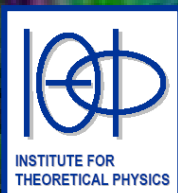


ITP 2006

Institute for Theoretical Physics
Vienna University of Technology
Annual Report 2006



Institute for Theoretical Physics
Vienna University of Technology
Annual Report 2006

Wiedner Hauptstraße 8-10, 1040 Wien

Tel.: +43/1/58801-13601

Fax.: +43/1/58801-13699

<http://www.itp.tuwien.ac.at>

Editors: [Elfriede Mössmer](#), [Florian Aigner](#) and [Cornelia Deiss](#)

The background picture of the cover page shows results of a computer simulation of plasma instabilities in an anisotropically expanding quark-gluon plasma as produced in ultrarelativistic heavy-ion collisions (FWF project no. P19526). Time flows from bottom to top, the horizontal position corresponds to a (comoving) coordinate of the expanding plasma along the beam axis of the collision, and the color represents the internal degrees of freedom of so-called chromomagnetic fields. For more information and a different representation of such simulations in laboratory coordinates see Fig. 2 on page 18.

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Executive Summary: Key data 2006

• Positions:	Faculty positions ^(a) :	14,5
	Externally funded scientific staff:	28

• Budget:	Operating budget available to the institute:	EUR	98.780
	External funds attracted in 2006:	EUR	1.837.148

• Research:	Publications in peer-reviewed journals:	49
	Invited talks at international conferences:	17

• Teaching:	Course hours/week taught by faculty during the academic year 2005/06:		
	Mandatory core courses:	30	
	Special lectures:	378	
	Total:	408	

• Degrees Awarded:	Diploma:	6
	Doctorate:	2
	Habilitation:	1

(a) 2 of which are vacant

Foreword

The year 2006 offered our institute a mixed bag of good and bad news. On the downside, our first choice for filling the vacancy left by the retirement of Prof. Kummer, Dominik Schwarz (University of Bielefeld), turned down the offer late last year. That meant at least another year of continued shortage of personnel for teaching and research. We are still cautiously optimistic that the second round will be more successfully completed before the end of 2007. Two senior members of the institute, a. o. Univ. Prof. Rainer Dirl and Univ. Prof. Manfred Schweda, reached their retirement or emeritus status during 2006. They have significantly contributed over several decades to the work of the institute in both teaching and research. We celebrated their accomplishments during our annual institute "fest" in December. Unfortunately, replacements for them are currently not in sight. Fortunately for us, however, Manfred Schweda has volunteered to continue giving his mandatory lecture "Mathematical Methods" for the time being. Clearly, this situation is not sustainable.

On the brighter side, our institute was remarkably successful in 2006 in attracting extramural funding reaching an all-time high of 1.8 Mio. Euros, a truly remarkable figure for a small theory institute with a very limited number of (in part, vacant) scientific staff positions. The level of scientific output in terms of 49 peer-reviewed research papers, 17 invited presentations, and 37 contributed papers at international conferences during 2006 continues to be excellent. The strong emphasis on teaching and training of young scientists is documented by a total of 9 awarded academic degrees. We are also proud that the "Diplomarbeitspreis der Stadt Wien" was awarded to one of our graduates, Johannes Feist.

All staff members deserve credit for their important contributions and their enthusiasm that helped to keep up this level of productivity. 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.

Finally, I would like to thank Cornelia Deiss and Florian Aigner for their editorial work on this annual report.

Vienna, October 2007

Joachim Burgdörfer
(Director of Institute)

In memoriam



Wolfgang Kummer (15.10.1935 - 15.7.2007)

During the completion of this annual report, we unexpectedly received the sad news of Wolfgang Kummer's passing away after a long and courageous battle with cancer. Just a few days earlier, Wolfgang had given in a phone conversation with the author of these lines an up-beat assessment of a new treatment he was receiving and to which he responded well. He was looking forward to a further improvement of his condition and he made already plans to return to the institute on a more regular basis. Sudden heart failure prevented his plans and wishes from coming true.

We mourn the loss of a great scientist, of an academic teacher and researcher of highest calibre, and of a key figure that helped shaping the scientific profile and reputation of our institute. He was appointed full professor of Theoretical Physics in 1968 as one of the youngest full professors in Austria and served in this capacity for 36 years until reaching emeritus status in 2004. His teaching career began even earlier when he became university assistant (or assistant professor) in 1958. Over a period of almost half a century, interrupted by several research visits abroad, Wolfgang taught theoretical physics at our institute.

His desire to specialize in the "modern" topics of high-energy physics and quantum field theory was, ironically, in part motivated as contrast program to the dominant research activity at the institute, represented by his supervisor and chair of Theoretical Physics at the time, Walter Glaser, which was firmly rooted in classical dynamics. Glaser, who died already in 1960 at the age of 54 did not live to see the high recognition his joint research with his experimental collaborator and winner of the 1988 Nobel prize Ernst Ruska would eventually receive. Glaser's theoretical contributions to electron beam optics played a crucial role in the developments of the high resolution electron microscope, as Ruska noted in his Nobel lecture.

Wolfgang Kummer received strong support and tutelage by Walter Thirring, University of Vienna, who secured for him a Ford fellowship and brought him in contact with the high-energy physics community. Kummer joined Victor Weisskopf, then director-general of CERN, first as a Ford fellow, later as a CERN fellow and as his scientific assistant from 1961 to 1964. Kummer became the founding director of the institute for high-energy physics of the Austrian Academy of Science in 1966, which he led until 1971. Over many years, he was member of the CERN council. He served as its vice president from 1980 to 1983 and as its president from 1985 to 1987. On December 26, 1985 Wolfgang became a victim of a terrorist attack on Vienna airport when he suffered multiple injuries from hand grenade splinters and shrapnel. Even though his injuries were life threatening and he spent eleven days in intensive care, he quickly recovered and resumed his duty as council president within weeks.

Wolfgang held over the years numerous administrative positions both within Vienna University of Technology and in national and international scientific organizations. Kummer's foremost achievement during his tenure as full professor at our university is undoubtedly the build-up of a strong theoretical high-energy physics group covering a broad range of topics in quantum field theory, string theory and (mainly 2D) quantum gravity. Kummer made fundamental contributions to quantum gauge field theory, in particular by using ghost-free non-covariant gauge fixing. Since the early 1990's, he mainly worked on two-dimensional gravity and he was unceasingly productive well beyond his official retirement in 2004.

Kummer's contributions to the institute and the university were by no means limited to science. He exemplified the role model of an enthusiastic teacher, of an unselfish and supporting mentor of his younger colleagues, and of a colleague of impeccable integrity. He will be remembered for his unfailing dedication to the cause of science, displayed even under adverse conditions of deteriorating health.

We are grateful for the time we were privileged to share with him. Our thoughts are with his wife of 47 years, Dr. Lore Kummer.

Joachim Burgdörfer

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.

Chapter 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.

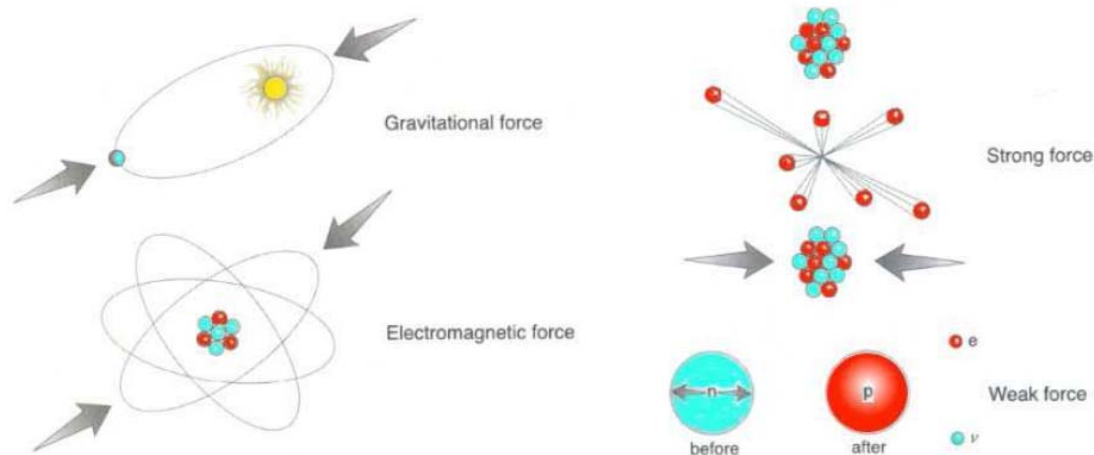


Fig. 1: Schematic presentation of fundamental interactions

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.

1.1 Non-Commutative Gauge Theory with the Slavnov Term

Staff: **Daniel N. Blaschke**, **Manfred Schweda**

External: **François Gieres** (Univ. Claude Bernard (Lyon 1), France) **Stefan Hohenegger** (CERN, Switzerland) **Olivier Piguet** (Univ. Federal do Esp rito Santo (UFES), Brasil)

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 natural, 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 leading to so-called loop corrections.

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 interaction vertices are described by local field products if the underlying geometry is commutative. It was suggested very early by Snyder [8] 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.

Non-Commutative Gauge Field Theory (NCGFT)

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. Here, we consider the simplest case of 3+1 dimensional θ -deformed Minkowski space-time $\mathbb{M}_\theta^4$, with the commutation relation

$$[\hat{x}^\mu, \hat{x}^\nu] = i\theta^{\mu\nu} \quad (1)$$

for the (operator-valued) space-time coordinates (cf. [8, 9], see also [10] for a review). The non-commutativity parameter $\theta^{\mu\nu} = -\theta^{\nu\mu}$, which implements the deformation, is assumed to be constant and in order to avoid difficulties with time-ordering in the field theory, we choose the special case where $\theta^{0\mu} = 0$. In order to construct the perturbative field theory formulation, it is more convenient to use fields $A(x)$ (which are functions of ordinary commuting coordinates) instead of operator valued objects like $\hat{A}(\hat{x})$. One therefore introduces the so-called Weyl-Moyal $\star$ -product

$$A_1(x) \star A_2(x) = e^{\frac{i}{2}\theta^{\mu\nu}\partial_\mu^x\partial_\nu^y} A_1(x)A_2(y) \Big|_{x=y}, \quad (2)$$

in order to implement non-commutativity. It has the important property of invariance under cyclic permutations of the integral which implies, that bilinear terms are unaffected by the star product. For a field theory this means that interaction vertices gain phases, whereas propagators remain unchanged. In constructing Feynman graphs one has to deal with so-called planar and non-planar diagrams [11]. While planar diagrams have the same ultraviolet divergences known from commutative field theory, the non-planar ones are finite due to phase factors. These phases act as UV-regulators, but since this regulating effect can only take place for non-vanishing external momentum, a new infrared divergence appears. This is the origin of the *UV/IR mixing* problem [12, 13].

Due the star product, even a non-commutative $U(1)$ gauge field is endowed with a non-Abelian structure, which leads to a generalization of the usual Abelian Maxwell theory - and thus to an extended non-Abelian gauge symmetry (BRST symmetry). As shown by several authors [7, 15, 16], the corresponding action leads to an IR singular vacuum polarization, whose quadratic IR divergent term is gauge fixing independent. Feynman graphs with such an insertion are IR divergent.

The Slavnov Term

In order to get rid of IR divergences, Slavnov [4, 5] has proposed a modification of Yang-Mills theories, adding to the action a further term with a multiplier field λ . This term implies a constraint for the field strength which has the effect of making the gauge field propagator transversal with respect to $\theta^{\mu\nu}k_\nu$, where k_ν denotes the momentum. Hence, initially IR divergent Feynman graphs become *finite*.

There is, however, a catch: One has additional Feynman rules, namely a λ propagator, a mixed λ -photon propagator and a λ -photon vertex, and hence numerous additional Feynman graphs. Since the additional propagators are not transversal with respect to $\theta^{\mu\nu}k_\nu$, Slavnov's trick does not work for certain diagrams, unless a special gauge fixing is used:

In order to avoid unitarity problems [14] we choose the non-commutativity tensor spacelike and choose the gauge fixing to be of an axial type [17, 18] with gauge fixing vector n^μ in the plane of the non-commutative coordinates. With these choices the Slavnov term, together with the gauge fixing terms, have the form of a 2-dimensional topological BF model (cf. [1, 2, 6] and references therein).

Symmetries & Consequences

In addition to its invariance under the usual BRST symmetry, the action S is also invariant under a (non-physical) *linear vector supersymmetry* (VSUSY). Since the VSUSY-operator δ_i lowers the ghost-number by one unit, it represents an antiderivation (very much like the BRST operator s which raises the ghost-number by one unit). It is important to note that *only the interplay of appropriate choices for $\theta^{\mu\nu}$ and axial gauge fixing vector n^μ lead to the existence of the VSUSY*.

In contrast to the pure topological theories, we have an additional vectorial symmetry. This further symmetry is in fact a (non-linear) symmetry of the gauge invariant action. Its existence is due to the presence of the Yang-Mills part of the action. The algebra involving all three symmetries and the (x_1, x_2) -plane translation generator ∂_i closes on-shell (cf. [1, 2]).

We shall now summarize the consequences of the linear VSUSY: From the Ward identity describing the linear vector supersymmetry, one can easily derive that all loop graphs involving the λ -photon vertex vanish. This is the reason, why the model is free of the most dangerous, i.e. the quadratic, infrared singularities, as pointed out by Slavnov [5] for the special case of $n^\mu = (0, 1, 0, 0)$.

Finally, we should note, that one also has a linear vector supersymmetry in the case of more general $\theta^{\mu\nu}$ and gauge fixing vector n^μ , provided one introduces stronger Slavnov constraints, i.e. a Slavnov term of BF type [3].

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1.2 Gravitation

Staff: **Herbert Balasin, Daniel Grumiller, Wolfgang Kummer**

External: **Peter Aichelburg** (Uni Wien), **Dimitri Vassilevich** (Uni Leipzig)

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 an non-Euclidean geometry.

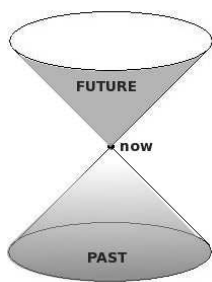


Fig. 1: Light-cone of an event representing its causal past and future.

But 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

Singularities in spacetimes are inevitable consequences of classical General Relativity as proven by Penrose and Hawking [1] in their by-now famous singularity theorems. They represent rips in the fabric of spacetime, which in the most prominent cases correspond to the beginning (big-bang) and endings of time (black-holes) respectively.

