



# Institute for Theoretical Physics Vienna University of Technology Annual Report 2005



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The image on the cover shows simulation snapshots of a system of particles interacting via a soft, bounded, and purely repulsive potential (for details cf. section 3.3.1). On the upper left, the system at low density is in the fluid phase, while on the lower right it has formed an ordered cluster phase: overlapping particles have formed clusters which themselves are arranged in a regular fcc lattice. The close-up picture shows one selected cluster. For details see B.M. Mladek, D. Gottwald, G. Kahl, M. Neumann, C.N. Likos, Phys. Rev. Lett. 96, 045701 (2006).

Institute for Theoretical Physics, Vienna, October 2006

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## Chapter 1

# Executive Summary: Key data 2005

• Positions:	Faculty positions: <sup>(a)</sup> Externally funded scientific staff:	$14,5 \\ 30$	
• Budget:	Operating budget available to the institute: External funds attracted in 2005:	EUR EUR	64.540,00 600.431,00
• Research:	Publications in peer-reviewed journals: Invited talks at international conferences:	$75\\16$	
• Teaching:	Course hours/week taught by faculty during the academic year 2004/05: Mandatory core courses: Special lectures: Total:	28 432 460	
• Degrees Awarded:	Diploma: Doctorate: Habilitation:	6 6 1	

(a) 2 of which are vacant

## Foreword

The year 2005 brought for our Institute of Theoretical Physics, Vienna University of Technology, many exciting developments, some of them less welcome than others. The implementation of the new university law and of the newly acquired autonomy of our university continued to be less than smooth and posed considerably challenges for all of us. For example, managing the financial affairs of an institute when definite figures for the operating budget for the calender year became only available in late October (when it was almost over) constituted one of the many unpleasant adventures. I am grateful to all members of the institute, most notably to our administrative staff, Mrs. Mössmer and Unden, for their extraordinary effort to keep our institute running smoothly nevertheless.

We were saddened by the loss of two senior scientists who were associated with our institute for several decades. Prof. Alfred Locker, a retired faculty member, passed away on February 12, 2005. Prof. Dieter Sigmar, a graduate and external lecturer of our institute and a retired MIT faculty member passed away on July 31, 2005.

On the bright side, our institute has established an excellent record in teaching and research that was maintained during 2005. 75 publications in international scientific journals (i.e. 6 publications per faculty member and year), a significant presence at international conferences with more than 50 contributions, many of which invited, and the award of 13 academic degrees under the supervision of our faculty members attest to the high scientific productivity and to the strong emphasis on teaching. All staff members deserve credit for their important contributions and their enthusiasm that helped to keep up this level of productivity.

During 2005, the role of our institute within the multidisciplinary and multi-institutional special research program advanced light sources (ADLIS) encompassing institutes from the Vienna University of Technology, the University of Vienna, as well Universities in Germany (Würzburg, Hamburg, Munich) was enhanced with the relocation of its central coordination project to our institute and the appointment of the institute director as spokesperson.

One of the highlights of this year was undoubtedly the celebration of the promotion to Professor Emeritus of Wolfgang Kummer. A well-attended symposium dedicated to Wolfgang's contributions to physics was organized by our institute and held on January 28, 2005, in the "Festsaal" of the VUT. Speakers included, among others, two Nobel prize winners, Carlo Rubbia and Jack Steinberger (CERN), Peter van Nieuwenhuizen (Stony Brook), and Roman Jackiw (MIT, Cambridge) and the President of the Austrian Academy of Sciences, Prof. Herbert Mang. A few visual impressions of this event are displayed on the following pages. It is my pleasure to acknowledge the generous support for this event by the Rektor of the Vienna University of Technology, Prof. Peter Skalicky.

Almost one year after the retirement of Prof. Kummer, a search to fill this position got finally underway during fall of 2005. Despite a considerable delay we are now hopeful that a successor to Prof. Kummer who will strengthen the area of fundamental physics and high-energy physics will be appointed in the not so distant future.

Finally, I would like to thank Johannes Feist and Elfriede Mössmer for their editorial work on this annual report.

Vienna, October 2006

Joachim Burgdörfer (Director of Institute)

## Chapter 2

# "Das Wolfgang-Fest"

CELEBRATION AND COLLOQUIUM ON THE OCCASION OF WOLFGANG KUMMER'S PROMOTION TO PROFESSOR EMERITUS

("WOLFGANG FEST")

FRIDAY, JANUARY 28, 2005, 15:30

FESTSAAL DER TU WIEN, KARLSPLATZ 13 A 1040 WIEN

#### PROGRAM

Welcome:

Director, Institute for Theoretical Physics Adresses: Peter Skalicky

Joachim Burgdörfer

President, Vienna University of Technology

Herbert Mang President, Austrian Academy of Sciences

Jack Steinberger, CERN, Geneva "Wolfgang Kummer, a valued colleague, teacher, musician and ski-instructor..."

Roman Jackiw, MIT, Cambridge "Elaborations on 2-d gravity"

Carlo Rubbia, University Pavi and CERN, Geneva "The quest for dark matter"

Peter van Nieuwenhuizen, SUNY at Stony Brook "Supergravity as a gauge theory"

**Dominik Schwarz**, University Bielefeld "The next generation"

Concluding remarks: Wolfgang Kummer







## CHAPTER 2. "DAS WOLFGANG-FEST"



## Chapter 3

## Research

The purpose of this report section is to feature a few research highlights during the year 2005. It is meant as an "appetizer" and is, by no means, complete. A complete listing of published and presented research results are given in the appendix. Interested readers are referred to the web page of the institute (http://www.itp.tuwien.ac.at/) where more information can be found.

The research program at our institute is characterized by a remarkable diversity covering a broad spectrum of topics ranging from high-energy physics and quantum field theory to atomic and condensed matter physics. As a focus area, non-linear dynamics of complex systems including aspects of quantum cryptography and quantum information plays an important role. Many of the research topics make use of and belong to the subdiscipline "computational physics". Keeping the available and accessible computer infrastructure competitive remains, in view of budgetary constraints, a constant challenge.

The breadth of activities at our institute provides advanced students as well as young researchers with the opportunity to be exposed to a multitude of state-of the art research directions and to receive a broad-based academic training. It is our intention to maintain and further develop our institute as an attractive place of choice for aspiring students and post-docs. The few highlights featured below may convey this message.

## 3.1 Fundamental Interactions

According to our present knowledge there are four fundamental interactions in nature: gravity, electromagnetism, weak and strong interaction with electromagnetism and weak interaction unified in the electroweak theory. Gravity as well as electromagnetism are macroscopic phenomena, immediately present in our everyday life, like falling objects and static electricity. Weak and strong nuclear interactions, on the other hand, become only important on the microscopic, atomic and subatomic level.



Schematic presentation of fundamental interactions

The most important aspect of the strong interaction is that it provides stability to the nucleus overcoming electric repulsion, whereas the transmutation of neutrons into protons is the most well-known weak phenomenon. The aim of fundamental physics may be described as obtaining a deeper understanding of these interactions, and penultimately finding a unified framework, which understands the different interactions as different aspects of a single truly fundamental interaction.

### 3.1.1 Quantum Field Theory and Non-Commutative Geometry

Staff: Manfred Schweda, Daniel N. Blaschke

External: Harald Grosse (Vienna University, Austria), Francois Gieres (Université Claude Bernard, Lyon I, France), Olivier Piguet (Universidade Federal do Espirito Santo (UFES), Vitória, Brazil), Raimar Wulkenhaar (MPI für Mathematik in den Naturwissenschaften, Leipzig, Germany)

Describing the interactions on a more fundamental level the concepts of relativistic quantum field theories are employed. With the advent of quantum mechanics in the first decades of the 20th century it was realized that the electromagnetic field, including light, is quantized and can be seen as a stream of particles, the photons. This implies that the interaction between matter is mediated by the exchange of photons. The concept of relativistic quantum field theory is very simple, unifying a classical field theory with the concepts of quantum theory and special relativity.

Within quantum electrodynamics (QED) — a unified quantum theory of Dirac particles (fermions) and photons (bosons) — the forces between fermions are realized by the exchange of massless photons. Additionally, QED is characterized by gauge invariance.

It turns out that also the strong and weak forces can be formulated in terms of quantized gauge fields. This implies the existence of quantized non-abelian gauge theories — a generalization of the quantized Maxwell theory containing self-interactions of the gauge bosons. The quantum field theory for the strong interaction is quantum chromodynamics (QCD) which also allows to form strongly bound states. The weak interactions are mediated by the exchange of massive gauge bosons with very short ranges.

The second half of the last century was dominated by the quest for a unified quantum gauge field theories leading to the Glashow-Weinberg-Salam model, the Standard Model. In the realm of string theories and with the concepts of supersymmetry also gravity may be included in the unification.

An important concept in any quantized field theory is its perturbative realization with quantum corrections described in terms of Feynman-graphs.

Fig. 1 contains all one-loop corrections of the propagation of a nonabelian gauge boson (vacuum polarization).

Samment + mmm . ....

Fig 1: Full Propagator in terms of free propagation and self-energy corrections

The wavy line represents the gauge field propagator which describes the free propagation.

The one-loop corrections contain products of propagators, i.e. products of distributions. Since such products are ill-defined also the corresponding Feynman-integrals in the momentum representation are divergent for high internal loop-momenta leading to the so-called ultraviolet (UV) divergences. These UV infinities demand a regularization scheme characterized by cutoffs in order to make the Feynman integrals meaningful and a corresponding renormalization program for the definition of physical quantities (physical masses, wave-functions renormalization and renormalized couplings) is needed.

The appearance of the UV singularities is caused by the fact that the interactions vertices are described by local field products if the underlying geometry is commutative.

It was suggested very early by Snyder [1] in the pioneering days of quantum field theory that one could use a noncommutative structure for space-time coordinates at very small length scale to introduce an effective UV cutoff. This was motivated by the need to control the divergences of quantum loop-corrections.

#### Noncommutative Quantum Field Theory (NCQFT)

In describing fundamental physics space and time are unified by the principle of Special Relativity into a four-dimensional space-time:  $x^{\mu} = (ct, \vec{x})$ . Usually, one assumes that the  $x^{\mu}$  are ordinary commuting 4-dimensional coordinates leading to the concepts of commutative geometry. In the context of commutative geometry one can discuss the fundamental interactions.

There are many hints that the concepts of space-time as a differentiable manifold cannot be extrapolated to the physics at short distances. Simple heuristic arguments forbid a naive unification of the principles of General Relativity with local quantum theory. It is impossible to locate a particle with an arbitrary small uncertainty. On the other hand, our understanding of the theories of fundamental interactions and General Relativity is strongly related to standard commutative differential geometry.

The failure of standard commutative differential geometry demands a replacement. Following Filk [2], the commuting space-time coordinates  $x^{\mu}$  of flat space are replaced by hermitian operators  $\hat{x}^{\mu}$  respecting in the simplest case the following algebra

$$\begin{bmatrix} \hat{x}^{\mu}, \hat{x}^{\nu} \end{bmatrix} = i\theta^{\mu\nu}, \begin{bmatrix} \theta^{\mu\nu}, \hat{x} \end{bmatrix} = 0.$$

 $\theta^{\mu\nu}$  is a real, constant and antisymmetric matrix — the deformation parameter. In natural units, where  $\hbar = c = 1$ , its mass dimension is -2, where the relevant scale is expected to be the Planck mass. We call a space with the above commutation relations as a noncommutative space.

In order to construct the perturbative NCQFT, it is more convenient to use fields  $\phi(x^{\mu})$ (which are functions of ordinary commuting space-time coordinates) and not operator-valued objects like  $\hat{\phi}(\hat{x}^{\mu})$ . The transition to fields which respect the noncommutative algebra is realized in redefining the multiplication law of functional (field) space. This is achieved by the so-called Moyal-Weyl correspondence for arbitrary fields

$$\hat{\phi}_{1}\left(\hat{x}\right)\hat{\phi}_{2}\left(\hat{x}\right) \Longleftrightarrow \phi_{1}\left(x\right) \star \phi_{2}\left(x\right),$$

where the star product is defined by

$$\left(\phi_1 \star \phi_2\right)(x) = e^{\frac{i}{2}\theta^{\mu\nu}\partial^x_{\mu}\partial^y_{\nu}}\phi_1\left(x\right)\phi_2\left(y\right)|_{x=y}.$$

For ordinary commuting  $x^{\mu}$  the star commutator gives

$$[x^{\mu}, {}^{\star}x^{\nu}] = x^{\mu} \star x^{\nu} - x^{\nu} \star x^{\mu} = i\theta^{\mu\nu},$$

which is a representation of the above mentioned algebra.

Thus, through the star product it is now possible to reformulate any quantum field theory in terms of ordinary commuting coordinates as a "deformed quantum field" theory  $\equiv$ NCQFT. The very simple recipe demands the replacement of field products by star products in any action. However, the presence of the  $\star$  in the bilinear part has no effect — therefore the propagators of the field models remain unchanged, whereas the polynomial interaction products of the fields develop additional phases responsible for the so-called UV/IR-mixing [3]. This means that these phases act as a regularization for high internal momenta but produce a new IR-singularity for small external momenta in one-loop corrections. These new types of IRsingularities represent a severe obstacle for the renormalization program at higher order and therefore lead to inconsistencies. The IR singularities are produced by the so-called UV finite nonplanar one-loop graphs in U(N) gauge models and also in scalar field theories. One also has to stress that the usual UV divergences may be removed by the standard renormalization procedure.

Additionally, due to the noncommutativity of the star product the U(1)-Maxwell theory becomes a nonabelian structure [4]

$$F_{\mu\nu} = \partial_{\mu}A_{\nu} - \partial_{\nu}A_{\mu} - i\left[A_{\mu} \star A_{\nu}\right],$$

with the gauge field  $A_{\mu}$  which is the noncommutative extension of the Maxwell field. The present research activities are devoted to find solutions for the UV/IR-mixing problem of noncommutative gauge field models. In order to respect the effects of noncommutativity (implied by the non-Abelian structure) a consistent treatment demands the use of the BRSquantization procedure even for a U(1) deformed Maxwell theory.

In three recent papers [5][6][7] it was shown that the non-commutative structure of spacetime has severe restrictions with respect to the (non-)Abelian gauge theory. Even for a U(1)pure gauge model — in the extended model of Slavnov quantized in the axial gauge — we have discovered new symmetry structures. It was surprising that a new kind of supersymmetry is devoted to solve the problem of renormalizability of a simple U(1)-gauge model. In the extension of Slavnov we have found that renormalizability, at least at the two loop level, is possible and that it is possible to solve the so-called UV/IR mixing problem of non-commutative gauge field theories.

Additionally, we have shown that the non-planar IR singularities are independent of the gauge fixing. This was demonstrated with the help of an interpolating gauge [6][7].

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### 3.1.2 Gravitation

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Since the groundbreaking work of Einstein, gravitation is conceived as defining the geometry of spacetime – even defining the very concepts of time and space itself. Planetary motion as well as the motion of massless particles, that is to say light, become the straightest possible paths in a non-Euclidean geometry.



