathin films gained increasing importance recently because of their many applications. For instance, the capacity of the films to structure themselves in the nanometer range renewed the interest in the dynamics of such films. At present the basic behavior of one-layer films is well understood, however, little is known about transitions between different 'simple' modi of behaviour and more complex systems like multi-layer films or reacting films. We first present selected results for one-layer films in different situations. After introducing the basic model we discuss the different possible geometries and the transitions between them, i.e. from homogeneous to inhomogeneous, or from horizontal to inclined substrates. We then focus on thin film systems where more degrees of freedom have to be taken into account. In the simplest case, two coupled evolution equations instead of only one are needed to model the dynamics. On general grounds one can distinguish two situations: (i) The second field beside the film thickness profile represents also a conserved quantity like for a two-layer ultrathin film or (ii) the second field corresponds to a non-conserved quantity like for chemically driven running droplets. We conclude the work with a short outlook.

One-layer systems

A layer of liquid on a solid substrate with a free surface is called a *thin film* if its thickness is small compared to the typical length scales parallel to the substrate. This allows to simplify the governing Navier-Stokes equations and boundary conditions using a long-wave approximation [1]. One derives an evolution equation for the film thickness profile. It has the form of a continuity equation and writes for a two-dimensional situation in dimensionless form

$$\partial_t h \;=\; -\partial_x \left\{ Q(h)\, \partial_x \left[\partial_{xx} h - \partial_h f(h,x) \right] + \chi(h) \right\} \qquad (1)$$

where $Q(h) = h^3$ is a mobility factor. The term in square brackets represents a pressure consisting of the Laplace pressure $\partial_{xx} h$ and an additional pressure $-\partial_h f(h,x)$ written as the derivative of a local free energy to be specified for the respective studied problem. For inhomogeneous systems it may depend on position. Finally, $\chi(h)$ stands for an

additional driving force parallel to the substrate. The used scalings depend on the problem studied.
Based on substrate properties and acting forces one can distinguish four basic geometries:
(a) A film on a horizontal homogeneous substrate. Examples that we study are the different rupture processes in dewetting [2,3] and pattern formation due to a long-wave Marangoni instability on a heated substrate [4, 5].
(b) A film on a horizontal inhomogeneous substrate as encountered for dewetting on a chemically patterned substrate [6] or for a film on an inhomogeneously heated plate [7]. We especially discuss the influence of the heterogeneity on coarsening and transversal instabilities.
(c) A film on an inclined homogeneous substrate. In former work we studied the characteristics of sliding drops and other basic properties of this simple model of microfluidic transport [8], whereas now we focus of the dynamics of fingering instabilities [4, 9] and on the study of the transition from Cahn-Hilliard to Kuramoto-Sivashinsky behaviour for a film on a slightly inclined plane [9].
(d) A film on an inclined inhomogeneous substrate as encountered for a falling films on an locally heated plate [7].
In extension to the cases discussed above, we also work on the control of the structuring of thin soft matter films by means of different types of external disturbances [10], the influence of thickness variations on the domain formation in biological membranes [11], and the validity domain of the Benney equation for closed and open flows [12].
In the following we focus on thin film systems where the description requires more than a single evolution equation because where more degrees of freedom have to be taken into account. In the simplest case, two coupled evolution equations instead of only one are needed to model the dynamics. One distinguishes the case where the second field beside the film thickness profile is also a conserved quantity and the case where it is not.

Two-layer systems

The first example represents a system where the model consists in two coupled conserved fields. A two-layer film allows for richer dynamics than a one-layer system because, both, the free liquid-liquid and the free liquid-gas interface evolve in a coupled way. The evolution for ultrathin films is driven by the effective molecular interactions between *all* the three interfaces separating the four material layers: substrate, liquid 1, liquid 2 and ambient gas. The most intricate question for the first stage of dewetting of a two-layer system is *which* interface will become unstable and *where* does the film rupture. This will determine the final morphology of the film. Fig. 1 illustrates two different pathways of the unstable evolution leading to rupture of the upper and lower layer, respectively.
We determine evolution equations for the film thicknesses h_1 and h_2 in long-wave approximation [13]

$$\begin{aligned} \frac{\partial h_1}{\partial t} &= \nabla\left(Q_{11}\nabla\frac{\delta F}{\delta h_1} + Q_{12}\nabla\frac{\delta F}{\delta h_2}\right) \\ \frac{\partial h_2}{\partial t} &= \nabla\left(Q_{21}\nabla\frac{\delta F}{\delta h_1} + Q_{22}\nabla\frac{\delta F}{\delta h_2}\right), \end{aligned} \tag{2}$$

where $\delta F/\delta h_i$ with $i = 1, 2$ denotes functional derivatives of the total energy of the

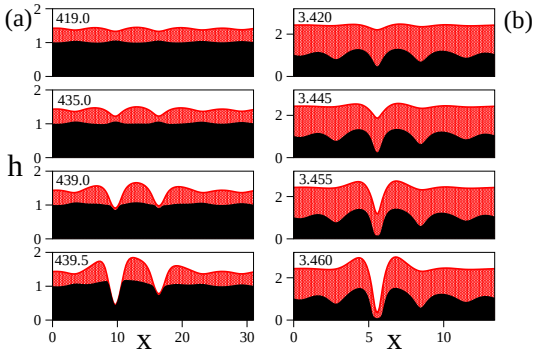

Figure 1: *Snapshots from time evolutions of a Si/PMMA/PS/air system at times as shown in the insets. (a) At $d = 1.4$ a varicose mode evolves leading to rupture of the upper layer. (b) At $d = 2.4$ a zigzag mode evolves and rupture of the lower layer. The domain lengths are 5 times the corresponding fastest unstable wave length and $\mu = \sigma = 1$.*

system, and the Q_{ik} represent the mobility matrix. The derived model is apt to describe a broad variety of experimentally studied two-layer systems. Studying Eqs. (2) by means of linear analysis one distinguishes two different types of unstable modes, namely, varicose and zigzag modes that also determine the non-linear evolution. In the model without stabilising short-range interactions studied in [13] they lead to rupture at the substrate or at the liquid-liquid interface (see Fig. 1). Both modes are asymmetric since the deflection amplitudes of the two interfaces are normally different. We show that the mobilities have no influence on the stability threshold, but determine mode type and the length and time scales of the dynamics.

Chemically driven running drops

The second example represents a system where one has to couple a conserved and a non-conserved field to model the dynamics. Recent experiments found chemically driven running droplets on solid substrates. There, a driving wettability gradient is produced by a chemical reaction at the substrate underneath the drop [14]. A simple theoretical argument [15], predicts a monotone increase of the droplet velocity with the droplet length and the reaction rate, in line with early experimental observations [14]. Recent experiments [16] show also the opposite trend; the velocity decreases with increasing drop sizes and reaction rate. In Ref. [17] we propose and analyse a dynamical model for self-propelled running droplets that allows to explain the different experimental findings as representing a reaction-limited and a saturated regime (see Fig. 2).

It consists of coupled evolution equations describing the interdependent spatiotemporal dynamics of the film thickness h and of the concentration of an adsorbate α that decreases the substrate wettability:

$$\partial_t h = -\nabla \left\{ h^3 \nabla \left[\Delta h - \partial_h f(h,\alpha) \right] \right\} \quad (3)$$

$$\partial_t \alpha = R(h,\alpha) + d\,\Delta\alpha. \quad (4)$$

The first equation describes the evolution of the film thickness profile. It is based on Eq. (1) with $\chi = 0$, and incorporates a disjoining pressure whose short-range part depends not only on h but changes linearly with the adsorbate concentration α The second equation (4) models the evolution of the chemical concentration of the adsorbate using a reaction-diffusion equation. The function $R(h,\alpha) = r\Theta(h - h_0)\,(1-\alpha)$ describes the reaction that changes the wettability of the substrate and the second term

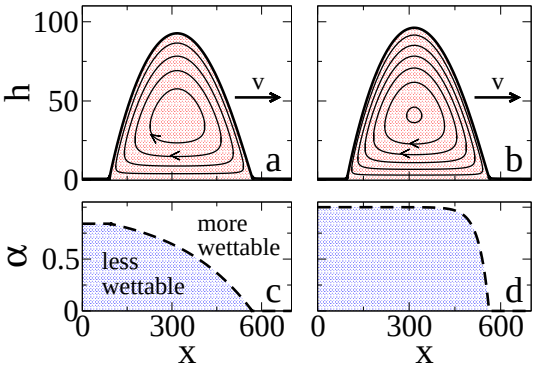

Figure 2: *Characterization of the two qualitatively different running droplet regimes. Shown are droplet and wettability profiles (a) and (c) in the reaction-limited regime at* $r = 0.0001$ *and (b) and (d) in the saturated regime at* $r = 0.001$ *The streamlines indicate the convective motion inside the droplet. The remaining parameters are* $g = 1.0, d = 0.0, b = 0.5$.

allows for a (usually small) diffusion of the chemical species along the substrate. The main results, however, are obtained without diffusion. The model Eqs. (3) and (4) is capable of reproducing the experimentally found regimes. In particular, varying the reaction rate or drop volume we identify two distinct regimes of running drops illustated in Fig. 2. For small reaction rate (or droplet size), the chemical gradient in the drop is limited by the progress of reaction. In contrast for a fast reaction (or large droplets), the chemical concentration at the receding end saturates at a maximum value. We show that the velocity of reaction-limited droplets increases, while the velocity of saturated droplets decreases with increasing reaction rate and drop size. Specifically, the velocity of the droplets may increase [14] or decrease [16] with their volume.
These two examples show the rich behaviour that can be found for these apparently simple systems. In the future the presented approach can be extended towards the incorporation of complex fluids like copolymers that allow for a coupling of liquid transport and structural phase transitions or liquid crystals and binary mixtures that require the description of the dynamics of an additional internal degree of freedom.

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3.2 PhD Program

The training of PhD students is one of the central educative tasks of the mpi**pks**. Prospective PhD students have several options of contacting scientific advisors at mpi**pks**. PhD position openings funded through external grants are advertised in scientific journals and on the internet pages of the institute. In addition there is a permanent advertising of PhD positions funded through the Visitors Program on the internet pages of the institute and in several information booklets. Finally, a significant part of PhD students is recruited through personal contacts with potential scientific advisors at mpi**pks**.

The success of this strategy is well documented in previous scientific reports of mpi**pks**. In 2003 we had a total of 25 PhD students at mpi**pks**, including 8 students from abroad (these numbers count all students, i.e. including those who finished their PhD studies or just started their studies during that year). The respective numbers for 2004 were a total of 26 PhD students at mpi**pks**, including 7 students from abroad. We counted 3 successful final PhD exams for the year 2003 and 8 exams for the year 2004.

Besides their scientific work at mpi**pks** our PhD students use several further types of activities to strengthen their academic and communicative skills. In addition to lecture courses offered at the TU Dresden the mpi**pks** provides lecture courses on modern topics of theoretical physics on a regular basis. PhD students can join workshop talks and seminar lectures of the Workshop and Seminar Program of mpi**pks**. Many of them participate actively in these events by presenting short talks or posters. Our institute organizes annual PhD Student Days (1-2 days). All students of mpi**pks** participate in this meeting and present short talks on their current research results. A PhD student exchange program with East European countries like Poland or Czech Republic, which is supported by the Max Planck Society, allows our students to visit cooperating research groups and to present talks, as well as to coach visiting PhD students from those groups at mpi**pks**. The mpi**pks** offers financial and logistic support for joining German language courses for our PhD students from abroad in order to help with integration into the German speaking community.

A growing number of PhD students pass the final PhD exams at the TU Dresden. Still, some students are obtaining the PhD degree from various universities throughout Germany. After obtaining the PhD degree most of our students continue their research

work by accepting PostDoc positions at research institutions in various countries. A significant part is also successfully applying for positions in companies in such areas as applied research, informatics, finance and consulting. The mpi**pks** organizes regular alumni meetings of former PhD students with discussion rounds to provide a transfer of experience for our present PhD students.

3.3 Workshop and Visitors Program

The Visitors Program of mpi**pks** hosts guest scientists for a period of usually up to two years. Excellent working conditions are offered to the qualified, mostly young, scientists. This also includes logistic help, e.g., for finding suitable accommodation, solving visa problems etc. The close collaboration with administrative units responsible for, e.g., the computational and technical equipments of the offices allows the guest scientists to fully concentrate their efforts on research. Informal Tea Seminars and financial support for joining German language courses help to integrate our guest scientists fast and easily into the local community. Many guest scientists participate actively in the events of the Workshop and Seminar Program of mpi**pks**.

During 2003 the mpi**pks** hosted 119 guest scientists with contracts for at least three months, and 92 during the year 2004. At the same time we enjoyed a large number of senior scientists who used their sabbatical time for long-term research stays at mpi**pks**. This led to an enhancement of transfer of experience to young scientists at the institute. The guest scientists are typically in close collaboration with the research groups at mpi**pks**. Otherwise they conduct more independent research, which leads to synergetic effects, including recent temporary collaborations at the institute on *Bose-Einstein condensation*. Synergetic effects are also enhanced due to the possibility to listen to talks and lectures within the Seminar and Workshop Program of mpi**pks** (see p. 134).

In addition to the regular positions of the Visitors Program the institute annually offers a Distinguished PKS Postdoctoral Position for experienced postdoctoral scientists for up to three years. PKS Fellows do research in areas related to but not directly represented by the work done in the mpi**pks** research groups. Three PKS Fellows are currently working at mpi**pks**: *Dr. Abhik Basu* on *Statistical Dynamics of Nonequilibrium Systems*, *Dr. Benjamin Lindner* on *Modelling of Nonequilibrium Processes in Biological Physics* and *Dr. Joachim Brand* on *Physics of Bose-Einstein Condensates*, see report on p. 129 Two PKS fellows have left the institute: *Dr. Rainer Klages Statistical Dynamics of Nonequilibrium Systems* accepted a lectureship at University of London, and *Dr. Manfred Lein* (*Molecular Quantum Dynamics*) took a C3 group leader position at the Max Planck Institute for Nuclear Physics at Heidelberg.

To strengthen the transfer of knowledge and experience at mpi**pks**, the institute awards annually the Martin Gutzwiller Fellowship to a senior scientist with exceptional contributions in the area of the physics of complex systems. Gutzwiller Fellows spend up to one year at mpi**pks** and have the possibility to nominate a young guest scientist for the Visitors Program. The 2003 and 2004 fellows were *Prof. Raymond Kapral* and *Prof. Antonio Politi* (see report on p. 131).

A considerable number of guest scientists leave the institute for permanent positions in the academic sector, besides many others who continue with postdoctoral positions at other institutions in Germany or abroad. Several guest scientists leave for positions in

the non-academic sector, such as applied research, informatics, finance or consulting. In addition to the long-term guest scientist positions the Visitors Program also hosts many short-term visits (for up to three months). These visits are usually due to research collaborations of the research groups at mpi**pks** with other institutes. Their number continued to grow from 144 during the year 2003 to 155 during the year 2004.

3.3.1 PKS-Fellowship

Report by *Dr. Joachim Brand:* Physics of Bose-Einstein condensates
The physics of quantum degenerate atomic gases has become an exciting and strongly growing field since the first experimental achievement of Bose-Einstein condensation in 1995. Interest in the field is documented by the strong participation in the two conferences, which I organised at mpi**pks**: "Atomic Physics 2003" in December 2003 with focus on "Nonlinear Phenomena in Quantum Degenerate Gases" (co-organised with J.-M. Rost) had 60 participants and "Mesoscopic Phenomena in Ultracold Matter" in October 2004 (co-organised with K. Burnett and P. Schmelcher) had more than 100 participants, who had to be chosen from more than 130 applicants. These workshops were the first in the field of quantum degenerate gases held at mpi**pks**.
During my stay at mpi**pks** since May 2002 I collaborated with I. Häring and J.-M. Rost from the Finite Systems group and with A. Kolovsky from the group "Nonlinear Dynamics in Quantum Systems". I am further coordinating a small group of researchers interested in degenerate quantum gases consisting of the guest scientist A. Yu. Cherny and the postdocs Ch. Lee, S. Sinha, and D. Kovrizhin. The group holds a weekly discussion meeting. Apart from these collaborations within mpi**pks**, I have maintained and started external collaborations with the experimental group of Lene Hau at Harvard University (Cambridge US), Lincoln Carr at JILA (Boulder, US), the Theoretical Condensed Matter group at the University of Cambridge (UK), and the University of Athens (Greece). At the Technical University of Dresden I am lecturing for advanced undergraduate students on the physics of Bose-Einstein condensates during the winter term of 2004/2005.
At this place I want to express my gratitude toward mpi**pks** for creating a wonderfully stimulating working environment and for giving me the opportunity to develop the described activities. In particular I want to thank J.-M. Rost whom I also had the pleasure to collaborate with scientifically, F. Jülicher and P. Fulde. I am also gracious for the support of Ms. G. Makolies and the staff of the visitor's programm, the computer department, and the administration of mpi**pks**.