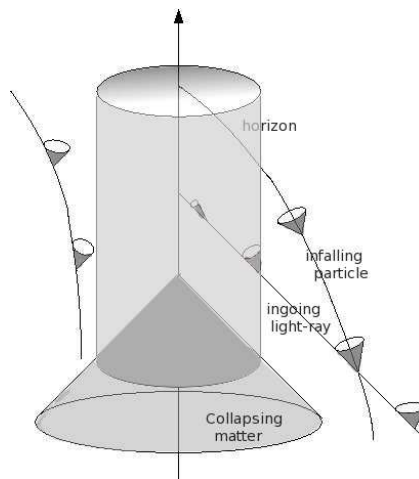


Fig. 2: Geometry of a black hole formed by a collapsing pulse of radiation

Quite recently progress in understanding the structure of singularities has been made within a systematic quantization of General Relativity (Loop Quantum Gravity). In a certain class of systems, which comprises both cosmological (big-bang) as well as isolated systems (black-holes), these results indicate that it is possible to (quantum-mechanically) evolve past the classical singularities. It seems therefore worthwhile to investigate these singularities on a (semi)classical level. The necessary mathematical framework is provided by the theory of (non-linear) generalized functions [2]. It turns out to be possible to assign energy-momentum distributions to the singular regions of all stationary black-hole solutions [3], thereby identifying the singular regions as part of spacetime in contrast to the usual classical treatments. Aside from the semi-classical aspect the localized energy distributions proved to be an important stepping stone for the (unambiguous) construction of so-called ultrarelativistic limit geometries. They represent spacetimes as they appear to a (ultra)fast-moving observer. In

particular they describe the geometry of black-holes that move at the speed of light. In a recent monograph [4], Barrabes and Hogan have provided a complimentary treatment of these gravitational shock-wave based upon the limit of the full spacetime curvature. In order to elucidate the connection with the energy-momentum tensor approach their limit-technique has been applied to the Curzon geometry, which represents short cosmic string, thereby obtaining a double-pulse gravitational wave in the limit.

Dark matter and General Relativity

In the usual approach the flat (non-Keplerian) rotation curves of galaxies are taken as evidence for the existence of non-luminous (dark) matter. Quite recently stationary axis-symmetric models within General Relativity (GR) have been put forward [5] which claimed to explain this behaviour. Although it turned out that the original model contained unphysical matter the basic idea of using GR rather than the Newtonian approximation to explain part of the rotation curve behaviour seems to be possible [6].

Quantized pp-waves

Since an exact treatment of the full theory of quantized gravity is in general not possible in closed form it seems useful to try to gain some insight via more simple (symmetry-reduced) models. The important task of such a reduction is to find the balance between an analytic treatment and the physical relevance of the system.

A simple class of gravitational fields, namely gravity-waves with plane wave-fronts (pp-waves) provide such a system. They are rich enough since in the ultrarelativistic limit all stationary black-holes become gravitational (pp-)shock-waves. On the other hand due to their light-like nature (propagation with the speed of light) they are simple enough a system to allow a classical treatment in closed form. Unfortunately, the simplicity comes at a price that renders quantization difficult. Namely, the very light-like nature entails the vanishing of the Lagrangian for the whole class of geometries. Thereby a Hamiltonian treatment, as prerequisite for quantization, seemed unfeasible. Recent progress [7] has removed this “road-block” on the way to a quantum treatment. The idea is to start from the non-trivial equations of motion for the metric and re-construct both the canonical variables, as well as the Hamiltonian that re-produces the correct dynamics. This new canonical formulation opens the road to a full quantization of the system within a geometric framework.

Two-dimensional Quantum Gravity

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

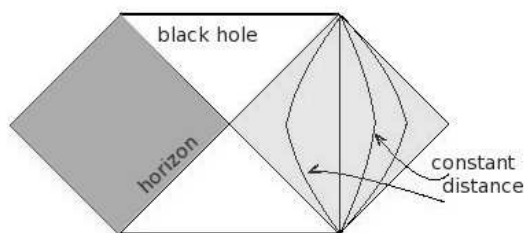


Fig. 3: Spherically symmetric black hole

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 these 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 [8]. 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 [9]. 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 [10].

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1.3 Quark-gluon plasma

Staff: **Max Attems**, **Ulrike Kraemmer**, **Anton Rebhan**, **Stefan Stricker**

External: **Jean-Paul Blaizot** (ECT*, Trento), **Andreas Ipp** (MPI Heidelberg), **Edmond Iancu** (CEA Saclay), **Keijo Kajantie** (University of Helsinki), **Paul Romatschke** (Uni Bielefeld), **Michael Strickland** (FIAS Frankfurt), **Aleksi Vuorinen** (University of Washington, Seattle)

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 color-neutral 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 lose 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 2×10^{12} Kelvin (100,000 times the temperature in the interior of the sun), 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.

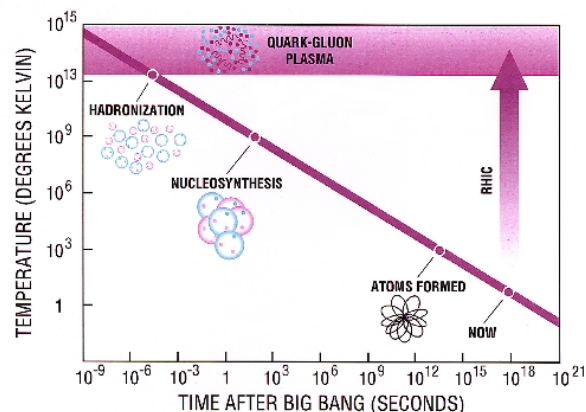


Fig. 1: Thermal history of the Universe from the time when it was filled by a quark-gluon plasma until now.

At present there are experiments being carried out in the Relativistic Heavy Ion Collider (RHIC) at the Brookhaven National Laboratory (BNL), 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. From 2008 on, 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, which however involved a couple of surprises.

One of the surprises was the extremely fast apparent thermalization of the quark-gluon plasma and its extremely low shear viscosity (as judged from hydrodynamical model simulations), which would make the quark-gluon plasma the most perfect fluid ever to be produced in the laboratory (at BNL one can now get coffee mugs with the inscription “RHIC serves the perfect fluid”).

Using string theory methods, hydrodynamical properties of strongly coupled (supersymmetric) gauge theories have been obtained which are conjectured to give a lower bound on the ratio of shear viscosity over entropy density, and the quark-gluon plasma seems to come close to this bound.

However, it is still not excluded that these phenomena could be due to weak-coupling physics involving quark-gluon plasma instabilities, which are nonabelian generalizations of the so-called Weibel instabilities in ordinary plasma physics [2]. One of the first results on their dynamics have been obtained by our group [3], with follow-up work by other groups from the US and Europe [4]. 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. These studies have so far been done for plasmas with a stationary anisotropic particle distribution and have now been generalized to the case of a longitudinally expanding quark-gluon plasma fireball [5]. Fig. 2 visualizes just the color degrees of freedom in collective fields as they evolve from small initial fluctuations in such a fireball. The horizontal axis is the spatial direction in which there is expansion of the plasma with the speed of light, with fields taken as constant with respect to transverse directions (out of the plane), and time flows from bottom to top (see the cover page for a representation using a comoving coordinate along the beam axis).

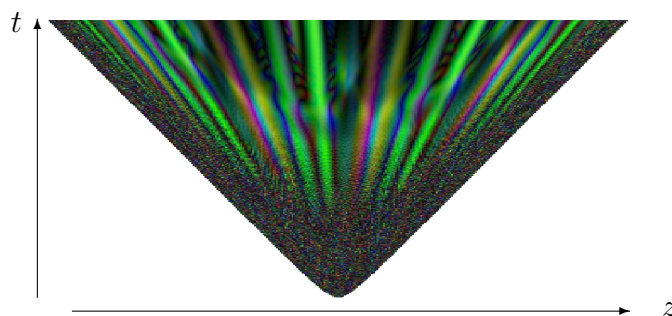


Fig. 2: The time evolution of the color degrees of freedom in the chromomagnetic field associated with instabilities in a longitudinally expanding quark-gluon plasma fireball.

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 absolute amplitudes of the fields are not shown). After these perturbations

have grown such that nonabelian self-interactions come into the play, there is a certain disturbance in the color distribution along a hyperbolic shell after which the color inhomogeneities are enhanced. The crucial finding, which cannot be read from this plot, is that the near 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.

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,

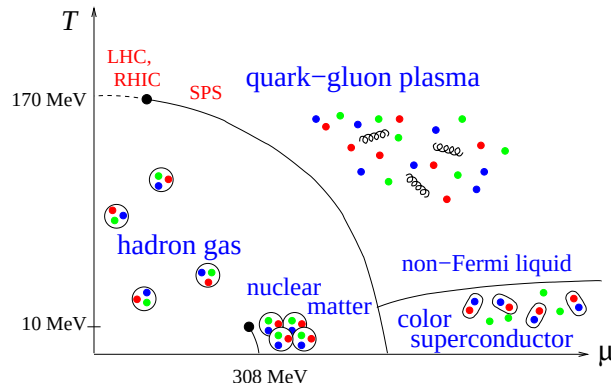


Fig. 3: Qualitative sketch of the phase diagram of quark-gluon matter as a function of temperature T and quark chemical potential μ . Solid lines denote first-order phase transitions, the dashed line a rapid crossover.

where T is the temperature in MeV ($1 \text{ MeV} \approx 10^{10} \text{ K}$), and μ 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]. One focus is on properties at small μ and high temperatures, which are relevant for relativistic heavy ion colliders and the physics of the early universe, and this has now been extended for all temperatures and chemical potential which allow a weak-coupling expansion [7], covering also high μ and smaller temperatures 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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1.4 String theory

Staff: Maximilian Kreuzer, Rashid Ahmad, Sebastian Guttenberg, Christoph Mayrhofer, Michal Michalcik

External: Victor Batyrev (U. Tübingen), Volker Braun (Pennsylvania U.), Stefan Hohenegger (CERN), Albrecht Klemm (Univ. of Washington-Madison), Johanna Knapp (CERN), Benjamin Nill (Freie U., Berlin), Burt A. Ovrut (Pennsylvania U.), Emanuel Scheidegger (Piemonte Orientale U., Alessandria)

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 build black holes. The separate description of the forces is quite accurate by now. This is summarized in the standard model of particle physics.

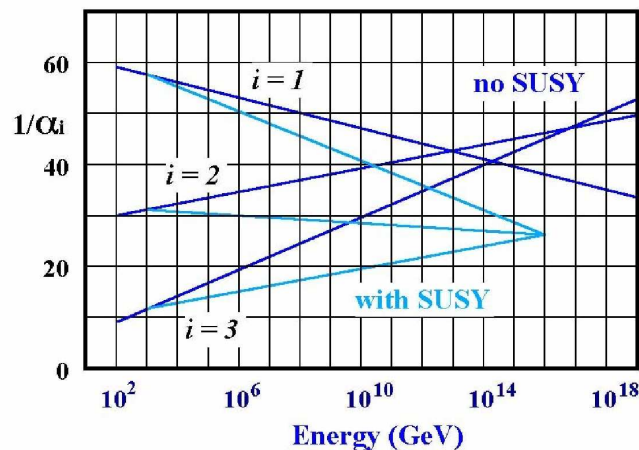


Fig. 1: Grand unification. $i=1$: Electromagnetism, $i=2$: weak interactions, $i=3$: strong interactions

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, whose coupling constant is far weaker still at this high energies. The theory, which 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'. Probably in mid-2008, the new accelerator LHC (large hadron collider) at CERN will start high energy collisions and try to produce the Higgs boson and the superparticles mentioned above and will therefore also be a first 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 Heisenberg's 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 consider extreme situations like black holes consistently, one also needs to treat the gravitational field 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'.

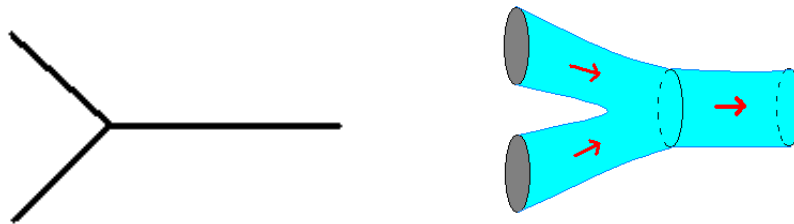


Fig. 2: Left: Point particle interaction, Right: Closed string interaction, note the smooth interaction surface

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.

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. 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. In addition to mirror symmetry, there is also a nonperturbative duality which relates fundamental strings with solitonic background solutions (the D-branes). Those in turn can be sources of so-called RR-fluxes. The effective physics in four dimensions depends very much on how one curls up (compactifies) the 6 additional dimensions.

The simplest class of phenomenologically interesting models is obtained when the six-dimensional compactification manifold is what mathematicians call a Calabi Yau space. In recent years it turned out, however, that phenomenological requirements like supersymmetry breaking and moduli stabilization require the presence of certain fluxes that are similar to electromagnetic fields but exist only in higher dimensions (string theory predicts the existence of such fluxes, which after compactifications give rise to the types of particle interactions that we are used to). Strong background fields of this type can have a strong influence on the geometry of the hidden dimensions. A detailed analysis of the resulting equations lead to a generalization of the Calabi-Yau condition known as "generalized complex geometry" [3], and the study of the resulting new mathematics is still in its infancy. On the physics side of this story, the description of the background fluxes has become feasible with "Berkovits' pure spinor formulation of the superstring" [4], whose development began roughly at the same time.

The study of Calabi-Yau compactifications and the generalizations required by the presence of fluxes are also the main subjects of our work. In the project “Non-perturbative effects in string compactifications” (FWF P18679) we continue our work on the classification of Calabi-Yau spaces [5,6], and explore their application to topological strings (with implications to the statistical mechanics of black holes), superpotentials generated by D-branes, as well as other phenomenological aspects of string compactifications. In the project “Generalized geometries of effective actions” (FWF P19051) we study flux induced generalizations of geometry using mainly the pure spinor formulation of the superstring. In particular, various aspects of the above mentioned generalized complex geometry and their appearance in string theory are considered [7].

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Chapter 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).

2.1 Quantum information

Staff: **Karl Svozil**

External: **Cristian Calude** (Auckland Univ.)

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 one-to-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-Bell-type 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.