Fig. 1: Light-cone of an event representing its causal past and future

Not only geometry and curvature rely on the gravitational field. The causal structure is completely determined by the so called light-cone that separates events that can be influenced from those that cannot, thus embodying the principle of a finite maximum speed. In contrast to the usual (quantum) field theories this structure is no longer fixed, i.e. given a priori, but in Einstein's General Theory becomes a dynamical entity of its own device which is responsive to the distribution of other matter fields, resulting in the curvature of spacetime.

General relativity is a very successful theory. Its predictions range from the deflection of light by massive bodies which distort spacetime (Einstein-lensing) to that of gravitational radiation carrying away energy in the form of "ripples" in spacetime (Hulse-Taylor binary pulsar), as well as to the expansion of the universe (microwave background radiation). Still, the geometric theory of gravity suffers also from severe problems. Namely the inevitable occurrence of spacetime singularities, which was proven by Penrose and Hawking in their famous singularity theorems. Physically this means that spacetime contains regions where the curvature grows without a bound. The most prominent examples are the singularities at the "center" of black holes, where time itself comes to an end as well as the so-called initial singularity that occurs at the "Big Bang" the beginning of time. Other difficulties arise from the unification of gravity with quantum theory which governs the atomic and subatomic regime. Although several promising proposals for such a unification have been promoted, like Ashtekar's Loop Quantum Gravity and String Theory, to name just the most prominent ones, many problems have so far remained unresolved. It is therefore useful to focus on these central problematic aspects of gravity.

#### **Distributions and General Relativity**

Spacetime singularities belong to the big stumbling blocks of the classical theory and are therefore usually excluded from the definition of spacetime itself. From the point of view of quantum theory, which considers not only the classical evolution between a given initial and final three-geometry, they may just be the sheet-lightning of a change in topology of spacetime [1]. Due to their strong localization the concept of distributions (generalized functions)



Fig. 2: Geometry of a black hole formed by a collapsing pulse of radiation.

suggests itself as the mathematical structure being able to handle these singular regions. The simplemost example of a geometry with distributional curvature may be derived from the image of a cone taken to be the limit of a hyperbolic shell whose curvature concentrates more and more on the tip. The limit geometry is flat with all its curvature concentrated in a Dirac deltafunction at the location of the tip. In spite of the non-linear structure of general relativity, it is still possible to construct distributional curvature quantities associated with the singular regions and beyond of all the known stationary black-holes [2]. The discussion of a continuation of the geometry of a black hole beyond its curvature singularity has to transgress the boundaries of "classical" distribution theory and make use of the so-called Colombeau-algebra of new generalized functions [3] which allows for a systematic multiplication of distributional objects. It is therefore important, both from the quantum as well as the classical point of view, to get a better understanding of these structures.

#### **Two-dimensional Quantum Gravity**

Deeper insights into the structure of physical systems have often been achieved by the imposition of symmetries.



Fig. 3: Spherically symmetric black hole.

This usually breaks the problem down into simpler building blocks which ideally allow a complete solution. Gravity is no exception to this rule since the prototypic black-hole solution, the Schwarzschild geometry (actually the first exact non-trivial solution of the Einstein-equations), has been found precisely along theses lines, i.e. upon imposing spherical symmetry.

It is therefore natural to pursue a similar plan of attack for the quantization of gravity. The corresponding models become gravitational theories in a 1+1 dimensional spacetime coupled to the area of the two-sphere which becomes a dynamical variable in the reduced theory. As shown by work in our group in the absence of additional matter all such models turn out to be exactly soluble classically and allow even a background independent ("exact") quantization in terms of the so-called first order formalism, which takes the normalized dyad and its parallel displacement as fundamental variables [4]. Coupling to matter allows the description of scattering within an exactly soluble gravitational sector thereby leading to the concept of virtual black holes, as intermediate states, which hopefully sheds some light on the process of Hawking-evaporation of four-dimensional black holes [5]. The richness of the two-dimensional structure allows also the discussion of a supersymmetric extension of the original dilaton model thereby incorporating fermionic degrees of freedom in a particularly natural form. Here new insights regarding closely related problems in String Theory have been gained [6].

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### 3.1.3 Quark-Gluon plasma

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Quantum chromodynamics (QCD) is the accepted theory of the strong interactions responsible for the binding of quarks into hadrons such as protons and neutrons, and the binding of protons and neutrons into atomic nuclei. The fundamental particles of QCD, the quarks and gluons, carry a new form of charge, which is called color because of its triplet nature in the case of the quarks (e.g. red, green, blue); gluons come in eight different colors which are composites of color and anticolor charges. However, quarks and gluons have never been observed as free particles. Nevertheless, because quarks have also electrical charge, they can literally be seen as constituents of hadrons by deep inelastic scattering using virtual photons. The higher the energy of the probing photon, the more the quarks appear as particles propagating freely within a hadron. This feature is called "asymptotic freedom". It arises from so-called nonabelian gauge field dynamics, with gluons being the excitations of the nonabelian gauge fields similarly to photons being the excitations of the electromagnetic fields, except that gluons also carry color charges. Asymptotic freedom is well understood, and the Nobel prize was awarded to its main discoverers Gross, Politzer, and Wilczek in 2004.

Much less understood is the phenomenon of "confinement", which means that only colorneutral bound states of quarks and gluons exist. This confinement can in fact be broken in a medium if the density exceeds significantly that of nuclear matter. When hadrons overlap so strongly that they loose their individuality, quarks and gluons come into their own as the elementary degrees of freedom. It is conceivable that such conditions are realized in the cores of certain neutron stars.

Moreover, lattice gauge theory simulations have demonstrated that deconfinement also occurs at small baryon densities for temperatures above approximately  $2 \times 10^{12}$  Kelvin, corresponding to mean energies of about 200 MeV. According to the Big Bang model of the early universe, such temperatures have prevailed during the first few microseconds after the Big Bang as shown in Fig. 1.



Fig. 1: Thermal history of the Universe from the time when it was filled by a quark-gluon plasma until now.

At present there are experiments being carried out in the Relativistic Heavy Ion Collider (RHIC) at the Brookhaven National Laboratory, where a tiny fire-ball with temperatures larger than the deconfinement temperature can be produced and the resulting "quark-gluon plasma" [1] can be investigated. Starting in 2007, similar experiments at even larger energies and thus higher temperatures will be carried out at the European collider center CERN in Geneva. There is now ample evidence for the generation of a new state of matter in these experiments, although much remains to be understood.

One recent problem is the surprisingly fast apparent thermalization of the quark-gluon plasma. This seems to be much faster than can be accounted for by calculations of elastic and inelastic scattering events. This issue has been the topic of a workshop organized by A. Rebhan (ITP) and C. Fabjan (CERN and Atominstitut of the VUT) August 10–12, 2005 which took place immediately after the big Quark Matter 2005 conference in Budapest and attracted about 70 experimental and theoretical physicists.

A possible explanation of the fast apparent thermalization problem is that what is being observed experimentally is just early isotropization. The latter could be due to nonabelian variants of plasma instabilities that are familiar from ordinary plasma physics [2]. First results from our group which support this picture have appeared in the 18 March 2005 issue of Physical Review Letters [3]: Numerical simulations of collective chromomagnetic and -electric fields in an anisotropic quark-gluon plasma show exponential growth of unstable modes which in the nonlinear regime lead to complicated dynamics, eventually leading to fast isotropization of the plasma. Fig. 2 visualizes just the color degrees of freedom in collective fields as they evolve from initial fluctuations. The horizontal axis is the spatial direction in which there is momentum-space anisotropy in the plasma, and fields are taken as constant with respect to transverse directions. Time flows from bottom to top, with initial conditions (at the bottom) corresponding to random color fluctuations in initially tiny collective fields.



Fig. 2: The time evolution of the color degrees of freedom in the chromomagnetic field associated with instabilities in an anisotropic quark-gluon plasma. The horizontal axis is the spatial direction (z) in which there is a momentum-space anisotropy in the quark-gluon plasma.

In this plot one can see how the initial random fluctuations are swamped by the exponentially growing collective modes which involve a characteristic wavelength and locally fixed color charges (the amplitudes of the fields are not shown). After these perturbations have grown such that nonabelian self-interactions come into the play, there is rapid color precession in time (upper half of the plot), and a certain amount of spatial "abelianization" (i.e. finite domains of fixed color). The crucial finding, which cannot be read from this plot, is that exponential growth of these intrinsically nonabelian plasma instabilities continues until the collective fields give significant backreaction on the plasma constituents, rapidly eliminating their momentum-space anisotropies. This isotropization is much faster than the processes leading to thermalization, which occur somewhat later in the evolution of the fireball created in relativistic heavy-ion collisions. A still open question is the fate of nonabelian plasma oscillations when there is also nontrivial dynamics in the transverse directions. First results involving 3+1-dimensional lattice simulations have appeared almost simultaneously by a US group [4] and by our group [5]. Further work in this direction, which also takes into account the expansion of the quark-gluon plasma is presently carried out using the BEN supercomputer at ECT<sup>\*</sup>, Trento (Italy).

After local thermalization has taken place, the physics of hot and dense quark-gluon matter can be described by the following sketch of a phase diagram,



Fig. 3: Qualitative sketch of the phase diagram of quark-gluon matter as a function of temperature T and quark chemical potential  $\mu$ . Solid lines denote first-order phase transitions, the dashed line a rapid crossover.

where T is the temperature in MeV (1 MeV  $\approx 10^{10}$  K), and  $\mu$  is the quark chemical potential characterizing the density of net baryon number. (Nuclear densities correspond to about 308 MeV quark chemical potential.) "SPS, RHIC, and LHC" mark the regions of this phase diagram accessible by the older CERN experiment SPS, the present RHIC collider in Brookhaven, and the future LHC collider at CERN.

Another main activity of our group is the development of improved analytical techniques to calculate the thermodynamical properties of the quark-gluon plasma [6,7]. One focus is on properties at small  $\mu$  and high temperatures, which are relevant for relativistic heavy ion colliders and the physics of the early universe. Another case of interest is high  $\mu$  and smaller temperatures, which is of relevance to the physics of neutron stars and proto-neutron stars.

At comparatively low temperatures, quark matter is known to form Cooper pairs and turns into a color superconductor [8]. Also at temperatures just above the superconductivity phase new phenomena appear, which reflect that quark matter has strong deviations from an ideal Fermi liquid. In particular, there is anomalous behaviour in the low-temperature specific heat, which has been calculated for the first time systematically by our group [9]. Together with new results on dispersion laws of quarks obtained by our group [10], this has already found application in revised calculations of the cooling behavior of young neutron stars [11].

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### 3.1.4 String theory

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The names of the fundamental forces are related to their strength. The strong force is much stronger than electromagnetism and is thus able to overcome the repulsive force between objects with the same electrical charge (protons or quarks). The weak force is weaker than electromagnetism but still much stronger than gravity. The reason that we almost only recognize gravity in everyday life is that the macroscopic objects are neutral. They don't carry an effective color charge and they carry - if at all - only very small electric charges. For gravity there is no negative charge (negative mass), so that all the small gravitational effects add up to something which is strong enough to move galaxies and to build black holes. The separate description of the forces is quite accurate by now. This is summarized in the standard model of particle physics.



Fig. 1: Grand unification. i=1: Electromagnetism, i=2: weak interactions, i=3: strong interactions

There is only one particle (the Higgs boson), which is predicted by the standard model and has not yet been found. A measure for the strength of a force are the coupling constants of the corresponding theory. They are, however, not constant, but depend on the energy level one is dealing with. If one extrapolates their values to high energies, one discovers that the couplings of electromagnetism, strong and weak force meet at a certain energy level almost in one single point (see Figure 1). This supports the idea that those three forces could be just different aspects of one and the same universal force. There are several theories which try to describe this unification. They are called GUTs, 'grand unified theories'. However, to be really 'grand', such a unification should also include gravity, which is still weaker, even these high energies. The theory that will manage to unify all forces, including gravity, is sometimes called TOE, "theory of everything". String theory is one candidate, and at present actually the only one for this TOE.

Before going to explain a little bit what string theory roughly is, let us have a second look at Figure 1, where it is shown that with 'SUSY', the lines not only almost meet in one point, but they meet exactly (within present precision) in one point [1]. 'SUSY' stands for supersymmetry and means that there is an exchange symmetry between fermionic particles (like quarks and electrons) and bosonic ones (like photons and even gravitons, if one includes gravity into the considerations). It does, however, not relate the already known particles, but it predicts new supersymmetric partners to the known particles (called e.g. squarks, selectrons, photinos and gravitinos). So far none of those superparticles has been discovered, but there are a lot of theoretical reasons for believing in supersymmetry, one of them being Figure 1. Supersymmetry is an integral part of string theory, or more precisely 'superstring theory'. In about two years, the new accelerator LHC (large hadron collider) at CERN will start and try to produce the Higgs boson and the superparticles mentioned above and will therefore also be a test for string theory.

Gravity is described by Einsteins general relativity which explains the gravitational force as being an effect of curved space-time. It is an extremely beautiful, successful and revolutionary theory, but it is classical in the following sense: the gravitational field is smooth and one can in principle measure arbitrarily small distances. However, time evolution of the gravitational field is governed by the matter content - or more specifically - by the fields that are described by the Standard Model. The Standard Model, on the other hand, describes quantum fields, i.e. the fields consist of quanta - the particles - whose position and momenta underly Heisenbergs uncertainty relation. In a macroscopic limit, one can still think of the fields being classical smooth fields and for this reason General Relativity is extremely successful in describing large scale physics. But in order to avoid inconsistencies and to consider extreme situations like black holes and the big bang correctly one needs to treat the gravitational field, like the other interactions described earlier, as a quantum field. There is a standard procedure how to make quantum fields out of classical ones. This procedure, called quantization, unfortunately fails for gravity. The reason is that interactions of point particles produce singularities (infinite values in at least intermediate steps on the way to compute probabilities of particle collisions). Those singularities can be dealt with in the standard model, but the standard (perturbative) approach fails for 'quantum gravity'. It is thus reasonable to avoid those singularities from the beginning by treating the elementary objects not as point particles, but as extended objects, which are called strings [2]. In Figure 2 one can see that the collision of two strings - joining to a single one - produces a smooth surface, while the same process for point particles is not smooth and therefore produces singularities. Considering a string instead of a point particle is a simple idea, but it has extremely far-reaching consequences. The first consequence is that a string has more degrees of freedom. It can oscillate in different modes like a guitar string. The different tones then correspond to different particles which makes it possible to describe the complete spectrum of particles by one fundamental object! While taking open or closed strings as starting point apparently leads to different string theories with different particle spectra, the very same string can start as an open one and become a closed one during some scattering processes.