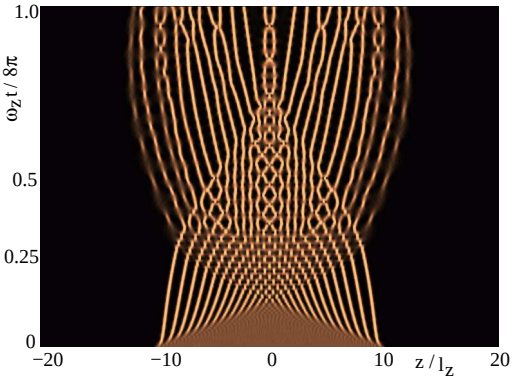

Figure 1: *Simulation of the formation and subsequent collisions of bright solitons in a quasi-1D Bose-Einstein condensate after atomic interactions were tuned from repulsive to attractive with a Feshbach resonance [3].*

The nonlinear dynamics of solitons and vortices is one of my main interests in the physics of ultracold gases. During my stay at mpi**pks**, this interest has led to a proposal for a pulsed atom laser emitting bright matter-wave solitons [5] and to the explanation of a related experiment at the Rice University (Texas) [3]. The interactions of vortex rings and solitons are the subject of a collaboration with the experimental group of Lene Hau at Harvard [6] and Stavros Komineas at Cambridge, UK. The subject of solitons in Bose-Einstein condensates has already evolved into a field of its own with the first conference entirely on this subject being organised in Almagro (Spain) in February 2005 where I will give an invited talk. While at mpi**pks** I gave 10 invited talks at international conferences and institutions including the Laser Physics meetings of 2002 and 2004, and the BEC summer programme in Trento 2002.
Another subject of my research performed at mpi**pks** is the properties of the 1D Bose gas in the strongly interacting regime. The generic perturbative approach relies on the coupling strength being a small parameter. With this approach, corrections to the effective coupling due to tight confinement can be found [4] but the regime of strong interactions can hardly be accessed. Density-functional theory, however, can be applied successfully and give a consistent and intuitive picture of the dramatic change from a weakly interacting Bose gas to strongly correlated fermionized gas of impenetrable particles [2]. Close to the fermionic limit, we were able to show that detailed information about correlation functions is attainable from a newly developed pseudopotential approach [7]. Thus new predictions for the fundamental properties of the 1D Bose could be made, which should become within the reach of experimental verification very soon.

Articles written at mpipks

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3.3.2 Gutzwiller-Fellowship

Report by *Prof. Dr. Antonio Politi*

The rapidly evolving organization of public research activity in Italy has obliged me to limit the Gutzwiller fellowship for the year 2004 to approximately six months divided into two periods, the first one from the middle of September 2004 until a few days before Christmas. Further three months are planned in the first half of year 2005.

I can hardly overestimate the importance of having been offered the chance to work in a quiet environment, surrounded by motivated and curious researchers. All of this has been indeed offered to me while being at the mpi**pks** in Dresden and has contributed to obtaining new results, in a way I was no longer used in the recent past. Moreover, in an epoch like the present one, when a researcher is too often forced to describe in advance the achievements of her/his research and even to identify intermediate milestones, I find worth spending some words to stress the importance of accidental discussions, when they occur in a lively environment among people whose main motivation is first to make progress and then to write a further paper. At the mpi**pks**, it was, indeed, by "chance", after an informal seminar, that I happened to realize (by discussing with a long term guest, *Dr. S. Denisov*) that my old and never-published results about the dynamics of a simple chain of hard–point particles could be explained by invoking an analogy with Levy flights, thereby bridging together two classes of models (namely, many-body and single-particle), I previously considered as substantially unrelated with one another. This connection will hopefully open a new route to understanding heat conductivity in classical low-dimensional systems.

The above is the most remarkable example, during my stay at the mpi**pks**, of how important is the environment a researcher is embedded in, but it is not the only one. It is still early to draw definite conclusions, but I can anticipate that an unplanned interaction with yet another young visitor at mpi**pks**, *Dr. P.K. Mohanty*, is perhaps leading to the development of a new approach to investigate the behavior of globally coupled oscillators. Once again, everything started from a discussion with a participant to one of the many Workshops organized at the mpi**pks**, *Prof. A. Pikovsky*. At the moment, our collaboration limits to investigating the much simplified case of equal rotators, but I expect that any progress made in this direction should shed some light about the general mechanisms linking micro- to macro-scopic dynamical properties in globally coupled systems. Further useful discussions have occurred with other scientists passing through or working stably at the mpi**pks** with benefits, I hope, in either direction. The touched arguments include among others: (i) phase synchronization and analytic (though perturbative) estimation of Lyapunov exponents, a subject on which I have been able to make a significant progress upon interacting with a former student of mine, now in Würzburg (*Dr. F. Ginelli*) and two scientists who are, respectively, in Berlin at the Weierstrass Institute (Dr. S. Yanchuk) and in Julich (*Prof. Y. Maistrenko*); (ii) modellization of cell division, a subject discussed with a PhD. student at the mpi**pks** (*G. Meacci*).

An important reason why many unforseen discussions proved so effective is the existence at the mpi**pks** of a competent technical and administrative staff which has smoothly solved all problems that unavoidably accompany a person when s/he has to settle into a new environment, as well as the less expected difficulties that arise when a scientist must keep links with an unpredictable and turbulent environment such as that of my

own country. Furthermore, by no means, I wish to devalue the importance of planning in doing good research: the generous terms of the Gutzwiller Fellowship allowed me to recommend the award of a postdoctoral fellowship for a collaborator during my stay. External difficulties have prevented a perfect synchronization between the arrival of my collaborator (*Dr. M. Perrin*) and my first sojourn in Dresden. Nevertheless, we have already established a contact with an experimental group in Tübingen (*Dr. Ph. Courteille*) which has recently performed a beautiful experiment to show the spontaneous self-organization of an ensemble of cold atoms interacting with a coherent electromagnetic field: this is a subject I have recently studied because of its relationship with synchronization in globally coupled systems and that I plan to further investigate with M. Perrin to possibly arrive at an experimental verification of the instabilities that we have numerically observed at relatively large intensities of the pump field.
Moreover, I have exploited my sojourn in Dresden to deliver seminars both internally at the mpi**pks** and in different Institutes all over Germany. Locally, I have given two informal talks about the current state of the art on the problem of heat conductivity in classical low-dimensional systems and about the phenomenon of the so-called "stable chaos" that, after having been discovered in artificial systems, has been recently observed in more realistic models. Later in year 2005, the formal mpi**pks** Colloquium for the Gutzwiller Fellowship will be given on the connection between microscopic and macroscopic dynamics in many-component systems. Out of Dresden, I have visited the MPI for Mathematics in the Sciences in Leipzig, where I have given a seminar on synchronization in spatially extended systems and had the chance to discuss with several scientists on the dynamics of neural networks. I also enjoyed visiting Berlin twice to give a seminar on "The collective behaviour of a gas of cold atoms" at the Fritz Haber Institute while attending a symposim on "Komplexe Nichtlineare Prozesse", and at the Weierstrass Institute within a Workshop about "Synchronization and high-dimensional chaos in coupled systems". Further seminars and colloquia are already planned in the second period in Oldenburg, Würzburg and Göttingen.
Although we live in an electronic era, with the information able to travel very rapidly all over the world, direct human contacts are not (yet?) superseded by the many high-tech tools which surround us. Indeed, what I have mostly benefitted from while being at the mpi**pks**, is the interactions both with scientists working stably there and all kinds of visitors. In particular, I wish to thank *Dr. Holger Kantz* and his group for discussions on Hamiltonian systems and *Dr. Sergej Flach* for exchanges of ideas about the dynamics of nonlinear chains. Finally, it is a pleasure to thank the whole administrative and technical staff for the kind hospitality and specifically *Uta Gneisse*, *Katrin Lantsch*, and *Mandy Lochar* for their support.

Articles completed and written at mpipks:

- *Studies of thermal conduction in FPU-like lattices*, S. Lepri, R. Livi, and AP, invited contribution on a special issue of CHAOS.
- *Relationship between heat conductivity in one-dimensional systems and Levy walks*, P. Cipriani, S. Denisov, and AP, in preparation.

3.3.3 Collaboration with Experimental Physics Groups

A number of joint collaborations with experimental physics groups in Germany, Europe and the US has been partially supported by mpi**pks**. The following list summarizes these collaborations for the period 2003-2004.

- *Physics of DNA-chips* with A. Ott (Bayreuth)
- *Biophysics of mechanosensory hair cells* with P. Martin (Paris)
- *Self-organization of active gels and motor-filament systems* with A. Bernheim-Groswasser (Beer-Sheva)
- *Biophysics of insect hearing* with M. Göpfert (Köln)
- *Biophysics of the cytoskeleton, cell division and the physics of motor proteins* with J. Howard (Dresden)
- *Biophysics of cell division in C. elegans* with A. Hymann (Dresden)
- *Formation of morphogen gradients in the fruit fly Drosophila* with M. Gonzales-Gaitan (Dresden)
- *Segmentation of vertebrates through oscillating and spatio-temporal gene expression patterns* with A. Oates (Dresden)
- *Mechanics and checkpoints in cytokinesis, orientation of the cell division plane* with M. Bornens (Paris)
- *The physics of contractile rings and the dynamics of the cytskeletion in plant cells* with M. Dogterom (Amsterdam)
- *Strukturbildung in katalytischen Oberflächenreaktionen* with R. Imbihl (Hannover)
- *Lipid-Protein Wechselwirkung und Membrandomänen.* with J. Käs (Leipzig)
- *Rennende Flüssigkeitstropfen in dünnen Filmen.* with R. Magerle (Chemnitz)
- *Dreidimensionale Strukturbildung in chemischen Reaktionen* with S. C. Müller (Magdeburg)
- *Dynamik von Ferrofluidoberflächen* with I. Rehberg (Bayreuth)
- *Dynamik dünner Filme* with H. Riegler (Potsdam)
- *Fronten in getriebenen Systemen* with H. H. Rotermund (Berlin)
- *Kollektive Dynamik in Mycobakterienkolonien* with L. Sogaard-Andersen (Marburg)
- *On the characterization of surface roughness* with J. Peinke (Oldenburg)
- *Ultracold glasses* with H. Strehlow (Berlin)
- *Spin-current control* with P. Mohanty (Boston)
- *Filamentation of High-Power Femtosecond Laser Pulses in Air* with S. L. Chin (Quebec)
- *Electron-Electron Momentum Exchange in Strong Field Double Ionization* with P. B. Corkum (Ottawa) and R. Dörner (Frankfurt)

- *Influence of self-action effects on fragmentation of toluene by femtosecond laser pulses* with P. Agostini (Berlin) and S. L. Chin (Quebec)
- *Ionization of C_{60} in intense laser pulses* with I. Hertel (Berlin)
- *Dynamics of cell migration: Analysis on different time scales* with P. Dieterich (Dresden), R. Preuss (München), V. Deval, C. Stock, A. Schwab (Münster)

3.3.4 Conferences, Workshops and Symposia 2003-2004

1. *Minerva Meeting of Young Researchers on Semiclassics, Quantum Chaos, and Mesoscopic*
   Workshop: January 20 - February 2, 2003 54 participants
   Scientific coordinators: S. Fishman, H. Schomerus, U. Smilansky

2. *Korrelationstage 2003*
   Workshop: February 24 - 28, 2003 160 participants
   Scientific coordinators: B. Büchner, P. van Dongen, P. Horsch

3. *Functional Renormalization in Interacting Quantum Many-Body Systems*
   Workshop: March 10 - 21, 2003 61 participants
   Scientific coordinators: S. Kehrein, A. Mielke, G. S. Uhrig, F. Wegner

4. *Modern Aspects of Quantum Impurity Physics*
   Workshop/Seminar: March 31 - April 18, 2003 69 participants
   Scientific coordinators: R. Bulla, D. E. Logan, A. Schiller

5. *Off-Shell Effects in Quantum Transport*
   Workshop/Seminar: May 5 - 16, 2003 50 participants
   Scientific coordinators: P. M. Oppeneer, M. Richter

6. *Classical and Quantum Barrier Transport in Complex Systems*
   Workshop: May 20 - 24, 2003 78 participants
   Scientific coordinators: J. Ankerhold, P. Reimann, T. Geisel

7. *Field Theory in Condensed Matter and Particle Physics*
   Workshop: June 02 - 06, 2003 51 participants
   Scientific coordinators: B. Altshuler, K. Efetov, L. Frankfurt, K. Goeke, M. Strikman

8. *Fermi-Liquid Instabilities in Correlated Metals*
   Workshop: June 11 - 13, 2003 50 participants
   Scientific coordinator: H. von Löhneysen

9. *Collective Phenomena in the Low Temperature Physics of Glasses*
   Workshop: June 16 - 21, 2003 54 participants
   Scientific coordinators: C. Enss, S. Hunklinger, R. Kühn

10. *Quantum Phase Transitions*
    Workshop/Seminar: June 23 - July 25, 2003 92 participants
    Scientific coordinators: D. Belitz, T.R. Kirkpatrick, T. Vojta

11. *Biological Information and Statistical Physics*
    Symposium: July 14 - 15, 2003 — 8 participants
    Scientific coordinators: F. Jülicher

12. *Quantum Transport and Correlations in Mesoscopic Systems and QHE*
    Seminar: July 28 - August 22, 2003 — 70 participants
    Scientific coordinators: V. Falko, B. Altshuler, A. Ludwig

13. *Trends in Pattern Formation: From Amplitude Equations to Applications*
    Workshop/Seminar: August 24 - September 19 , 2003 — 114 participants
    Scientific coordinators: M. Bär, H. Engel, E. Schöll, A. Torcini

14. *Non-Equilibrium Statistical Physics in Low Dimensions and Reaction Diffusion Systems*
    Seminar: September 21 - October 10, 2003 — 59 participants
    Scientific coordinators: P. Grassberger, M. Henkel, H. Hinrichsen, U. Schollwöck

15. *Motion, Sensation and Self-Organization in Livin Cells*
    Workshop/Seminar: October 20 - 31, 2003 — 90 participants
    Scientific coordinators: K. Kruse, F. Jülicher, J. Howard, J. Prost

16. *PhD Students Representatives Meeting*
    November 5 - 7, 2003 — 57 participants
    Scientific coordinators: G. Klein, F. Mintert

17. *4. Dresdner Herbstseminar des Arbeitskreises Nichtlineare Physik*
    Workshop: November 9 - 12, 2003 — 76 participants
    Scientific coordinators: T. Geisel, S.C. Müller, H. Pleiner

18. *Atomic Physics 2003*
    Workshop: December 1 - 5, 2003 — 68 participants
    Scientific coordinators: J.-M. Rost

19. *Resonances - From physics to mathematics and back*
    Workshop: January 26 - 30, 2004 — 68 participants
    Scientific coordinators: A. Buchleitner, R. Hempel

20. *Advances in molecular electronics: From molecular materials to single molecule devices*
    Workshop: February 23 - 27, 2004 — 126 participants
    Scientific coordinator: G. Cuniberti, G. Fagas, K. Richter

21. *Rydberg physics*
    Workshop/Seminar: April 19 - May 14, 2004 — 102 participants
    Scientific coordinator: R. Cote, T. Pattard, M. Weidemüller

22. *Complex dynamical processes in electroreceptors and hair cells*
    Workshop: May 17 - 21, 2004 — 52 participants
    Scientific coordinator: H. Braun, M. Hofmann, F. Jülicher, F. Moss, D. Russel

23. *Cooperative Phenomena in Optics and Transport in Nanostructures*
    Workshop/Seminar: May 31 - June 25, 2004 — 95 participants
    Scientific coordinators: M. Portnoi, R. Römer, T. Shahbazyan

24. *Structural approaches to sequence evolution: Molecules, networks, populations*
    Workshop: July 5 - 10, 2004 86 participants
    Scientific coordinators: U. Bastolla, M. Porto, H. E. Roman, M. Vendruscolo

25. *From many-particle to multi-agent systems*
    Thematic Institute of Exystence - the Network of Excellence for Complex Systems
    Workshop/Seminar: July 19 - September 17, 2004 80 participants
    Scientific coordinators: E. Ben-Jacob, D. Helbig, F. Schweitzer

26. *Symposium on Physics of Biological Systems*
    Symposium: August 4 - 6, 2004 20 participants
    Scientific coordinators: F. Jülicher, J. Howard

27. *Pattern formation through instabilities in thin liquid films: From fundamental aspects to applications*
    Workshop: September 21 - 28, 2004 79 participants
    Scientific coordinators: A. Nepomnyashchy, G. Reiter, U. Thiele

28. *Stochastic resonance: New horizons in physics and engineering*
    Workshop: October 4 - 7, 2004 50 participants
    Scientific coordinator: P. Hänggi, L. Schimansky-Geier

29. *Mesoscopic phenomena in ultracold matter: From single atoms to coherent ensembles*
    Workshop: October 11 - 15, 2004 104 participants
    Scientific coordinators: J. Brand, K. Burnett, P. Schmelcher

30. *German-Russian Symposium "Novel materials with electronic correlations, strong coupling and different dimensionalities"*
    Symposium: October 21 - 31, 2004 30 participants
    Scientific coordinators: M. Huth, J. Wosnitza

31. *5. Dresdner Herbstseminar des Arbeitskreises Nichtlineare Physik*
    November 7 - 10, 2004 88 participants
    Scientific coordinators: B. Eckardt, T. Geisel, H. Pleiner, W. Zimmermann