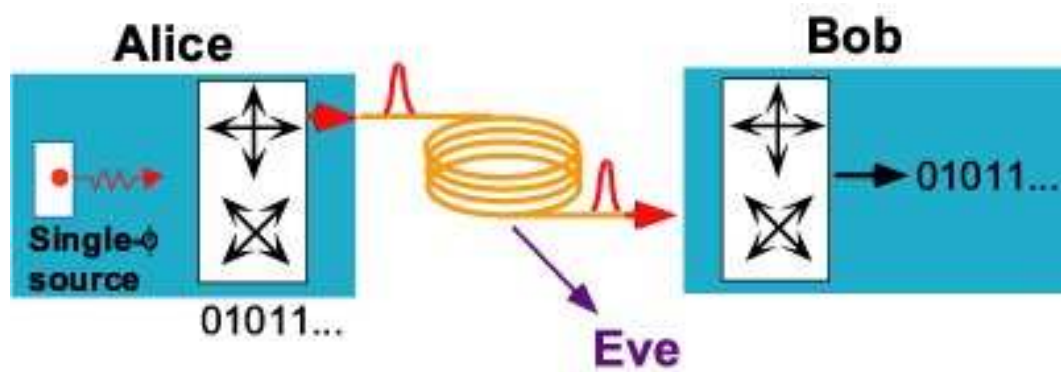


Fig. 1: Quantum cryptography using single-photon sources.
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2.2 Coherence, Decoherence, and Echoes

Staff: Shuhei Yoshida, Emil Persson, Joachim Burgdörfer

External: F. B. Dunning (Rice University, Houston, Texas, USA)

and C. O. Reinhold (Oak Ridge National Laboratory, Oak Ridge, Tennessee, USA)

The word “coherence” is now becoming one of the most important keywords in the research of quantum dynamics. All dynamical systems are coupled to a typically uncontrolled environment. Due to interactions with the environment it becomes very difficult to predict how the system evolves. Put it differently, from the final state we cannot trace back the initial state or the time reversibility of the system is lost. This deviation of the “real” dynamics from the dynamics of the “isolated” system, *i.e.*, without the coupling to the environment, is called “decoherence” [1]. The control and, if possible, the suppression of decoherence or the preservation of coherence (or reversibility) is important for many applications. For example, reversibility implies that the information stored initially in the system is maintained during the time evolution. For the quantum information processing where quantum systems are used as information registers [2], the preservation of the stored information is a crucial problem [5]. Or, in engineering, it is quite useful if a target state can be produced efficiently by enhancing a certain quantum mechanical transition in a controlled manner [3]. In this case, uncertainties in the outcome induced by decoherence reduces the efficiency of the control. Therefore, coherence is essential to keep control of the dynamics of the system.

The dynamics of the system as a whole should always be reversible. This does not, however, apply to subsystems interacting with the environment. For example, we consider the dynamics of a pendulum (Fig.1a). Assuming that it experiences only the gravitational force of the earth, the equation of motion is given by $m\ddot{\theta} = -mgL\theta$. Its time evolution shows oscillations $\theta(t) = \theta(0) \cos(\sqrt{gL}t)$ (Fig.1b, dashed line). The motion of the pendulum is affected by the interaction with the air surrounding it. It is quite cumbersome to study the detailed dynamics of each molecule in the air and, instead, the coupling to the air can be approximated as friction, *i.e.* the averaged collisional forces between the pendulum and molecules. The dynamics of the air is “hidden” by this averaging and the air becomes the environment. In fact, a friction force decelerates and damps the oscillations of the pendulum (Fig.1b, solid line) and breaks the time-reversal symmetry of the isolated system.

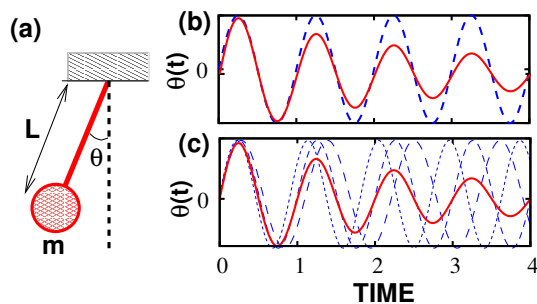


Fig. 1: (a) Schematic illustration of a pendulum, (b) time evolution of θ with (dashed) and without (solid) damping, and (c) time evolution of θ for an ensemble of pendulums (solid). Dashed lines are $\theta(t)$ of individual pendulum. (Only a few are plotted).

In practice, measurements are performed on an ensemble of microscopic objects, such as atoms, molecules, quantum dots or by repetitive measurements on a single atom. The coherence within the ensemble provides the information on how isolated the system is from the environment and also from the other members of the ensemble. The coherence of the system can be measured through the so-called “echo” technique. The dephased ensemble can be rephased by reversing the “arrow of time”. The resulting echo state is identical to the initial

state for a perfectly reversible (coherent) system. Thus, in general, the deviation of the echo state from the initial state can be used as a measure of decoherence, *i.e.* the irreversibility of the dynamics. In a real system, time reversal is impossible unless a “time machine” is invented. Therefore, an operation mimicking the time reversal is required. The spin echo is one of the examples known for the study of nuclear magnetic resonance (NMR) [4]. The concept of spin echo can be easily understood using the analogy to a horse race. Initially all horses are aligned at starting gate (Fig.2a). After time τ faster horses advance more and horses are spread along the race track (Fig.2b). Upon a signal all horses turn around and run towards the starting gate with the same speed but in opposite direction (Fig.2c). At $t = 2\tau$, all horses are aligned again and back in the starting gate simultaneously (Fig.2d). Coupling to the environment is not time-reversed by the π -pulse. Therefore, “the realignment” will not be perfect. Those interactions are considered to be the sources of decoherence induced in an ensemble of isolated spins in a magnetic field.

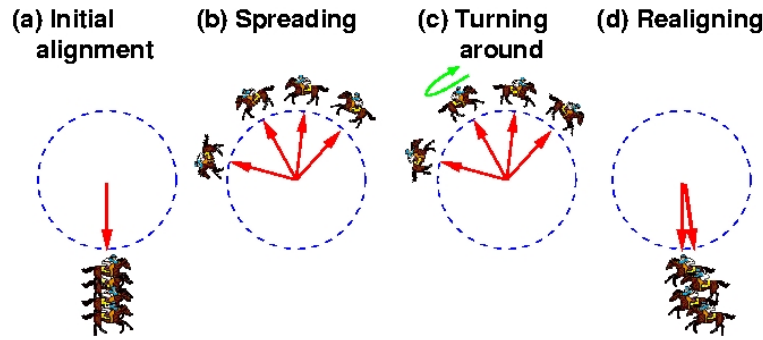


Fig. 2: Schematic drawing illustrating how the electric dipole echo works. Initially aligned dipoles (a) precess with different frequencies and spread in angle (b). Upon a field reversal their precession orientation is reversed (c). Finally the initial alignment is recovered (d). A small misalignment is due to decoherence.

More than 50 years after the invention of spin echo, the generation of echoes in the electric dipole moment of a Rydberg wavepacket has become possible [7]. An electric dipole moment precesses about a static electric field similar to the precession of a spin. Realization of echoes in the electric dipole moment is more challenging because of the faster electron motion and the stronger coupling to the environment.

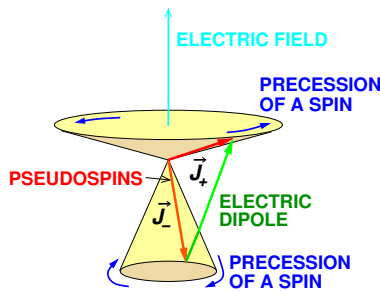


Fig. 3: Pseudospins (red) precess about the electric field (light blue) following Eq. (1). The direction of the precession is proportional to the electric field $\omega_{\pm} = \pm(3/2)nF$ and can be reversed by the field reversal $F \rightarrow -F$.

We consider here a hydrogenic Rydberg atom. The electron evolves around the nucleus following an elliptic orbit. The dipole moment averaged over an orbital period (Fig.3, green arrow) precesses about the static field applied ($\vec{F} = F\hat{z}$, light blue). More precisely, the so-called

pseudospins $\vec{J}_{\pm} = (\langle \vec{L} \rangle \pm n \langle \vec{A} \rangle)/2$ which are the sum of the angular momentum $\vec{L}$ and the Runge-Lenz vector $\vec{A}$ (approximately proportional to the dipole moment) obey an equation similar to that governing the dynamics of a spin in a magnetic field

$$\frac{d}{dt} \vec{J}_{\pm} = \omega_{\pm}(F) \vec{J}_{\pm} \times \hat{z}. \quad (1)$$

and precess around the electric field conserving their magnitude, $n/2$.

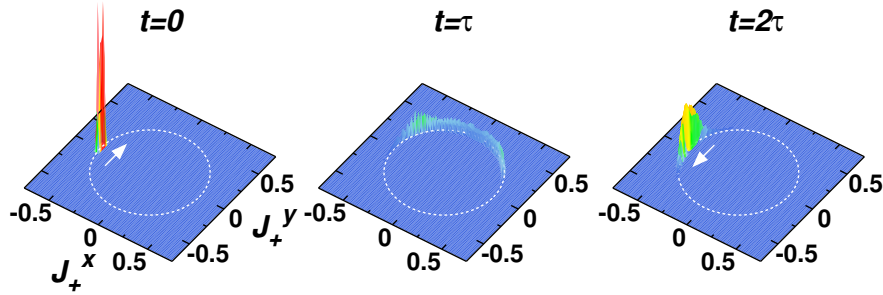


Fig. 4: Time evolution of the pseudospin distribution. As the pseudospin precesses about the static field, the initial distribution ($t = 0$) dephases during the evolution and spreads ($t = \tau$). At the field reversal, the direction of the precession is reversed and the distribution is refocused ($t = 2\tau$).

Similar to the spin echo, the reversal of the applied field $F \rightarrow -F$ reverses the direction of the precession $\omega_{\pm} \rightarrow -\omega_{\pm}$ and thus the time-reversal of the dynamics can be achieved. Quantum mechanically, wave-like nature implying that the orientation of the pseudospin can be determined only with a certain probability and has a spread in its magnitude and orientation. Since the precession frequency depends on the spin-magnitude n , the distribution (ensemble) of pseudospin dephases. After the time-reversal, this dephased distribution can rephase and exhibit an echo of the initial state (Fig.4). This echo of an electric dipole has been theoretically predicted and experimentally demonstrated [7] and is considered to be one powerful tool to realize quantum information registers using Rydberg atoms.

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2.3 Atoms in ultrashort laser fields

Staff: **Johannes Feist**, **Stefan Nagele**, **Klaus-Michael Schiessl**, **Emil Persson**, **Joachim Burgdörfer**

External: **Diego Arbó** (IAFE, University of Buenos Aires, Argentina), **Lee Collins** (Los Alamos National Laboratory, USA), **Kenichi Ishikawa** (University of Tokyo, Japan), **Xiao-Min Tong** (University of Tsukuba, Japan), **Barry Schneider** (National Science Foundation, USA)

Recent progress in laser technology has lead to shorter and shorter pulse durations. Nowadays, infrared laser pulses with a duration of a few femtoseconds (10^{-15} s), which is near the single-cycle limit at these wavelengths, are routinely available. Additionally, peak intensities that are well beyond the over-the-barrier ionization limit of most atoms can be reached. Sub-cycle ionization dynamics can be studied and taken advantage of in experiments. Due to the short timescales involved, measurements on a femtosecond or even attosecond (10^{-18} s) timescale become possible. Here, the direct imaging of a light wave's electric field in the near-infrared may serve as one outstanding example [1]. Time-domain observations of electron dynamics, which is even faster, are now experimentally feasible through the use of attosecond XUV pulses that can be produced through high harmonic generation [2]. Through this process, pulses in the XUV energy range (tens to hundreds of eV) with durations down to less than 200 as can be generated.

Dramatic enhancement of high-harmonic generation

High-harmonic generation (HHG) is the workhorse of many experiments in ultrafast optics. The basic mechanism of HHG is divided in two steps: First, the outermost electron is ionized by the strong electric field of the laser (tunneling through the distorted atomic potential). Then, the electron driven by the laser rescatters with the parent atom and can eventually recombine. Recombination with the remaining atomic core leads to high-frequent radiation on an attosecond timescale. Due to the periodicity of recombination events in a multi-cycle laser pulse a spectrum peaking at the harmonics of the driving frequency emerges. This radiation can be used to synthesize attosecond pulses needed for time-resolved experiments[1].

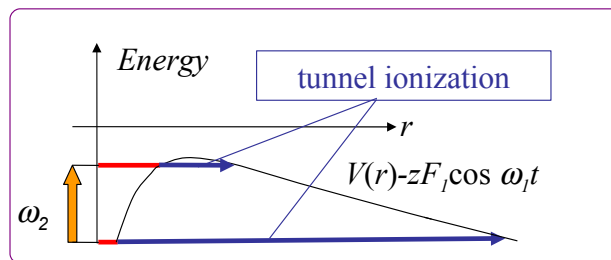


Fig. 1: Scheme of HHG with a resonant two-color laser pulse. The weak but (nearly)-resonant second color (ω_2) efficiently populates some excited state out of which tunnel ionization by the principal color (ω_1 , F_1) can take place much more easily, thus facilitating the first step of HHG.

One major difficulty is the low conversion efficiency of the incident laser to the high harmonics. A novel experimental setup suggested by Ishikawa [3] involves driving of HHG by two-color fields where one of the latter is weak but (near-)resonant to an intra-atomic excitation. Such a scheme allows to boost the high-harmonic output by several magnitude via enhancement of the first step of HHG - the ionization step (see figure 1).

As previous calculations [3] only covered the single-atom response of simple atoms such as hydrogen and singly-ionized helium, we have extended calculations to rare gases that are regularly used in HHG experiments. Multi-electron atoms have been treated in the framework of the single-active-electron approximation which allows one to calculate the quantum-mechanical response and the HHG spectrum.

The mechanism is found to work best in a regime of intermediate driving intensities, where the second resonant photon (color) provides the most efficient ionization channel in the system. At larger intensities tunneling ionization directly out of the ground state becomes the most efficient ionization channel, thus the net enhancement due to the second color becomes negligible.

In order to go one step further to possible experimental realization, we have developed a one-dimensional laser pulse propagation algorithm that is based on the full solution of the time-dependent Schrödinger equation for the atom in the laser field [4]. This method is capable of simulating the propagation of the light field and its harmonics in a dilute gas of atoms.