Fig. 2: Left: point particle interaction, Right: closed string interaction, note the smooth interaction surface

According to an old idea of Kaluza and Klein (KK) it should be possible to describe also the other forces in a purely geometrical way, as it was done for gravity. Indeed they managed to produce electromagnetism by starting with a five dimensional gravity and then curling up one dimension on a very small radius, so that gravity effectively becomes four-dimensional. Components of the gravitational field belonging to the fifth dimension then show up as an electromagnetic field. The KK method needs 11 dimensions in order to describe all the fundamental forces but it never worked out to give the correct matter content. Superstring theory, on the other hand, *predicts* ten dimensions. Hence one has to curl up six dimensions in order to end up with a four-dimensional observable space-time. In contrast to point particles, strings have the new feature that they can wind around the curled up dimensions, thus extending the spectrum of physical states. With string, it turns out, the matter content of the Standard Model indeed fits into 10 dimensions.

When string theory is compactified on a circle there is a 'dual' inverse radius for which we obtain exactly the same spectrum of particles, so that the full quantum theory is indistinguishable from the first one. This implies a smallest observable scale, a feature that should be expected from any consistent quantum theory of gravity. Going below that scale would mean that one ends up with something that is actually bigger! This is only one example of a number of dualities connecting string theories that are at first sight completely different. The above radius duality led to the discovery of other extended objects, which are not just strings but can have more dimensions and are called D-branes. They are dynamical objects on which open strings end. Gauge fields, the fields that also appear in the standard model, are restricted to those D-branes, while gravity is diluted because it can spread out into ten dimensions. This would explain the large difference between the values of the coupling constants of the standard model and of gravity, respectively: we are just living on a brane!

The duality mentioned above, relating big and small radii, can be generalized to curved spaces and is then called mirror symmetry. The curled up six-dimensional spaces have to fulfill certain properties and are mathematically called Calabi-Yau spaces. A major work of our group goes into examining and classifying those Calabi-Yau spaces [3], exploring the consequences of dualities [4], and physical properties of D-branes therein.

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## **3.2** Nonlinear Dynamics, Physics of Complex Systems

The physics of complex systems has developed into one of the rapidly growing "hot" subfields of physics, as reflected in the foundations of several institutes worldwide dedicated to this topic. The faculty of physics has recognized this field in its development plan as one of its strategic key areas. Complexity refers, one hand, to "large" multi-scale systems whose dynamics cannot be reduced to simple independently evolving building blocks. Examples range of biophysical systems to the weather pattern. One of the exciting discoveries is that complexity does necessarily require a large system but can likewise be observed in "small" systems with as few as two degrees of freedom. Non-linearity of the underlying dynamics is the root cause for the ensuing complexity in such seemingly simple systems.

The notion of physical complexity is closely related to information-theoretical concepts of complexity. The underlying question is how much information or how long a data string is required to uniquely characterize the state of a system and its future. It is the hallmark of classically chaotic systems that the required data string is infinity long. In remarkable contrast, their quantized counterparts ("quantum chaos") have been found to lack this "exponential complexity". The transition from classical to quantum dynamics is therefore accompanied by a fundamental change in information density. This observation is one of the keys to the current interest in "quantum information" and "quantum computation". Research at our institute focuses on quantum-information theoretical aspects and on the classical-quantum transition in chaotic few-degree systems. A recent addition is the investigation of non-linear phenomena in the interactions of atoms and solids with strong optical fields which is part of the FWF-funded special research program advanced light sources (ADLIS).

### 3.2.1 Quantum information

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Suppose we would be able to unleash the power of the quantum world in ways which would have been unthinkable only a few years ago. For instance, we could use quantum superposition, the possibility for a quantum bit to contain all conceivable and mutually excluding classical states in itself. Then, in a single computational step, we could realize the parallel processing of all these classical states, whose number grows exponentially with the number of classical bits involved, through the quantum state evolution of this single state. That is the vision of quantum parallelism, which is one of the driving forces of quantum computing, and at the same time one of the fastest growing areas of research in the last decade or so. These strategies have all been made possible with new techniques capable to produce, manipulate, and detect single quanta, such as photons, neutrons and electrons.

There are other prospects as well. Quantum processes and in particular the quantum state evolution in-between irreversible measurements are one-to-one, i.e., reversible. The "message" encoded into a quantum state merely gets permuted and transformed such that nothing gets lost. Thus, processes such as state copy or state deletion, which appear so familiar from classical computing, are not allowed in quantum information theory. Copy, for instance, is oneto-two, or one-to-many. Deletion is many-to-one. As a consequence, information transmission has to rely on processes which are strictly one-to-one. This elementary, innocently looking fact of quantum state evolution, can be put to practical use in areas such as cryptography, where it is tantamount to keep a secret secret; i.e., by not allowing potential eavesdroppers to divert, copy, and resubmit messages. Actually, quantum cryptography uses another mind-boggling quantum feature: complementarity; the impossibility to measure all classical observables of a state at once with arbitrary accuracy. So it is the scarcity of the quantum processes which could be harvested for new technologies. Even potential cryptanalytic techniques – such as man-in-the-middle attacks on quantum cryptography – could be perceived as a challenge to cope with the structure of the quantum world in detail.

The basis of these potential exciting new technologies is the quantum world and its relation to the performance of classical systems. Already George Boole, one hundred and fifty years ago, mused over issues which became most important today. He figured out that there are some constraints on the joint frequency of classical events which come from the requirement of consistency.

Suppose someone claims that the chances of rain in Vienna and Budapest are 0.1 in each one of the cities alone, and the joint probability of rainfall in both cities is 0.99. Would such a proposition appear reasonable? Certainly not, for even intuitively it does not make much sense to claim that it rains almost never in one of the cities, yet almost always in both of them. The worrying question remains: which numbers could be considered reasonable and consistent? Surely, the joint probability should not exceed any single probability. This certainly appears to be a necessary condition, but is it a sufficient one? Boole, and much later Bell – already in the quantum mechanical context and with a specific class of experiment in mind – derived constraints on the classical probabilities from the formalization of such considerations. In a way, these bounds originate from the conception that all classical probability distributions are just convex sums of extreme ones, which can be characterized by two-valued measures interpretable as classical truth values. They form a convex polytope bounded by Boole-Belltype inequalities.

Remarkably, quantum probability theory is entirely different from classical probability theory, as it allows a statistics of the joint occurrence of events which extends and violates Boole's and Bell's classical constraints. Alas, quantum mechanics does not violate the constraints maximally, quantum bounds fall just "in-between" the classical and maximal bounds.

The question is: how much exactly and quantitatively does quantum mechanics violate these bounds? We have derived numerical as well as analytical bounds on the norm of quantum operators associated with classical Bell-type inequalities can be derived from their maximal eigenvalues. This quantitative method enables detailed predictions of the maximal violations of Bell-type inequalities, and generalizes Tsirelson's result  $2\sqrt{2}$  for the maximal violation of the Clauser-Horn-Shimony-Holt inequality.

We have also developed new protocols for quantum cryptography using interferometers. Thereby, we have considered sets of quantum observables corresponding to *eutactic stars*. Eutactic stars are systems of vectors which are the lower-dimensional "shadow" image, the orthogonal view, of higher-dimensional orthonormal bases. Although these vector systems are not comeasurable, they represent redundant coordinate bases with remarkable properties. One application is quantum secret sharing. The Figure below depicts a typical configuration.



Fig. 1: Quantum cryptography using single-photon sources. (copyright) http://www.epfl.ch

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### 3.2.2 Atoms in ultrashort laser fields

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Since the first working laser device was built by Maiman in 1960, the progress in laser technology has been tremendous. The intensity of the lasers has been increased by many orders of magnitude. Intensities reach presently well above  $10^{20}$ W/cm<sup>2</sup>, where plasma effects as well as relativistic effects are important. In the near future, laser intensities may even reach the critical field strength to directly produce positron-electron pairs.

At the same time, the length of the shortest pulses has decreased by more than 10 orders of magnitude (Fig. 1). While the first lasers had a pulse length of some  $100\mu$ s, very short pulses can nowadays be produced by mode-locking. In 1990, Zewail et al. [1] managed to generate pulses as short as several femtoseconds, which meant that snapshots of chemical reactions could be taken directly. This opened up the field of femto-chemistry.



Fig. 1: Decrease of pulse duration as a function of time.

To take time-resolved pictures of atomic processes, even shorter pulses down to the attosecond regime are needed. Such short laser pulses can be produced by the process of high harmonics generation (HHG): the time-dependent field of a strong femtosecond laser may ionize an atom and accelerate the electron in one direction. As the field changes direction, the electron might get accelerated back and emit radiation by "bremsstrahlung" as it hits the nucleus. The frequency of the radiation may be hundreds of times higher than the driving field. By filtering out a narrow region of the highest frequencies produced, pulses as short as some hundreds of attoseconds can be generated [2].

Such electromagnetic pulses still subtend several periods of the XUV-carrier oscillation within the envelope and is capable of delivering a photon ( $\leq$ keV) on a sub-fs timescale. By contrast, a half-cycle pulse (HCP) contains ideally no additional oscillatory structure inside its envelope. If the width  $\tau_P$  of such a pulse is short compared to the typical time scale  $T_n$  of the driven system, the HCP is impulsive, i.e. it delivers a linear momentum to an electron. Such pulses are ideal tools to shape, drive, control and probe wave packets in momentum space. We study the full macroscopic response of a gas of atoms to a strong two-color laser field with frequencies  $\omega$  and  $2\omega$ . Carefully choosing the parameters of the driving pulse and assuming that the amplitudes and phases of the driving components can be adjusted after the propagation, a train of unidirectional HCPs emerge (Fig. 2) [3].



Fig. 2: Train of u-HCP after propagation. Left panel: train after 9mm. The train has an intensity of  $I_{HCP} = 4.2 \times 10^{12} W/cm^2$  and width  $\tau_P = 650$ as of the individual HCP's. Right panel: Build up of train with propagation length. The intensity and wavelength of the driving field are  $I = 10^{14} W/cm^2$  and  $\lambda = 1064$ nm, respectively.

The possibility of driving an atom by a femtosecond laser as well as the usage of high harmonics generation to produce the shortest pulses presently available challenges our current understanding of the processes taking place in the atom. Insights can be gained from doublydifferential  $(k_z, k_\rho)$  momentum distributions. At large values of |k| semicircles of fixed energy can be seen corresponding to above-threshold ionization peaks (Fig. 3). The radius of each semicircle corresponds to an energy given by  $U_j = E_0 + j\omega$ , where  $E_0$  is the ground state energy of the atom, and j the number of photons absorbed. The iso-energy circles are modified in the low momentum region to radial "finger like" structures. The latter represent Ramsauer-Townsend diffraction pattern [4] in the angular distribution experimentally observed for the first time in laser-atom interactions.



Fig. 3: Doubly differential momentum distributions. T = 2 fs and the pulse contains about 8 cycles. (a)  $I = 5 \times 10^{13}$ W/cm<sup>2</sup>, (b)  $I = 1 \times 10^{14}$ W/cm<sup>2</sup>, (c)  $I = 2 \times 10^{14}$ W/cm<sup>2</sup>.

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### 3.2.3 X-ray generation by laser-cluster interaction

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The study of the interaction of intense short and ultra-short laser pulses with clusters has received much attention during the last decade [1]. This interaction results in the emission of highly energetic ions, electrons and x-ray photons. For the production of keV photons, rare-gas clusters unite the advantages of both solid and gaseous targets: like solids they can provide large yields, yet they are relatively debris-free, just like gas targets.

In a simple picture, the dynamics during the laser-cluster interaction can be summarized as follows (Fig. 1): the atoms of the cluster are first ionized by the incident laser pulse (inner ionization) and a cold "nano-plasma" of solid density is formed. The quasi-free electrons take part in a collective oscillation driven by the laser field and moreover interact with the field of the surrounding particles. Electron-impact ionization of cluster ions produces additional quasi-free electrons and inner-shell vacancies which are at the origin of x-ray radiation. As a fraction of the electrons leaves the cluster (outer ionization), a net positive charge is left behind and the cluster begins to expand before disintegrating completely in a Coulomb explosion.

Recent experiments [2] found an unexpectedly low laser intensity threshold for x-ray production. When irradiating large clusters with N > 10000 argon atoms with infrared  $(\lambda = 800nm)$  laser pulses of duration  $\tau = 60 fs$  at FWHM, characteristic x-ray radiation could be measured for laser peak intensities as low as  $I_{th} \simeq 2.2 \cdot 10^{15} \text{Wcm}^{-2}$ . At this intensity, the ponderomotive energy  $U_P = F^2/(4\omega^2)$  (atomic units are used unless otherwise stated) associated with the oscillatory motion of a free electron in a laser field with field strength Fand frequency  $\omega$  is  $U_P \simeq 130 \text{eV}$ . This value is more than one order of magnitude below the



Fig. 1: Stages of cluster dynamics (see text)

binding energy  $E_K \simeq 3.1 \text{keV}$  of K-shell electrons in argon. This raises questions as to the additional heating mechanisms at play in a cluster environment, which allow the electrons to be effectively accelerated well beyond the ponderomotive energy.

Due to the large size of the clusters (N > 10000 atoms), a full ab-initio simulation seems still impractical. We therefore opt for a simplified theoretical description of the dynamics of the laser-cluster interaction [3,4]. The many-electron system is treated as an open effective meanfield one electron system, in which many-particle effects are included via stochastic processes. We could show that elastic electron-ion scattering is an effective electronic heating mechanism, allowing an electron to gain energy in the laser field well beyond the ponderomotive energy. The estimate of the efficiency of this mechanism depends crucially on appropriate differential scattering cross-sections. Our model results in a high-energy tail of the electron distribution being sufficient to produce K-shell vacancies. We find good quantitative agreement with the experimentally measured effective x-ray yields (Fig. 2).

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Fig. 2: Experimental x-ray yields ( $\circ$ ) for argon clusters with N = 280000 atoms, excited by 60 fs,  $\lambda = 800$ nm laser pulses. With a Coulomb scattering cross-section ( $\blacksquare$ ) the yield is too small. With a more realistic ionic potential ( $\bullet$ ) the results lie within the experimental error estimates.

### 3.2.4 Engineering Highly Polarized Rydberg states

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In recent years there has been increasing interest in the control and manipulation of atomic wave functions. The engineering of wave functions promises applications in many areas of physics, such as quantum computing [1], promotion of chemical reactions towards any preferable direction [2], or optimization of high harmonic generation [3]. Theoretically any wave function can be formed as a coherent superposition of energy eigenstates. In practice, however, it is not an easy task to prepare a preselected target state experimentally. Thus there are increasing demands for establishing easy protocols to produce preferable designer states starting from the states which are experimentally accessible. Recently a few protocols have been suggested to create and manipulate wave packets. Due to the relatively large time and spatial scale ( $t \sim n^3$  and  $r \sim n^2$ ) of Rydberg atoms with quantum number n, Rydberg wave packets are known to be among the best explored quantum objects which approximately follow the dynamics of the corresponding classical particle and serve as benchmark for probing the crossover between classical and quantum dynamics [4]. With recent advances in ultra-short pulse generation it has become possible to engineer wave packets using Rydberg atoms [5]. With a properly tailored sequence of short pulses, so-called half-cycle pulses (HCPs) a Rydberg wave packet can be transiently localized leading to a highly polarized Rydberg wave packet [6].