32. *Prospects in cellular biophysics*
    Workshop: November 18 - 19, 2004 44 participants
    Scientific coordinators: K. Kruse, P. Martin, G. Romet-Lemonne

33. *Atomic Physics 2004*
    Workshop: November 29 - December 3, 2004 79 participants
    Scientific coordinators: J.-M. Rost, U. Saalmann

3.3.5 Workshop Participation and Dissemination of Results

Statistics of Workshop participation

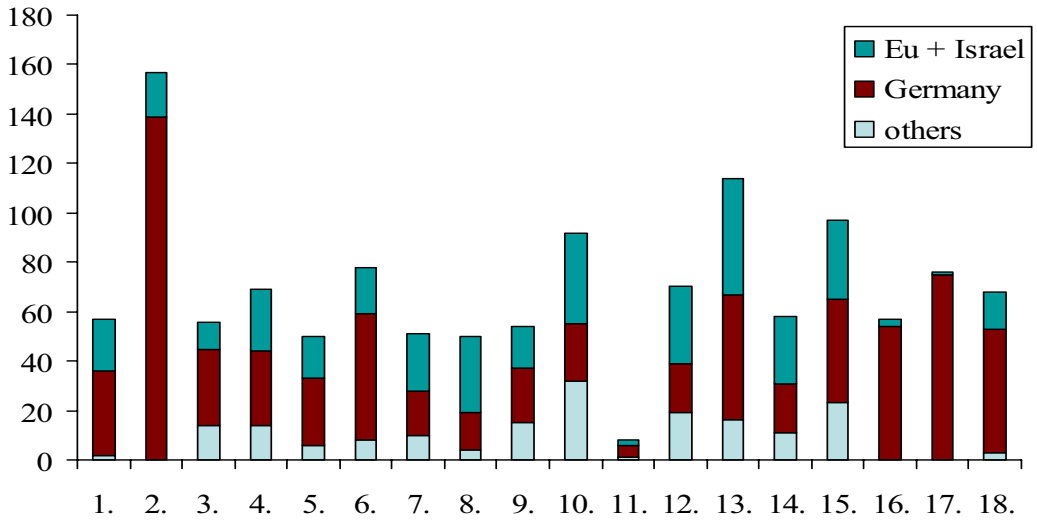

Figure 1: *Workshop/Seminar participantnumber in the year 2003.*

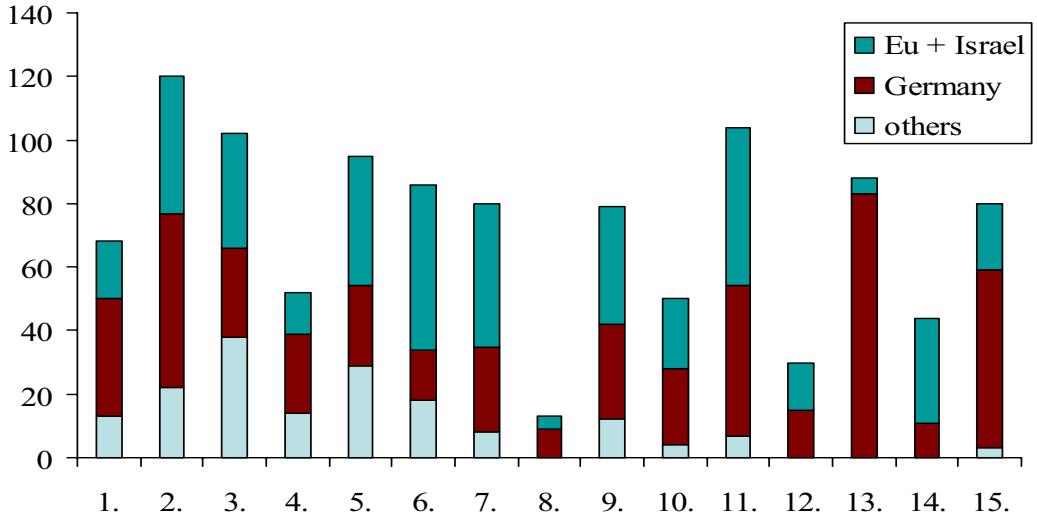

Figure 2: *Workshop/Seminar participantnumber in the year 2004.*

Dissemination of Workshop Results

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

- Workshop:
  Rydberg physics
  Journal of Physics B **38**, 1 - 421 (2005)
- Workshop:
  Trends in Pattern Formation: From Amplitude Equations to Applications
  Physica D **199**, 1 - 277 (2004)
- Workshop:
  Advances in molecular electronics: From molecular materials to single molecule devices
  G. Cuniberti, G. Fagas, K.Richter, Springer: (to be published)
- Workshop:
  Structural approaches to sequence evolution: Molecules, networks, populations
  U. Bastolla, M.Porto, H.E.Roman, M. Venduscolo, Gene: (to be published)

3.3.6 Workshop-Reports

Minerva Meeting of Young Researchers on Semiclassics, Quantum Chaos and Mesoscopic

Workshop, scientific coordinators: S. Fishmann, H. Schomerus, U. Smilansky

The purpose of this conference was to bring together young and senior researchers from Israel, Germany, and other countries, in order to discuss results and exchange ideas in the fields of semiclassics, quantum chaos, and mesoscopic physics.
Most important to the success of this meeting have been three aspects concerning the compilation of the participants:
a) The majority of the participants have been the about 40 young researchers at graduate student and young postdoc level.
b) Each field was well represented by senior researchers (advanced postdocs and professors) with international reputation in active scientific research.
c) Besides about twenty participants working in Israel and an equal number of external participants working in Germany (plus a few from other countries), an international group of about twenty local researchers from the mpipks and the TU Dresden took part in this meeting. The involvement of these participants considerably helped to enrich the program by their active contributions, and also attests to the benefit from this event for the host institution itself.

The 31 presentations (lasting 50 min each) and 18 posters (discussed in a lively Saturday-evening poster party) mainly have been given by the younger participants, while senior researchers were actively involved in the discussions and chairing the sessions. Presentations and posters encompassed topics from atoms and fields, chaotic scattering, mesoscopic transport, mixed and pseudointegrable systems, quantum pumps and ratchets, quantum computation, spectral correlations, and wavefunctions. All these fields share distinct quantum effects as common concepts, like resonances, coherence and interference, which advanced an atmosphere of mutual apprehension in quite different physical contexts. The participants listened attentively to each other's contributions, and exposed their own advanced and timely research in high-quality presentations. The scientific discussion was lively, both following the talks as well as in the breaks and after the program.
This meeting was co-sponsored by the Minerva Center for Nonlinear Physics, the Minerva Foundation, and the mpi**pks** .

Korrelationstage

Workshop, scientific coordinators: B. Büchner, P. van Dongen, P. Horsch
The main focus of the conference was to discuss properties of glasses at low temperatures, roughly 30 years after the discovery of the universal glassy low-temperature anomalies. It gathered in total 54 participants, 24 of them experimentalists and 30 of them theorists, which together represented a significant portion of the core of the international community working in the field. A number of PhD students or young post-docs participated in the workshop and had the opportunity to present their results.
The program consisted of 35 talks, 14 poster presentations and two dedicated discussion sessions. Main topics covered at the conference were dissipation and relaxation phenomena, elastic and thermal properties, magnetic field effects, dielectric properties, relations to spin-glass physics, memory effects, theoretical and experimental approaches to Bose-peak phenomena, optical investigations, microscopic and computational approaches, and metallic glasses.
Progress was reported at the conference for instance on numerical methods for dissipative quantum systems (Grabert), the understanding of nonlinear effects in dielectric response (Polishchuk, Ladieu), the clarification of the origin of magentic field effects on dielectric echoes (due to nuclear quadrupoles), both experimentally (Nagel, Enss, Hunklinger), and theoretically (Würger, Fleischmann, Enss), on memory effects in glasses (Ludwig, Osheroff), the computational exploration of energy landscapes in glasses (Heuer, Schober), or universal aspects of interaction induced restructuring of vibrational-mode spectra (Parshin) with implications on Bose peak physics.
Concerning the old question of universality of glassy low-temperature physics, complementary approaches were presented, one based on a renormalization group argument (Burin) taking a system of interacting quantized excitations (tunneling systems) as its starting point. The *Korrelationstage* bring mathematical physicists, phenomenologists, experts on various numerical approaches, and experimentalists working on a broad spectrum of highly correlated materials together with the purpose that they interact and exchange their research experiences.

Participants

The *Korrelationstage* were attended by many prominent and important physicists from Germany and several of its neighboring countries. The list of participants from Germany included: K. W. Becker, W. Brenig, G. Czycholl, H. Eschrig, H. Fehske, J. Fink, P. Fulde, F. Gebhard, C. Gros, G. Güntherodt, W. Hanke, K. Held, D. Ihle, E. Jeckelmann, B. Keimer, H. Keiter, A. Klümper, P. Kopietz, Th. Kopp, V. Meden, W. Metzner, H. Monien, E. Müller-Hartmann, K.-H. Mütter, A. Muramatsu, R. Noack, I. Peschel, M. Potthoff, Th. Pruschke, J. Richter, K. Samwer, A. Schadschneider, K. Scharnberg, K. Schönhammer, U. Schollwöck, D. Schotte, F. Steglich, J. Stolze, L.H. Tjeng, G. Uhrig, R. Valenti, H. von Löhneysen, M. Vojta, D. Vollhardt, W. Weber, R. Zeyher, K. Ziegler, G. Zwicknagl. Some prominent participants from outside Germany were: A. M. Oles, J. van den Brink, P. van Loosdrecht, D. Khomskii, H. G. Evertz, B. Normand, J. Schliemann. In accordance with tradition, the conference language of the *Korrelationstage* 2003 was German.

Scientific newcomers

The newcomers at the *Korrelationstage* 2003, i.e., advanced PhD-students and young postdocs, presented themselves in a variety of ways. Most of the newcomers presented their work in the form of posters. These poster contributions raised a lot of attention and generated vivid discussions. Other newcomers were given the chance to present their work in talks, some of which were absolutely brilliant. One young participant (P. Gegenwart, an experimentalist) was invited to hold the mpi**pks** Colloquium.

Scientific results

Among the scientific results of the *Korrelationstage*, that should be highlighted, are the new theoretical and experimental results on orbital physics and on heavy fermion systems, the progress made in developing powerful numerical algorithms, the new insights gained concerning the thermodynamic and transport properties of low dimensional systems, recent developments in density funcional theory and high-T_c superconductivity, and the insights gained concerning metal-insulator transitions. The *Korrelationstage* 2003 were generally considered to be so successful, that the participants had no doubts about the necessity of a follow-up conference. The next *Korrelationstage* are now scheduled for 2005.

Functional Renormalization in Interacting Quantum Many-Body Systems

Workshop, scientific coordinators: S. Kerein, A. Mielke, G. S. Uhrig, F. Wegner Renormalization (RG) is a powerful tool to focus on the relevant degrees of freedom in a systematically controlled way. In recent years there has been considerable progress in the renormalization of quantum many-body systems both on the conceptual and on the applied level. The workshop brought together the experts in the field in order to discuss recent advances as well as future directions of research. The comparison of various approaches, i.e. the assessement of their strengths and weaknesses, was one main focus. Another important aim was to disseminate the know-how of modern renormalization methods among younger scientists.
Important presentations were delivered by V. Bach (spectral properties with math-

ematical rigor), C. DiCastro (constraints on RG couplings from Ward identities), J. Fröhlich (mathematical foundations of bosonization and theorems on magnetism), M. Imada (path-integral renormalization), W. Metzner (two-dimensional Hubbard-model by Wick-ordered RG), M. Salmhofer (foundations of fermionic RG), K. Schönhammer (transport through interacting wires), R. Shankar (pedagogical introduction to RG), T.M. Rice (colloquium on the diversity of electronic states) and C. Varma (concepts for high-temperature superconductivity). The method of continuous unitary transformation of Hamiltonians (flow equations) was presented by the scientific coordinators.

Besides the important contributions from well-established and renowned colleagues the workshop has benefitted much from the dedicated input of young scientists. In particular, we wish to mention the talks by B. Binz (RG for the two-dimensional Hubbard model), T. Domanski (fermion-boson models), C. Honerkamp (temperature flow RG and itinerant ferromagnetism), A. Katanin (RG for the two-dimensional Hubbard model), V. Meden (transport through interacting wires), V. Oganesyan (nematic order in metals), T. Pruschke (Kondo-model by flow equations), A. Rosch (non-equilibrium transport through a Kondo impurity), A. Schwenk (RG in nuclear physics), K. Wiese (functional RG for disorder). Furthermore, also the PhD students participated in the discussions. Many participants stated that they have profited significantly from the workshop.

The topics presented ranged from mathematical rigorous statements to applications of the formalism to various physical question where strong correlations dominate. An excellent overview over the possible rigorous statements and over the possible applications has been obtained. The workshop succeeded to trigger vivid discussions on the potential of renormalization methods. It turned out that fixed points and the asymptotic behaviour at the lowest energies only are no longer the main objective for the application of renormalization. The current aim is to use renormalizing approaches to obtain quantitatively reliable results for various experimentally quantities on different energy and length scales. The aim is to derive effective models by renormalization-enhanced perturbation theory. It can be achieved by considering expectation values (Green functions) or effective hamiltonians (flow equation approach). The former approach is by now well established; more insight in the foundations of the latter is still desirable.

Further work is called for to overcome the difficulties to treat strong-coupling situations in extended models. Conceptual questions remain in the treatment of non-equilibrium problems. The workshop provided first ansätze also for these issues which we expect to stimulate future research.

Modern Aspects of Quantum Impurity Physics

Workshop and Seminar, scientific coordinators: R. Bulla, D. E. Logan, A. Schiller

The field of quantum impurity physics has recently seen a strong resurgence of interest. Important experimental advances have for example been made in the preparation and controlled interrogation of quantum impurity systems, spawning growth areas in nanoscience that include quantum dots, the study of magnetic adatoms on surfaces *via e.g.* STM experiments and so on. Recent years have likewise seen significant progress in

theoretical methods for handling quantum impurity and related models, encompassing almost the entire spectrum of physical properties, from thermodynamic to dynamic. Recognising the emergent modern era of quantum impurity physics, the intent of the workshop/seminar was to bring together a wide range of workers in the field; with a central aim of promoting communication and cooperation between researchers in different communities, and between theorists and experimentalists. In addition to general issues in the physics of quantum impurity systems, topics covered at the workshop/seminar included: • quantum dots and the many sides of Kondo physics, both in and out of equilibrium; • the Kondo effect on surfaces; • developments in theoretical approaches to quantum impurity and related models; • from impurity to lattice systems, including aspects of heavy fermions and dynamical mean-field theory; • magnetic impurities in correlated hosts and unconventional superconductors.

The mpi**pks** was an ideal place in every respect: location, facilities and support, as well as the superb organisation that underpinned the event. The workshop/seminar was certainly an international activity: researchers from 18 countries were present, with more than 70 participants in total. Highlight lectures included a joint Colloquium with mpi**pks** and TU-Dresden, given by M. Crommie (Berkeley) on STM studies of surface Kondo impurities and clusters; and the opening lecture of the Seminar by H. R. Krishnamurthy (Bangalore) giving an overview of quantum impurity physics. In addition, results, perspectives and insights on a diverse array of subjects were given by a range of 'senior scientists', including N. Andrei, T. Costi, J. von Delft,

P. Fulde, L. Glazman, A. Hewson, K. Ingersent, M. Jarrell, H. Kroha, H. Manoharan, L. Oliveira, T. Pruschke, A. Schneider, K. Schönhammer, M. Vojta and A. Zawadowski. One aim of the workshop/seminar was also to encourage active, but younger or less established researchers. They were well represented on the speaker's list, and included F. Anders, S. de Franceschi, M. Glossop, W. Hofstetter, C. Hooley, E. Jeckelmann, H.-A. Krug von Nidda, E. Lebanon, L. Limot, J. Nygard, Y. Oreg, B. Paulus, D. Quirion, F. Reinert and N. S. Vidhyahiraja. Participants also had the opportunity to present their work in two poster sessions — one each during the workshop and Seminar — and preceded by short oral presentations of the work. With the same aim in mind overview/tutorial lectures, as well as short research talks, formed an integral part of the workshop programme; although care was also taken to leave sufficient time for the individual discussions that are central to science, and which were able to thrive in the stimulating and friendly atmosphere that prevailed throughout.

Judged by the reaction of participants the workshop/seminar was a definite success. Many felt that a new and 'needed' community had been helped to crystallize, and our hope (indeed expectation) is that this will continue into the future. The organisers would simply like to express their grateful thanks to the mpi**pks** for the hospitality and generous support that made the venture possible.