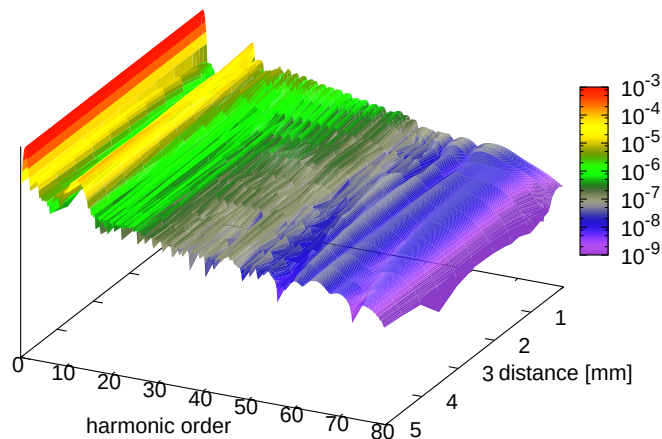


Fig. 2: Color plot of the intensity spectrum for a resonant two-color pulse propagating in a gas of xenon atoms. The principal intensity is $I_1 = 2 \times 10^{13} \text{W/cm}^2$.

An example for harmonic output in the case of two-color driving is presented in figure 2. We plot the yield as a function of the harmonic order and the propagation length. Observing the “smooth” growth of harmonics near the cut-off shows that the enhancement scheme remains intact also when accounting for pulse propagation [4]. Proof-of-principle experiments approaching this phenomenon under similar conditions are currently in progress [5].

Two-photon above-threshold double ionization of helium

Most research on ultrashort laser-atom interactions uses the Single Active Electron (SAE) approximation. This assumes that only one electron responds to the electrical field of the laser. In this picture, all other electrons are taken account of by using effective potentials to represent their influence on the active electron. While the SAE has been successfully used for a wide range of applications, it can not describe processes where more than one electron participates in the dynamics. This means that any processes in which electron correlation plays a role, e.g. double ionization, can not be described within this approximation. The simplest atom showing correlation effects is helium.

By using the ultrashort attosecond XUV pulses which are now available by High Harmonic Generation (HHG), it is possible to probe time-dependent processes governed by electron correlation for the first time. To investigate such processes, we have developed an ab initio numerical simulation based on integrating the Time-Dependent Schrödinger Equation (TDSE). The full wave function $\Psi(\vec{r}_1, \vec{r}_2)$ (without spin) in helium is six-dimensional. By using the fact that there is cylindrical symmetry in a linearly polarized laser field, this can be reduced to five active dimensions. Even then, this is a numerically very challenging problem which quickly gets too big for single processor workstations. We have therefore parallelized our code, enabling us to harness the power of modern supercomputers.

One of the effects of an intense XUV pulse impinging on helium is two-photon double ionization [6,7]. In this process, two photons interact with the two electrons, freeing both electrons from their binding to the nucleus. In the limit of a long laser pulse, this would be a two-step process: (1) The first photon frees one of the electrons, leaving a singly charged ion He^+ and a free electron at energy $\epsilon_1 = \hbar\omega - I_1$, where $I_1 \approx 24.6 \text{ eV}$ is the single ionization potential of helium. (2) The second photon interacts with the singly charged ion some time later, freeing the second electron, which is released at energy $\epsilon_2 = \hbar\omega - I_2$, with $I_2 \approx 54.4 \text{ eV}$ being the ionization potential of He^+ . This would give two sharp lines in the electron energy spectrum. When an ultrashort pulse with a duration of just a few hundred attoseconds is used, there are two modifications to this simple picture: (1) Because of Fourier broadening, the pulse does not have a sharply defined energy anymore - this leads to a corresponding Fourier broadening of the peaks in the electron spectrum. (2) The shorter the pulse, the higher the possibility that both photons interact with the atom within such a short period that both electrons are still close to the nucleus and close to each other when they are ionized. In this case, the ejection process for both electrons is modified through correlation. This leads to an additional component in the electron energy spectrum which is strongest at equal energy sharing, i.e. when both electrons acquire the same energy and stay close to each other during the ejection process.

In Fig. 3, we show (a) the probability distribution as a function of the distances (r_1, r_2) of the two electrons and (b) the energy spectrum of double ionization of He after exposure to a 225 attosecond, 91 eV XUV pulse with a peak intensity of 10^{15} W/cm^2 . In the radial probability distribution, two main parts can be identified: (i) The part of the wave function close to the two axes represents the singly ionized part, where one electron is close to the nucleus (i.e., r_1 or r_2 is small). (ii) The part near the diagonal $r_1 \approx r_2$ is the doubly ionized part, where both electrons are some distance away from the nucleus. By calculating the energy distribution of the doubly ionized part, we obtain Fig. 3(b). As the two-photon process dominates here, the observed distribution is close to the line where the total energy of the electrons is equal to twice the photon energy minus the energy $I_1 + I_2$ required to free both

electrons from the field of the nucleus, i.e. $E_1 + E_2 = 2\hbar\omega - I_1 - I_2 \approx 103$ eV. Fig. 4 shows the energy spectrum of Fig. 3(b), integrated over one of the electron energies. Here, an additional component between the two peaks is clearly visible, showing the contribution of non-sequential two-photon double ionization for ultrashort XUV pulses.

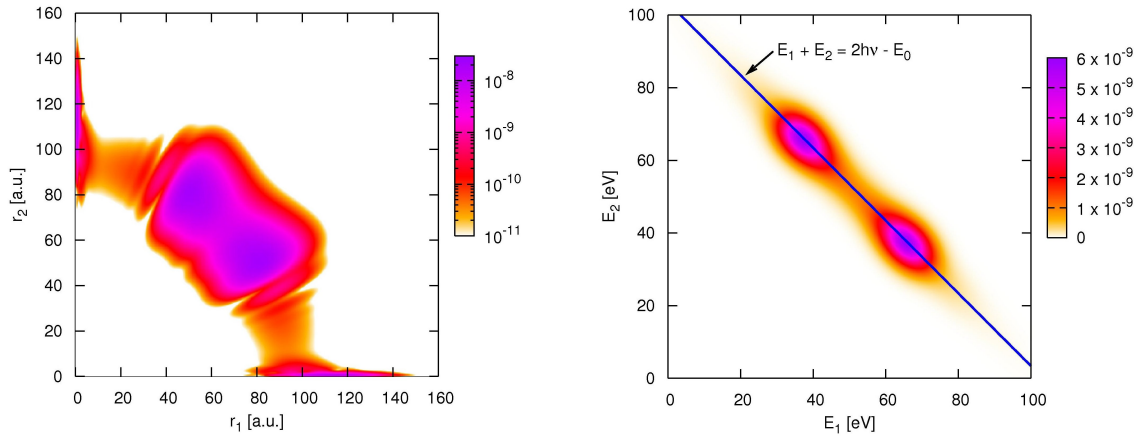


Fig. 3: Helium after exposure to a 225 as, 91 eV XUV pulse with intensity 10^{15} W/cm²: (a) Probability density $|\Psi|^2$ in radial space (r_1, r_2) , for total angular momentum $L = 2$. (b) The part of the same wave function that was doubly ionized by two photons, shown in energy space (E_1, E_2) (i.e., the two-electron spectrum).

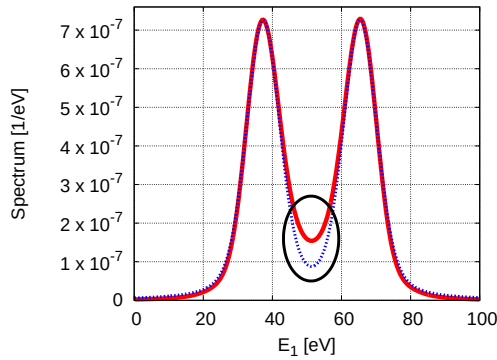


Fig. 4: Single electron spectrum after the same pulse as in Fig. 3. The red line is the numerically calculated spectrum (Fig. 3(b) calculated over E_2), while the blue line is a fit to the sequential double ionization peaks (peak shape as in [6]). At equal energy sharing (around 51 eV), the anomalous component is clearly visible.

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2.4 The dynamics of strong-laser cluster interaction

Staff: **Cornelia Deiss, Joachim Burgdörfer**

External: **Emily Lamour, Christophe Prigent, Jean-Pierre Rozet, Dominique Vernhet** (INSP, Univ. Paris 6 et 7, France)

Clusters are nanoparticles consisting of anything between a few hundred and several million atoms agglomerated at solid densities. When irradiated by intense (intensities above 10^{15}Wcm^{-2}) femtosecond laser pulses, rare gas clusters can emit keV x-ray photons, combining advantages of both solid and gaseous targets: the conversion of the incident infra-red laser into x-rays takes place with a high efficiency just like in solids, yet is relatively debris-free which is a typical advantage of gas targets [1]. Similar advantageous behavior has been observed for the emission of energetic electrons or highly charged ions, thus making the interaction of intense short and ultra-short laser pulses with clusters receive a lot of attention during the last decade [2].

The description of this system unites aspects of atomic physics, plasma physics, as well as solid-state and surface physics. In a simple picture [3], the dynamics during the laser-cluster interaction can be summarized as follows: 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.

The size of the system and the abundance of mechanisms at play provide challenges for the theoretical description of the interaction. Due to the large number of atoms ($N > 10000$) in a large cluster, 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]. The many-particle system is treated as an open effective mean-field one-particle system, in which many-particle effects such as elastic electron-ion scattering or electron impact-ionization are included via stochastic processes [4]. The mean field is evaluated at each time step by solving the field equations on a grid. Furthermore, we employ a classical-trajectory Monte Carlo (CTMC) test particle discretization with a typical representation fraction of $\alpha \simeq 0.1$, thereby drastically reducing the number of test particles to be followed thus achieving reasonable computation times even for clusters as large as $N \sim 10^6$. The roles played by different effects such as cluster polarization, surface disintegration and microscopic atomic dynamics (elastic electron-ion scattering, electron-impact ionization etc.) can thus be studied. Particular emphasis is put on the inclusion of various ionization mechanisms such as field ionization, electron-impact ionization, two-step ionization (impact excitation followed by impact ionization) or barrier suppression by neighboring ionic potentials [5].

The benchmark for our simulation results are experimental data from x-ray spectroscopy. The measurements of the 3.1 keV characteristic K-shell x-ray radiation emitted from argon clusters [1] provide an excellent yard stick to calibrate the dynamics of the interaction on the short time-scale of the irradiating laser pulse ($\tau > 60 \text{fs}$). As hot electrons create inner-shell vacancies in the cluster ions by impact ionization, the production of x-ray photons directly probes the high energy tail of the electron energy distribution. A comparison of simulation

results with experimental data is shown in figure 1. We achieve good agreement for the intensity dependence of the total x-ray yield, as well as for the evolution with varying laser pulse length.

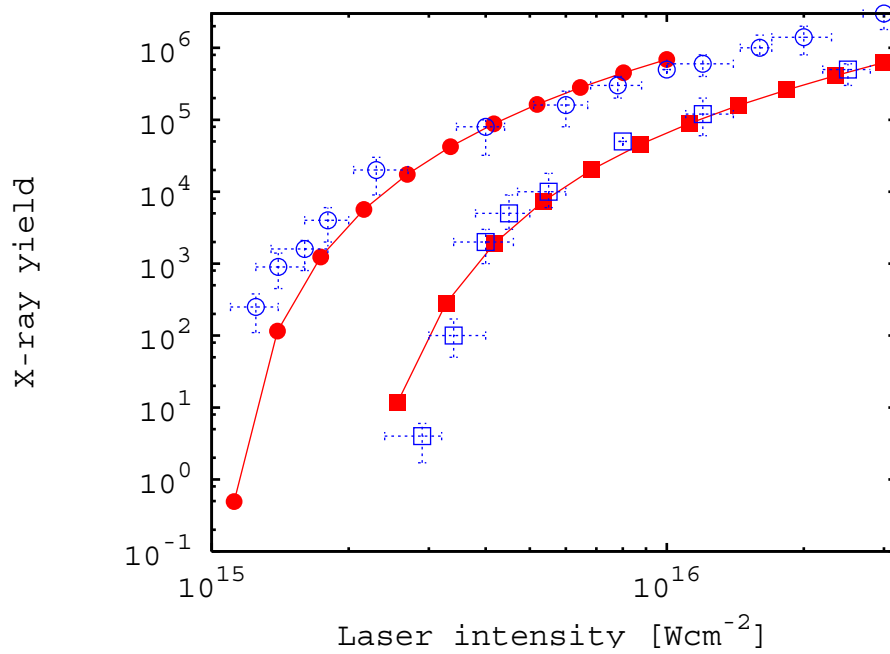


Fig. 1: Intensity dependence of the total x-ray yield from clusters with $N = 4 \times 10^4$ argon atoms irradiated by a pulse of duration (FWHM) 60fs (squares) or 150fs (circles). The simulation results (full symbols) compare well to the experimental data (empty symbols).

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Chapter 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.

3.1 Many-Particle Systems Under Gravity

Staff: **Christian Tutschka**

External: **Karl Grill** (Institut für Statistik und Wahrscheinlichkeitstheorie, TU Wien)

Recently, we uncovered a well-delineated phase separation for a one-dimensional classical fluid with next neighbor interactions in a weak gravitational field [2]. We showed that one can identify, with probability tending to one as the size of the system approaches infinity, three regions: a dense part at the bottom, which we called the condensate, a dilute part at the top, called the gas, and in between these two phases an interface whose relative width goes to zero as the number of particles goes to infinity.

The next step was clearly to drop the nearest neighbor assumption. The global effect of weak gravitational forces on the equilibrium structure of hard rods with finite-range interactions has been studied in [1]. It turned out that the overall qualitative behavior we found for the special class of next neighbor interactions prevails in this more general situation. That is, the phenomenon appears to be robust with respect to changes in the interactions.

The purpose of the paper [3] was to extend this work to D -dimensional space. To allow for the phenomenology without unnecessary structural details, we considered a particle system in a subset Λ of the D -dimensional integer lattice $\mathbb{Z}^D$, with finite-range forces, and in a weak external (gravitational) field.

The corresponding Gravitational Phase Separation Theorem is stated and proved in [3].

An illuminating application of our theory is depicted in Figure 1. It shows a typical isothermal equilibrium state of the next neighbor lattice gas under gravity in a 2D container $\Lambda = [1, 1000] \times [1, 2000]$, with a density of $\rho = 0.25$, a reciprocal temperature $\beta = 2$, and an acceleration due to gravity g set equal to 0.00141565.