Fig. 1: Time evolution of the phase space distribution for Rydberg atoms subject to a sequence of a weak localization HCP (a), a strong excitation HCP (b), and a periodic train of HCPs (c-f). The results are calculated using CTMC. White solid lines indicate energy manifolds for Rydberg states with n = 350 and n = 600. k is the number of kicks applied.

Initially we photoexcite alkali atoms in a weak dc field to generate an incoherent mixture of several parabolic Stark states  $(n \simeq 350, n_1 \simeq 320, m = 0)$  oriented parallel to the applied dc field. This oriented state is, in fact, highly polarized and excited Rydberg wave packet. However, our aim is to demonstrate how to generate an even more highly  $(n \sim 600)$  excited wave packet without losing the polarization by applying a tailored sequence of HCPs. When a Rydberg atom is subject to a half-cycle pulse (HCP) [7] whose duration is much shorter than the Kepler period of the Rydberg electron, the atom experiences an impulsive momentum transfer or "kick" given by

$$\Delta p = -\int F_{\rm HCP}(t) \tag{1}$$

at the moment of the kick. For example, when the momentum of the electron and the direction of the kick are parallel to each other, the electron is accelerated and gains energy. When they are anti-parallel, the decelerated electron loses a part of its energy. When a single HCP is applied to a stationary Rydberg state, several energy levels are excited. Since the orbital frequency of the electron motion depends on the energy, this small spread of the energy distribution, *i.e.* a small variation of orbital frequency, keeps the dynamics of the electron ensemble coherent. After a proper amount of time delay an even more localized wave packet can be transiently realized [8]. This localized wave packet is easier to manipulate by further application of kicks and therefore this weak localization is necessary to create a highly excited polarized state by a further application of HCPs.

As a next step, a relatively strong HCP is applied to the transiently localized wave packet in order to excite electrons to even higher Rydberg levels  $(n \sim 600)$  (see Fig. 1b). This strong kick broadens the energy distribution of the wave packet. In such a broad energy distribution, the pieces of the wave packet with different orbital frequencies start dephasing and the resulting wave packet disperses. This energy dependent variation of the orbital frequency elongates the wave packet as seen in Fig. 1c. In order to narrow the energy distribution broadened by the excitation kick, we apply a periodic sequence of HCPs polarized anti-parallel to the previous



Fig. 2: Time evolution of the energy distribution for Rydberg atoms subject to a sequence of a weak localization HCP at t = 0, a strong excitation HCP at t = 6 ns, and a periodic train of HCPs. The results are calculated using CTMC.

excitation kick, *i.e.* towards the nucleus. As shown in the Fig. 1c a high energy tail of the wave packet resides in the positive momentum space. This *negative* kick decelerates the electron and the energy is lowered. On the other hand, the low energy tail with negative momenta is accelerated and gains energies. Thus, by choosing a proper size of kicks, the energy spread of the wave packet can be reduced. (A more accurate description in terms of stable and unstable manifolds of the periodically kicked atom can be found in Ref. [6].) When a few kicks are applied, the wave packet is brought almost parallel to the energy manifold of a single state (Fig. 1e). The energy distribution is thus narrowed and focused as illustrated in Fig. 2.

Using a properly tailored sequence of HCPs, very high excited and polarized Rydberg wave packets can be prepared. This is only an example of how to engineer the Rydberg wave packet. Further control and manipulation of wave packets are currently under investigation.

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### 3.2.5 Enhanced Electron-Ion Recombination in Ion Storage Rings

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Electron-ion recombination plays an important role in many areas of physics, such as astrophysics, plasma physics, and accelerator physics. With the aid of electron coolers in ion storage rings it has become possible to measure the recombination rate at very low energies (typically < 1 meV). In these experiments the incident ion beam is merged with a cold and magnetically guided beam of electrons in the electron cooler. The electrons provide not only the cooling medium for the ion beam but also supply a very cold target for electron-ion recombination. For the experiments involving bare ions, the dominant recombination mechanism has been attributed to radiative recombination (RR). The measured rates [1] show, however, a significant enhancement beyond the theoretical prediction for RR [2,3] (see, for example, Fig. 1). To understand the surprising discrepancy between the measured recombination rates and the theoretical prediction there have been a number of studies focusing on a variety of aspects ranging from the influence of three-body recombination [4] and density enhancement due to plasma screening effects [5] to the effect of a magnetic field on the cross section by considering the chaotic dynamics caused by a magnetic field in the electron cooler [6]. None of these models can, so far, account quantitatively for the observed enhancement. We have recently identified another recombination mechanism in the merging section of the electron cooler [7]. In the merging section a toroidal magnetic field guiding the electron beam is not aligned with the ion beam. Therefore the ions are exposed to a magnetic field transverse to their direction of motion, *i.e.*, to a motion-induced transient electric field in their rest frame. This induced field opens an additional pathway for free-bound transitions of electrons and plays an important role to explain the gap seen between measurements and the theory.



Fig. 1: Recombination rate for C<sup>6+</sup> ions at B = 42 mT as a function of relative energy between electrons and ions. The standard RR theory (line), the experimental data [1] ( $\blacktriangle$ ) and the rate including FIR ( $\bigcirc$ ) are shown. The longitudinal and perpendicular temperatures of the electron beam are  $kT_{\parallel} = 0.2$  meV,  $kT_{\perp} = 10$  meV.
In the electron cooler (Fig. 2b) a longitudinal magnetic field is applied in order to suppress the spatial spreading of the electron beam due to its space charge. The field guides the electrons through a curved (toroidal) section into a straight (solenoidal) section aligned to the ion beam. Electrons and ions interact under quasi-stationary conditions at nearly matched beam velocities ( $\vec{v}_e \sim \vec{v}_{ion}$ ) until the beams are demerged in a second toroidal section. In the rest frame of an ion crossing the toroidal region, these magnetic field components give rise to a motional transverse electric field which is a time-varying, transient field as the electron propagates through the toroid (Fig. 2a). This electric field tilts the ionic Coulomb potential such as to form a Stark saddle (Fig. 2c). Initially free electrons can pass over the saddle and thus become trapped in the Coulomb potential when the transient electric field is switched off at the entrance of the solenoid (Fig. 2d). This non-radiative, *i.e.* field-induced mechanical recombination due to time-dependent electric fields opens an alternative pathway to recombination specific to devices such as storage rings that competes with radiative recombination.



Fig. 2: (a) Schematic picture illustrating the different field configurations in the labframe and the rest frame of ion. (b) Geometry of the electron-ion interaction in the cooler of a storage ring. In the solenoidal region a constant magnetic field B is present. (c)-(f) Field induced recombination mechanism followed by either radiative stabilization (e) or reionization at the demerging section (f).

Radiative decay of these transiently formed Rydberg states inside the solenoid can stabilize a fraction of these weakly bound electrons (Fig. 2e) thereby preventing field ionization in the toroidal demerging section (Fig. 2f). In the case of  $C^{5+}$  ion, the radiative lifetime of such a high Rydberg state is about 0.1 milliseconds, much longer than the propagation time of the ion beam through the solenoid ( $\sim 60$  ns). Thus, only a miniscule fraction will have radiatively decayed to a state sufficiently deeply bound to escape the demerging toroid without field ionization. However, such a small fraction cannot be neglected since the radiative recombination rate itself is a very small quantity and comparable to the field induced recombination rate.

Figure 1 shows the recombination rate calculated using CTMC including the effect of the field-induced recombination followed by radiative stabilization. The magnetic field and the ion charge dependences of the measured recombination rate is also well reproduced by simulating the effect of the motion-induced electric field [7]. This new path to recombination appears to close the gap between measurements and theory.

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### 3.3 Condensed Matter Theory

The research topics within the field of condensed matter theory at our institute reflect the fact that condensed matter physics is a central facet of the research portfolio at the faculty of physics at a technologically oriented university. At the same time, it mirrors the diversity of the field itself, ranging from mathematical, specifically group-theoretical, aspects of crystalline solids, and equilibrium properties of soft matter and liquids to dynamical interactions with surfaces. Several joint collaborations with experimental activities at the Faculty of Physics of the VUT and other institutions exist and emphasize the synergistic potential of the research in this field.

### 3.3.1 Formation of ordered cluster phases in soft matter systems

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#### Introduction

Both from theoretical and experimental investigations there is clear evidence that soft matter shows a distinctively different behaviour under compression than atomic (or 'hard') systems. It is in particular the richness of spontaneously forming complexes, exceeding the dimensions of the individual mesoscopic macromolecules, that is so characteristic for soft matter systems. Indeed, the macromolecules can self-organize in a variety of ways, giving rise to so-called hypermolecular structures that encompass a large number of mesoscopically sized entities. In many cases the underlying physical mechanism that drives the emergence of hypermolecular structures is widely believed to rest on the existence of competing interactions, i.e, the presence of short-range attractions and long-range repulsions in their effective interparticle potentials [1]. However, there is another mechanism that can give rise to a distinct type of formation of aggregates of particles (which we term clusters) and which does not rest on the explicit existence of competing interactions. This cluster formation occurs even in the complete absence of attractive forces and might seem counterintuitive at first sight [2,3].

In our investigations we have considered particles that are allowed to spatially overlap and interact purely repulsively. Both conditions are readily fulfilled for various types of polymeric macromolecules, e.g., polymer chains, polyelectrolytes, or dendrimers. Under certain general conditions of the properties of the Fourier transform  $\tilde{\Phi}(q)$  of the potential,  $\Phi(r)$ , the particles are able to form aggregates that further organize into regular crystals with multiple site occupancy. We will refer to this scenario as formation of ordered cluster phases.

#### Model and methods

For simplicity we have assumed a simple model potential  $\Phi(r)$  that features above properties which we term generalized exponential model of index n (GEM-n), given by

$$\Phi(r) = \epsilon \exp[-(r/\sigma)^n],\tag{1}$$

 $\epsilon$  and  $\sigma$  being energy- and length-parameters. We point out that above model can also show – depending on the value of n – the so-called re-entrant melting scenario. Here, the solid phase can re-melt again under compression. In the following we focus on the cluster phase phenomenon, which – according to a general criterion derived in literature [3] – is guaranteed for n > 2. To be more specific we restrict ourselves to n = 4.

The properties of the fluid phase are calculated within the mean spherical approximation, i.e., a liquid state theory that is known to provide accurate results for soft systems [4]. The ordered cluster phases are treated within classical density functional theory where we have assumed for the free energy functional,  $\mathcal{F}[\varrho]$ , a mean-field format for the excess (over ideal) contribution. For the density profiles,  $\varrho(\mathbf{r})$ , we have used a Gaussian shaped distribution, localized at the lattice sites  $\{\mathbf{R}_i\}$  and characterized by the width,  $\alpha$ , and the occupancy number (or cluster size),  $n_c$ . Minimization of  $\mathcal{F}[\varrho]$  with respect to  $\alpha$  and  $n_c$  provides the equilibrium values of  $\varrho(\mathbf{r})$ .

In addition, Monte Carlo (MC) computer simulations have been carried out [5] in various thermodynamic ensembles. Typically we used systems of several thousands of particles and extended the computer experiments to 150 000 MC sweeps. Considerable speed-up was achieved by implementing a discretized simulation technique [6].

#### Results

From our simulations we found evidence of spontaneous clustering and crystallization; this is demonstrated by the simulation snapshots in Fig. 1, all of them taken at the same temperature  $[T^* = (\beta \epsilon)^{-1} = 0.4]$ , but different densities. At  $\rho^* = \rho \sigma^3 = 2.5$  the system is obviously in the fluid phase; still (and since we are close to the phase boundary – see below and Fig. 2) clusters of particles have formed. As the density is increased to  $\rho^* = 3.5$  a (first order) phase transition takes place: clusters of particles form which are located on a reagular structure. A quantitative analysis [7] reveals that this structure is a (slightly distorted) fcc lattice. As the density is further increased ( $\rho^* = 7$ ) the clusters become more compact, they grow in size, and the fcc lattice is nearly perfect. Further investigations of the simulation data, that are fully consistent with the DFT results, reveals striking features of the cluster phase that will be discussed below.



Fig. 1: Three simulation snapshots of a GEM-4 system at  $T^* = 0.4$  and for  $\varrho^* = 2.5$ , 3.5, and 7 (from left to right). Particle diameters are not drawn to scale but are chosen to optimize the visibility of the structures.

Due to the high computational cost of the simulations a more comprehensive picture of the cluster phenomenon can be obtained via liquid state theory and density functional theory. The theoretical prediction of the phase diagram is shown in Fig. 2; the thermodynamic data obtained in simulation for selected state points fully confirm the theoretical results [8]. From the phase diagram in Fig. 2 we see that at low densities the system is in the fluid phase where already some clusters have formed (see snapshot in Fig. 1). Upon compression, a first order clustering transition occurs, leading at sufficiently high densities to the fcc stucture. Above the triple temperature,  $T_{\rm tr}^* = k_{\rm B}T/\epsilon \sim 0.4$ , a wedge-shaped cluster bcc region intervenes between the fluid and the cluster fcc. Thus, the system also shows polymorphic transitions between cluster solids. In agreement with theoretical predictions [3], the freezing and the melting curves are almost straight lines. The DFT calculations provide results for  $\alpha$  and  $n_c$ which can easily be compared to the data extracted from simulations; again we find excellent agreement between the two sets of data. Finally, the density profiles of the particles in the clusters,  $\rho(r)$ , as extracted from the simulations are within high accuracy indeed Gaussians, which justifies a posteriori our assumption for  $\rho(r)$  within the DFT scheme.



Fig. 2: The phase diagram of the GEM-4 model (temperature vs. density), as obtained by DFT. The shaded area represents the coexistence region of the liquid and the cluster bcc phase.

A quantitative analysis of the simulation and the DFT data reveals the following striking effects: (i) despite the complete absence of attractive forces, formation of stable clusters is indeed possible. On the level of the free energy this can be understood as a competition of the ideal and the intra-cluster contributions on the one hand, and inter-cluster contributions, on the other. (ii) Upon compression, the lattice and the lattice constant of the hyperstructure remains invariant. If we increase the density at fixed volume by inserting more and more particles, these join the already existing clusters, leaving the hyperstructure (both with respect to its symmetry as well as to its lattice constant) unchanged. Thus, the cluster size increases linearly with density. This is in striking contrast to atomic systems where the lattice constant shrinks with increasing density.

Our investigations [8] have been commented in the scientific community [9] and were also presented in Austrian newspapers [10].

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# 3.3.2 Genetic algorithms – an attractive tool in condensed matter theory

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#### Introduction

The search for solid equilibrium structures in liquid-solid transitions in condensed matter systems is still an unsolved problem. The conventional approach proceeds along the following lines: first – relying on experience, intuition, or plausible arguments – a set of possible candidate structures for the solid phase(s) is preselected. Then, using one of the methods proposed in literature, the free energies of the competing phases are calculated and for a given state point the one with the lowest free energy is considered to be the stable one. In the last step, phase boundaries are determined via the coexistence relations, taking now also the fluid phase into consideration. The inherent weak point of this approach lies in the first step, i.e., the preselection process, which always bears the risk of simply forgetting possible candidate structures.