Off-Shell Effects in Quantum Transport

Workshop and Seminar, scientific coordinators: P. Lipavsky, K. Morawetz

Vom 05.05.03 bis 16.05.03 fand am Max-Planck-Institut für Physik komplexer Systeme in Dresden ein internationaler Workshop statt, der sich mit den Erscheinungen auf kürzesten Zeitskalen beschäftigte. Im Rahmen dieses zweiwöchigen Workshops gelang es, hochrangige internationale und nationale Wissenschaftler der Festkörper- und Kern-

physik zusammenzubringen und sowohl aufregende experimentelle Resultate als auch neue theoretische Ansätze auszutauschen. Hierbei hat es sich bewährt, die 50 Vorträge auf zwei Wochen zu verteilen, so daß an jedem Tag 5 Vorträge am Vormittag gehalten und die Nachmittage für Diskussionen freigehalten wurden. Obwohl es von einigen Teilnehmern sehr bedauert wurde, nicht alle Vorträge hören zu können, da sie z.T. nur eine Woche anwesend sein konnten, war die Atmosphäre und der Freiraum Nachmittags außerordentlich stimmulierend für Diskussionen über das eigene Fachgebiet hinaus. Als ein erstes unmittelbares Resultat des Workshops wird im November ein Europäisches Netzwerk beantragt werden. Herausragende Experimente zu kürzesten Laserpulsen bis hin zu Kernstößen wurden vorgestellt, die an die Grenzen unserer Erkenntnis reichen. International herausragende Experimentatoren und Theoretiker versuchten, in den zwei Wochen dem Rätsel Zeit näherzukommen. Wie klein läßt sich die Zeit unterteilen? So beobachtet man auf den kürzesten erreichbaren Zeitskalen neuartige Phänomene, die auf der nicht wirklich stattfindenden ("virtuellen") Bewegung von Teilchen beruhen, bevor diese tatsächlich als reale (also nicht mehr virtuelle) Teilchen auftreten. In der Fachsprache heißt dies "off-shell". Das Thema "Off-shell" Effekte erwies sich als ein sehr geeigneter roter Faden durch das Programm, da sich zum einen die Festkörperphysiker mit Untersuchungen zu inkoherenten Anteilen im Transport und transienten Effekten genauso wiederfanden wie die Kernphysiker, wenn Teilchenproduktionen abseits der Massenschale beschrieben werden. Obwohl es eine gute Mischung des Programmes gab, war die erste Woche etwas mehr den Problemen der Quantenoptik, der ultraschnellen Propagation von Exzitonen und den ultrakleinen Nanostrukturen, wie z.B. Quantenpunkten gewidmet. Die zweite Woche legte den Schwerpunkt dann auf kernphysikalische Probleme von Phasenübergängen in Kernstößen und Transporteigenschaften auf kürzesten beobachtbaren Zeitskalen. Besondere Höhepunkte waren die experimentellen Resultate zur Femto-Sekunden Dynamik in Festkörpern durch entsprechende Kurzzeitlaser sowie die Messungen an künstlichen Atomen wie Quantenpunkten, wobei die Dynamik von geladenen Exzitonen im Quante-Hall Regime große Aufmerksamkeit erregte. Als Brücke zur Kernphysik kann man die hervorragenden Experimente an kleinen Metallclustern an sehen. Experimentatoren der Schwerionenreaktionen zeigten neuartige Verfahren der Datenanalyse, die den Schluß eines Phasenüberganges im Bereich der Multifragmentation nahelegen. Im Gegesatz zu dem bereits lange diskutierten Flüssig-Gas Phasenübergang scheint es möglich, daß eher eine Art Konfigurationswechsel der Materie stattfindet. Diese genaueren Analysen sind durch die nunmehr hervorragenden Daten vom GANIL möglich geworden, die erstmals wirklich erlauben dynamische Modelle zu testen. Von theoretischer Seite her wurde der gegenwärtige Stand der Quantentheorie des Nichtgleichgewichtes diskutiert und verschiedene Zugänge dargestellt, um transiente Effekte auf kurzen Zeitskalen sowie Korrelationen einzubeziehen. Hierzeigt sich, daß unser theoretisches Verständnis weit hinter den experimentell erreichbaren Aussagen zurückbleibt. Dieses hat allen Beteiligten eine neue Motivation gebracht, die offenen Fragen des Quantentransportes anzugehen. Hier sind in den nächsten Jahren entscheidende Entwicklungen in der quantenkinetischen Theorie für endliche Quantensystemen zu erwarten. Abschließend kann man feststellen, daß der Workshop unter dem Titel "Off-shell effects in quantum transport" Vorstellungen der Quantentheorie mit Theorien zur Beschreibung von Systemen im Nicht-Gleichgewicht sehr fruchtbar vereinte. Nicht zuletzt soll hier die außerordentlich effektive Organisation durch Claudia Poenisch hervorgehoben werden.

Ohne Abstriche an der wissenschaftlichen Qualität des Workshops machen zu müssen gelang es, mit ca 80% der zugesagten Mittel auszukommen.

Field Theory in Condensed Matter and Particle Physics

Workshop and Seminar, scientific coordinators: B. Altshuler, K. Efetov, L Frankfurt, K. Goeke, M. Strikman

This conference on quantum field theory in particle and condensed matter physics took place in the week 2.-6. June 2003. The topics were modern common applications and perspectives simultaneously in both fields. The workshop was organized by theoretical physicists from Germany (K. Efetov and K. Goeke, Ruhr-University of Bochum), USA (B. Altshuler, Princeton University, and M. Strikman, Pennsylvania State University) and Israel (L. Frankfurt, Tel Aviv University). The technical organization was done by Mrs. K. Lantsch from the Max-Planck-Institute.The objective of the workshop was to connect two fields of physics, which developed separately in the last years, but showed in recent times noticeable methodological similarities: Physics of condensed matter, mesoscopic physics and statistical physics on one hand and particle physics, hadronic physics and nuclearphysics on the other. The workshop, opened by E. Dreisigacker (Heraeus-Foundation) und P. Fulde (Max-Planck-Institute), offered in 27 talks by leading experts and by ample discussions and poster sessions the opportunity to connect both fields in a convincing way with future aspects and clear perspectives. The topics which turned out to be most relevant for both fields with great potentiality were: random matrix theory, supersymmetry, superbosonisation, conformal mappings, instantons, localization, spontaneous symmetry breaking, solitons and exotic states, quantum anomalies, gauge symmetries, lattice gauge theories, systemsof various space-time dimensions, theories of non-equilibrium processes and phase transitions, random-combinatorics. Those topics were covered in review talks by D. Diakonov (NORDITA), Y. Dokshitzer (U. Paris-VI), D. Khmelnitskii (U. Cambridge), V. Kravtsov (U. Trieste), A. Tsvelik (Brookhaven Nat.Lab.), A. Vainshtein (U. Minnesota), J. Verbaaschot (U. Stony Brook), J. Wess (U. Munich), P. Wiegmann (U. Chicago), A. Zamolodchikov (Rutgers U.), M. Zirnbauer (U. Cologne),etc. The seminar has been financed by the Wilhelm und Else Heraeus-Foundat ion und received further support by the Alexander von Humboldt-Foundation (Wolfgang Paul and Sofja Kovalevskaja-Programs) and the Max Planck Gesellschaft. The discussions were extraordinary lively and all participants were fond of the good technical service and the quiet and relaxed atmosphere of the Max-Planck-Institute.

Classical and Quantum Barrier Transport in Complex Systems

Workshop, Scientific coordinators: J. Ankerhold, T. Geisel, P. Reimann

The main focus of the workshop has been on the recent theoretical progress and spectacular experimental achievements regarding the role of transport in the presence of potential barriers for physical, chemical, and biological systems. Phenomena on scales ranging from ensembles of atoms to structures in biological cells have attracted an interdisciplinary community of 76 participants. Their contributions – even though quite different in detail – has led to a substantial exchange of ideas and methods between

practitioners in atomic, condensed matter, statistical, and chemical physics. The three methodological cornerstones of the workshop were: (i) classical/quantum mechanical dissipative transport across/through potential barriers, (ii) Brownian motors, molecular motors, ratchet systems, and (iii) deterministic quantum transport in periodic structures. An explicit aim and achievement has been to provide a platform for younger scientists in order to present their results in about 1/3 of the 50 invited lectures an in some 20 very fine poster contributions. A further goal of the workshop has been a sound mixture of experimental and theoretical participants and has indeed lead to numerous very promising new contacts.
The organizers wish to cordially thank the mpipks for the generous support of the meeting and especially the conference secretary Mandy Stiegler for the extremely enjoyable and professional collaboration.

Fermi-liquid instabilities in correlated metals

Workshop, scientific coordinators: H. von Löhneysen
This Workshop was the final Annual Workshop of the European Science Foundation (ESF) Programme "Fermi-Liquid Instabilities in Correlated Metals (FERLIN)" which was initiated 1998 by a Steering Committee headed by H. v. Löhneysen, Karlsruhe, and was funded by research funding agencies of 9 European countries. Focus of the ESF programme and also of the workshop were the various forms of Fermi-liquid instabilities occurring in different classes of metals with strong electronic correlations, in particular f-electron systems and transition-metal oxides, notably cuprate superconductors. While there are various microscopic origins of Fermi-liquid instabilities, an important scenario is the proximity to a quantum critical point (QCP) separating a magnetically ordered and a Pauli-paramagnetic ground state. Manifestations of a QCP may be found in unusual thermodynamic and transport properties deviating from the predictions of a Fermi liquid. However, microscopic measurements and spectroscopy tools are necessary to unravel the nature of the fluctuations determining the quantum critical behavior. Consequently, the workshop was organized in the following sessions covering these aspects: Non-Fermi-liquid behavior and quantum critical points in f-electron systems, Fermi-liquid instabilities as investigated by electron, neutron, μSR and optical spectroscopy, Theory of quantum criticality, Quantum critical points in HTSC, and Ferromagnetic superconductors, with a total of 27 invited talks of 30 min. each, complemented by a session with 6 short contributions and an evening poster session with 16 posters. The workshop was attended by 52 registered participants but also attracted a number of scientists of the Max-Planck-Institutes in Dresden. Among the important participants were Z. Fisk, addressing the topic "Probing the Fermi lattice", J. A. Mydosh "The many high field phases of URu_2Si_2", M. B. Maple "Supercondctivity near quantum critical points in f-electron materials", A. Georges "So me remarks on the puzzle of non-Fermi liquid behaviour at a quantum critical point", S. Sachdev "Understanding correlated electron systems by a classification of Mott insulators", and Z. X. Shen "Competing interactions in cuprate superconductors". Scientific newcomers presented short contributions and/or posters. Although this was the last workshop of the series within the ESF programme FERLIN, it was felt by many participants that this research field continues to be a very lively and topical subject. The workshop was honored by Professor Fulde officially opening the workshop. The scientific organizers

are indebted to the Max-Planck-Institut für Physik Komplexer Systeme for hosting this workshop and supporting it, together with the ESF. Finally, the efficient and friendly organization of the workshop, including a magnificant excursion to Schloss Pillnitz with a wine tasting party, by Claudia Pönisch is gratefully acknowledged.

Collective Phenomena in the Low Temperature Physics of Glasses

Workshop, Scientific coordinators: C. Enss, S. Hunklinger, R. Kühn

The main focus of the conference was to discuss properties of glasses at low temperatures, roughly 30 years after the discovery of the universal glassy low-temperature anomalies. It gathered in total 54 participants, 24 of them experimentalists and 30 of them theorists, which together represented a significant portion of the core of the international community working in the field. A number of PhD students or young post-docs participated in the workshop and had the opportunity to present their results.

The program consisted of 35 talks, 14 poster presentations and two dedicated discussion sessions. Main topics covered at the conference were dissipation and relaxation phenomena, elastic and thermal properties, magnetic field effects, dielectric properties, relations to spin-glass physics, memory effects, theoretical and experimental approaches to Bose-peak phenomena, optical investigations, microscopic and computational approaches, and metallic glasses.

Progress was reported at the conference for instance on numerical methods for dissipative quantum systems (Grabert), the understanding of nonlinear effects in dielectric response (Polishchuk, Ladieu), the clarification of the origin of magentic field effects on dielectric echoes (due to nuclear quadrupoles), both experimentally (Nagel, Enss, Hunklinger), and theoretically (Würger, Fleischmann, Enss), on memory effects in glasses (Ludwig, Osheroff), the computational exploration of energy landscapes in glasses (Heuer, Schober), or universal aspects of interaction induced restructuring of vibrational-mode spectra (Parshin) with implications on Bose peak physics.

Concerning the old question of universality of glassy low-temperature physics, complementary approaches were presented, one based on a renormalization group argument (Burin) taking a system of interacting quantized excitations (tunneling systems) as its starting point — an approach initiated by Yu and Legget (both also present at the conference) — and another one that investigates the glassy interacting many body system with an eye towards the *emergence* of a particular spectrum of quantized low energy excitations (Kühn), the latter also leading to a tentative explanation of the so-called quantitative universality. First steps at formulating a quantum field theory for the description of glassy low-temperature physics were also discussed (Schirmacher)

Lastly, contributions which may perhaps have opened wider perspectives for the field were those pointing out the possible relevance of quantum spin-glass concepts for the understanding of ultra-cold glasses (Rieger), or the considerable potential that noise-spectra could have in helping to understand the low-temperature physics of structural glasses.

Quantum Phase Transition

Workshop, Scientific coordinators: D. Belitz, T. R. Kirkpatrick, T. Vojta

Quantum phase transitions are a central topic in modern condensed matter physics. They occur at zero temperature as a function of a non-thermal order parameter, and are thought to be of crucial importance for the understanding of such diverse topics as metal-insulator transitions, heavy fermions, the quantum Hall effects, or high-temperature superconductivity.

This Seminar, built around a three-day Workshop, has brought together 88 researchers from 17 countries and 3 continents. Main topics covered by the workshop, and the corresponding invited speakers, were,

- Metal-insulator transitions and related quantum phase transitions in two-dimensions (Popovic, Pudalov, Shahar)
- Quantum ferromagnets, antiferromagnets, and spin glasses (Chubukov, Julian, Nicklas, Pfleiderer, Rieger, Young)
- Heavy fermions and new types of quantum criticality (Geibel, Si, M. Vojta) item Exotic superconductivity and superconducting transitions (Huxley, Kapitulnik, Maple)
- Transitions in quantum Hall systems (Jiang)
- General aspects of strongly correlated electrons (Marston)
- Quantum dots (Shankar)

In addition, two "precursor talks" by Frank Steglich (on heavy fermions) and Hilbert von Löhneysen (on quantum antiferromagnets) provided high-profile contributions from two speakers who were unable to attend the workshop proper. The focus of the workshop was deliberately on the experimental side, to provide the mainly theoretically oriented seminar with the latest experimental results. Lively discussions ensued, which helped shed light from various angles on the presented results. A poster session that remained in place throughout the workshop gave all participants, and in particular young researchers, a chance to present their work to an international audience of experts.

The seminar was centered around informal talks, on average once a day. Almost all of the participants took advantage of this opportunity. In addition, the seminar contributed an Institute Colloquium, which was given by Ian Affleck on Luttinger liquids. Every Monday an informal get-together ensured that newly arrived participants could introduce themselves to the group and briefly outline their research interests. These organized activities were deliberately held to a minimum, to give the participants ample time for spontaneous discussions. Judging from the lively use of the discussion and meeting rooms, this model worked very well. Apart from providing a venue for researchers, both established and emerging, from all over the world to exchange ideas and obtain feedback on their work, this seminar/workshop has underscored the common physical phenomena that underly seemingly unconnected phenomena in strongly correlated electron systems. One of the main scientific results of the event has been a heightened awareness that soft modes, which determine the critical behavior at phase transitions, are likely responsible for a host of interesting phenomena, both close to and

far away from quantum critical points. In summary, this was a highly successful event, in large part due to the generous support provided by the mpipks both in financial terms and through the efforts of the Institute's expert staff.

Quantum Transport and Correlations in Mesoscopic Systems and QHE

Workshop, scientific coordinators: V. Falko, B. Altshuler, A. Ludwig

This workshop has brought together experts in field-theoretical treatment of classical and quantum transport problems in chaotic and disordered systems and self-organisation in complex systems. The main focus of this meeting was on the interplay between interactions and complex dynamics in quantum dots (such as Kondo effect and Luttinger liquid discussed in talks by Y. Nazarov, J. von Delft, T. Giamarchi, P. Brouwer, M. Pustilnik, D. Polyakov, Y. Alhassid), on the issue of coherence and de-coherence on the single-particle and many-body level and of the noise and charge/energy transfer statistics in quantum transport devices (discussed in talks by D. Loss, L. Glazman, I. Lerner, A. Lamacraft, C. Beenakker, L. Faoro, F. Marquardt, N. d'Ambrumenil, D. Saraga). The studies of these two topics are crucially important for the development of a realistic theory of quantum computation and finding ways to create a solid state realisation of qubits and qubits networks. We have also discussed the development of new analytical techniques applicable to disordered systems (the use of functional renormalisation group approach has been discussed in the talk by P. Le Doussal and K. Wiese), and O. Agam and I. Gruzberg have given a series of talks and informal lectures on the application of Leowners equation to the description of fractal structures emerging in the self-organising systems in physics and biology and in the patter formation (talk by E. Brener). The notes prepared by I. Gruzberg for his lectures have recently appeared on the web: cond-mat/0309292. Few talks also discussed the recent progress in the quantum Hall effect and localisation (M. Raikh, M. Zirnbauer, S Ryuu, A. Mirlin, M. Ortuno Ortin).