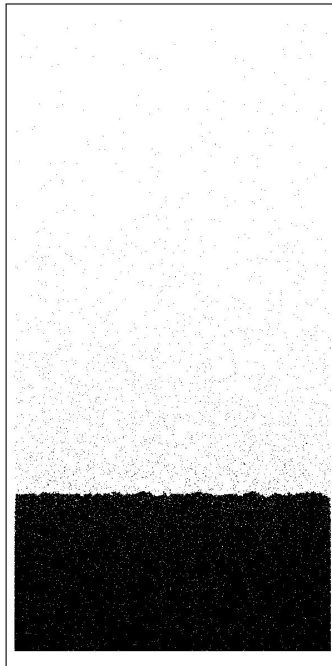


Fig. 1: Typical isothermal particle configuration of the nearest neighbor lattice gas under gravity on a 2D lattice of 1000×2000 gridpoints (particles in black). The gravity acts along the vertical axis. $\rho = 0.25$, $\beta = 2$, and the acceleration due to gravity g taken to be 0.00141565.

Notice, first, that we can see a condensed phase at heights below 500 which contains only small bubbles of a gas phase. At relative heights greater than 0.25, we find a gaseous phase with only small drops of condensate and, in addition, we have an approximate barometric equation (see, e.g., Kittel [5]).

Both the condensate and the gas use up an almost fixed fraction of the available space, whereas the width of the interface where the two phases mix is small, i.e., of order $1/\log N$, in comparison to the total height N of the system.

Moreover, it can be shown that if we want a gaseous phase, the smallest order that can be achieved for the relative width of the interface is $1/\log N$.

Finally, we point out that many-particle systems with a density profile going from minimum to maximum density over a relatively small interval arise in gravitational astrophysics and space science, as well (see, e.g., Stahl, Kiessling, and Schindler [6]). There, local particle densities of core-atmosphere type signify the low temperature phase of a gravitational phase transition. The existence of a gravitational phase transition has been proved by Kiessling in 1989 [4].

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3.2 Cross-over phenomena in the critical behavior of simple liquids

Staff: **Gernot J. Pauschenwein**, **Gerhard Kahl**

External: **Elisabeth Schöll-Paschinger** (Institut für Experimentalphysik, Universität Wien), **Jean-Jacques Weis** and **Jean-Michel Caillol** (Laboratoire de Physique Théorique, Université Paris-Sud, France)

The exact determination of the critical properties of a fluid in terms of the location of its critical point and of its universality class represents a formidable challenge both to theoretical approaches as well as to computer simulations. During the past decades significant progress has been made in the development of liquid state theories that remain reliable even in close vicinity to the critical point. This concerns not only the localization of the gas-liquid coexistence branches; also the resulting critical exponents reproduce the exact ones rather well. The most prominent representatives of these advanced liquid state theories are the Hierarchical Reference Theory (HRT) [1] and the Self-consistent Ornstein-Zernike Approximation (SCOZA) [2,3]. While HRT successfully merges concepts of liquid state theory with renormalization group theory, SCOZA imposes thermodynamic self-consistency between different thermodynamic routes [4].

Motivated by recent experimental investigation on charged colloids which interact via long-range effective interactions of variable range [5] we have posed the question if liquid state theories are able to trace a possible change in the critical behavior of such a system as the range of the interaction varies. To this end we have considered a simple model fluid where the potential $\Phi(r)$ is a linear combination of two interactions, exhibiting different, but well-established critical behavior. The first one belongs to the three-dimensional Ising (IS) universality class, while the other one displays a mean field (MF) behavior. The total interaction is assumed to be given by

$$\Phi(r) = \Phi_{\text{IS}}(r) + \xi^2 \Phi_{\text{MF}}(r), \quad (1)$$

where the dimensionless parameter ξ^2 represents the relative weight of the two contributions: as we vary ξ^2 we expect to observe a cross-over in the critical behavior of the system which we can trace via the critical exponents.

For the reference system we have considered the restricted primitive model (RPM), i.e., an equimolar binary mixture of equally-sized and oppositely charged hard spheres of diameter σ and charges $\pm q$:

$$\Phi_{\text{IS}}(r) = \begin{cases} \infty & r \leq \sigma \\ \pm \frac{q^2}{r} & r > \sigma \end{cases} \quad (2)$$

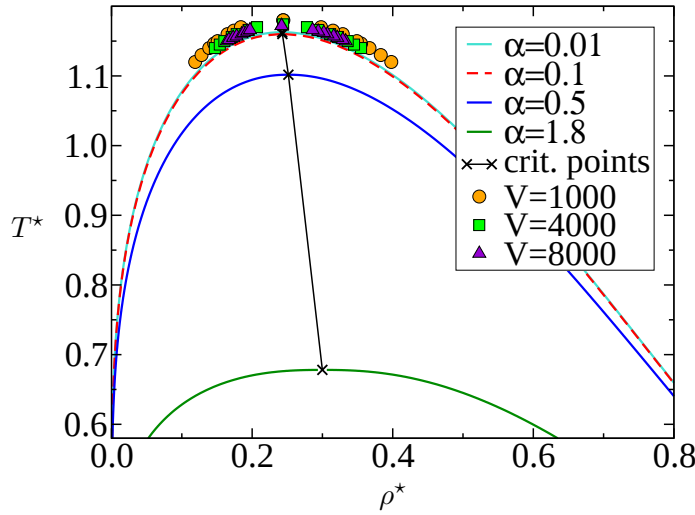


Fig. 1: Coexistence curves for our model system [cf. (1)] for $\xi^2 = 1$ and different values of α as indicated in the legend (in units of σ^{-1}); SCOZA results – lines, simulation results – symbols. The critical points are indicated by the crosses and are connected with the solid black line. For decreasing α the curves converge against the simulation data, obtained for different sizes of the simulation box and $\alpha = 0$. The following reduced units are used: $T^* = k_B T / \Phi(\sigma)$ and $\rho^* = \rho \sigma^3$.

('+' for particles with equal charges, '-' for different charges). For the system that belongs to the MF universality class we have chosen a Yukawa potential where the screening length becomes infinite (which corresponds to the Kac limit [6]), i.e.,

$$\Phi_{\text{MF}}(r) = - \lim_{\alpha \rightarrow 0} \frac{q^2}{r} \alpha^2 e^{-\alpha r / \sigma}. \quad (3)$$

Note that as $\alpha \rightarrow 0$, the screening length becomes infinitely long, while the strength vanishes with α^2 , keeping, however, the field content (3D integral) finite.

Our choice for these potentials is on one side motivated by the fact that the rather intricate formalism of SCOZA simplifies for Yukawa potentials to some extent. On the other hand, this type of potential approximates the effective interaction between the charged colloidal particles rather accurately.

To confirm the SCOZA results our collaborators in Paris have performed grand-canonical Monte Carlo simulations. A detailed account of the results is given in [7].

In Figure 1 we show the phase diagram of our model system for $\xi^2 = 1$. While the simulations can be performed for exactly $\alpha = 0$ by adding a MF-term to the energy (for details see [7]), SCOZA can only be applied to systems with a finite α -value. The coexistence curves, calculated for α from 1.8 down to 0.01, display the tendency that the SCOZA results 'converge' with decreasing α towards the data of the Kac potential. In particular, for the smallest α value, agreement with the simulation data is already excellent indicating the reliability of the SCOZA results.

In an effort to identify the critical behavior of our system we have calculated with SCOZA the thermodynamic properties and have extracted from these data the critical exponent γ . To be more specific, we have recorded the isothermal compressibility, χ_T , as we approach

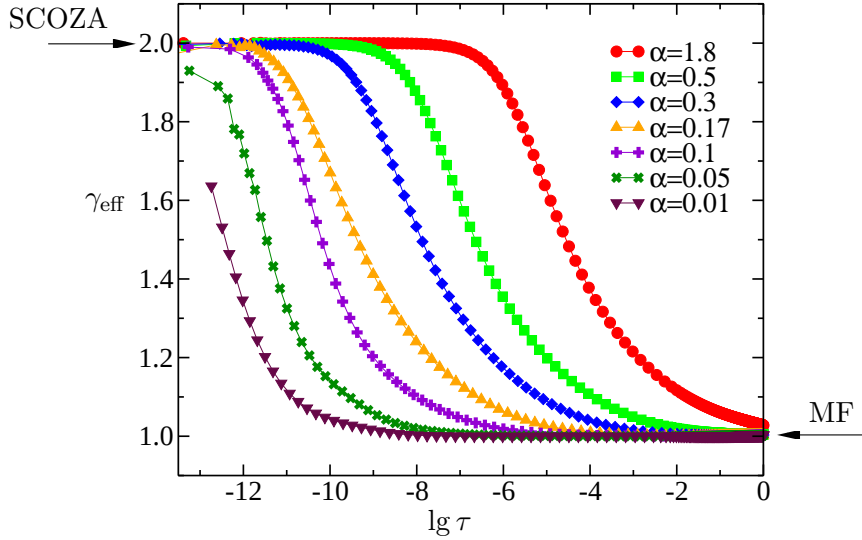


Fig. 2: Effective critical exponent γ_{eff} for different values of α as indicated in the legend (in units of σ^{-1}) versus $\tau = (T - T_c)/T_c$ obtained from SCOZA calculations.

the critical point along the critical isochore from above. As T tends towards the critical temperature T_c from above, we define an effective critical exponent γ_{eff} via

$$\gamma_{\text{eff}} = -\frac{\partial(\log \chi_T)}{\partial[\log(T - T_c)]}. \quad (4)$$

γ_{eff} is displayed in Figure 2 as a function of $\tau = (T - T_c)/T_c$, calculated for different α -values ranging from 1.8 down to 0.01. We observe that γ_{eff} varies between 1, representing γ_{MF} , and 2, i.e., γ_{SCOZA} as we approach the critical temperature, i.e., as $\tau \rightarrow 0^+$. For $\alpha = 1.8$ we find $\gamma_{\text{eff}} = 2$ for $\tau \lesssim 10^{-4}$, i.e., we observe a critical behavior that is obviously non-MF like. However, as α becomes smaller, the MF character of the potential becomes dominant; concomitantly, a MF critical behavior can be identified via γ_{eff} for τ down to 10^{-10} . We note that for small α -values the calculations become very time-consuming and are prohibitively expensive for $\alpha \lesssim 0.01$. Thus we conclude that the critical behavior is likely to be MF over the *entire* τ range at $\alpha = 0$, as expected in the Kac limit [6,8].

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3.3 The role of diffraction in transport interference effects through quantum billiards

Staff: Iva Brezinova, Stefan Rotter and Joachim Burgdörfer

External: **Christoph Stampfer** (Solid State Physics Laboratory, ETH Zürich, Switzerland), **Ludger Wirtz** (Inst. for Electronics, Microelectronics and Nanotechnology, Villeneuve d'Ascq, France)

Phase coherent electron transport through mesoscopic systems gives rise to several effects not explainable in the framework of a classical theory. This is due to the fact that electrons display quantum interference. Quantum mechanically, the paths connecting the entrance and exit lead of the electron billiard carry along a phase which is equivalent to the classical action S_q , in which the length and directed enclosed area of the path enters. As a consequence not only the paths themselves, but the information on their relative phases affects transport through ballistic systems. At zero magnetic field, the constructive interference of paths of time-reversal symmetry always produces an enhancement of the resistance of the billiard compared to the classical prediction for ballistic transport. This effect is known as weak localization. The resistance decreases upon applying a perpendicular magnetic field B giving rise to the characteristic peak as function of B . Due to current conservation, increased resistance leads to reduced conductance, which is proportional to transmission within the Landauer formalism for ballistic transport. For the weak localization dip in conductance an intuitive picture of the underlying mechanism has been lacking, since in transmission there are, in general, no symmetry related classical paths.

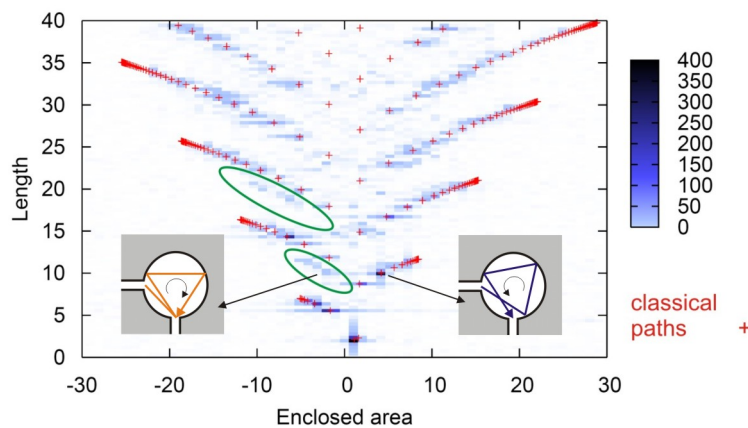


Fig. 1: The absolute square of the Fourier transform of the quantum mechanical transmission amplitude $t_{22}(k, B)$ for the circular billiard from mode 2 to 2 in the leads. The weights of the quantum mechanical transmission amplitude are compared to the lengths and directed enclosed areas of classical paths (red crosses). Inset: A classical (right) and a diffractive path (left) are assigned to the corresponding weighting in the length-area distribution.

In contrast to previous proposals applicable only to chaotic billiards [1], we implement a theory based on diffraction at the open lead mouths [2,3] and thus succeed in reproducing weak localization in a regular billiard for the first time via explicit path interference. Diffraction at the leads has been neglected up to now although it is prominently present in real experiments operated at moderate Fermi wave lengths.

By analyzing quantum mechanical data for the circular billiard (regular system) we identify in the spectrum of lengths and directed enclosed areas of quantum mechanical probability amplitudes diffractive paths which are responsible for interference and weak localization (Fig. 1). To quantitatively establish the importance of diffraction we calculate weak localization by explicitly including diffractive paths. We reach remarkably good agreement with quantum mechanical data (Fig. 2). We conclude that diffraction is a crucial process for weak localization in quantum billiards. The work in progress is to extend our diffractive semiclassics to chaotic billiards .

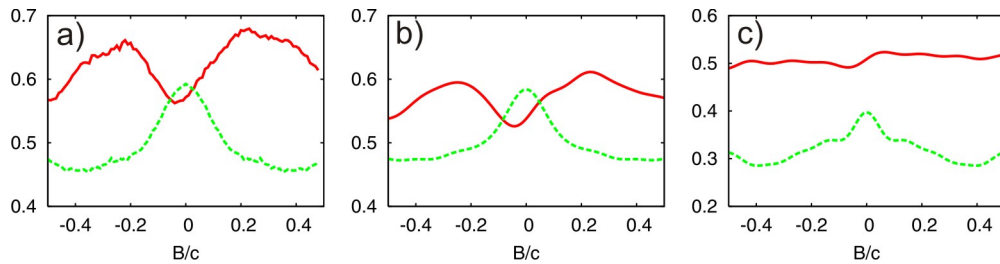


Fig. 2: Weak localization of conductance (red solid line) and resistance (green dashed line): (a) Quantum mechanical data. (b) Semiclassical theory using classical paths and diffractive paths. (c) Semiclassical theory using classical paths only. All calculations contain only pathlengths up to $L_{max} = 40$ leading to broken unitarity.