We have introduced genetic algorithms (GAs) in our investigations of liquid-solid transitions in (soft) condensed matter systems to address this problem. GAs were originally developed for engineering sciences and have later been extended to different fields (such as economics) where they have meanwhile become a very attractive tool [1]. In the following we give evidence that GAs can indeed be a very useful, efficient, and reliable tool in physics. We will demonstrate their potential, power, and merits in their application to the liquid-solid transition in condensed matter theory.

#### The basic idea of genetic algorithms and their implementation

GAs are optimization strategies that can be viewed as an implementation of Darwin's process of evolution, using thus features of evolutionary processes as key elements to find the optimal solution for a problem. The basic quantity is an *individual* which represents a candidate solution. Individuals are evaluated via a problem-specific fitness function in the sense that a better (or fitter) individual has a higher fitness value. A large number of individuals forms a *generation*. After selecting – according to their fitness values – parents in one generation, individuals of the subsequent generation are formed via simple operations (such as recombination and mutation). Iterating through several generations, retaining in each generation the individual with the highest fitness value, and taking in the end the one with the absolutely highest fitness value leads to the optimized solution.

In our application of GAs to the liquid-solid transition, an individual represents the primitive vectors that form a simple lattice in a suitably coded form; eventually the individual will also include positions of further particles in non-simple lattices (or other parameters that characterize additional internal degrees of freedom of the system). To this end, we have introduced a standardized parametrization of a simple lattice. The coding of these parameters (which is realized via their binary representation) defines the individual,  $\mathcal{I}$ , that represents this particular lattice. A large, but fixed number of individuals forms a generation  $\mathcal{G} = \{\mathcal{I}\}$ . Further, a positive-definite fitness function  $f(\mathcal{I})$  is introduced which evaluates the individual in the above mentioned sense. For our problem we specify the fitness function as follows: since the crystal structure with the lowest free energy is considered to be the stable one, the fitness function is related to the energy of the lattice represented by the individual  $\mathcal{I}$ . We now start an iterative process that creates from the individuals of generation  $\mathcal{G}_{[i]}$  the individuals of the subsequent generation,  $\mathcal{G}_{[i+1]}$ . Choosing according to their fitness values two individuals,  $\mathcal{I}'_{[i]}$ and  $\mathcal{I}''_{[i]}$ , as parents, we create via a so-called one-point crossover operation two individuals of the subsequent generation,  $\mathcal{I}'_{[i+1]}$  and  $\mathcal{I}''_{[i+1]}$ . Further, we perform mutations with a certain probability on the individuals which avoids inbreeding and represents at the same time reintroduction of new or lost genetic information. We evaluate the free energy of all individuals of the new generation,  $\mathcal{G}_{[i+1]}$ , and denote the one with the highest fitness value by  $\mathcal{I}_{[i+1]}^{\star}$ . The sequence of  $\mathcal{I}_{[i]}^{\star}$  is recorded and the converged solution of the GA,  $\mathcal{I}^{\star}$ , is considered to be the individual among the  $\mathcal{I}_{[i]}^{\star}$  with the highest fitness value. The optimized solution to the problem is found by an additional hill-climbing optimization, starting from  $\mathcal{I}^{\star}$ , compensating thus for the limited accuracy in the encoding step. Further details are compiled in [2].

Applications of this nice tool outlined in the following demonstrate that GAs are indeed able to search in an unbiased and parameter-free way basically among *all* possible candidates for equilibrium structures, avoiding thus the risk of 'forgetting' a candidate lattice in the preselection process.

#### Examples

Liquid-solid transitions in soft matter systems – In typical soft matter systems the effective interparticle interactions are often bounded or weakly diverging at the origin, reflecting the fact that – as a consequence of their loose internal structure – the mesoscopic particles can overlap or even intertwine. This is in striking contrast to typical atomic (or hard) matter systems, where the interparticle interaction is characterized at short distances by a strong repulsion. Thus, as we investigate the solid phases in liquid-solid transitions in soft matter

systems we can no longer rely on the experience acquired for atomic systems (with the usual suspects of solid equilibrium structures, such as fcc, bcc, or hcp).

As an example we consider a system of (neutral) star polymers. The center of a star polymer particle is a colloidal particle to which f polymer chains are grafted [3]. In literature an (effective) interaction  $\Phi(r)$  has been derived between two such complex aggregates;  $\Phi(r)$ diverges logarithmically at short distances. For simplicity we look at the zero temperature phase diagram. In this case and since the effective interaction is athermal, the free energy is identical to the lattice sum L; for f = 64 it is depicted in Fig. 1. We observe that rather unconventional solid equilibrium structures are predicted by the GA, such as the trigonal, the diamond, or the hexagonal lattice; at higher densities (not displayed) the exotic A15 structure is predicted. In addition, the figure visualizes the risks of the conventional approach mentioned above: preselection – based on more or less plausible arguments – of a set of candidate structures bears the risk to exclude *a priori* lattices that turn out to be energetically more favourable than the preselected ones. We point out that also in other applications to liquid-solid transitions in soft matter systems GAs have proven to be a very useful and efficient tool [4,6].



Fig. 1: Dimensionless lattice,  $\beta L$ , for star polymers with functionality f = 64 as a function of the reduced density  $\rho^* = \rho \sigma^3$ , evaluated for the equilibrium structures found in the conventional approach [5] (red line) and for the equilibrium structures predicted by the GA (green line); at low and intermediate densities the two curves coincide within linethickness. The inset shows the difference in  $\beta L$  between the bco and the trigonal structure for  $1.3 \leq \rho^* \leq 2.2$ .

Minimum energy configurations of hard-core particles in two and three dimensions – Extension of the GA to colloidal systems with hard-core repulsion (as they are for instance encountered for polymethylmethacrylate – PMMA – particles in appropriate solvents [7]) is rather tricky. The key-problem is now to create individuals (i.e., candiates for equilibrium structures) in such a way that particle overlap is excluded right from the beginning. This problem has meanwhile been solved for the two-dimensional case. Application to a model system of hard-core particles of diameter  $\sigma$  that interact via an additional repulsive (square-)shoulder of range  $\sigma/2$  demonstrates that the variety of possible minimum energy configurations is much richer than the simple hexagonal lattice that one would intuitively expect. The examples shown in Fig. 2 give an idea about the rich wealth of two-dimensional non-simple lattices that are proposed by the GA as minimum energy configurations for this particular system.



Fig. 2: Minimum energy configurations of a two dimensional system of hard-core particles (of diameter  $\sigma$ ) that interact via a repulsive (square-)shoulder interaction of range  $\sigma/2$ . The following packing fractions  $\eta = \rho \sigma^2$  ( $\rho$  being the number density) have been investigated: 0.524 (top-left), 0.780 (top-right), 0.874 (bottom-left), and 1.024 (bottom-right). The dark particles form the (underlying) simple lattice, while the light particles represent the basis particles.

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#### 3.3.3 Ballistic quantum transport through nanostructures

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A major aim in ballistic transport theory is to simulate and to stimulate experiments in the field of phase-coherent electron conductance through nano-scaled semiconductor devices [1]. However, even for two-dimensional quantum dots ("quantum billiards") the numerical solution of the Schrödinger equation has remained a computational challenge. This is partly due to the fact that many of the most interesting phenomena occur in a parameter regime of either high magnetic field B or small de Broglie wavelength  $\lambda_D$ . Under the influence of a high magnetic field, one can study the Quantum Hall effect [1], de Haas-van Alphen oscillations [2], the "Hofstadter butterfly" [3] and electronic Mach-Zehnder interferometry [4]. In the regime of small  $\lambda_D$  the main interest is focused on the transition from quantum to classical dynamics [5,6] and related topics such as "quantum chaos" [7] and localization [8].



Fig. 1: (a) Illustration of the conventional tight-binding discretization employed in the *Recursive Green's Function Method* for transport through a circular quantum dot with infinite leads. Our modular approach as illustrated in (b) leads to increased efficiency in the numerical calculations.

However interesting they may be, these parameter ranges are difficult to handle from a computational point of view. This is because in the "semi-classical regime" of small  $\lambda_D$  as well as in the "quantum Hall regime" of high magnetic fields B, the proper description of the transport process requires a large number of basis functions. As a result, the theoretical models which are presently being employed eventually become computationally unfeasible or numerically instable.

At the Institute for Theoretical Physics an extension of the widely used *Recursive Green's Function Method* (RGM) [1] was developed which can bypass several of the limitations of conventional techniques. Key ingredient of this approach [9] is the decomposition of the scattering geometry into separable substructures ("modules") for which all the numerical procedures can be performed very effectively. All the modules are eventually connected with each other by

means of matrix Dyson equations such that they span the entire scattering region (see Fig. 1). In this way we reach a high degree of computational efficiency. Adapting our *Modular Recursive Green's Function Method* (MRGM) [9] to different scattering scenarios we are able to study a variety of different transport phenomena in previously unexplored parameter regimes. We highlight in the following three areas we focused on in 2005.

#### Andreev billiards

At a clean interface between a normal-conducting (N), ballistic quantum dot and a superconductor (S), phase coherent scattering of electrons into holes takes place. This phenomenon is known as Andreev reflection [10]. A N-S hybrid structure consisting of a superconducting lead attached to a normal ballistic cavity (see Fig. 2) is called an Andreev billiard [11]. Due to the peculiar properties of the N-S boundary, the hole is retroreflected into the direction the electron came from [see Fig. 2(a)]. As a consequence, the classical dynamics in these systems feature continuous families of periodic orbits, consisting of retracing electron-hole trajectories [see Fig. 2(b)].

Quantum mechanically the eigenstates of Andreev billiards are governed by the BogolioubovdeGennes equation, i.e. two coupled Schrödinger equations for electron and hole. If the classical picture of retracing electron-hole orbits holds, these electron and hole components should closely resemble each other: by comparing the eigenfunctions of electron and hole, one can thus directly assess the validity of the classical retracing picture.



Fig. 2: (a) Andreev reflection at a SN boundary (b) Retracing electron-hole trajectory in a normal-conducting (N) square billiard with a superconducting (S) lead attached ("Andreev billiard"). (c)-(e) Andreev eigenstates featuring different degrees of correspondence between electron (left column) and hole (right column) (see text)

Many wavefunctions feature indeed not only a close correspondence between electron and hole eigenstates, as expected by the classical retracing electron-hole orbits, but additionally pronounced density enhancements along the classical periodic orbits. These "superscars" are engraved in the quantum wavefunctions of Andreev states, as shown in Fig. 2(c) [12]. As the quantum mechanical nature of the underlying wave mechanics starts to emerge, discrepancies between electron and hole start to appear. We have identified three distinct mechanisms responsible for this breaking of particle-hole symmetry: i) resonant eigenstates of the normal conducting billiard [see Fig. 2(d)], ii) quantum diffraction at corners of the structure [see Fig. 2(e)] and iii) divergence of electron and hole path for long orbits [13]. Work on the time dependent evolution of wavepackets in Andreev billiards is in progress.

#### Noiseless scattering states in mesoscopic quantum dots

When one investigates a physical quantity fluctuating in time, noise is usually an unwanted feature. In transport through mesoscopic systems, however, the time-dependent noise of the electrical conductance carries important and interesting information [14].

At room temperature, thermal fluctuations are a strong source of noise, but even at zero temperature, some noise remains. This residual noise, the *quantum shot noise*, is due to the fact that charge is transmitted in portions of single electrons, and not as a continuous fluid-like current. Consider a wavepacket being split up into a transmitted and a reflected part at a barrier: Even if the wavepacket is always prepared in exactly the same initial quantum state, it will sometimes be measured as a transmitted particle and sometimes as a reflected particle. This leads to noise in the conductance which cannot be explained classically.

If the quantum dot supports one open quantum channel, the quantum shot noise is proportional to T(1-T), where T is the transmission probability. A classical particle always has transmission probability of either 0 or 1, and therefore classical transport is noiseless.

Inspired by recent experiments [15], we numerically study the crossover from stochastic quantum transport to deterministic classical transport in mesoscopic systems. We consider quantum dots with tunable openings, which allow us to control the dwell time of the electron. Inside the quantum dot, we add a random disorder potential of tunable strength and short correlation length. That way, we can observe two independent sources of quantum shot noise.

If we switch off the disorder completely, we find two different classes of transmission eigenstates: States which closely correspond to very short classical trajectories may travel through the quantum dot without being split up into a transmitted and a reflected part and therefore lead to transmission probabilities close to 0 or 1 (*noiseless scattering states*). Other states spread across the whole cavity and may yield any transmission probability between 0 and 1. In the classical limit, all transmitted states are noiseless scattering states.

The number of noiseless scattering states is governed by the weight of short classical trajectories in phase space. In the case of large shutter openings (short dwell times), noiseless scattering states play a dominant role (see Fig. 3c). As we reduce the size of the shutter openings, electron transport becomes more and more stochastic, until all noiseless scattering states are destroyed.

In the presence of a disorder potential the number of noiseless scattering states is drastically reduced (Fig. 3d), even if the disorder potential is very weak (much smaller than the Fermi energy).

These results demonstrate that noise and the statistics of transmission probabilities reflect the deterministic (classical) or stochastic (quantum) nature of electron transport. Furthermore, it allows us to distinguish between diffraction at the lead openings and diffraction at the disorder.



Fig. 3: (a) Rectangular quantum dot with tunable shutter openings and tunable bulk disorder. (b) Experimental setup [15] (c) Noiseless scattering states (transmission probability T > 0.999) as a function of the shutter opening width. For smaller shutter openings, the ratio of noiseless states decreases gradually. (d) Noiseless states as a function of strength of the disorder potential (For technical details see [16]).

#### Nanowires with surface disorder

In most materials, the conductance (or lack of it) is governed by disorder. For example, the strength and distribution of disorder determine whether a wire behaves like a "normal" wire, where the conductance decreases inversely with length, or like an insulator, where conductance is exponentially suppressed with length [1]. With modern semiconductor technology, materials with almost vanishing *bulk* disorder, such as disorder from crystal defects or impurities, can be fabricated. In this case, it is possible to create two-dimensional structures, called nanowires, with conductance properties that are governed by the *surface* disorder, instead. We have studied a special case of such a nanowire, the nanowire with one-sided surface disorder in a magnetic field (see Fig. 4, inset) [17,18].