In the middle of the workshop, we have arranged for a special event, the Zero-Resistance Day focused on the recently discovered phenomenon of a zero-resistance state observed in the 2DEG subjected simultaneously to a magnetic field and the high-intensity microwave irradiation. R. Mani has presented the experimental side of this finding of von Klitzings group at MPI-FKF in Stuttgart, and I. Aleiner has offered an overview of theoretical activities in this field. These two scheduled talks have been followed by several informal afternoon seminars (by A. Mirlin and Klesse) and intense discussions. For scientific newcomers to present themselves, we have run one poster session, where all willing participants have presented posters. With enough free time left for discussions and the time of talks not rigidly restricted, everyone had a chance to ask questions and to bring the subject to the level of mutual understanding. The main goal of this meeting was to provide participants with an opportunity to collaborate and the newcomers - with the chance to meet leading experts in the field of quantum transport and to initiate work with them. That is why the programme of talks filled only half of each day. There was, therefore, ample time for work, and several groups have emerged themselves and built the foundations for future collaborations. There were many examples, and there was at least one paper submitted during the meeting itself that would not be completed otherwise, cond-mat/0308052. The discussions during the Zero-Resistance Day have initiated collaborations between I. Aleiner (Columbia) with

A. Mirlin (Karlruhe) and with R. Klesse and F Merz (Koln). Joint interest have been also found by J. Robinson and Falko from Lancaster and M. Kennet and N. Cooper from Cambridge, who are already preparing a paper on surface acoustic wave induced magneto-resistance in 2DEG.

Trends in Pattern Formation: From Amplitude Equations to Applications

Workshop, Scientific coordinators: M. Bär, H. Engel, E. Schöll, A. Torcini
Main focus: The conference focussed on new developments in pattern formation. During the first period the focus was on amplitude equations, phenomenological approaches and fluid dynamics, while in the second half applications in biology, chemical reactions and applied physics were highlighted. Altogether ca. 60 invited speakers, 50 participants (out of 75 applications) and the 4 coordinators participated in the meeting.
Senior participants: E. Knobloch, I. G. Kevrekidis, W. Zimmermann, D. Barkley, E. Meron, L. van Hemmen, R. Friedrich, W. van de Water, A. Politi, T. Geisel, R. Goldstein, H. Meinhardt, W. van Saarloos, H. Levine, K. Showalter, J. Socolar, L. Bonilla, T. Arrechi, L. Schimansky-Geier, L. Pismen, R. Kapral, A. Mikhailov, V. Hakim, J. Hudson, S. Müller, H. G. Purwins, C. Denz, U. Ebert, M. Fromhold.
Young scientists: 26 out of a total of 74 talks given in the two workshops and the seminar were presented by young scientists in postdoctoral position without tenure. Also the majority of the posters has been presented by young people at the Ph. D. or postdoc level. Young scientists made the two seminar weeks a very stimulating experience.
Scientific results: During the first workshop a lively dialogue between experimentalists mostly from fluid dynamics and theoreticians emerged that has already led to first new collaborations. Highlights were talks that showed a detailed access and understanding to complex patterns in convection, optical systems, thin film dynamics and a variety of complex fluids. A second notable development is the fruitful application of amplitude equation concepts developed for fluids and chemical reactions to a variety of fields including ecology, technical processes, biophysics and granular materials. The seminar dealt with general concepts for complex systems and advances in the stability analysis of nonlinear waves. The second workshop provided an excellent overview of developments in biological systems, chemical pattern formation and physical applications. Interdisciplinary sessions addressed the control of patterns and the treatment and influence of noise in experiments and models (ESF sponsored session on Wednesday). As a result of the meeting a special issue of the Physica D on the topic ,,Stability, Fluctuations and Control in Pattern Forming Systems" with ca. 25 original papers will be published.
Acknowledgements: We would like to thank the MPI for Physics of Complex Systems for generous support and the ideal environment as well as Mandy Lochar for her efficient and dedicated organization of the whole meeting. We are also very grateful to the SFB 555 ,,Complex nonlinear processes" and the ESF programme ,,Stochdyn" for enabling us to extend the scope of the meeting and supporting the participation of many young scientists among the applicants.

Non-Equilibrium Statistical Physics in Low Dimensions and Reaction Diffusion System

Seminar, Scientific coordinators: P. Grassberger, M. Henkel, H. Hinrichsen, U. Schollwöck

The study and comprehension of collective phenomena of systems with many strongly coupled degrees of freedom and out of equilibrium is one of the great challenges at present. The motivation for this International Seminar was to bring together experts from non-equilibrium statistical physics in low dimensions, in particular researchers working on exactly solvable systems, novel field-theory methods, and new methods in computational non-equilibrium physics. The aim was to allow for a cross-fertilization in these different fields, in order to achieve deeper physical insight into the physics of scale-invariant strongly interacting systems with many degrees of freedom.

One major focus of the seminar was the study of driven diffusive systems as well as coarsening and phase separation (including the talks by Y. Kafri, D. Mukamel, G. M. Schütz, R. Zia). As a remarkable result it was shown how to formulate a general criterion under which conditions phase separation in one dimension can be expected. Applications to specific models have provided insight beyond the capabilities of pure numerical simulation.

A number of talks focused on the so-called diffusive pair contact process which exhibits an unusual type of critical behaviour (G. T. Barkema, E. Carlon, H. Chaté, G. Ódor, H. Park). Since the numerical and approximative results are debated controversially two additional round-table discussions were arranged. As a promising direction towards a better unterstanding of this critical phenomenon, a novel type of field theory was presented by U. C. Täuber and F. van Wijland.

Significant progress has also been made in solving particular reaction-diffusion systems exactly (D. ben-Avraham, J.-M. Luck, E. Ben-Naim, S. Majumdar). Moreover, various talks were concerned with general methods of nonequilbrium statistical physics (B. Derrida, C. Godrèche, W. Janke, I. Jensen, Z. Racz, C. Sire) and the treatment of specific non-equilibrium models (E. Albano, J.F.F. Mendes, A. Vespignani). Other contributions emphasized the relation to different fields such as synchronization transitions (M. Muñoz) or heteroepitaxial growth (M. Biehl). Finally, the talks by B. Nienhuis and V. Rittenberg reported on recent breakthroughs in conformal field theory applied to non-equilibrium statistical physics.

One of the goals of the seminar was to stimulate discussions and to trigger new cooperations. For this reason the number of talks per day was limited, leaving enough time for mutual interaction among the participants.

In addition 20 posters were presented, allowing the younger participants to communicate their results. As the posters were located between the offices they attracted much more attention than in a separate poster session. Indeed, several papers are forthcoming from the common work carried out during the Seminar.

The seminar was a very fruitful platform for the exchange of ideas. These mutltiple exchanges reconfirm that the study of non-equilibrium statistical physics is a lively and promising field. It became clear that the complexity of the observed phenomena requires a joint effort from various directions, employing exact, field-theoretic, as well as numerical and approximative methods.

Motion, sensation and self-organization in living cells

Workshop, Scientific coordinators: Karsten Kruse, Frank Jülicher, Jonathon Howard, Jaques Prost

The goal of the workshop and seminar was to bring together biologists, and physicists in order to discuss recent advances in cell biology and cellular biophysics, as well as to define and identify prospects of future research. During the workshop week, thematic sessions covered gene expression, hearing, mitosis, flagellar motility, cellular force transduction, cell organization, motors and filament dynamics as well as actin dynamics. The sessions consisted of three to four talks, each of 45 min duration with 15 min of discussion. The presentations were given by outstanding senior scientists most notably Michael Fisher, Jim Hudspeth, Tim Mitchison, Julie Theriot, Raymond Goldstein and Michael Sheetz. The colloquium talk given by Jim Hudspeth from Rockefeller University, New York was a particular highlight of the conference. The workshop week was not only characterized by an exceptionally high quality of presentations, there were after each talk long and lively discussions, which would involve comments and insights from different diciplines

Young participants could present their work in a poster session on Tuesday evening. This poster session was a great success and lead to many stimulating discussions. In addition, contributed oral presentation were given by participants during the second seminar week. The second week was organized i n a less formal manner with the morning sessions consisting of several talks, while in the afternoon discussion sessions were organized. Thematically, the morning sessions covered hearing, actin, microtubules, and integral properties of cells. To name but two of the subjects discussed in the afternoons, cell locomotion and the formation of membrane tubes. The second seminar week kept a very high quality of presentations and discussions were lively and deep.

In summary, the workshop and seminar week was a very successful event judging from comments of many participants as well as the numerous discussions between speakers and participants of very diverse backgrounds.

Resonances - From physics to mathematics and back

Workshop, Scientific coordinators: A. Buchleitner, R. Hempel

Main focus of the conference The central purpose of the workshop was the exchange of concepts from Mathematics and Physics relevant for the characterization and analysis of unstable, decaying quantum states—so-called "resonances". In many cases these concepts complement one another and one community has developed efficient tools (mathematical or theoretical or experimental) while the other one holds a problem perfectly suited for an application of these tools. Here a key issue is the translation of community-specific "jargons" which too often hinder the communication.

Most important participants E. Brézin (Paris), J.-M. Combes (Marseille), E.B. Davies (London), P. Gaspard (Bruxelles), P. Hislop (Lexington), G. Kaindl (Berlin), W.P. Reinhardt (Seattle), J. Sjöstrand (Palaiseau), U. Smilansky (Rehovot), H.-J. Stöckmann (Marburg), K. Yajima (Tokyo), M. Zworski (Berkeley).

Presentation of scientific newcomers

The workshop program was specifically tuned to provide a stage for promising PhD students and young PostDocs, at each level: all speakers were given the same amount

of time for their presentation and younger speakers systematically appeared at prominent time slots (i.e., they were *not* relegated to "edge slots" like friday afternoon or the last slot of a long day). Furthermore, "tough" young colleagues have been chairing sessions, and two long poster sessions were given central time slots (Tuesday evening and Thursday afternoon).

Results
The workshop stimulated numerous fruitful and intense discussions during the breaks and also during the poster sessions (having set up a program with relatively generous breaks was instrumental for this strong interaction of the participants). Once more, the specific logistics offered by the mpi**pks** with its various discussion rooms proved to be perfectly suited. This stimulating and informal atmosphere led to the identification of common problems, e.g.

- between mathematicians and experimentalists interested in strong localization phenomena (of dynamical/Anderson type) in periodically driven, open quantum systems;
- between mathematicians and computational physicists struggling with spurious solutions of complex non-symmetric eigenvalue problems;
- mathematicians and theoretical physicists interested in the simultaneous description of coherent and incoherent coupling to different continua (imagine, e.g., an excited atomic or molecular level coupled, through coherent laser radiation, to an atomic/molecular continuum, and simultaneously to the electromagnetic vacuum);
- between mathematicians, theoretical physicists, computational physicists,and experimentalists working on statistical properties of resonances at high spectral densities, i.e., in the semiclassical regime.

The communication between the different communities present was considerably enhanced by "Dictionary Sessions", which we had first introduced during our "QRandom II" workshop in January 2002. On two afternoons we dedicated approximately one hour to the clarification and definition of "jargon words" expressing notions that are completely obvious to one group but remain totally opaque to the others without a five minute definition (e.g., "C-product", "F-product", "spectrum", "meromorphic continuation", "compact operator", "self-adjoint extensions", "Stark resonances", "dilation", "trace class operators", "Gutzwiller trace formula", "scattering length"). To the delight of the organizers, these dictionary sessions have once again been enthousiastically received by the participants; they contributed considerably to the truly constructive and illuminating discussions during and after the talks. From the feedback we received from various participants since the end of the conference, common research projects or at least intense scientific exchanges have been seeded by the meeting. Finally, a public evening lecture in the institute's large lecture hall was delivered by Peter Richter (Bremen) on "Schönheit und Chaos in der Kreiseldynamik", on thursday evening. Afterwards, discussions between interested laymen and workshop participants lasted for at least one more hour in the institute's lobby.

Advances in molecular electronics: From molecular materials to single molecule devices

Workshop, Scientific coordinators: G. Cuniberti, G. Fagas, K. Richter
The international Workshop on "Advances in Molecular Electronics", held atmpi**pks** Dresden, brought together most of the world leaders in Molecular Electronics, among them Prof. Mark Ratner, one of the founders of the field. The recent developments of this rapidly growing and highly multidisciplinary field were featured by a balanced selection of participants from Physics, Chemistry and Engineering. Both Theory and Experiments were presented. The thematic activities discussed at the workshop included: i. carbon nanotube-based molecular conductors ii. realization of single-molecule electronics iii. DNA-based devices iv. theory of electron transport and device modeling at the nanoscale v. organic molecular materials and organic optoelectronics. The mixed composition of internationally recognized experts in the field (Z. Bao, M. Di Ventra, J. Jortner, P. Hänggi, K. Leo, K. Likharev, A. Nitzan, S. Pantelides, M. Ratner, M. Reed, D. Tomanek, J. van Ruitenbeek, to name only a part), young postdocs and students guaranteed the valuable training of junior (andsenior) scientists who recently entered or are approaching Molecular Electronics. Several industrial research laboratories (Hewlett-Packard, Phillips, IBM) were also represented. With such an agenda, the envisaged number of 60 participants had been reached very soon and despite the generous extension of the participants number by the mpi**pks** administration, many highly qualified applicants had to be rejected. A total of 125 (including local scientists from the TU-Dresden and mpi**pks**) from 20 European and non-European countries (including USA, Japan, Canada, Brazil, Korea) attended the workshop. The scientific program comprised invited (33; 30 + 5 min discussions) and contributed talks (18; 15 + 5 min discussions), highlighted presentations (colloquium by M. Reed (Yale), evening lectures (3); 45-60 min), short and extended poster sessions (53 contributions), and a round table discussion (2+ hours). At the end of the conference a public lecture was delivered for the citizens of Dresden (in German). The lecturer, Dr. Siegmar Roth (MPI Stuttgart), disclosed recentadvances in Molecular Electronics at a popular science level in his vivid talkentitled: "Elektronik aus der Retorte?" (Schaltmoleküle und Nanoröhrchen für Superchips?). The rich combination of invited, plenary, and contributed accounts allowed for covering the various advances in the rapidly developing field and for presenting the most recent results of both, groups and scientists with track record in the field and researchers with new ideas from adjacent disciplines. Contributed talks were given by PhD students, junior and senior scientists. The poster sessions generated an additional exchange of ideas at the forefront of current developments. An extremely important complement of the formal presentations was the round table discussion which pointed out current trends andproblems in Molecular Electronics, followed by some brain-storming on the challenges ahead. The success of the Workshop is reflected in a questionnaire that was distributed (for internal use) to the participants.

Rydberg physics

Workshop, Scientific coordinators: R. Cote, T. Pattard, M. Weidenmüller
The International Workshop and Seminar on Rydberg Physics took place at the Max Planck Institute for the Physics of Complex Systems in Dresden from April 19^{th} to

May 14^{th} 2004. The purpose of the conference was to bring together theoretical and experimental physicists working with atoms or
molecules in highly excited states (Rydberg systems). The central event was a workshop week where all areas of Rydberg physics were covered, embedded within three weeks of seminars with lecture series devoted to specific aspects and targeted at PhD students and young Postdocs. The meeting was considered extremely fruitful by the conference participants. The workshop week assembled more than 90 participants from 22 different countries, with all the key players in the field attending. For the seminar weeks, renowned experts could be recruited for the lectures, which was reflected in the participation of on average 30 "students". Many more applications to participate had to be denied in order to keep the meeting within a reasonable limit.
The seminar weeks were determined by extended lecture series, as well as long subsequent discussions between the participants, which showed the high level of motivation of the seminar attendees. In the workshop week, more than 40 talks and two well-attended poster sessions reflected both the diversity of the field and the impressive progress that has been achieved in the last years. New directions in the field have been identified and new collaborations have been stimulated during the meeting. Moreover, research results presented at the workshop and the lectures given during the seminars will be published in a special issue of Journal of Physics B and a volume of the Springer "Lecture Notes in Physics" series, respectively, ensuring a lasting impact on the Rydberg physics community beyond the actual workshop.
The success of the workshop is intimately linked with the open atmosphere of the institute and its efficient and professional staff members. The organizers are very grateful for the hospitality of the institute as well as the financial and organizational support of the Max Planck Society, without which this workshop would not have taken place.