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3.4 Interaction of Ions and Atoms with Metal Surfaces

Staff: **Beate Solleder, Georg Wachter, Christoph Lemell, Joachim Burgdörfer**

External: **K. Tókési** (ATOMKI, Hungary), **L. Wirtz** (CNRS Lille, France)

The interaction of ions and atoms with surfaces results in the emission of a large number of secondary particles observed in experiment. These include sputtered target atoms, photons, and electrons. During the past year we have concentrated on the simulation of electron production by the interaction of projectiles with metal surfaces along their trajectory. For many scenarios we are now able to qualitatively *and* quantitatively compare our results with experimental data.

The three main contributions to the total electron yield are schematically depicted in Fig. 1: a) When an ion approaches a metal surface interaction with its own image charge shifts

its electronic levels upwards while at the same time lowering the potential barrier separating target and projectile. This initiates electron transfer from the target into highly excited projectile states. As a consequence of the subsequent deexcitation processes electrons are emitted (“potential electron emission” (PE), [1]). b) Upon touchdown on the surface direct scattering processes between target electrons and the projectile become possible. In such binary encounters the projectile transfers momentum on the electron which may lead to electron emission (“kinetic electron emission” (KE)). c) Finally, electrons produced by PE and KE processes may be emitted towards the surface from where they may be backscattered or may produce secondary electrons. Such processes are described at the end of this chapter.

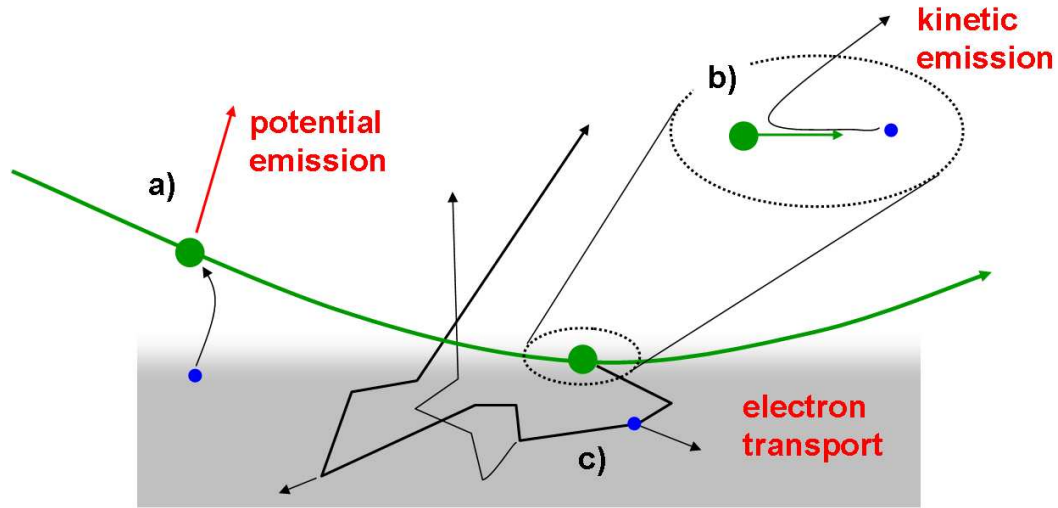


Fig. 1: Schematic picture of projectile-induced electron emission processes: a) electron transfer sets in at large distances from the surface leading to potential emission processes. b) Head-on collisions between projectile and target electrons cause kinetic electron emission. c) Electron transport through the target material generates secondary electron cascades and contributes to the total electron emission yield.

Potential electron emission

After the initial electron transfer from the target to highly excited projectile states a sequence of deexcitation processes leads to emission of a large number of electrons. Depending on the projectile’s distance from the surface different pathways to emission can be distinguished (Fig. 2): With decreasing ion-surface distance highly excited projectile levels may become unbound due to interaction with the projectile’s own image charge. This leads to “peeling off” of high lying energy levels while lower lying levels are populated by target electrons. An autoionization cascade at close distance to the surface also involving target electrons leads to filling of inner-shell holes.

Fig. 2 displays the electron emission characteristics caused by the impact of N^{6+} ions on an iron surface under a grazing angle of incidence. The small impact angle leads to the reflection of the ion trajectories at the topmost atomic layer. The emission spectrum includes electrons emitted during the approach of the ion to the surface as well as after reflection. Low-energy electron emission sets in at about 20 a.u. above the jellium edge by peeling off the projectile shell with primary quantum number $n = 8$. Subsequently, lower levels get depleted one after the other dominating the low-energy emission spectrum. Another contribution to this part

of the spectrum are Auger electrons from high- n levels ($n > 2$). L-Auger electrons (decay into $n = 2$) are emitted with energies above about 50 eV. At energies larger than > 250 eV, K-Auger electron emission (decay into $n = 1$) becomes increasingly important.

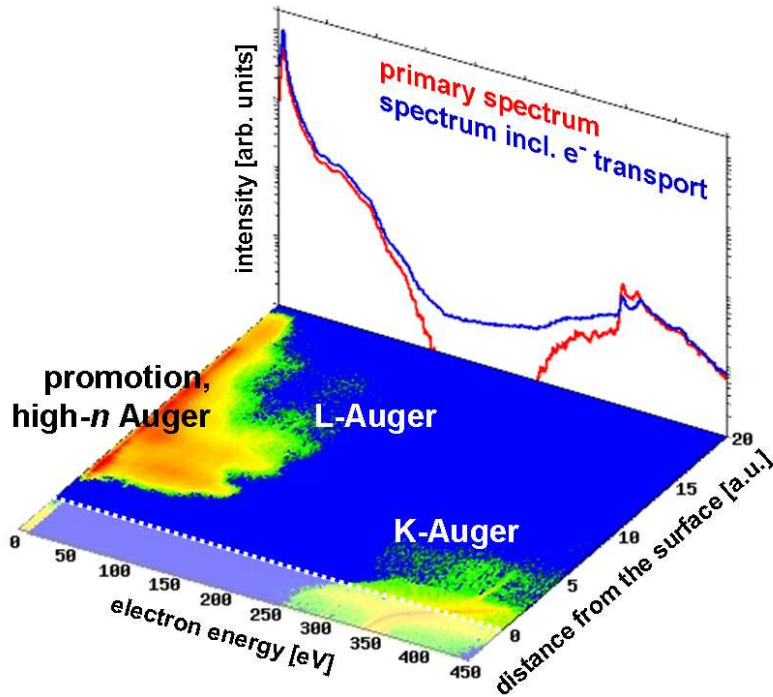


Fig. 2: Spatially and energy resolved potential emission spectrum of electrons during the impact of N^{6+} ions on a Fe surface. False color plot of the energy and point of emission (ion-surface distance) distribution. Integration over the distance of emission gives the primary spectrum (red curve in the projected spectrum). The total electron spectrum including electron transport in the solid is also shown (blue curve, cf. text).

Kinetic electron emission

Following up on our earlier work started in 2005 [2] we have simulated kinetic electron emission in grazing atom-surface interactions. Classically, the process can be described as elastic scattering of a target electron off the heavy projectile. For a head-on binary encounter, the maximum momentum transfer is given by $\Delta p_{max} = 2m_e v_p$, where m_e and v_p are the electron mass and the projectile velocity, respectively. If electrons in the target could be described by an ideal Fermi gas (i.e., electrons have kinetic energies between 0 and a maximum value $\varepsilon_F = m_e p_F^2 / 2$) a minimum projectile velocity would be required to allow the accelerated electron to escape the surface. The experimentally observed behavior does not show such a sharp threshold.

A detailed investigation of the momentum distribution of target electrons reveals that also states with momenta higher than the Fermi momentum p_F can be found due to correlation (electron-electron interactions not described by the theory of a non-interacting Fermi gas) and corrugation (lattice structure of the target) effects. Using ab-initio codes employing density-functional theory [3] we have calculated the electron densities near the target surface. We have derived the momentum distribution of electrons as a function of the distance from the surface (see Fig. 3). Based on these distributions we were able to reproduce experimental results [4].

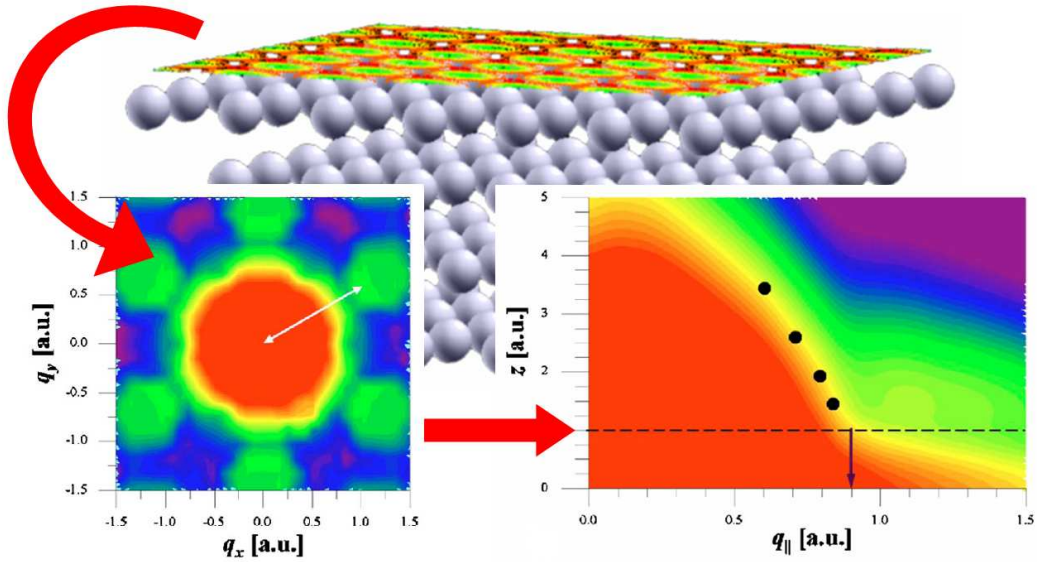


Fig. 3: From the electron density in front of metal surfaces we derive the momentum distribution as a function of the distance from the surface.

Electron transport

A substantial amount of electrons produced by the processes just described is emitted towards the surface. Most of them penetrate the solid where they can be either elastically or inelastically scattered in the target. Thereby, plasmons or electron-hole pairs are excited leading to the production of secondary electrons, if the excitation energy is high enough to raise the electrons above the vacuum level.

We have simulated electron transport through solids employing the classical trajectory Monte Carlo technique where we follow all trajectories of primary as well as subsequently produced secondary electrons until they are emitted from the surface or stopped in the bulk. Electron transport changes the original emission spectrum (red line in Fig. 2) dramatically. While the emission of high energy electrons is suppressed an increased amount of low energy electrons can be detected in experiments (blue line in Fig. 2).

Recently, spin dependent processes were included in our simulations of potential emission and electron transport to model the interaction of ions and electrons with magnetized surfaces. Good agreement between experimental data and our results was found [5]. In the near future, we will apply our model to simulate the transport of polarized electron beams through paramagnetic materials (first results are described in [6]).

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3.5 Ballistic quantum transport through nanostructures

Staff: **Florian Libisch, Florian Aigner, Johannes Feist, Bernhard Weingartner, Stefan Rotter, Joachim Burgdörfer**

External: **J. Cserti** (Eötvös University Budapest, Hungary), **A. Kormányos** (University of Lancaster, UK), **H. Schanz** (Göttingen University, Germany), **C. Stampfer** (ETH Zürich, Switzerland), **L. Wirtz** (CNRS Lille, France)

Time evolution of wave packets in chaotic systems

While the motion of a classical particle through a billiard system follows a well-defined trajectory, a quantum mechanical wavepacket spreads. This follows from the non-linear dispersion relation $E \propto k^2$ of a massive particle. As a consequence, the particle may be found at different, disjoint locations with nonvanishing probability. To investigate the consequence of this property of quantum mechanics, we calculate the time evolution of a particle incident on a mushroom-shaped billiard [see Fig. 1 (a)] [1].

From a classical point of view, after a time τ , the particle has either left the cavity [e.g. by following the blue, dashed trajectory indicated in Fig. 1 (a)], or is still inside [e.g. by following the green, dotted trajectory indicated in Fig. 1 (a)]. A quantum mechanical gaussian wavepacket describing the particle [see Fig. 1 (b)] will, however, split up, indicating finite probabilities for finding the particle either inside the mushroom head or outside [see Fig. 1 (c,d)]. In a sense, the particle is thus inside the mushroom head and in the lead at the same time, demonstrating the non-locality of quantum mechanics.

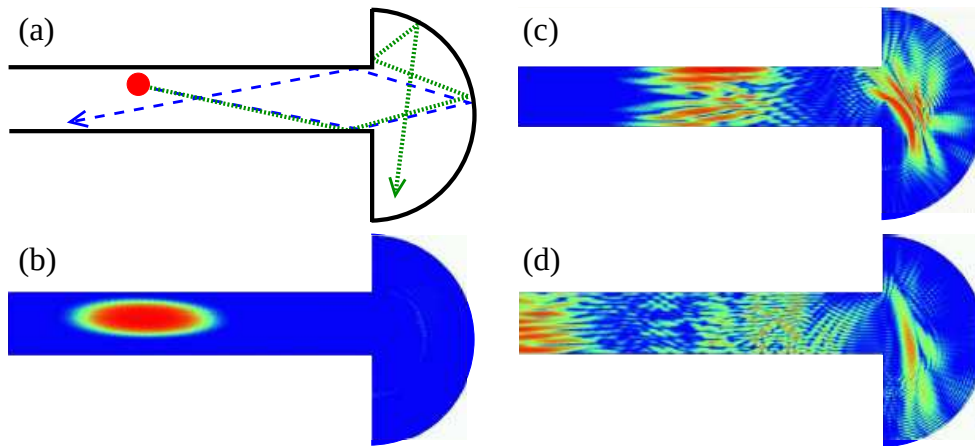


Fig. 1: (a) Classical mushroom billiard with one incident particle. Two possible classical trajectories featuring only a small difference in initial velocity are shown. (b) A quantum mechanical analogon of (a). (c) After evolving for a short time (the time it would take the classical particle to reach the end of the trajectories in (a)), the wavepacket has split into two disjoint regions. (d) The wavepacket has now spread out over most of the area.