As the classical dynamics in our system are determined only by the cyclotron radius (the radius of curvature of the electron paths), we can investigate the quantum-to-classical crossover in our (fully quantal) simulation by increasing the Fermi wavenumber  $k_{\rm F}$  (corresponding to energy) while keeping the cyclotron radius constant. We were able to show both numerically and analytically that the localization length increases exponentially with the Fermi wavenum-



Fig. 4: Localization length  $\xi$  for a wire with surface roughness vs  $k_{\rm F}W/\pi$ . Results are compared for wires with (i) one-sided disorder (OSD) with  $B \neq 0$  ( $\blacksquare$ ), (ii) OSD with B = 0 ( $\bullet$ ), and (iii) two-sided disorder with  $B \neq 0$  ( $\blacktriangle$ ). In (i) an exponential increase of  $\xi$  is observed in excellent agreement with Eq. (1) which has no adjustable parameters (dashed line).

ber, as shown in Fig. 4 [18]. We derived a simple analytical result for the localization length  $\xi$ ,

$$\xi(k_{\rm F}) \approx \left(a \, k_{\rm F}^{2/3} - b\right) \exp\left(c \, k_{\rm F} (1 - d \, k_{\rm F}^{-2/3})^{3/2}\right) \,, \tag{1}$$

where a, b, c, and d are system-dependent constants. Comparing Eq. 1 with the numerical result obtained with the MRGM in Fig. 4, we find excellent agreement. We stress that no adjustable parameters are involved. The observed exponential increase can be understood by studying the classical dynamics in our system: Without a magnetic field, all trajectories are eventually scattered off the disordered surface of the wire. But when turning on a magnetic field perpendicular to the 2D-structure, so-called "skipping" orbits appear. Such orbits do not reach the disordered surface but skip along the flat lower boundary wall without suffering any scattering (sketched in Fig. 4, inset). In terms of phase space, this leads to the emergence of a regular island. Around this regular island there is a chaotic sea, containing those trajectories that still reach the disordered surface. Our system thus has an overall mixed regular-chaotic phase space structure (see Fig. 5b).

In a classical description, the "localization length" of a wire with one-sided surface disorder would be infinite, as no scattering with the disordered surface ever occurs for skipping orbits. Quantum mechanically, a small but non-negligible part of the electron wave function extends through the classical barrier between the regular island and the chaotic sea. This process is called *tunneling*, more specifically "dynamical tunneling" when it occurs through a barrier in phase space.

The quantum phase space distributions (so called Poincaré-Husimi functions) for different transmission modes (e.g. within Fig. 5c) show that quantum mechanical tunneling can occur. Effectively, the modes in the regular island do interact with the disordered surface because of tunneling. For very long wires, this ultimately leads to localization and insulating behaviour even though the localization is suppressed exponentially with increasing Fermi wavelength.



Fig. 5: (a) Nanowire with the regular transverse modes (green) m = 4, 3, 2, 1 for  $k_F W/\pi = 14.6$ . The gray shaded part indicates the spatial region affected by disorder. (b) Poincaré surface of section of phase space showing a large regular island with outermost torus (dashed), a chaotic sea (blue dots) and quantized tori corresponding to the regular modes (green). (c) Poincaré–Husimi functions of these modes and their quantizing tori, i.e. the classical trajectories corresponding to these quantum waves.

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#### 3.3.4 Interaction of slow highly charged ions with solid surfaces

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External: Karoly Tőkési (ATOMKI, Debrecen, Hungary), Maite Alducin, Andres Arnau, Inaki Juaristi (DIPC and Univ. of the Basque Country, San Sebastian, Spain)

The current theoretical understanding of the neutralization sequence of highly charged ions interacting with solid surfaces is based on the classical over-the-barrier (COB) model developed by Burgdörfer and coworkers [1] and has been confirmed by many experimental findings since (e.g. [2, 3]). The scenario of the interaction sequence is depicted in Fig. 1: At large distances from the surface, the ion is attracted towards the surface by its own image charge. Starting from a critical distance  $d_c$  target electrons are captured by the projectile into highly excited projectile states which subsequently decay by Auger processes leading to electron emission or radiative deexcitation. Additional electrons are emitted by an upward shift of the energy levels upon approach of the projectile to the surface and by kinetic electron emission, the transfer of momentum to target electrons in binary encounter events with the projectile.

We have recently extended this description to include spin-dependent interactions of ions with magnetized and paramagnetic surfaces and for transmission of highly charged ions through insulating capillaries.

#### Electron emission from magnetized surfaces

When highly charged ions interact with magnetized surfaces, electrons transferred from the target to the projectile and emitted in a later stage of the neutralization will mirror the target polarization. This effect can be studied in two different ways: One can either look at the polarization of emitted electrons P defined by

$$P = \frac{N_{\uparrow} - N_{\downarrow}}{N_{\uparrow} + N_{\downarrow}},\tag{1}$$

with  $N_{\uparrow}$  and  $N_{\downarrow}$  being the number of electrons emitted with spin orientation parallel and antiparallel to the majority-spin direction as a function of their emission energy [5] or measure the relative importance of multiplet emission lines in the electron spectrum [6].



Fig. 1: Interaction of highly charged ions with surfaces: schematic picture of imagecharge acceleration (left), creation and deexcitation of so-called "hollow atoms", and neutralization upon scattering at the surface (from [4]).

We have performed Monte-Carlo simulations based on the COB model accounting for the spin dependence of electron-transfer and deexcitation channels. In addition to the original COB model which includes only resonant over-barrier electron transfer to the projectile, we also account for side feeding from target core states to inner levels of the projectile as well as Auger deexcitation and Auger neutralization processes.

Different sources contributing to different regions of the emission spectrum can be readily identified: electrons are emitted either by potential emission (potential energy of the projectile is converted in kinetic energy of the emitted electron) or by kinetic emission (momentum transfer to a conduction band electron in a binary collision with the projectile). The latter process will produce electrons with energies less than 60 eV. Electrons reaching the detector with energies between 100 and 300 eV were originally emitted towards the surface, have undergone multiple elastic and inelastic scattering processes in the target material, and have eventually escaped the surface. Potential-energy driven processes, in particular KLL Auger decay, dominate the spectrum at electron energies above 300 eV. Experimental data and COB model can be compared directly in this energy regime (see Fig. 2).

#### Electron emission from paramagnetic surfaces

The energy-dependent spin-polarization of the emitted electrons has been recently measured for 10-500 eV He<sup>+</sup> projectiles on Al(001), Au(001) and Cu(001) [7, 8]. At first glance surprisingly, even for paramagnetic target surfaces a nonzero spin-polarization of the emitted electrons can be observed. Analysis of the polarization of emitted electrons provides information on the electronic properties of the surface as well as on the local magnetization induced in the target by the projectile. For these paramagnetic surfaces, an average polarization of emitted electrons of around 30% was found, always parallel to the spin orientation of the electron bound to the incoming He<sup>+</sup> ion. Larger values of the polarization were measured at higher emission energies.

We have performed simulations for the neutralization of He<sup>+</sup> ions in paramagnetic materials (e.g. [9] and references therein). Spin-dependent Auger neutralization rates give an estimate for the spin orientation of electrons emitted in the neutralization process. These Auger electrons



Fig. 2: Polarization of emitted electrons a) and electron emission spectrum b) for emission energies  $E_{e^-} > 100$  eV. Full and open symbols in a) denote experimental and simulated data, respectively.

interact with the paramagnetic target surface and generate secondary electrons. The measured polarization is therefore a superposition of the original electron emission spectrum and the secondary electron spectrum which is unpolarized. The relative weight of the two spectra at different emission energies determines the measured polarization (see Fig. 3 for a comparison of experimental and simulated polarization for polarized He<sup>+</sup> atoms interacting with an Al surface).

#### Transmission of highly charged ions through insulating capillaries

The interaction of highly charged ions with insulator surfaces adds another aspect to the interaction sequence depicted in Fig. 4: if the surface is charged up due to the impact of projectiles in an earlier stage of the experiment, ions are deflected before electron transfer from the target can take place. This effect is exploited experimentally to guide highly charged ions through insulating microcapillaries.

Based on experimental data and our simulations [10] the following picture of the interaction process has emerged (see Fig. 4): Parts of the incoming ion beam  $(j_{in})$  hit the inner wall of the insulating material at the beginning of an experiment depositing charge on the capillary surface. Charges diffuse along the surface  $(j_{surf})$ , eventually reaching the grounded metallic layer on the front side of the foil; a thin coating of metal on the front and back side of the foil is necessary to avoid a global charge-up of the insulator foil during the experiment). Due to the small but finite bulk conductivity of the insulator, charges also diffuse into the bulk  $(j_{bulk})$ . The interplay between surface and bulk diffusion leads to the establishment of a dynamic equilibrium of a self-organized charge patch close to the entrance of the capillary and eventually to transmission  $(j_{tr})$ . It is important to note that our model does not contain any freely adjustable parameters. They can be deduced - at least in their order of magnitude - from material data of PET [11].



Fig. 3: Spin polarization of the integrated electron spectrum including all electrons emitted from Al with energy larger than E. Experimental data (open and closed symbols) from [8]. Typical error bars are included for selected data points.



Fig. 4: Possible pathways for charges entering the capillary  $(j_{in})$ . They can either be transmitted  $(j_{tr})$  or deposited on the surface from where they diffuse into the bulk  $(j_{bulk})$  or are partly transported on the surface to the gold layer  $(j_{surf})$  covering the front and back side of the foil.

Invoking this scenario we were able to reproduce a wide range of experimental findings, e.g., ion guiding even for large angles of incidence [12], the temporal decrease of transmission during beam-off times, and a relatively large angular spread of the transmitted beam [10].

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# Appendix A

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## Appendix B

## **External Speakers and Visitors**

- Ewald Balcar Institute for Atomic Physics, VUT Vienna, Austria RXS and the magic of nj-symbols, 18.10.2005
- Victor Batyrev Mathematical Institute, University of Tübingen Tübingen, Germany, 2.10.2005 - 9.10.2005 and 4.12.2005 - 11.12.2005
- Arnd Bäcker Institute for Theoretical Physics, University of Dresden Dresden, Germany, 9.02.2005 - 18.02.2005 *Chaos and order in quantum mechanics*, 10.02.2005
- Carlo Beenakker Lorentz Institute for Mesoscopic Physics, University of Leiden Leiden, The Netherlands Quantum shot noise, 17.01.2005
- Cristian Calude University of Auckland Auckland, New Zealand, 1.10.2005 - 10.10.2005
- Jozsef Cserti Eötvös University Budapest, Hungary, 7.02.2005 - 15.02.2005
   Electronic properties of Rashba billiards, 11.02.2005
- Alan Denton Department of Physics, North Dakota State University Fargo, USA, 11.06.2005 - 16.06.2005 Phase separation in suspensions of like-charged colloids
- Robert Evans H.H. Wills Physics Laboratory, University of Bristol, Bristol, UK, 17.11.2005 - 19.11.2005

- S.J. Gates jr. University of Maryland College Park, USA From 1D SUSY theory toward graphs and K-theory, 15.03.2005
- Daniel Greenberger The City University of New York (CUNY) New York, USA, 1.05.2005 - 10.05.2005
- Daniel Grumiller Institute for Theoretical Physics, University of Leipzig Leipzig, Germany An action for the exact string black hole: thermodynamic consequences, 22.06.2005
- H.H. von Grünberg Institute for Chemistry, Karl Franzens-University Graz Graz, Austria Hard physics of soft matter, 17.01.2005
- Roman Jackiw Massachusetts Institute of Technology Cambridge, USA, 26.01.2005 - 30.01.2005 *Elaborations on 2d gravity*, 28.01.2005
- Jan Jirsak
   E. Hala Laboratory of Thermodynamics, Academy of Sciences, Prague, Czech Republic, 13.12.2005 - 17.12.2005
   Thermodynamic properties of water
- Gerry McKeon Department of Applied Mathematics, University of Western Ontario London, Canada, 16.05.2005 - 24.05.2005
- Christos N. Likos Institute for Theoretical Physics II, Heinrich-Heine University Düsseldorf, Germany, 18.06.2005 - 24.06.2005 and 1.08.2005 - 6.08.2005
- René Meyer University of Leipzig Leipzig, Germany.
   Integrating out geometry in 2D dilaton gravity coupled to fermion, 27.10.2005
- Filip Moucka E. Hala Laboratory of Thermodynamics, Academy of Sciences Prague, Czech Republic, 13.12.2005 - 17.12.2005 Quantitative characterization of structural changes in the hard-disk fluid near freezing/melting conditions
- Michaela Oswald Department of Physics, University of Virginia Charlottesville, USA, 3.01.2005 - 14.01.2005

- Carlo Rubbia ENEA Frascati (Roma), Italy, 27.1.2005 bis 29.1.2005 The quest for the dark matter, 28.01.2005
- Peter van Nieuwenhuizen State University of New York, Stony Brook New York, USA The geometry of ordinary and harmonic superspace I, 10.01.2005
- Peter van Nieuwenhuizen State University of New York, Stony Brook New York, USA The geometry of ordinary and harmonic superspace II, 14.01.2005
- Peter van Nieuwenhuizen State University New York, Stony Brook New York, USA Supergravity as a gauge theory, 28.01.2005
- Francesco Sciortino Dipartimento di Fisica, Università di Roma "La Sapienza" Rome, Italy, 08.10.2005 - 12.10.2005 Mechanisms of dynamic arrest at low packing fraction: Cluster phases, gels, and Yukawa glasses in charged colloid-polymer mixtures
- Andrey Soldatov
   Steklov Mathematical Institute, Academy of Science of Russia Moscow, Russia, 27.07.2005 - 3.11.2005
- Michael Strickland Institute of Physics, University of Helsinki Helsinki, Finland, 2.05.2005 - 15.05.2005 and 9.08.2005 - 16.08.2005
- Josef Tkadlec Technical University Prague, Prague, Czech Republic, 14.06.2005 - 30.06.2005
- Dmitri Vassilevich Institute for Theoretical Physics, University of Leipzig Leipzig, Germany, 7.10.2005 - 14.10.2005
- Qun Wang Institute for Theoretical Physics, University of Frankfurt Frankfurt/Main, Germany, 5.05.2005 - 7.05.2005 Quark matter - the condensed matter physics of QCD, 06.05.2005
- Jean-Jacques Weis & Jean-Michel Caillol Laboratoire de Physique Théorique, Université Paris-Sud, Orsay, Paris, 19.11.2005 - 24.11.2005

- Frederik Witt Mathematical Institute, FU Berlin Berlin, Germany Generalized geometries and superstring theory of type II B, 13.09.2005
- Xu Hong Laboratoire de Physique des Milieux Denses, Université de Metz Metz, France, 14.04.2005 - 21.04.2005 Brownian dynamics simulations of wormlike micelles

 Anatoly Zagorodny Bogoliubov Institute for Theoretical Physics, National Academy of Sciences of Ukraine Kiew, Ukraine, 18.08.2005 - 19.08.2005
 Effective interactions in dusted plasmas: kinetic description and numerical simulation, 18.08.2005

## Appendix C

## Publications

### C.1 Articles in refereed journals

- F. Aigner, S. Rotter, J. Burgdörfer Shot noise in the chaotic-to-regular crossover regime Physical Review Letters, 94 (2005), 21680-1 - 21680-4.
- J. O. Andersen, M. Strickland *Three-loop Phi-derivable approximation in QED* Physical Review D, 71 (2005), 025011-1 - 025011-11.
- M. Attems, D. Blaschke, M. Ortner, M Weiretmayr, M. Schweda Gauge independence of IR singularities in non-commutative QFT - and interpolating gauges
   J. High Energy Phys., 07 (2005), 071; S. 1 - 9.
- I.F. Barna Coherent control calculations for helium atom in short and intensive XUV laser pulses Eur. Phys. J. D, 33 (2005), 307 - 311.
- I.F. Barna, A.C. Gagyi-Pálffy, L. Gulyás, K. Tökési, J. Burgdörfer Singly differential electron emission cross sections for ionization of helium by protons
   Nuclear Instruments and Methods in Physics Research B, 233 (2005), 176 - 181.
- I.F. Barna, K. Tökési, J. Burgdörfer Single and double ionization of helium in heavy-ion impact J. Phys. B: At. Mol. Opt. Phys., 38 (2005), 1001 - 1013.
- L. Bergamin Generalized complex geometry and the Poisson sigma model Modern Physics Letters A, 20 (2005), 13; 2 - 4.
- L. Bergamin, D. Grumiller, W. Kummer, D. Vassilevich *Classical and quantum integrability of 2D dilaton gravities in Euclidean space* Class. Quant. Grav., 22 (2005), 1361 - 1381.