Cooperative Phenomena in Optics and Transport in Nanostructures

Workshop, Scientific coordinators: M. Portnoi, R. Römer, T. Shahbazyan
The Seminar and Workshop on "Cooperative Phenomena in Optics and Transport in Nanostructures" (CoPhen04) took place at the mpi**pks** from May 31 to June 25, 2004. CoPhen04 was quite distinct from other conferences in the breadth of the topics covered and in the diversity of the research interests of the participants. The reasons for such a diversity of topics and people were spelled out in theconference announcement. In short, the main objectives of the event were (a) to bring together experimentalists and theorists from various fields in order tofacilitate the exchange of ideas between seemingly different topics and encourage collaborations and crosstalk between people of different interests and research fields; and (b) to mix together young scientists at the beginning of theirscientific careers with well-established leaders in the various fields with the aim of helping young scientists to get into the forefront of research in different areas - a crosstalk between generations. The feedback received from the participants during and after the event certifies that both goals were achieved.
The workshop has had a number of topical sections represented by leading and young researchers (both for experiment and theory). These represent much of the current research activities in condensed matter physics and the main topics (with leading topical speakers indicated) were Quantum Dots (Haug, Imamoglu, von Oppen, War-

burton), Quantum Computing (Dykman, Hawrylak), Transport in Mesoscopic Systems (Grundler, Lorke, Savchenko), Magnetoresistance/Quantum Hall Effect (Chalker, Dyakonov, Vignale), Nanoplasmonics (Citrin, Stockman, Vallee), UltrafastDynamics (Bigot, Elsaesser, Nurmikko, Wang), Photonics (Baumberg, Bergmann, Kavokin), Bose-Einstein Condensate (Butov, Littlewood, Snoke), Organic Materials (Di Carlo, Mukamel, Shklovskii, Turberfield, Vardeny).
The presence of leading researchers in each field resulted in intensive (and sometimes heated) discussions following the talks. These were particularly usefulfor young scientists to participate in. The Workshop Colloquium given by the distinguished researcher Boris Shklovskii was also very successful and had perhaps the largest audience of recent MPI Colloquia, at least according to opinionsexpressed by mpi**pks** in-residence scientists. The 3-week Seminar - into which the Workshop was embedded in week 2 - had been envisioned as a school for young scientists, postdocs, and students. For this purpose, the organisers asked several leading and young scientists to present a long (1.5 hours) lectures designed as an introduction into their respective fields. We are particularly grateful to Profs. Dzyubenko, Raikh, Apalkov, Falko, Chaplik, Cooper, Fogler, Shtengel, Lyanda-Geller, Kibis, Ulloa, and Raimondi whowere able to stay for an extended period to make the seminar a success. Young scientists, including postdocs and students, have complemented the Seminar by giving regular 1-hour talks held each afternoon on their current research. In order to ensure future access to the materials of CoPhen04 for participants and the larger scientific audience the programme of these events on the mpi**pks** website is complemented by the scripts for a large number of talks. The reaction of participants to the unusual diversity of conference topics was uniformly enthusiastic. Many participants expressed in strong terms their excitement by the number of new topics in the program as well as by the high scientific level of the discussions. A number of senior participants and especially yo ung scientists suggested that follow-up conferences would be quite useful to hold at mpi**pks** in the future. Also, various collaborations took place during Workshop and Seminar that we are convinced will lead to exciting research results in due course. The organizational part of the Workshop and Seminar, managed by Katrin Lantsch, was outstanding and won uniform praise from participants as well as organizers. All issues related to housing and last minute changes in participants plans were solved promptly and efficiently. The entertainment part of the Conference was excellent. On behalf of ourselves and the participants, we would like to sincerely thank the mpi**pks** for making this event possible and for the generous support provided.

Structural approaches to sequence evolution: Molecules, networks, populations

Workshop, Scientific coordinators: U. Bastolla, M. Porto, H. E. Roman, M. Vendruscolo

The goal of this workshop has been to bring together experts from different scientific communities working in the fields of molecular biology, bioinformatics, and mathematical modeling. The idea of the workshop started with the recognition that an interdisciplinary combination is indispensable to achieve the two main objectives of the study of molecular evolution, namely (i) to reconstruct the biochemical history of life, through the analysis of the macromolecules of existing organisms; and (ii) to understand the

determinants of the evolution at the molecular level. The increasing amount of data made available by genome sequencing projects are demanding an increasing integration of the abovementioned disciplines. In particular, progress in understanding the structural properties of biological entities at different levels, as molecules, networks, and populations, greatly contributes both to elucidate the mechanisms of evolution and to reconstruct its course. The synergies between experimental, theoretical, computational, and statistical analysis approaches are anticipated to improve our understanding of the processes and pathways of molecular evolution, and need to be pursued further. However, some of the fields that we considered in the workshop, such as those studying the structure and thermodynamics of biomolecules, gene networks, and the mechanisms of molecular biology, are not yet fully integrated in the field of molecular evolution and the need for a closer integration of these disciplines is becoming increasingly evident. Therefore, the central goal of the workshop has been to stimulate this integration, by bringing these different disciplines together and providing a framework for interaction. The workshop has been organized in three main units dedicated to three main levels of description: Biological macromolecules, macromolecular interaction networks, and biological populations. These three levels give a broad overview of the whole field of molecular evolution. In particular, as system biology is raisi ng more and more interest among experimental, computational, and theoretical biologists, we are witnessing a shift of focus from the evolution of single molecule properties to the evolution of the integrated properties of protein interaction networks, which lay at the core of cellular processes. Yet, this level is still not considered in more traditional approaches to molecular evolution. The workshop has been structured in ten sessions, namely 'RNA' (P. Schuster and P. Stadler), 'Proteins' (R. Goldstein, A. Lesk, and C. Orengo), 'Drift and Selection' (A. EyreWalker, H. Fraser, and T. Ohta), 'Mechanisms of Molecular Evolution' (L. Cowen, M. Nei, and J. Shapiro), 'Prokaryotic Genomes' (A. Moya), 'Eukaryotic Genomes' (G. Bernardi and L. Duret), 'Genomic Elements and Modules in Evolution' (T. Gojobori), 'Networks' (P. Bork, K. Jordan, M. Lässig, A. Valencia, and A. Wagner), 'Phylogenetic Trees' (P. Higgs, P. Li'o, and J. Lobry), and 'Populations' (E. L'azaro and L. Peliti). Besides the contributions of the invited speakers, the workshop has benefited enormously of very high level contributions from non-invited participants.

3 The friendly and communicative atmosphere that developed from the very beginning favored the discussion, which was also facilitated from the fact that most talks contained references to the work of other participants. Participants' reactions to our effort to integrate the so far separated disciplines into a single workshop and, possibly, into a common scientific community has been unanimously enthusiastic. Prof. Bernardi, who is one of the invited speakers of the workshop and editor-in-chief of the renowned journal 'Gene,' has offered to publish the work presented at the conference as a special issue of this journal. Furthermore, we plan to publish a tutorial book on the broad range of fields considered in the workshop, combining chapters written by the workshop's invited speakers. This book is suppose to strengthen the integration of the different approaches to molecular evolution, in particular those based on structural considerations. The organizers wish to express their sincere gratitude to the mpi**pks** for hosting and financing this workshop and for the very generous support.

From many-particle physics to multi-agent systems

Workshop, Scientific coordinators: E. Ben-Jacob, D. Helbig, F. Schweitzer
From July, 19 to September 17, 2004, the two-months seminar *From Many-Particle Physics to Multi-Agent Systems* (MULTI04) took place at the mpipks. The seminar was accompanied by two workshops *I: Driven Many-Particle Systems - Hopping Particles, Granular Media, and Colloidal Systems*, 26-29 July 2004, *II: Multi-Agent Systems - Swarms, Ecology, and Society*, 29 August - 3 September 2004. Both, the seminar and the workshops, were part of the activities of the European Network of Excellence (NoE) "Complex Systems" (EXYSTENCE) and were jointly financed by EXYSTENCE and the mpipks. The event attracted a total of 80 participants. 22 of them were staying at the mpipks for a longer period (2.5 - 4 weeks), while the others participated in two different workshops. The participants did not just come from all over Europe, the Americas, and Asia, they also represented a large variety of scientific areas, ranging from physics, biology, informatics, to economics, the social sciences, and the humanities.
The seminar/workshops mainly focused on transdisciplinary aspects of Complex Systems, in order to develop a commonality of concepts and methods applicable to different fields. In particular, the aim was at the transfer of methods developed primarily in statistical physics to deal with many-particle systems in other scientific areas – where they are often called multi-agent systems – such as biology, artificial intelligence, or social sciences.
The participants included leading experts in their field, such as H. J. Herrmann (U Stuttgart) or S. Luding (U Delft) for granular material, D. Rubenstein (Princeton U) or S. Simpson (Oxford U) for collective biological motion, E. Ben-Jacob (U Tel-Aviv) or J. L. Deneubourg (Free U Brussels) for bacterial and insect societies, E. Bonabeau (Boston) for management sciences, or K. Nagel (Technical U Berlin) for traffic simulations. But there were also many young scientists from different areas, interested in transdisciplinary topics, who mostly stayed for a longer period (2.5 - 4 weeks). Apart from contributing to the two different workshops, they presented their work during a series of talks at the mpipks. The close interaction among the senior and the junior participants (in shared offices), also resulted in many common scientific projects.
The scientific aim of the seminar/workshops – to establish collaborations between physicists who want to apply their methods to interdisciplinary problems and scientists from other fields interested in formal methods developed for interacting particle system – was fully matched. In particular, many participants from the social sciences for the first time got involved in intensive collaborations with physicists, and the other way round – which was considered as very fruitful. It is expected to have about 12 different journal publications (according to a survey among the participants). Further a book on "Collective Biological Motion" published with Springer (Eds. I. Couzin, F.S.) is planned, which to a large extent reflects the common viewpoints of the second workshop.

Pattern formation through instabilities in thin liquid films: From fundamental aspects to applications

Workshop, Scientific coordinators: A. Nepomnyashchy, G. Reiter, U. Thiele

The evolution of thin films of soft matter is investigated in a large number of different situations due to its importance in nature like, for instance, as tear film or lung lining *and* in many technical applications like coating or drying processes. Detailed studies were performed to understand (1) how to keep thin films stable and (2) how to break them in a controlled manner. Especial importance gained very recently also the replication of substrate patterns by a deposited liquid film or the control of surface properties by switchable coatings.

The scope of the workshop was to discuss recent developments and future directions of the rapidly evolving field of thin films of soft matter. A special aim was to bring together leading researchers working on quite different problems in the field of thin films in order to share experimental and theoretical approaches and methods *and* to foster future collaborations throughout Europe and the world. In order to make the exchange as fruitful as possible, we invited exceptionally active scientists of the different sub-fields. Long talks were given by renowned senior scientists like, for example, M. Bestehorn, A.-M. Cazabat, S. Davis, S. Dietrich, L. Limat, R. Lipowsky, L. Pismen, Y. Pomeau and A. Sharma, but also by outstanding young scientists as, for example, B. Audoly, L. Brush, G. Grün, L. Kondic, R. Magerle, A. Münch and H. Riegler. Furthermore, a number of short talks and two poster sessions allowed most participants to present their results. Nearly one third of the time for each talk was reserved for discussion, an opportunity that was well used. In a vivid additional 45 min discussion the participants identified openproblems and future challenges of the field.

During the workshop the recent developments in the individual sub-fields were presented, with a special emphasis on common properties and differences. Central subfields included, for instance, the dynamics of dewetting of ultrathin films of thicknesses smaller than one hundred nanometres, surface instabilities and dry spot formation in thin heated films, the description of surface waves on falling films, the interplay of pattern formation and phase changes in thin films, the movement of three-phase contact lines and their instabilities, the manipulation of liquid structures especially on heterogeneous substrates, instabilities of liquid rivulets, fingering instabilities under the influence of surface tension gradients, the mechanisms behind the movement of self-propelled running droplets and the influence of heterogeneities on the structure formation.

Although the main focus was the pattern formation in thin liquid films on solid substrates other relevant subjects were not excluded if the emphasis of the presentation was on their relation to the main subject of the workshop. This included, for instance, pattern formation in soft elastic films, the influence of wetting interactions on instabilities in thin solid films, the formation of structures in biological membranes, the drainage in metallic foams and soap films and nanostructures in thin films of mixed brushes and copolymers.

The interesting talks and the vivid poster sessions gave a strong evidence for the broad interest in this scientific area. The workshop united about seventy researchers from about 15 countries and more importantly it brought together mathematicians, experimental and theoretical physicists and engineers to discuss problems of common

interest. It is to expect that the workshop initiated future collaborations and was instrumental to identify future challenges for the investigation of thin films of soft matter.

Stochastic resonance: New horizons in physics and engineering

Workshop, Scientific coordinators: P. Hänggi, L. Schimansky-Geier

The theme of this international workshop had its focus on the phenomenon of Stochastic Resonance in nonlinear systems in physics, engineering sciences, geophysics and biological physics. In addition we made an attempt to feature also related fluctuation phenomena, such as fluctuation theorems, and more general noised-induced resonance phenomena in complex systems. The phenomenon of Stochastic Resonance (SR) is a paradigm for noise induced order: The transduction of feeble information can be improved when an optimal dose of noise assists the system dynamics. The goal of this workshop was also to identify -in the spirit of SR - new ideas, guiding novel advances and presenting novel applications within those differing, although related, areas of sciences. The meeting itself took place during October 4 - 7, 2004.

Much to the regret of all participants, Professor E.G.D. Cohen, - the recipient of the Boltzmann medal in 2004 - could not attend the workshop and report on interesting, recent findings for the theme of fluctuation theorems. The colloquium was given by Professor Fabio Marchesoni (Camerino): He presented a most illuminating and exciting overview of Stochastic Resonance and its role in physics, biology and engineering. Some highlights included, among others, the presentations by M. Morillo (Sevilla) on nonlinear Stochastic Resonance, by S. Rahmsdorf (Potsdam) on Stochastic Resonance in abrupt glacial climate changes, by T. Klinger (Greifswald) on Stochastic resonance in plasma experiments, and by F. Marin (Firenze) on SR-experiments in bistable optical cavities. This selection also underpins the multidisciplinary character of SR after 23 years from its discovery in 1981 have passed. New theoretical approaches using correlated noise were discussed by P. Gora (Krakow). Y.-C. Lai (Tempe, USA) and A. Pikovsky (Potsdam) elucidated the connection between SR phenomena and synchronization features.

A group of younger scientists presented professional presentations on a variety of timely topics. Carmen Schmitt (Stuttgart) presented SR-features for a set of new experiments in colloidal systems. The nontrivial challenge of SR in non-Markovian systems was mastered by I. Goychuk (Augsburg). T. Prager (Berlin) and N. Stocks (Warwick, U.K.) introduced the participants to the latest advancements of SR-phenomena for excitable systems involving neuronal activity.

The world of quantum dynamics and quantum information processing has by now also entered the phenomenon of SR. The set of the three given lectures by S. Huelga (Herts, UK) on quantum information and SR-assisted quantum computing, by T. Wellens (Nice) on quantum Stochastic Resonance per se and by S. Kohler (Augsburg) on quantum Brownian motors prove the case.

These above comments give clear evidence that the topic of Stochastic Resonance cannot be considered as "solved". In summary, the field of SR-physics and SR-phenomena is very much alive and lots of challenges still need to be addressed and mastered.

Mesoscopic phenomena in ultracold matter: From single atoms to coherent ensembles

Workshop, Scientific coordinators: J. Brand, K. Burnett, P. Schmelcher

Since the first experimental achievement of Bose-Einstein condensation in atomic vapors in 1995, the physics of quantum degenerate atomic gases has become an exciting and strongly growing field. Popularity of the subject is documented by the strong interest in the workshop MESUMA05 with over 130 applicants even though this was the first conference at mpi**pks** devoted entirely to this topic. Here we want to express our gratitude towards the management and the staff of the visitors program, who made it possible by generous funding and superb organizational support to accommodate more than 100 participants from 17 countries, although the workshop had originally been devised only for 70 participants.

The intention of the organizers was to bring together experts in "quantum engineering" of ultracold coherent matter covering both the many-body aspects as well as the properties and interaction of single atoms. The workshop evolved into a busy and exciting week with the discussion of many spectacular new developments. The conference colloquium was given by Georgy Shlyapnikov (Orsay) who commented on the theoretical background of the only very few month-old breakthrough in achieving fermionic superfluidity in atomic gases and the Bose-Einstein condensation of molecules.

Many more exciting talks were given by a total of 29 invited speakers. The 15 contributed talks and two poster sessions gave many young researchers the opportunity to present their work. Pairing in degenerate fermionic gases was certainly one of the dominant topics of the workshop highlighted by the presentation of the pioneering experimental work of the Innsbruck group of Rudi Grimm given by Johannes Hecker-Denschlag. The two-body scattering physics involved in the formation of molecules in ultracold gases was discussed in depth in the theoretical talks of Chris Greene (Boulder) and Paul Julienne (Gaithersburg) and the experimental talk of Eberhard Tiemann (Hannover) while the many-body aspects of the expected BEC-BCS crossover were investigated by Yvan Castin (Paris) and Carlo Strinati (Camerino) while Sandro Stingari (Trento) discussed collective oscillations in such gases. A beautiful overview of the close links between condensed matter model systems and Bose-Einstein condensates in optical lattices proposing novel quantum phase transitions was given by Maciej Lewenstein (Hannover).

Considerable progress towards the Bose-Einstein condensation of metastable Neon in Hannover was reported by Wolfgang Ertmer. Similar efforts towards the condensation of Chromium atoms and the exciting prospects due to its strong and tunable anisotropic and long-range dipole interactions were the subject of Tilman Pfau's talk. In, fact Bose-Einstein condensation of Chromium was first observed in Pfau's lab in Stuttgart only few weeks after the workshop in Dresden. Dieter Meschede (Bonn) and Gerhard Rempe (Munich) reported on substantial recent progress with respect to single atom manipulation while Jörg Schmiedmayer (Heidelberg) gave an overview of the variety of methods and the technical possibilities to control matter waves on atom chips. A breakthrough on the matter-wave interference in a chip trap with interesting prospects for the fabrication of acceleration sensors was reported for the first time at the MESUMA05 workshop by Claus Zimmermann (Tübingen). Further highlights of the meeting were the discussion of non-ideal Bose gases by Alain Aspect (Orsay), the

prediction of a surprising and counter-intuitive effect of the 'Ulm sparrow' in quantum scattering by Wolfgang Schleich, and the review on rotating condensates by Jean Dalibard (Paris).