Disordered 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 [2]. A N-S hybrid structure consisting of a superconducting lead attached to a normal ballistic cavity (see Fig. 2) is called an Andreev billiard [3]. Due to the peculiar properties of the S-N 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 [5]. Accordingly, the corresponding wavefunctions for electron and hole sheet closely resemble each other [see Fig. 2(a)].

If disorder is introduced into such a system, diffractive scattering destroys these retracing properties. We investigate the transition from a perfectly regular system of periodic orbits to a chaotic one by increasing the strength of the disorder potential. We find that a relatively weak disorder is already sufficient to significantly reduce the similarity between electron and hole wavefunctions [see Fig. 2(b)]. Furthermore, the prominent condensation of the wavefunction along bundles of classically periodic orbits vanishes in the case of disordered Andreev billiards [4].

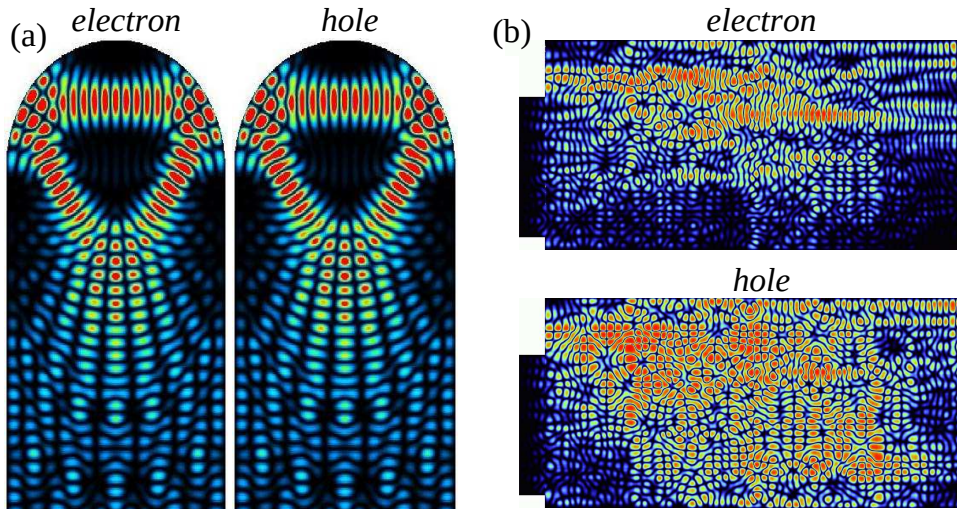


Fig. 2: (a) Electron and hole wavefunction of a regular half-circle Andreev billiard. The wavefunctions closely resemble each other, and are enhanced along a classically periodic orbit. (b) Electron and hole wavefunction of a disordered rectangular Andreev billiard. The disorder strength is taken at 10% of the Fermi energy.

Nanowires with a mixed classical phase space

In most materials, the conductance (or the lack of it) is governed by disorder. For example, the strength and distribution of disorder determine whether a wire behaves like a “normal” wire in which the conductance decreases inversely with increasing length, or like an insulator, where conductance is exponentially suppressed with length [6]. 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 ballistic nanowire, the nanowire with one-sided surface disorder in a magnetic field [7,8]. Such a wire, where one side is perfectly flat while the other side has surface disorder, will possess a mixed classical phase space if the system is subjected to a perpendicular magnetic field. *Skipping* trajectories do not interact with the disordered surface and are thus perfectly transmitted. These trajectories form a so-called “regular island”. All other trajectories are chaotic, forming a “chaotic sea”. Classically, this leads to directed chaotic transport, where transport in one direction proceeds primarily in the regular island, while transport in the other direction proceeds in the chaotic sea. Nonetheless, the total transmission probability is the same regardless of direction, as this is an unbiased system [9].

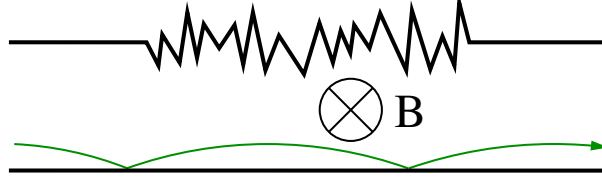


Fig. 3: (a) Schematic of a nanowire with one-sided surface disorder in a magnetic field. Shown is one skipping orbit (green).

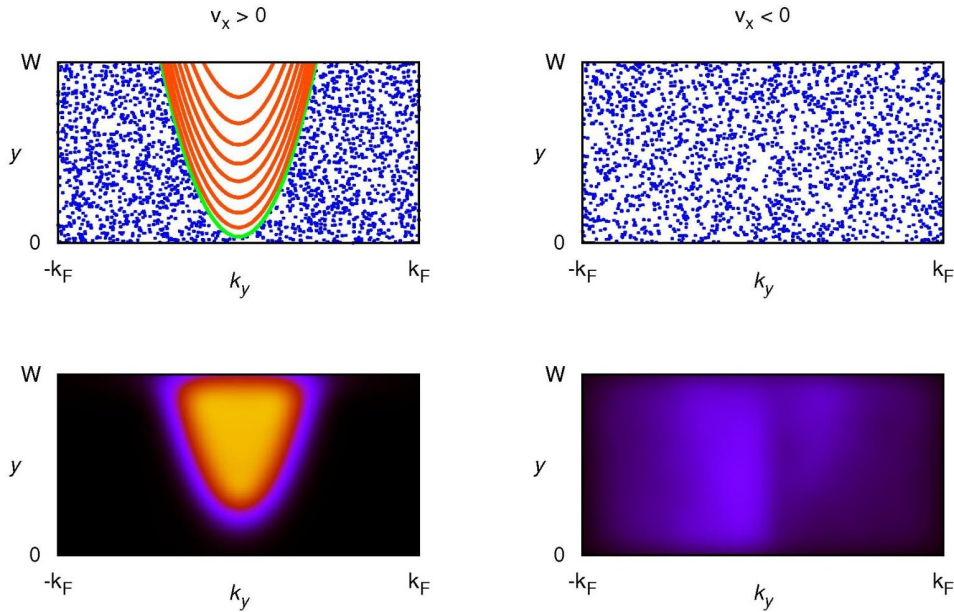


Fig. 4: (a) Classical phase space distribution of the wire with one-sided surface disorder (top) and corresponding quantum (Husimi) distribution (bottom) for electrons entering from the left ($v_x > 0$) or right side ($v_x < 0$).

We have investigated the signature of the mixed phase space in the quantum mechanical transport properties of such a system. While in classical mechanics, each starting point in phase space either leads to transmission or reflection, the situation is different in quantum mechanics: each of the transverse modes n in the leads has some transmission probability T_n . A simple picture for this is that due to the Heisenberg uncertainty relation, each quantum

mode corresponds to a finite cell of initial conditions in phase space, only some of which lead to transmission. According to this picture, one would only expect channels with transmission probability $T = 1$ if there is no random scattering for a significant portion of the trajectories belonging to that mode. This condition is fulfilled in the transport direction which contains the large regular island of skipping trajectories. Accordingly, the Husimi distribution (a quantum mechanical analogue of a phase space distribution) for all strongly transmitted modes closely mirror the regular island in phase space. In the direction which does not contain a regular island, the Husimi distribution is smeared out over the whole classically chaotic region.

Quantum-to-classical correspondence of transmitted states

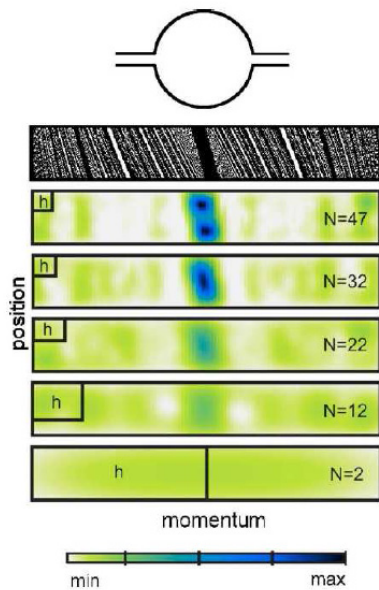


Fig. 5: Phase space analysis of a circular shaped billiard. Top: The classical phase space consists of regions corresponding to full transmission (black) or full reflection (white). Quantum Husimi distributions of transmitted states correspond nicely to the black regions in the classical phase space. If the number of quantum states N in the phase decreases, these regions cannot be resolved any more, and the Husimi distributions become almost uniform (bottom).

Transport through a quantum system is characterized by a transmission- and a reflection amplitude for each quantum channel. By studying the statistics of a large set of these transmission amplitudes, one can determine important features of the quantum billiard, such as the average dwell time or the presence of surface disorder [10].

A chaotic quantum dot will show transmission and reflection amplitudes which are uniformly distributed. If the energy of the particle is high, and transport through the system is dominated by short trajectories, considerable deviations from a uniform distribution have been found [12]. Such systems exhibit an excess rate of transmission probabilities very close to 0 and 1 - instead of a stochastic mixture of transmission and reflection, system specific signatures resembling classical transport arise.

We study the correspondence of quantum transmission probabilities and classical trajectories. The best way to directly compare quantum transport to classical transport is to look at the phase space of the particle entering the cavity. Each classical trajectory passing through the system can be characterized by the transverse position in the lead and the transverse momentum at which it enters the quantum dot. In such a two-dimensional classical phase space (see Fig. 5), we find regions corresponding to transmitted trajectories (black) and regions corresponding to reflected trajectories (white).

The same phase space can also be investigated quantum mechanically: Similarities between the quantum Husimi distributions and the classical phase space are obvious: Strongly transmitted quantum states occupy those regions in phase space, which also in the classical phase space refer to transmission. (See also [13].)

The phase space has a volume of Nh , where N is the number of quantum states supported by the lead. A smooth crossover from quantum transport to classical transport, governed by the quantum number N . As the quantum number N is increased from 2 (Fig. 5, bottom) to $N = 47$ (towards the classical limit), more and more features of the classical phase space become visible in the quantum calculation. The classical phase space can be seen as the high-energy limit of the quantum Husimi distributions.

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Appendix A

Staff Members

Professors

Tel.: 01/58801 + Ext.

BURGDÖRFER Joachim
burg@concord.itp.tuwien.ac.at

Ext.: 13610

SCHWEDA Manfred
mschweda@tph.tuwien.ac.at

Ext.: 13640

Associate Professors

BALASIN Herbert
hbalasin@tph.tuwien.ac.at

Ext.: 13624

DIRL Rainer
(retired since 1/10/2006)
rdirl@tph.tuwien.ac.at

Ext.: 13617

KAHL Gerhard
gkahl@tph.tuwien.ac.at

Ext.: 13632

KRAEMMER Ulrike
on leave until 8/07/2007

KREUZER Maximilian
kreuzer@hep.itp.tuwien.ac.at

Ext.: 13621

LEMELL Christoph
lemell@concord.itp.tuwien.ac.at

Ext.: 13612

REBHAN Anton
rebhana@tph.tuwien.ac.at

Ext.: 13626

SVOZIL Karl
svozil@tuwien.ac.at

Ext.: 13614

Assistant Professors

Tel.: 01/58801 + Ext.

AIGNER Florian

(since 16/03/2006)

aigner@concord.itp.tuwien.ac.at

Ext.: 13633

DEISS Cornelia

cornelia@concord.itp.tuwien.ac.at

Ext.: 13633

FEIST Johannes

(since 16/03/2006)

feist@concord.itp.tuwien.ac.at

Ext.: 13627

LIBISCH Florian

florian@concord.itp.tuwien.ac.at

Ext.: 13618

PERSSON Emil

emil@concord.itp.tuwien.ac.at

Ext.: 13630

ROTTER Stefan

(on leave)

rotter@concord.itp.tuwien.ac.at

Ext.: 13618

YOSHIDA Shuhei

shuhei@concord.itp.tuwien.ac.at

Ext.: 13611

Administrative Staff**MÖSSMER Elfriede**

moessmer@pop.tuwien.ac.at

Ext.: 13601

UNDEN Roswitha

unden@tph.tuwien.ac.at

Ext.: 13602

HÖLLER Heike

(SFB 016 secretary)

adlis@tuwien.ac.at

Ext.: 13625

Professor Emeritus and Retired Faculty

ADAM Gerhard
gadam@tph.tuwien.ac.at
Tel.: 01/58801 + Ext.
Ext.: 13651

GRAU Dietrich
d.grau@kabsi.at

KASPERKOVITZ Peter
kasperko@tph.tuwien.ac.at
Ext.: 13632

KUMMER Wolfgang
wkummer@tph.tuwien.ac.at

NOWOTNY Helmut
hnowotny@tph.tuwien.ac.at
Ext.: 13634

External Lecturers

LANDSTEINER Karl
Instituto de Física Teórica, Universidad de Madrid

MAJEROTTO Walter
Institute for High Energy Physics of the Austrian Academy of Sciences

MARKYTAN Manfred
Institute for High Energy Physics of the Austrian Academy of Sciences

SCHALLER Peter
Bank Austria - Creditanstalt

SCHWARZ Dominik
University of Bielefeld

SEKE Josip
Institute for Theoretical Physics, VUT

SKARKE Harald
Bank Austria - Creditanstalt

WULKENHAAR Raimar
University of Münster

Scientific Coworkers

Tel.: 01/58801 + Ext.