- L. Bergamin, W. Kummer Two-dimensional N=(2,2) dilaton supergravity from graded Poisson-Sigma models I: complete actions and their symmetries Eur. Phys. J. C, 39 (2005), s1.41 - s1.52.
- L. Bergamin, W. Kummer Two-dimensional N=(2,2) dilaton supergravity from graded Poisson-Sigma models II: Analytic solution and BPS states Eur. Phys. J. C, 39 (2005), s1.53 - s1.63.
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## C.2 Articles in conference proceedings

 E. Benes, M. Gröschl, S. Radel, C. Hauser, H. Böhm, H. Nowotny, New simple mathematical model for the separation performance of ultrasonic cell filters in: "Proc. 2nd Congress of Alps-Adria Acoustics Association and 1st Congress of Acoustical Society of Croatia", Acoustical Society of Croatia, Zagreb/Croatia, 2005, ISBN 953-95097-0-X, 14 - 17.

### • S. Filipp, K. Svozil

Tracing the bounds on Bell-type inequalities in: "Foundations of probability and physics - 3", A. Khrennikov (ed.); American Institute of Physics, Melville, New York, 2005, ISBN: 0-7354-0235-3, S. 87 - 94.

### • A. Gerhold

Two aspects of color superconductivity: gauge independence and neutrality in: "Strong and electroweak matter 2004", K. J. Eskola, K. Kainulainen, K. Kajantie, K. Rummukainen (eds.); World Scientific, Singapore, 2005, ISBN: 981-256-135-8, 351 -355.

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Anomalous specific heat in ultradegenerate QED and QCD in: "Strong and electroweak matter 2004", K. J. Eskola, K. Kainulainen, K. Kajantie, K. Rummukainen (eds.); World Scientific, Singapore, 2005, ISBN: 981-256-135-8, 411 -415.

• D.M. Greenberger, K. Svozil

Quantum Theory Looks at Time Travel,

in "Quo Vadis Quantum Mechanics?", A. Elitzur, S. Dolev and N. Kolenda (eds.); Springer Verlag, Berlin, 2005, ISBN: 354-022-188-3, 63 - 72.

• A. Ipp

Thermodynamics of deconfined QCD at small and large chemical potential

in: "Strong and electroweak matter 2004", K. J. Eskola, K. Kainulainen, K. Kajantie, K. Rummukainen (eds.); World Scientific, Singapore, 2005, ISBN: 981-256-135-8, 256 - 260.

• U. Reinosa

Renormalization and gauge symmetry for 2PI effective actions

in: "Strong and electroweak matter 2004", K. J. Eskola, K. Kainulainen, K. Kajantie, K. Rummukainen (eds.); World Scientific, Singapore, 2005, ISBN: 981-256-135-8, 316 - 320.

• P. Romatschke, M. Strickland

Progress in anisotropic plasma physics

in: "Strong and electroweak matter 2004", K. J. Eskola, K. Kainulainen, K. Kajantie, K. Rummukainen (eds.); World Scientific, Singapore, 2005, ISBN: 981-256-135-8, 167 - 176.
• K. Svozil

On counterfactuals and contextuality

in: "Foundations of probability and physics - 3", A. Khrennikov (ed.); American Institute of Physics, Melville, New York, 2005, ISBN: 0-7354-0235-3, 351 - 360.

• P. Zeiner

Remarks on CSLs for cubic and hypercubic lattices

in: "Group Theoretical Methods in Physics, Proceedings of the XXV Intern. Colloquium on Group Theoretical Methods in Physics", G.S. Pogosyan, L.E. Vicent, K.B. Wolf (eds.); Institute of Physics; Institute of Physics Publishing, Bristol and Philadelphia, 2005, ISBN 0-7503-1008-1, 569 - 573.

## C.3 Invited talks

• J. Burgdörfer

Attosecond electronic dynamics in atoms Conference on Laser, Electrooptics and Quantum Electronics (CLEO Europe-EQEC 2005), International Congress Centre Munich, Germany; 12.06.2005 - 17.06.2005.

• J. Burgdörfer

Attosecond-time resolved Fano resonances High-Field Attosecond Physics Workshop of the Heraeus Foundation, Obergurgl, Austria; 09.01.2005 - 15.01.2005.

• J. Burgdörfer

Attosecond-time resolved Fano resonances Workshop on Attosecond Science, Cambridge, MA, USA; 02.05.2005 - 04.05.2005.

• J. Burgdörfer

Interaction of ultrashort pulses with matter: light-phase-sensitive photoemission and streaking

International Seminar on Atomic Processes, Shonan Village Center Zushi, Japan; 20.01.2005 - 23.01.2005.

• J. Burgdörfer

Ion-surface collisions 24th International Conference on Photonic, Electronic and Atomic Collisions (XXIV ICPEAC), Rosario, Argentina; 21.07.2005 - 27.07.2005.

• M. Kreuzer

String, branes and dualities

Lectures at Fundamental Problems in Modern Quantum Theories und Experiments, Sevastopol, Ukrain; 17.09.2005 - 21.09.2005.

• M. Kreuzer

Toric geometry, complete intersections and fundamental groups Math and Physics Colloquium, Penn State University, USA; 08.04.2005.

• C. Lemell

Interaction of slow multicharged ions with surfaces: Status of theoretical and experimental understanding Conference on Elementary Processes in Atomic Systems (CEPAS), Miskolc, Hungary; 01.09.2005.

• C. Lemell

Simulations on ion-surface interactions Joint EU-Collaboration Meeting, Munich, Germany; 27.05.2005.

- E. Persson, M. Lezius, K.-M. Schiessl, A. Scrinzi, X.-M. Tong, V.S. Yakovlev, J. Burgdörfer *Towards attosecond half-cycle pulses* Intense Laser-Matter Interaction and Pulse Propagation, MPI, Dresden, Germany; 01.08.2005 - 24.08.2005.
- A. Rebhan

Analytical approaches to the thermodynamics of deconfined quark-gluon matter Ohio Center for Theoretical Science Workshop: Effective Field Theories in Physics -From Nano to Tera, Columbus, Ohio; 17.06.2005.

• A. Rebhan

Thermodynamics of QCD at large quark chemical potential 29th Johns Hopkins Workshop in Theoretical Physics: "Strong Matter in the Heavens", Budapest, Hungary; 01.08.2005.

• K. Svozil

Quantum logic and related probabilistic aspects: A brief introduction to quantum logic 4th International Summerschool on Philosophy, Probability and Physics, Konstanz, Germany; 07.08.2005 - 13.08.2005.

• K. Svozil

Some remarks on quantum contextuality and quantum computing Special Workshop "What is Quantum in Quantum Computing", University of Konstanz, Konstanz, Germany; 19.05.2005.

### C.4 Contributed presentations

• F. Aigner, S. Rotter, J. Burgdörfer *Chaotic-to-regular crossover of shot noise in mesoscopic conductors* Dynamics Days 2005, Berlin, Germany; 25.07.2005 • D. Arbó

Ionization by short-laser pulses: Interference phenomena Int. Seminar on Intense Laser-Matter Interaction and Pulse Propagation, Dresden, Germany; 01.08.2005 - 24.08.2005

- D. Arbó, S. Yoshida, E. Persson, K. Dimitriou, J. Burgdörfer Ionization by short-laser pulses: complex low-energy structures 24th Int. Conf. on Photonic, Electronic and Atomic Collisions (XXIV ICPEAC), Rosario, Argentina; 20.07.2005 - 26.07.2005
- D. Arbó, S. Yoshida, E. Persson, K. Dimitriou, J. Burgdörfer Single ionization of atoms in the tunneling regime: Interference phenomena Intern. Workshop on Intense Laser-Matter Interaction and Pulse Propagation, Dresden, Germany; 15.08.2005 - 19.08.2005
- F. Aumayr, M. Fürsatz, S. Pleschko, I. Gebeshuber, HP. Winter, C. Lemell, N. Stolterfoht 2-D scattering distribution of multiply charged ions guided through nano-capillaries 24th Int. Conf. on Photonic, Electronic and Atomic Collisions (XXIV ICPEAC), Rosario, Argentina; 22.07.2005
- I.F. Barna, K. Tökési, L. Gulyás, J. Burgdörfer *Angular differential double ionization cross sections for anti Proton-Helium collisions*  24th Int. Conf. on Photonic, Electronic and Atomic Collisions (XXIV ICPEAC), Rosario, Argentina; 21.07.2005 - 27.07.2005
- L. Bergamin Dimensional reduction of Chern-Simons (super-)gravity XVII Workshop: Beyond the Standard Model, Bad Honnef, Germany; 14.03.2005
- L. Bergamin Global aspects of Chern-Simons supergravity and its kink
  8th European Meeting: from the Planck Scale to the Electroweak Scale, ICTP Triest, Italy; 27.05.2005
- C. Deiss, N. Rohringer, E. Lamour, C. Prigent, J. Rozet, D. Vernhet, J. Burgdörfer *Laser-cluster interaction: The role of electron-ion collision in the production of hot electrons* 24th Int. Conf. on Photonic, Electronic and Atomic Collisions (XXIV ICPEAC), Rosario, Argentina; 22.07.2005
- M.-J. Fernaud, G. Kahl, R. Roth A hard-sphere fluid exposed to the external field of two impenetrable spheres 6th Liquid Matter Conference 2005, Utrecht, Netherlands; 02.07.2005 - 06.07.2005

- S. Filipp, K. Svozil Analytic quantum bounds on bell inequalities Quantum Physics of Nature Conference, University of Vienna, Vienna, Austria; 23.05.2005
- D. Gottwald, G. Kahl, C.N. Likos Genetic algorithms - a powerful and efficient tool to predict equilibrium structures in freezing transitions
  6th Liquid Matter Conference 2005, Utrecht, The Netherlands; 02.07.2005 - 06.07.2006.
- D. Gottwald, C.N. Likos, G. Kahl Ordering of soft particles in quasi-two-dimensional geometries 6th Liquid Matter Conference 2005, Utrecht, The Netherlands; 02.07.2005 - 06.07.2005
- D. Gottwald, C.N. Likos, G. Kahl, H. Löwen Structure and phase behavior of ionic microgels 6th Liquid Matter Conference 2005, Utrecht, The Netherlands; 02.07.2005 - 06.07.2005
- M. Hörndl, S. Yoshida, A. Wolf, J. Burgdörfer Enhancement of low energy electron-ion recombination in a magnetic field: influence of transient field effects
  24th Int. Conf. on Photonic, Electronic and Atomic Collisions (XXIV ICPEAC), Rosario, Argentina; 21.07.2005 - 27.07.2005
- Yu.V. Kalyuzhnyi, G. Kahl, S.P. Hlushak, P.T. Cummings Liquid-gas phase coexistence in polydisperse liquid mixtures: application of the MSA 29th International Conference on Solution Chemistry, Portoroz, Slovenia; 21.08.2005 - 25.08.2005
- M. Kreuzer Statistics of toric Calabi-Yau fourfolds Strings05, Toronto, Canada; 11.07.2005 - 16.07.2005
- B.M. Mladek, D. Gottwald, G. Kahl, M. Neumann, C.N. Likos Evidence for clustering transitions in soft matter
   6th Liquid Matter Conference 2005, Utrecht, The Netherlands; 02.07.2005 - 06.07.2005
- B.M. Mladek, G. Kahl, G. Neumann Thermodynamically self consistent liquid state theories for the Gaussian core model 6th Liquid Matter Conference 2005, Utrecht, The Netherlands; 02.07.2005 - 06.07.2005

- M. Nigsch *Time-dependent scattering by arrays of elliptic cylinders*  Waves 2005, Providence, Rhode Island, USA; 21.06.2005
- G. Pauschenwein, E. Schöll-Paschinger, D. Levesque, J.-J. Weis, G. Kahl A thermodynamically self-consistent liquid state theory for the restricted primitive model of electrolytes
  6th Liquid Matter Conference 2005, Utrecht, The Netherlands; 02.07.2005 - 06.07.2005
- E. Persson, M. Lezius, K.-M. Schiessl, A. Scrinzi, X.-M. Tong, V.S. Yakovlev, J. Burgdörfer *Towards attosecond half-cycle pulses* Intense Laser-Matter Interaction and Pulse Propagation, MPI, Dresden, Germany; 01.08.2005 - 24.08.2005
- S. Pleschko, M. Fürsatz, I. Gebeshuber, HP. Winter, C. Lemell, N. Stolterfoht, F. Aumayr
   2-D scattering distribution of multiply charged ions guided through nano-capillaries
   348. WE-Heraeus-Seminar, Bad Honnef, Germany; 21.06.2005
- C.O. Reinhold, J. Burgdörfer, F.B. Dunning *Collisional decoherence of Rydberg wavepackets*  24th Int. Conf. on Photonic, Electronic and Atomic Collisions (XXIV ICPEAC), Rosario, Argentina; 21.07.2005 - 27.07.2005
- S. Rotter, B. Weingartner, F. Libisch, F. Aigner, J. Feist, J. Burgdörfer
   A modular method for the efficient calculation of ballistic transport through quantum billiards
   Large Scale Scientific Computing, Sozopol, Bulgaria; 07.06.2005
- A. Reiner, J.S. Hoye First steps towads a unification of HRT and SCOZA 6th Liquid Matter Conference, 2.07.2005 - 6.07.2005
- K.-M. Schiessl, C. Lemell, K. Töksi, J. Burgdörfer Simulation of guiding of highly charged projectiles through insulating nanocapillaries 24th Int. Conf. on Photonic, Electronic and Atomic Collisions (XXIV ICPEAC), Rosario, Argentina; 21.07.2005 - 27.07.2005

- K.-M. Schiessl, E. Persson, A. Scrinzi, Y. Yakovlev, J. Burgdörfer Enhancement of high harmonic generation by resonant two-color fields: propagation effects
   Workshop on Laser Matter Interaction and Pulse Propagation Dresden, Germany, 01.08.2005 - 24.08.2005
- M. Seliger, C.O. Reinhold, T. Minami, D.R. Schultz, S. Yoshida, J. Burgdörfer, E. Lamour, J. Rozet, D. Vernhet *Production and transport of electronic states in fast ions penetrating solids* 24th Int. Conf. on Photonic, Electronic and Atomic Collisions (XXIV ICPEAC), Rosario, Argentina; 21.07.2005 - 27.07.2005
- M. Seliger, C.O. Reinhold, T. Minami, J.Burgdörfer Open quantum system approach to coherence in ion-solid transport Workshop on Quantum Information, Max-Planck-Institut für Physik komplexer Systeme, Dresden, Germany; 26.09.2005 - 30.09.2005
- B. Solleder, C. Lemell, K. Tökési, J. Burgdörfer *Electron emission from a magnetized Fe surface under impact of N*<sup>6+</sup> ions 24th Int. Conf. on Photonic, Electronic and Atomic Collisions (XXIV ICPEAC), Rosario, Argentina; 21.07.2005 - 27.07.2005
- K. Svozil Is quantum contextuality a red herring?
  6th European QIPC Workshop, University of Vienna, Vienna, Austria; 22.05.2005
- K. Svozil