3.4 Externally Funded Research and Relations to Industry

3.4.1 DFG Projects

Individual Projects

- *Experimentelle und theoretische Untersuchung von räumlich lokalisierten Anregungen in nichtlinearen Gittern*, Dr. S. Flach
- *Der Einfluss viskoser und viskoseelastischer Eigenschaften auf die Stabilität von Ferrofluidschichten in statischen Magnetfeldern*, Dr. A. Lange
- *Probabilistische Verfahren zur Vorhersage raumzeitlicher Strukturen des Autobahnverkehres*, Prof. H. Kantz
- *Modellierung schneller chaoticher Freiheitsgrade durch stochastische Prozesse*, Prof. H. Kantz
- *Kohn-Sham Dichtefunktionaltheorie mit exaktem Austausch für Grund- und angeregte Zustände*, Dr. St. Kümmel
- *Moderne und universelle first-principles Methoden für Mehrelektronensysteme in Chemie und Physik*, Dr. U. Birkenheuer
- *Wechselwirkung in ultrakalten Atom- und Molekülgasen*, Prof. Jan-Michael Rost, Dr. Thomas Pattard

Schwerpunktprogramme

- *Zeitreihenanalyse von Bifurkationen elasto-plastischen Typs auf der Grundlage von extrem kurzen Zeitreihen (SPP 1114)*, Prof. Holger Kantz
- *Elektronenstruktur und Magnetismus (SPP 1153)*, Dr. U. Saalmann

Sonderforschungsbereiche, Forscher- und Nachwuchsgruppen

- *Emmy-Noether-Gruppe: Elektronische Struktur endlicher Systeme*, Dr. S.Kümmel
- *SFB 463 Seltenerd-Übergangsmetallverbindungen: Struktur, Magnetismus und Transport*, Prof. Peter Fulde
- *SFB 609 Modellierung von Erstarrungsvorgängen unter Magnetfeldeinfluss*, Prof. Holger Kantz
- Forschergruppe *Nanostrukturierte Funktionselemente in makroskopischen Systemen*, Dr. Markus Bär, Heiko Kühne

3.4.2 EU funding

- TMR-Network *Quantum transport on the atomic scale*, Dr. Andreas Buchleitner
- Marie Curie RTN *Unifying Principles in Non-Equilibrium Pattern Formation*, Dr. Uwe Thiele
- TMR-Network *Quantum Chemistry of the Excited State*, Prof. Peter Fulde
- TMR-Network *Localization by nonlinearity and spatial discreteness, and energy transfer, in crystals, biomolecules and Josephson arrays*, Dr. Sergej Flach
- ESF-Network *Arrays of quantum dots and Josephson junctions*, Dr. Sergej Flach

3.4.3 Additional external funding

- VW-Stiftung, Zusammenarbeit mit Natur- und Ingenieurwissenschaftlern in Mittel- und Osteuropa: *Entanglement measures and the influence of noise*, Dr. Andreas Buchleitner, together with Dr. K. Życzkowski, Polish Academy of Sciences, Warsaw
- VW-Stiftung, *Molekularsieblaser - Konglomerate im Infraroten*, Prof. Peter Fulde
- VW-Stiftung, *Faltenbildung als dynamische Instabilität bei der Blechumformung durch Drücken*, Prof. Holger Kantz
- VW-Stiftung, *Schleifbranderkennung durch Analyse von Schallemissionssignalen*, Prof. Holger Kantz
- DAAD (PROCOPE), *Spektrale Eigenschaften von Mehrelektronenatomen im elektromagnetischen Feld*, Dr. Andreas Buchleitner, together with Dr. D. Delande, Universite Pierre et Marie Curie, Paris
- GIF, *Self-organization phenomena in catalytic surface reactions: from nanoscale to microscale*, Dr. Markus Bär
- HLRB Grand Challenge Projekt: *Spectral Properties of Atomic Rydberg States in Intense Electromagnetic Fields*, Dr. Andreas Buchleitner
- HFSPO *Research Grant*, Dr. Prof. Jülicher
- Robert Bosch Stiftung, *Winterschule für Sächsische Gymnasien*, Prof. Holger Kantz, Uta Gneisse
- Robert Bosch Stiftung, *Netzwerk Lehrerweiterbildung in Sachsen*, Prof. Holger Kantz, Uta Gneisse
- Japan Society for the Promoting of Sciences, *Ultrafast Intense Laser Science*, Dr. Andreas Becker
- NSERC Canada, *Controlled electron rescattering: sub-A, sub-fs imaging of single molecules*, Dr. Andreas Becker

3.4.4 Stipends

- *Eduardo Altmann*, DAAD PhD stipend
- *Dr. Liliana Arrachea*, AvH research stipend

- *Dr. Fu Li Bin*, AvH research stipend
- *Rodriguez Pineda*, DAAD PhD stipend
- *Dr. Nilüfer Baba*, DAAD PhD stipend
- *Dr. Katrin Gelfert*, AvH research stipend
- *Dr. Nikolay Vitanov*, AvH research stipend

3.4.5 Cooperations with Industry

Prof. Holger Kantz: Wind speed predictions and more specifically the prediction of turbulent gusts is of high potential use for wind energy conversion. With the help of Garching Innovation, the technology transfer branch of the Max Planck Society, we have established contacts to the spanish manufacturer GAMESA in Pamplona in order to explore the technological usefulness of our patented gust prediction algorithm.
Automatic speech recognition suffers strongly from environmental noises superimposed to the recording of human voice. Together with LINGUATEC in Munich we are exploring how far the recognition rate of human speech, using commercial speech recognition systems, can be enhanced by our noise reduction technique.

3.4.6 Patents and Licences

- *Dr. Mario Ragwitz, Prof. Holger Kantz*
  Verfahren und Vorrichtung zur Steuerung von Windenergieanlagen, since 2000
- *Prof. Holger Kantz*
  Verfahren und Vorrichtung zur Vorhersage von Strömungsparametern turbulenter Medien, since 2002

3.5 Teaching and Education

3.5.1 Lectures at Universities

Wintersemester 02/03

Introduction to thermodynamics and statistical mechanics - Dr. R. Everaers, Uni Mainz

Grundlagen der Laserkühlung - Dr. Th. Pattard, TU Dresden

Sommersemester 03

Semiclassical Quantisation and Chaos - Prof. H. Kantz, Uni Wuppertal

Introduction to Biophysics - Dr. K. Kruse, TU Dresden

Physik der weichen Materie - Dr. M. Bär, TU Dresden

Strukturbildung II-Musterbildung in räumlich ausgedehnten Systemen - Dr. U. Thiele, BTU Cottbus

Wintersemester 03/04

Nonlinear Pulse Propagation - Dr. A. Becker, Uni Bielefeld

Stochastic processes - Prof. H. Kantz, Uni Wuppertal

Physik 1 für Mechatroniker - Dr. K. Kruse, TU Dresden

Strukturbildung II - Einführung in die nichtlineare Dynamik - Dr. U. Thiele, BTU Cottbus

Einführung ins Quantenchaos -Dr. A. Buchleitner, Uni Halle

Transport in Nanostrukturen -Dr. U. Saalmann, TU Dresden

Sommersemester 04

Kontrolle quantenmechanischer Prozesse - Dr. A. Becker, Uni Bielefeld

Numerical, Statistical and Stochastic Aspects of Hydrodynamic Turbulence - Prof. H. Kantz, Uni Wuppertal

Theoretische Biophysik - Dr. K. Kruse, TU Dresden

Lecture series on correlated electrons - Prof. P. Fulde, Uni Wroclaw

Theoretische Quantenoptik - Dr. A. Buchleitner, Uni München

Dichtefunktionaltheorie - Dr. St. Kümmel, TU Dresden

Wintersemester 04/05

Physikochemische Hydrodynamik - Dr. U. Thiele, BTU Cottbus

Physik der Bose-Einstein Kondensate - Dr. J. Brand, TU Dresden

Grundlagen der Laserkühlung - Dr. Th. Pattard, TU Dresden

3.5.2 Degrees

Habilitations

- *Becker, A.: Nonlinear-interaction of atoms and molecules with intense laser fields.* Bielefeld 2003
- *Everaers, R.: Computer simulations and scaling concepts in polymer physics,* Mainz 2003
- *Klages, R.: Microscopic Chaos, Fractals, and Transport in Nonequilibrium Steady States,* Dresden 2004
- *Thiele, Uwe.: Microscopic Chaos, Fractals, and Transport in Nonequilibrium Steady States,* Dresden 2004

Dissertations

- *Miroshnichenko, A.: Spectroscopy of discrete breathers,* Dresden 2003
- *Risler, T.: Comportement critique d oscillateurs couples,* Paris 2003
- *Sczyrba, M.: Semiclassical approximations for single eigenstates of quantum maps,* Dresden 2003
- *Börner, U.: Modeling Myxobacterial Rippling: Pattern Formation in a Multicellular System,* Dresden 2004
- *Häring, I.: Atomic scattering from Bose-Einstein condensates,* Dresden 2004
- *Korabel, N.: Deterministic Transport: From Normal to Anomalous Diffusion,* Dresden 2004
- *Madronero, J.: Spectral Properties of Planar Helium under Periodic Driving,* München 2004
- *Mintert, F.: Measures and Dynamics of Entangled States,* München 2004
- *Nadrowski, B.: Mechanical properties of active hair bundles,*Paris 2004
- *Wimberger, S. M.: Chaos and Localisation: Quantum Transport in Periodically Driven Atomic Systems,* München and Como 2004
- *Zerec, I.: Electronic structure and tunneling states in clathrates,* Dresden 2004

3.5.3 Appointments and Awards

Appointments

- *Prof. Erich Runge* accepted the offer for a C4 professorship at the University Ilmenau.
- *Dr. Rainer Klages* accepted the offer for a Lecturer in Physics at the University London.
- *Dr. Markus Bär* accepted the offer for a Group Leader at the Physikalisch-Technische-Bundesanstalt.
- *Dr. Manfred Lein* accepted the offer for a Group Leader at the Max Planck Institute for Nuclear Physics.
- *Dr. Henning Schomerus* accepted the offer for a Reader in Physics at the University Lancaster.

Awards

- *Risler, T.:* Otto-Hahn-Medaille 2003

3.6 Public Relations

3.6.1 Long Night of Sciences

On June 27th, 2003 and June 25, 2004 the institute participated in the *Long Night of Sciences* jointly with the Technische Universität Dresden and many other research institutes in Dresden. We opened the doors for everyone interested in visiting our institute from 6pm to 12pm. The members of our institute conveyed the importance and fascination of their research to a broad audience with various talks, video shows, a physics show, a physics quiz, a science cinema and poster presentations. The resonance was very good with about 2800 visitors counted at each event.

3.6.2 Science in the City Hall

The mpi**pks**, the Technische Universität Dresden and the City of Dresden are running a series of public lectures (about 3 per year) called *Wissenschaft im Rathaus*. The following lectures were delivered during the period 2003-2004:

- 26 Februar 2003, Prof. Dr. Günther Hasinger, *Schicksal des Universums*, about 500 participants
- 28 Mai 2003, Prof. Dr. Stefan Kaufmann, *Gene und Klone: Die Wiederkehr der Seuchen*, about 250 participants
- 26 November 2003, Prof. Dr. Peter Berthold, *Faszination Vogelzug*, about 350 participants
- 4 März 2004, Prof. Dr. Axel Ullrich, *Vom Gen zur Krebstherapie*, about 250 participants
- 16 September 2004, Prof. Dr. Karsten Danzmann, *Dellen in Raum und Zeit - Mit Gravitationswellen dem Universum zuhören*, about 350 participants
- 2 November 2004, Prof. Dr. Kurt Biedenkopf, *Welche Zukunft hat unsere Gesellschaft*, about 500 participants

3.6.3 mpipks school contact program

The mpi**pks** offers workshops on modern aspects of physics research for high school physics teachers. On September 9 2004 we conducted a workshop on *Biophysik*.
On the 28th of April 2004 we hosted the first *Girls Day - Mädchenzukunftstag* at mpi**pks**. It was aimed at young female high school students to get information on the spot about career opportunities and challenges when pursuing a scientific career. About 45 female students participated in that event.
mpi**pks** conducts Praktika for interested high school students, with durations from 2 weeks to several months. At the moment there are six students enrolled.
In addition mpi**pks** offers lecturing at high schools on a permanent basis. High school teachers receive updated lists of available lecture topics offered. About twenty five lectures are given annually.

3.6.4 Winter School for high school students

Together with the Fetscher Gymnasium (a high school in Pirna), we have applied for and obtained funding from the Robert Bosch foundation within a program called "Nat-Working". This program aims at establishing links between academia and high schools. Our joint project consists in a series of three winter schools for high school students. For about 60 participants, we arranged an entertaining and educating mixture of scientific talks on a level accessible for interested students in the final two years of a high school, interactively designed exercises, and discussions on issues concerning science relevant for future studies and professional careers. Responding to the increasing interest in biological physics, we make use of the excellent facilities of the Hygienemuseum (museum for hygienics), and in particular of their experimental labs. This school was extremely well received from both students and teachers.

3.7 Budget of the Institute

Figures 1 and 2 show a breaking down of the budget for personnel and for research for the years 2003 and 2004

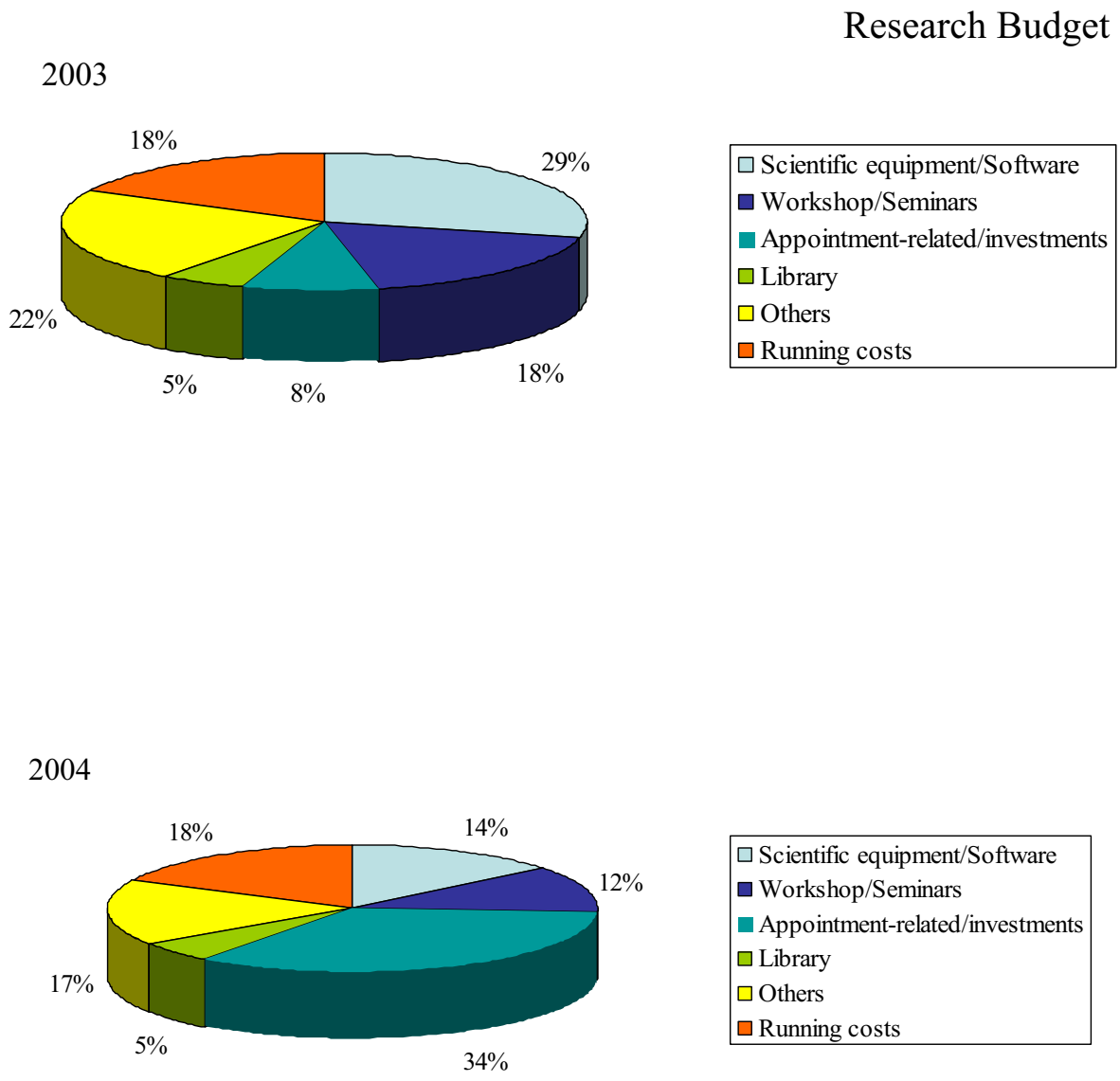

Figure 1: *Research budgets during the past two years*

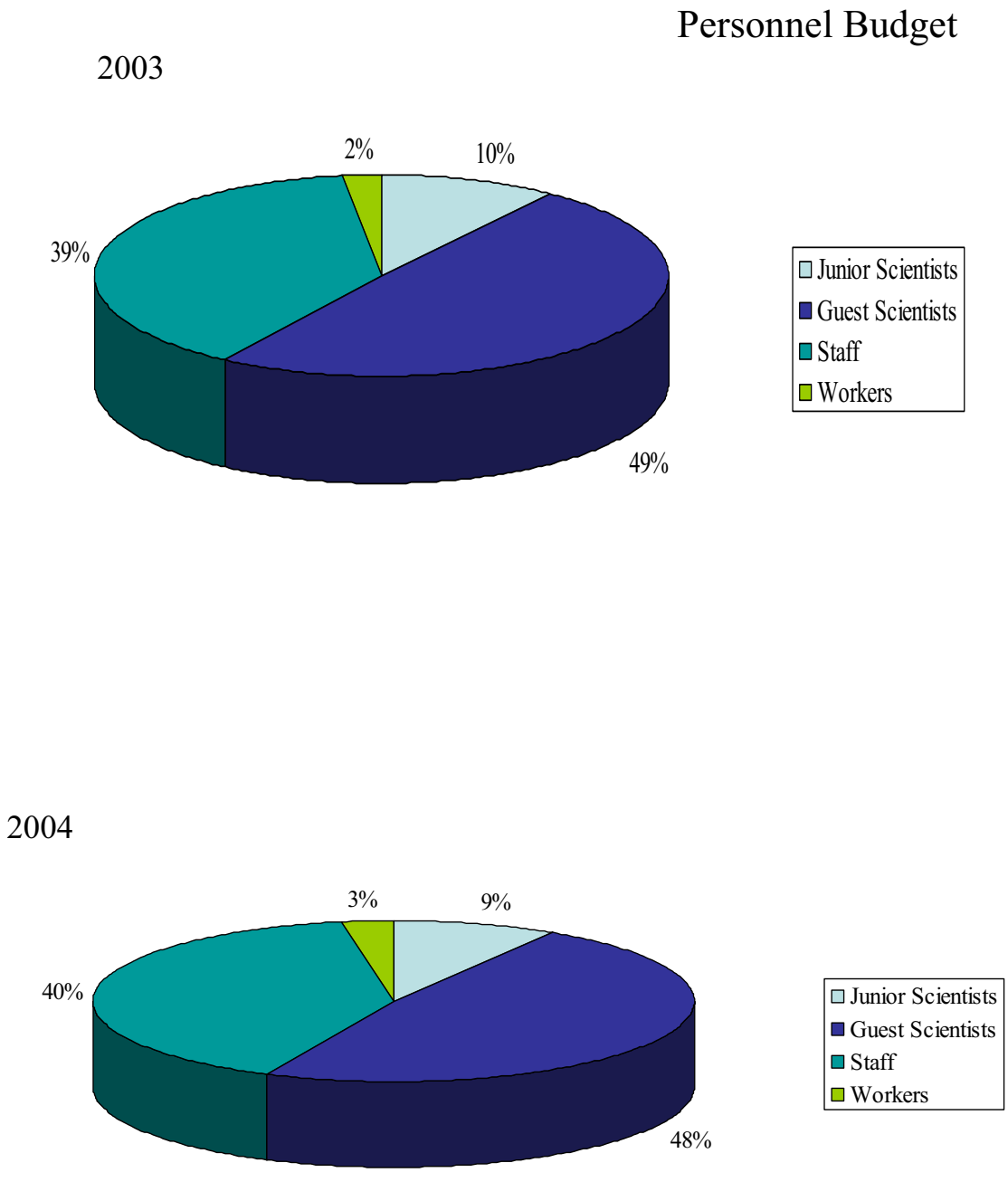

Figure 2: *Budgets for personnel*

3.8 Equipment and Premises

3.8.1 Computer Facilities

The computer requirements in our institute are mainly characterised by a very high demand for computing power and relatively moderate requests for graphics. This implies that most offices are equipped with X-Terminals while nearly all the compute servers are located in server rooms. At present the institute has approximately 330 computers with a total of 600 CPU's. New to our equipment are two parallel clusters with 64 CPU's each and a Myrinet interconnect plus a smaller cluster with 32 CPU's for the development of parallel applications. This latest increase of our computing power was only possible due an improved and enlarged air conditioning system for our server rooms which was generously and unbureaucratically planned and paid by the Max Planck Society. The computers offer from one to four CPU's and a maximum of 64 Gigabytes of main memory and six Terabytes of local disk space. We use both Gigabit and Fast Ethernet as a local area network interconnect. By the end of 2004 about 80 % of the computing power available was based on Linux systems, 20 % on computers running Tru64 Unix. In order to maximize the computational throughput in our computing cluster, we run a network queuing system which achieves an overall average utilization of more than 90 % of the available CPU time. Besides the unix cluster there are about 20 PC's in our institute, running a Windows operating system, mainly for office applications. We also offer about 30 Laptops for our scientists in order to give them the possibility to continue their work while they are abroad. Furthermore we are running a Windows Terminalserver in our network in order to offer access to a Windows environment from every desktop. For numerical and analytical calculations there are various software packages available for our scientists. During the last years we noticed a tendency towards integrated software environments while fewer people are writing their own programs using programming languages like C or Fortran.
For our short-term guests that participate in seminars and workshops we run a separate small cluster. We offer those guests the possibility to connect their own laptops to our network or use X-Terminals to access that cluster. The separation was introduced for both greater convenience and higher security.
We are connected to the Internet using a bandwidth of 34 MBit/s which we share with our neighboring institute.
The computer department is run by four employees with their respective main tasks being unix and networks, web and windows, hardware and general user support. Smaller to medium programming tasks are done by our staff and two students who are working part-time in the computer department. Larger programming tasks have to be given to external companies.

Future

Linux will continue to be the main operating system for our number crunchers in the near future, running mainly on AMD Opteron based hardware. By 2007 we will have to decide which way to go with our main servers. If Linux has become mature by then, it will be tempting to leave the proprietary operating system - Tru64 Unix from HP (formerly Compaq, formerly Digital) - in order to become independent from hardware

vendors and still having the option to run the same flavor of operating system on all hardware.

History

In 1996 the institute occupied three buildings in Dresden and an outpost in Stuttgart. Before we moved to our new building, a further office in Dresden was needed. This implied that the interconnection of the offices and running the distributed infrastructure made up the biggest part of the work of the two employees in the computer department at that time. Moving to the new building in 1997 implied a boost in local network bandwidth from shared ethernet to ATM and an increased bandwidth of our internet connection from 128 kBit/s to 2 MBit/s. While during the first years nearly all the computing power was covered by workstations, starting from 2000 we switched to small and medium sized servers. 2002 was the first year to see an inhomogeneous unix cluster in our institute when we introduced linux on standard PC systems. By the end of 2002 we even decided to give away our 16 processor server in favor of a Linux based PC cluster that delivers several times the cpu performance of that server. The following table shows the development of the computer resources at our institute over time.

year	computers	GFlops	main memory (GB)	disk space (TB)
1996	33	15	13	0.5
1997	49	30	30	1.0
1998	66	60	60	2.0
1999	68	100	190	5
2000	95	140	310	8
2001	138	220	420	10
2002	162	400	590	22
2003	261	1200	1150	32
2004	327	2100	2600	90

3.8.2 Library

The library is a specialized library offering services firstly to scientists working at the institute. Scientists from outside the institute are welcome and may use the library. The library is permanently accessible for members of the institue including guests and provides the scientists with media and scientific information in many forms.
The annual growth rate in 2003/2004 of the library holdings increased in line with the budget and our holdings list consists of 3304 monographs, 12.545 bound journal volumes and 78 (54) scientific journals subcriptions. Books or references, which are not available in the library can be ordered through document delivery. The scientists receive articles within 24 hours as email files. With an automatic lending system all users can borrow literature themselves 24 hours a day. There are two special scanners available for books and journals only. The members of the library committee discuss new developments in quarterly meetings. Via the homepage of the library up-to-date electronical access to journals, databases and information of the services of the Max-Planck-Society is offered.
The discussion of the future of both electronic and printed media is still ongoing. Contracts between the Max-Planck-Society and Elsevier, Springer, Wiley, Kluwer, AIP

and IOP have been signed, other publishers will follow. The policy of our library is - the scientists should have the possibility to use the electronic resources whenever they need them.

3.8.3 Guest Houses

To accommodate the large number of short- and long-term visitors, the Max Planck Institute for the Physics of Complex Systems provides three guest houses with different apartment types for up to 42 guests in total.
Guest house 1 comprises 20 single and 5 double rooms (with two separate bedrooms). All of them have a bathroom, a telephone and a terrace or a balcony. The guests are able to use the fully equipped communal kitchen and two meeting rooms, one of them with a small library, the other one with a TV set.
Guest house 2 offers ten apartments with kitchen for up to two persons and three large apartments with two bedrooms, a living room, bathroom and kitchen for up to three persons (e.g. families). All apartments have TV connection ports, telephones and a balcony or a terrace. In the basement of guest house 2, two washing machines and a tumble dryer are available. They are accessible from all three guest houses.
Guest house 3 allows to accommodate guests in four large apartments similar to the ones in guest house 2. They are situated on the second floor, the apartments on the first floor have been transformed into offices. Like in the two other guest houses, guest house 3. offers TV connection ports, telephones and balconies.
The guest house rooms and apartments are regularly cleaned and towels and bed linen exchanged. Additionally, the institute provides free of charge rental service for cots and TV sets.

3.9 Committees

3.9.1 Scientific Advisory Board

According to the statutes of the Max Planck Society the mpipks has a Scientific Advisory Board. The members of the Board advise the board of directors concerning the research at the institute. The Board assesses the research direction of the institute, the scientific relevance and chances for success of the research projects, as well as the collaborations among members of the institute, with universities, other research institutions and with industry. The Scientific Advisory Board evaluates the results of the research work presented by the board of directors in the biannual research report and prepares, usually every two years, a report for the President of the Max Planck Society on the research of the institute.
Currently the Scientific Advisory Board has the following members:

Bensimon, D.
Professor Dr.

Laboratoire de Physique Statistique
Ecole Normale Superieure
24, rue Lhomond, 75231 Paris cedex 05
Frankreich

Efetov, K.
Professor Dr.
Institut für Theoretische Physik III
Ruhr-Universität Bochum
Universitätsstrasse 150, 44801 Bochum

Haake, F.
Professor Dr.
Fachbereich Physik
Universität Duisburg-Essen
Universitätsstrasse 2, 45141 Essen

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

Ketzmerick, R.
Professor Dr.
Technische Universität Dresden
Helmholtzstr. 10
01069 Dresden

Lhuillier, C., J. C.
Professor Dr.
Physique Theoretique des Liquides
Universit Pierre & Marie Curie
4, Place Jussieu, 75252 Paris Cedex 05
Frankreich

Pietronero, L.
Professor Dr.
Dipartimento di Fisica
Universita degli Studi di Roma
La Sapienza
Piazzale Aldo Moro 2, 00185 Roma
Italien

Stark, J.
Professor Dr.
Department of Mathematics
University College London
Gower Street, WC1E 6BT, London
Grossbritannien

Sznajd, J.
Professor Dr.
Institute of Low Temperature and Structure
Research
Polish Academy of Sciences
ul. Okolna 2,
50-422 Wroclaw
Polen

3.9.2 Board of Trustees

In accord with the statutes of the max planck society the mpi**pks** has formed a board of trustees. the board members discuss and consult the proposed budget, the annual report, and the budget of the last year of mpi**pks** together with the directors. the board of trustees advises the institute on important issues and promotes the connection of the institute to research oriented circles in the society. the board of trustees had the following members during the period of this report (current membership is until December 31 2006):

Birgel, D.	Chefredakteur Dresdner Neueste Nachrichten Hauptstrasse 21, 01097 Dresden
Eschelbacher, H. C. Dr.-Ing.	Ministerialdirigent a. D. Hauptstrasse 124, 53604 Bad Honnef
Freiesleben, H. Professor Dr.	Fachrichtung Physik Technische Universität Dresden Zellescher Weg 16, 01062 Dresden
Harter, J. Dr.	Geschäftsführer Infineon Technologies Dresden Gmbh & Co.OHG Königsbrücker Str. 180, 01099 Dresden
Junker, F. Dr.	Mitglied des Vorstandes König & Bauer Ag Friedrich-List-Str. 47-49, 01445 Radebeul
Kokenge, H. Professor Dr.	Rektor der Technischne Universität Dresden Mommsenstrasse 13, 01069 Dresden
Ludwig, B.	Sächsische Staatsministerin für Wissenschaft und Kunst Wigardstrasse 17, 01097 Dresden
Mehlhorn, A. Professor Dr.	Fachrichtung Chemie Technische Universität Dresden Mommsenstraße 13, 01069 Dresden

Müller, H. Dr.	Mitglied des Vorstandes Dresdner Bank AG Jürgen-Ponto-Platz 1, 60329 Frankfurt/M.
Reichard, Ch. Dr.	Mitglied des Bundestages Bürgerbüro Rähnitzgasse 10, 01097 Dresden
Rossberg, I. Dr.	Oberbürgermeister Landeshauptstadt Dresden, Dr.-Külz-Ring 19, 01067 Dresden
Tschira, K. Dr.	Geschäftsführender Gesellschafter Klaus Tschira Stiftung gGmbH Schloss Wolfsbrunnenweg 33, 69118 Heidelberg
Weber, St. Dr.	Mitglied des Vorstandes Sächsische Aufbaubank Pirnaische Strasse 9, 01069 Dresden

3.10 Members of the MPI for the Physics of Complex Systems

(as of December 2004)

1. **mpipks positions**		**41**
1.1 Scientific personnel		
Scientific members	3	
Research staff (including four junior research groups)	14	
1.2 Technical staff	5	
1.3 Administration and infrastructure staff	19	
2. **Externally funded research staff**		**5**
3. **PhD students**		**28**
3.1 German PhD students (MPG funding)	19	
3.2 Foreign PhD students (MPG funding)	7	
3.3 PhD students (external funding)	2	
4. **Guest scientists**		**56**
4.1 German guest scientists	14	
4.2 Foreign guest scientists (MPG funding)	42	

The research positions are generally limited in time. Only *Prof. H. Kantz*, head of the group "Time Series Analysis" is employed on a permanent C3 position. Furthermore, *Priv. Doz. Dr. S. Flach*, head of the Visitors and Workshop Program, is a permanent staff member of the scientific service with a BATIb position.

Chapter 4

Publication List 2003-2004

4.1 Light-matter interaction

2003

Aközbek, N., A. Becker, M. Scalora, S.L. Chin and C.M. Bowden: Continuum generation of the third-harmonic pulse generated by an intense femtosecond IR laser pulse in air. Applied Physics B **77**, 177 - 183 (2003).

Barna, I.F., N. Grün und W. Scheid: Coupled-channel study with Coulomb wave packets for ionization of helium in heavy ion collisions. European Physical Journal D **25**, 239 - 246 (2003).

Barna, I.F. and J.M. Rost: Photoionization of helium with ultrashort XUV laser pulses. European Physical Journal D **27**, 287 - 290 (2003).

Emmanouilidou, A., T. Schneider and J.M. Rost: Quasiclassical double photoionization from the $2^{1,3}S$ excited states of helium including shake-off. Journal of Physics B **36**, 2717 - 2724 (2003).

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Jaron, A. and A. Becker: Laser-assisted and laser-induced electron-impact ionization during nonsequential double ionization of He. Physical Review A **67**, 035401 (2003).

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Magunov, A.I., I. Rotter and S.I. Strakhova: Fano resonances in the overlapping regime. Physical Review B **68**, 245305 (2003).

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Pattard, T., T. Schneider and J.M. Rost: On the role of shake-off in single-photon double ionization. Journal of Physics B **36** , L189 - L195 (2003).

Pohl, T., W. Ebeling and M.Y. Romanovsky: Recoil ion momentum distributions from laser-induced double ionisation. Physics Letters A **311**, 396 - 402 (2003).

Requate, A., A. Becker and F.H.M. Faisal: Limits of a stationary phase method for ionization of atoms in strong laser fields. Physics Letters A **319**, 145 - 149 (2003).

Saalmann, U. and J.M. Rost: Ionization of clusters in intense laser pulses through collective electron dynamics. Physical Review Letters **91**, 223401 (2003).

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4.3 Semiclassics and chaos in quantum systems

2003

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Wellens, T. and A. Buchleitner: Quantum State Control in Cavity QED. In: Dynamics of Dissipation. Ed. by P. Garbaczewski. Springer Verl.; S. 351 - 376 (2003).

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4.4 Atomic and molecular structure

2003

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2004

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4.5 Electronic structure

2003

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