Quantum computation by state identification Conference on Quantum Theory: Reconsideration of Foundations-3, Vaxjö, Sweden; 06.06.2005 - 11.06.2005

- W. Zhao, J.J. Mestayer, J. Lancaster, F.B. Dunning, S. Yoshida, C.O. Reinhold, J. Burgdörfer *Engineering Rydberg atom wavefunctions* 24th Int. Conf. on Photonic, Electronic and Atomic Collisions (XXIV ICPEAC), Rosario, Argentina; 21.07.2005 - 27.07.2005
- W. Zhao, J.J. Mestayer, J. Lancaster, F.B. Dunning, S. Yoshida, C.O. Reinhold, J. Burgdörfer *Exploring the ultra-fast ultra-intense regime at nanosecond timescales* using very-high-n Rydberg atoms
  24th Int. Conf. on Photonic, Electronic and Atomic Collisions (XXIV ICPEAC), Rosario, Argentina; 21.07.2005 - 27.07.2005

## C.5 Talks at other institutions

• D. Arbó

Electron distribution in ionization of atoms by short and strong laser pulses Max-Planck-Institut für Kernphysik, Heidelberg, Germany; 09.11.2005

• H. Balasin

Beyond the singularity curvature structure of the extended Schwarzschild geometry Institute for Theoretical Physics, University of Leipzig, Leipzig, Germany; 06.12.2005

- L. Bergamin 2D dilaton supergravity as a graded Poisson-Sigma model University of Hannover, Hannover, Germany; 22.03.2005
- C.G. Böhmer Static perfect fluid spheres with cosmological constant Hungarian Academy of Sciences (RMKI) Budapest, Hungary; 17.03.2005
- J. Feist *Transport through nano-wires with surface disorder* TU Dresden, Dresden, Germany; 21.06.2005
- P. Fischer *Quantum gravity in extra dimensions*  University of Bielefeld, Bielefeld, Germany; 20.04.2005
- P. Fischer *Quantum gravity in extra dimensions* University of Geneva, Geneva, Switzerland; 11.03.2005
- M. Hörndl

Classical Dynamics of Low Energy Electron-Ion Recombination in Storage Rings Max-Planck-Institutt für Kernphysik, Heidelberg, Germany; 20.10.2005

• G. Kahl

Genetic algorithms - an attractive tool in soft condensed matter theory Laboratoire de Physique des Milieux Denses, Université de Metz, Metz, France; 14.02.2005 - 18.02.2005

- M. Kreuzer Geometry and string theory University of Hannover, Hannover, Germany; 24.05.2005
- M. Kreuzer *Toric geometry and Calabi-Yau compactification* Bogoliubov Institute for Theoretical Physics, Kyiv, Ukraine; 16.09.2005
- W. Kummer *Progress and problems in quantum gravity* Bogoliubov Institute, Academy of Sciences of Ukraine, Kyiv, Ukraine; 16.09.2005
- B.M. Mladek Formation of clustered crystals in soft matter in the absence of attractive forces AMOLF 2005, Amsterdam, The Netherlands; 11.10.2005
- A. Rebhan Quark-gluon-plasma instabilities in the hard-loop approximation Brookhaven National Laboratory, Upton, New York; 30.09.2005
- U. Reinosa 2PI effective action and non-perturbative thermodynamics Laboratoire de Physique Théorique d'Orsay, Université Paris-Sud XI, Orsay, France; 17.03.2005
- U. Reinosa 2PI effective action and non-perturbative thermodynamics Centre de Physique Théorique Marseille, Marseille, France; 30.03.2005
- U. Reinosa 2PI effective action and non-perturbative thermodynamics LAPPTH Annecy, Annecy-le-Vieux, France; 31.03.2005
- U. Reinosa 2PI effective action and non-perturbative thermodynamics Physics Department, University of Technology, Munich, Munich, Germany; 03.06.2005
- S. Rotter Quantenmechanisches Schrotrauschen in mesoskopischen Systemen TU Dresden, Dresden, Germany; 23.06.2005

• S. Rotter

Quantum shot noise in mesoscopic conductors University of Zaragoza, Zaragoza, Spain; 08.09.2005

• E. Schöll-Paschinger

Phasenverhalten von einfachen Flüssigkeiten und ihren Mischungen Institute for Experimental Physis, University of Vienna, Vienna, Austria; 11.01.2005

• M. Seliger

Open quantum system approach to coherence in ion-solid transport International Summer School on Quantum Information, Max-Planck-Institut für Physik komplexer Systeme, Dresden, Germany; 06.09.2005

• B. Solleder

Electron emission from a magnetized Fe surface under impact of  $N^{6+}$  ions Seminar Talk, Institute of Nuclear Research, ATOMKI, Debrecen, Hungary; 23.09.2005

• B. Solleder

Electron emission from a magnetized Fe surface under impact of  $N^{6+}$  ions Seminar Talk at IEMN (Institute d'electronique, de microelectronique et de nanotechnologie), Dept. ISEN, Lille, France; 17.11.2005

- K. Svozil Aesthetics and Scarcity: A physics perspective Data Ecologies05, Linz, Austria; 13.05.2005
- K. Svozil

Quanten-Kryptographie - und wie man sie (vielleicht) knacken kann Institute for Photonics, Vienna University of Technology, Vienna, Austria; 16.03.2005

- K. Svozil Quantum correlations & beyond University of Gdansk, Gdansk, Polen; 19.10.2005
- K. Svozil Quantum correlations and beyond Institute for Theoretical Physics, University of Tübingen Tübingen, Germany; 28.11.2005

- K. Svozil Randomness & undecidability in physics Perimeter Institute for Theoretical Physics, Waterloo, Ontario, Canada; 09.12.2005
- K. Svozil Zufall und Bestimmtheit in der Physik
  10. Naturwissenschaftlicher Tag am G 19, Vienna, Austria; 22.02.2005
- S. Yoshida Enhancement of low energy electron-ion recombination in storage rings Oak Ridge National Laboratory, Oak Ridge, Tennessee, USA; 10.08.2005
- S. Yoshida *Probing a phase space distribution using a train of kicks*, Rice University, Houston, Texas, USA; 30.08.2005

• S. Yoshida Steering Rydberg wave packets using a chirped train of half-cycle pulses Kansas State University, Kansas, USA; 31.03.2005

# Appendix D

## Graduates

## D.1 Master degrees (Diploma)

### • F. Aigner Quantum shot noise in mesoscopic conductors Supervisors: J. Burgdörfer, S. Rotter

- T. Baier On periodic Schrödinger operators and the infinite volume limit Supervisor: R. Dirl
- C. Deiss Laser-cluster interaction: production of hot electrons by short laser pulses Supervisors: J. Burgdörfer, N. Rohringer
- K.-M. Schiessl Resonant effects and propagation in high harmonics generation Supervisors: J. Burgdörfer, E. Persson
- R. Schöfbeck *The quantum Bogomol'nyi bound in supersymmetric Yang-Mills theories* Supervisor: A. Rebhan
- M. Weiretmayr Slavnov method of noncommutative U(1) theory Supervisor: M. Schweda

## D.2 Doctorates

- P. Fischer Quantum gravity, extra dimensions and the exact renormalisation group Supervisor: W. Kummer
- A. Gerhold Aspects of cold dense quark matter Supervisor: R. Rebhan
- D. Gottwald Genetic algorithms in condensed matter theory Supervisor: G. Kahl
- M. Hörndl Classical dynamics of low energy electron-ion recombination in storage rings Supervisors: J. Burgdörfer and S. Yoshida
- N. Rohringer

A quantitative test of time-dependent density functional theory Supervisor: J. Burgdörfer

• M. Seliger

Open quantum system approach to transient coherence in ion-solid transport Supervisors: J. Burgdörfer, C.O. Reinhold

## D.3 Habilitation

• R. Wulkenhaar

Renormalization of noncommutative  $\phi_4^4$ -theory to all orders Supervisor: M. Schweda

# Appendix E

## Projects

### E.1 Projects started in 2005

 Joachim Burgdörfer together with Hannspeter Winter Ion technoloy and spectroscopy at low energy ion beam facilities European Commission (EC) Project-Nr.: JRA6 Amount: EUR 66.000,00 01.01.2006 - 31.12.2009

 Gerhard Kahl Phasenübergänge in der weichen Materie Fonds zur Förderung der wissenschaftlichen Forschung (FWF) Project-Nr.: P17823-N08 Amount: EUR 192.381,00 01.03.2005 - 29.02.2008

 Gerhard Kahl Phase behaviour of a symmetrical binary mixture in a field Österreichischer Akademischer Austauschdienst (OEAD) Project-Nr.: (BC) Amount: EUR 1.466,00 01.01.2005 - 31.12.2005

 Gerhard Kahl, Rainer Dirl *Computational Material Science*  Fonds zur Förderung der wissenschaftlichen Forschung (FWF) Project-Nr.: WK004 Amount: EUR 288.060,00 30.04.2006 - 01.05.08
  Wolfgang Kummer Hawkingflux
 Fonds zur Förderung der wissenschaftlichen Forschung (FWF)
 Project-Nr.: P17938-N08
 Amount: EUR 52.524,00
 01.01.2005 - 28.02.2006

## E.2 Current projects and projects completed in 2005

- Wolfgang Kummer *Quantum gravity*  Österreichischer Akademischer Austauschdienst (OEAD) Project-Nr.: 349-1/2004 Amount: EUR 8.460,00 01.10.2004 - 30.06.2005
- Wolfgang Kummer Dilaton supergravity
   Fonds zur Förderung der wissenschaftlichen Forschung (FWF)
   Project-Nr.: P16030-N08
   Amount: EUR 41.772,00
   01.11.2004 - 31.07.2005
- Joachim Burgdörfer Simulation of chaotic Andreev Billards Fonds zur Förderung der wissenschaftlichen Forschung (FWF) Project-Nr.: P17359-N08 Amount: EUR 188.622,00 01.11.2004 - 31.10.2007
- Joachim Burgdörfer together with Friedrich Aumayr (E 134) How do insulator surfaces react to highly charged ions Fonds zur Förderung der wissenschaftlichen Forschung (FWF) Project-Nr.: P17449-N02 Amount: EUR 123.711,00 01.11.2004 - 31.10.2007

 Gerhard Kahl Structure, thermodynamics, and phase transitions in polydisperse liquid mixture Bundesministerium für Bildung, Wissenschaft und Kultur (BM:BWK) Project-Nr.: GZ45.492/1-VIII/B/8a/2000 (D13600040500) Amount: EUR 26.889,00 14.11.2000 - 31.12.2006

- Shuhei Yoshida Enhanced recombination in low temperature magnetized plasmas Fonds zur Förderung der wissenschaftlichen Forschung (FWF) Project-Nr.: P15025 Amount: EUR 155.168,00 01.07.2001 - 30.06.2006
- Gerhard Kahl *Atomic-scale computational materials science* European Commission (EC) Project-Nr.: IHP-MCHT-01-1 Amount: EUR 66.000,00 6.08.2001 - 30.06.2007
- Joachim Burgdörfer *Ion TMP facilities for highly charged heavy ions*  European Commission (EC) Project-Nr.: HPRI-CT-2001-50036 Amount: EUR 176.617,00 1.11.2001 - 31.10.2005
- Manfred Schweda Supersymmetry in commutative and non commutative QFT Fonds zur Förderung der wissenschaftlichen Forschung (FWF) Project-Nr.: P15015 Amount: EUR 121.380,00 10.10.2001 - 30.09.2006
- Maximilian Kreuzer Non-commutative structures in the open string theory Fonds zur Förderung der wissenschaftlichen Forschung (FWF) Project-Nr.: P15553 Amount: EUR 144.171,00 11.03.2002 - 28.02.2005
- Maximilian Kreuzer D-branes on Calabi-Yau manyfolds
   Fonds zur Förderung der wissenschaftlichen Forschung (FWF)
   Project-Nr.: P15584
   Amount: EUR 126.070,00
   11.3.2002 - 30.04.2005

Manfred Schweda
 Mitarbeiter: P. Fischer, M. Wohlgenannt
 Non-commutative gauge field theories
 Fonds zur Förderung der wissenschaftlichen Forschung (FWF)
 Project-Nr.: P15463
 Amount: EUR 93.468,00
 11.3.2002 - 30.09.2006

- Rainer Dirl, Gerhard Kahl, Peter Kasperkovitz *Computational materials science*  Fonds zur Förderung der wissenschaftlichen Forschung (FWF) Project-Nr.: WK W004 Amount: EUR 245.921,00 19.03.2002 - 30.04.2005
- Gerhard Adam

Nachweis der Inkonsistenz der konventionellen Renormierungstheorie und Ausarbeitung sowie Anwendung eines neuen konsistenten Renormierungskonzepts in der Quantenelektrodynamik Österreichische Akademie der Wissenschaften (OEAW) Project-Nr.: EST-254/2002 Amount: EUR 104.640,00 10.5.2002 - 31.12.2005

### • Gerhard Kahl

Phase behaviour and critical behaviour in simple liquids Fonds zur Förderung der wissenschaftlichen Forschung (FWF) Project-Nr.: P15758 Amount: EUR 138.802,00 21.5.2002 - 31.12.2005

### • Gerhard Kahl

Phase transitions in colloids Jubiläumsfonds der Stadt Wien (JSW) Project-Nr.: H-1080/2002 Amount: EUR 4.000,-17.10.2002 - 31.12.2006

### • Joachim Burgdörfer

Advanced light sources - interaction of ultrashort pulses with matter theory Fonds zur Förderung der wissenschaftlichen Forschung (FWF) Project-Nr.: F 1610. Amount: EUR 220.020,00 01.04.2003 - 30.03.2006

### • Anton Rebhan

Colour superconductivity Fonds zur Förderung der wissenschaftlichen Forschung (FWF) Project-Nr.: P16387-N08 Amount: EUR 154.014,00 06.03.2003 - 31.03.2006

- Gerhard Kahl Simple and complex fluids in disordered porous media Ministerio de Educacíon, Cultura y Deporte (MECD) Project-Nr.: EX2003-0580 Amount: EUR 36.542,00 01.12.2003 - 30.11.2005
- Joachim Burgdörfer Study of normal-superconducting hybrid nanostructures Österreichischer Akademischer Austauschdienst (OEAD) Project-Nr.: A-2/2003 Amount: EUR 11.730,00 30.11.2003 - 31.12.2005