ARBÓ Diego
diego@iafe.uba.ar

ATTEMS Maximilian
mattens@hep.itp.tuwien.ac.at Ext.: 13637

BARNA Imre
barnai@sunserv.kfki.hu

BERGAMIN Luzi
bergamin@tph.tuwien.ac.at

BLASCHKE Daniel
blaschke@hep.itp.tuwien.ac.at Ext.: 13653

DIMITRIOU Konstantinos
kostas-dimi@yahoo.com

FERNAUD María-José
fernaud@tph.tuwien.ac.at Ext.: 13631

FORNLEITNER Julia
fornleitner@cmt.tuwien.ac.at Ext.: 13631

GUTTENBERG Sebastian
basti@hep.itp.tuwien.ac.at Ext.: 13623

GRUMILLER Daniel
grumil@hep.itp.tuwien.ac.at Ext.: 13623

HOFMANN Daniel
hofmann@hep.itp.tuwien.ac.at

HÖRNDL Maria
maria.hoerndl@yahoo.com

IPP Andreas
andreas.ipp@mpi-hd.mpg.de

KÖFINGER Jürgen

MLADEK Bianca
mladek@tph.tuwien.ac.at Ext.: 13631

NIGSCH Martin
nigsch@cmt.tuwien.ac.at Ext.: 13616

ORTNER Michael
michael.ortner@uibk.ac.at

PAUSCHENWEIN Gernot
pauschenwein@cmt.tuwien.ac.at Ext.: 13631

REINER Albert
areiner@tph.tuwien.ac.at Ext.: 13631

REINOSA Urko
reinosa@hep.itp.tuwien.ac.at

SCHEIDEGGER Emanuel
esche@hep.itp.tuwien.ac.at

SCHIESSL Klaus-Michael
klaus@concord.itp.tuwien.ac.at Ext.: 13627

SELIGER Marek
marek@concord.itp.tuwien.ac.at

SOLLEDER Beate
beate@concord.itp.tuwien.ac.at Ext.: 13612

STRICKER Stefan
stricker@hep.itp.tuwien.ac.at Ext.: 13637

TUTSCHKA Christian
tutschka@tph.tuwien.ac.at Ext.: 13616

WICKENHAUSER Marlene
wick@concord.itp.tuwien.ac.at Ext.: 38785

Appendix B

External Speakers and Visitors

- Anton Arnold
Institute for Analysis and Scientific Computing, VUT
Vienna, Austria
Transparent boundary conditions in the simulation of quantum waveguides, 4.4.2006.
- Jessica Barrett
University of Iceland
Reykjavik, Iceland, 26.6.2006 - 9.7.2006.
- Paul Bartlett
School of Chemistry, University of Bristol
Bristol, UK, 25.6.2006 - 27.6.2006
Can maximizing entropy explain the self-assembly of proteins? - Insights from colloids, 26.6.2006.
- Victor Batyrev
Mathematical Institute, University of Tübingen
Tübingen, Germany, 24.4.2006 - 30.6.2006.
- Nikola N. Bogolubov
Steklov Mathematical Institute, Academy of Sciences of Russia
Moscow, Russia, 1.8.2006 - 6.10.2006.
- Christian Calude
University of Auckland
Auckland, New Zealand, 4.10.2006 - 15.10.2006.
- F. Barry Dunning
Rice University
Texas, USA, 14.9.2006 - 15.9.2006.
- El Bahloul El Mendour
Université de Metz, Laboratoire de Physique des Milieux Denses
Metz, France, 18.1.2006 - 20.1.2006.

- Daniel Grumiller
Institute for Theoretical Physics, University of Leipzig
Leipzig, Germany, 1.2.2006 - 8.2.2006.
- Kenichi L. Ishikawa
Department of Quantum Engineering & Systems Science,
School of Engineering, University of Tokyo
Tokyo, Japan, 1.3.2006 - 31.3.2006.
- Noel Jakse
Université de Metz, Laboratoire de Physique des Milieux Denses
Metz, France, 18.1.2006 - 20.1.2006.
- Gabor Kunstatter
University of Winnipeg
Winnipeg, Manitoba, Canada, 6.4.2006 - 15.4.2006
Highly damped quasinormal modes of Black Holes: Universality and quantumrelevance,
11.4.2006.
- Martin Lísal
E. Hála Laboratory of Thermodynamics, Institute of Chemical Process Fundamentals,
Academy of Sciences of the Czech Republic
Prague, Czech Republic
*Alignment of Lamellar Diblock copolymer phases under shear. Insight from dissipative
particle dynamics simulations*, 28.11.2006.
- Neil Lane
Department of Physics & Astronomy, Rice University Houston
Houston, USA, 23.3.2006 - 28.3.2006
Science policy in the US, 27.3.2006.
- Chii-Dong Lin
Kansas State University Manhattan
Kansas, USA 6.6.2006 - 10.6.2006
Probing atomic and electronic dynamics with sub-10 fs and attosecond light pulses,
9.6.2006.
- Frederica Giulia Lo Verso
Institute for Theoretical Physics II, Heinrich Heine University of Düsseldorf
Düsseldorf, Germany, 5.3.2006 - 18.3.2006, 19.6.2006 - 23.6.2006 and 12.11.2006 - 19.11.2006.
*Star polymers with tunable attractions: Cluster formation phase separation, reentrant
crystallization*, 15.3.2006. *Star-like polymeric micelles: Conformation, structural prop-
erties and phase behavior*, 13.11.2006.
- Ivo Nezbeda
E. Hála Laboratory of Thermodynamics, Academy of Sciences of the Czech Republic
Prague, Czech Republic, 4.10.2006 - 8.10.2006.

- Benjamin Nill
Freie Universität Berlin
Berlin, Germany, 26.6.2006 - 30.6.2006.
- Josep Pamies
Institute for Atomic and Molecular Physics (AMOLF)
Amsterdam, The Netherlands, 18.4.2006 - 31.5.2006.
- Radoslav Rashkov
Universtiy of Sofia
Sofia, Bulgaria
The state of the art and a few projects on AdS/CFT, 29.6.2006.
- Carlos O. Reinhold
Oak Ridge National Lab.
Tennessee, USA, 9/2006.
- A. Robin
KVI Atomic Physics, Rijksuniversiteit Groningen
Groningen, The Netherlands, 20.2.2006 - 25.2.2006
Surface spin polarization investigated by slow hollow atoms, 21.2.2006.
- Paul Romatschke
Faculty of Physics, University of Bielefeld
Bielefeld, Germany, 30.1.2006 - 3.2.2006.
- Andrey V. Soldatov
V.A. Steklov Mathematical Institute of the Russian Academy of Sciences
Moscow, Russia, 1.9.2006 - 10.10.2006.
- Christoph Stampfer
ETH Zürich
Zürich, Switzerland
Spatially resolved Raman spectroscopy of single-and few-layer graphene, 24.10.2006.
- Michael Strickland
Frankfurt Institute for Advanced Studies
Frankfurt/Main, Germany, 31.1.2006 - 3.2.2006.
- Xiao-Min Tong
Institute of Material Sciences, University of Tsukuba
Tsukuba, Japan, 11.7.2006 - 16.7.2006
Molecular tunneling ionization theory and its applications, 14.7.2006.
- Karoly Tökési
ATOMKI Debrecen
Debrecen, Hungary, 27.1.2006 - 5.2.2006.
- Peter van Nieuwenhuizen
State University of New York, Stony Brook
New York, USA, 2.1.2006 - 22.1.2006.

- Pierre Vanhove
SPhT CEA Saclay
France, 12.2.2006 - 19.2.2006
A pure spinor approach to multiloop amplitudes in string 11 D, 15.2.2006.
- Maxim Vasilov
Department of Applied Physics, Yale University
New Haven, USA
Electron energy spectrum in an Andreev billiard
22.8.2006.
- Jean-Jacques Weis
Laboratoire de Physique Théorique, Université Paris-Sud
Orsay, France, 16.6.2006 - 22.6.2006 and 10.12.2006 - 15.12.2006.
- Nigel Wilding
University of Bath
Bath, UK, 23.1.2006 - 24.1.2006.
- Robert Wimmer
Institute for Theoretical Physics, University of Hannover
Hannover, Germany, 2.1.2006 - 15.1.2006.
- Primož Ziherl
Department of Physics, Jozef Stefan Institute, University of Ljubljana
Ljubljana, Slovenia, 26.11.2006 - 28.11.2006
Condensed phases of soft colloids with a hard core, 27.11.2006.

Appendix C

Publications

C.1 Articles in Refereed Journals

- D. Arbó, E. Persson, J. Burgdörfer
Time double-slit interferences in strong-field tunneling ionization
Physical Review A, 74 (2006), 063407-1 - 063407-6.
- D. Arbó, S. Yoshida, E. Persson, K. Dimitriou, J. Burgdörfer
Interference oscillations in the angular distribution of laser-ionized electrons near ionization threshold
Physical Review Letters, 96 (2006), 143003-1 - 143003-4.
- H. Balasin
Singular null hypersurfaces in general relativity. Light-like signals from violent astrophysical events
General Relativity and Gravitation, 38(3) (2006), 541 - 543.
- I. Barna, J. Wang, J. Burgdörfer
Angular distribution in two-photon double ionization of helium by intense attosecond soft-x-ray pulses
Physical Review A, 73 (2006), 023402-1 - 023402-7.
- L. Bergamin, D. Grumiller, W. Kummer, D.V. Vassilevich
Physics-to-gauge conversion at black hole horizons
Class. Quant. Grav., 23 (2006), 3075 - 3101.
- J.-P. Blaizot, A. Ipp, A. Rebhan
Study of the gluon propagator in the large- N_f limit at finite temperature and chemical potential for weak and strong couplings
Annals of Physics, 321 (2006), 2128 - 2155.
- J.-P. Blaizot, A. Ipp, A. Rebhan, U. Reinosa
The Entropy of hot QCD at large N_f : Successfully testing weak coupling techniques
Romanian Reports in Physics, 58 (2006), 43 - 47.
- D. Blaschke, F. Gieres, O. Piguet, M. Schweda
A vector supersymmetry in noncommutative $U(1)$ gauge theory with the Slavnov term
J. High Energy Phys., 05 (2006), 059-1 - 059-16.

- C. Deiss, N. Rohringer, J. Burgdörfer, E. Lamour, C. Prigent, J. Rozet, D. Vernhet
Laser-cluster interaction: X-ray production by short laser pulses
Physical Review Letters, 96 (2006), 13203-1 - 13203-4.
- J. Feist, A. Bäcker, R. Ketzmerick, S. Rotter, B. Huckestein, J. Burgdörfer
Nanowires with surface disorder: Giant localization lengths and quantum-to-classical crossover
Physical Review Letters, 97 (2006), 116804-1 - 116804-4.
- V.A. Gopar, S. Rotter, H. Schomerus
Transport in chaotic quantum dots: Effects of spatial symmetries which interchange the leads
Physical Review B, 73 (2006), 165308-1 - 165308-4.
- K. Grill, C. Tutschka
Lattice gas with finite-range interaction under gravity
Journal of Statistical Physics, 125/3 (2006), 717 - 726.
- M. Hörndl, S. Yoshida, A. Wolf, G. Gwinner, M. Seliger, J. Burgdörfer
Classical dynamics of enhanced low-energy electron-ion recombination in storage rings
Physical Review A, 74 (2006), 052712-1 - 052712-5.
- J.S. Høye, A. Reiner
Self-consistent Ornstein-Zernike approximation for molecules with soft cores
J. Chem. Phys., 125 (2006), 104503.
- A. Ipp, K. Kajantie, A. Rebhan, A. Vuorinen
Pressure of deconfined QCD for all temperatures and quark chemical potentials
Physical Review D, 74 (2006), 045016-1 - 045016-28.
- J. Köfinger, G. Kahl, N.B. Wilding
Phase behaviour of a symmetrical binary mixture in a field
Europhys. Lett., 75 (2006), 234 - 240.
- J. Köfinger, N.B. Wilding, G. Kahl
Phase behaviour of a symmetrical binary fluid mixture
J. Chem. Phys., 125 (2006), 234503.
- W. Kummer
Missbrauch physikalischer Begriffe in den sogenannten Alternativwissenschaften
Imago Hominis, 13 (2006), 199 - 210.
- W. Kummer, D. Hofmann
IR renormalization of general effective actions in 2D gravity theories
European Physical Journal C, 48 (2006), 291 - 301.
- F. Libisch, S. Rotter, J. Burgdörfer
Non-retracing orbits in Andreev billiards
Physical Review B, 73 (2006), 045324-1 - 045324-8.

- B. Mladek, D. Gottwald, G. Kahl, M. Neumann, C.N. Likos
Formation of polymorphic cluster phases for a class of models of purely repulsive soft spheres
 Physical Review Letters, 96 (2006), 45701-1 - 45701-4.
- B. Mladek, G. Kahl, M. Neumann
Thermodynamically self-consistent liquid state theories for systems with bounded potentials
 Journal of Chemical Physics, 124 (2006), 064503-1 - 064503-10.
- E. Persson, S. Fürthauer, S. Wimberger, J. Burgdörfer
Transient localization in the kicked Rydberg atom
 Physical Review A, 74 (2006), 053417 -1; 053417-10 - 10.
- E. Persson, K.-M. Schiessl, A. Scrinzi, J. Burgdörfer
Generation of attosecond unidirectional half-cycle pulses: Inclusion of propagation effects
 Physical Review A, 74 (2006), 013818-1 - 013818-8.
- A. Rebhan, T. S. Biro
Foreword - Quark-Gluon-Plasma Thermalization
 European Physical Journal A, 29 (2006), XI.
- A. Rebhan, P. van Nieuwenhuizen, R. Wimmer
Quantum mass and central charge of supersymmetric monopoles: anomalies, current renormalization, and surface terms
 J. High Energy Phys., 0606 (2006), 056-0 - 056-40.
- C. O. Reinhold, S. Yoshida, J. Burgdörfer, W. Zhao, J.J. Mestayer, J. Lancaster, F.B. Dunning
Realization of the kicked atom at high scaled frequencies
 Physical Review A, 73 (2006), 033420-1 - 033420-6.
- N. Rohringer, S. Peter, J. Burgdörfer
Calculating state-to-state transition probabilities within time-dependent density-functional theory
 Physical Review A, 74 (2006), 042512-1 - 042512-7.
- P. Romatschke, A. Rebhan
Plasma instabilities in an anisotropically expanding geometry
 Physical Review Letters, 97 (2006), 252301-1 - 252301-4.
- K.-M. Schiessl, E. Persson, A. Scrinzi, J. Burgdörfer
Enhancement of high-order harmonic generation by a two-color field: Influence of propagation effects
 Physical Review A, 74 (2006), 053412-1 - 053412-8.
- E. Schöll-Paschinger, A. Reiner
Soft core thermodynamics from self-consistent hard core fluids
 J. Chem. Phys., 125 (2006), 164503.

- A. Soldatov, J. Seke, G. Adam
On the Fourier transforms of the spinor components of relativistic eigenfunctions of hydrogen-like atoms
 Int. J. Mod. Phys. B, 20/9 (2006), 1123 - 1138.
- C. Stampfer, S. Rotter, J. Burgdörfer
Comment on "Dynamic range of nanotube- and nanowire-based electromechanical systems"
 Applied Physics Letters, 88 (2006), 036101-1 - 036101-2.
- K. Svozil
Are simultaneous Bell measurements possible?
 New J. Phys., 8 (2006), 39-1 - 39-5.
- K. Svozil
Staging quantum cryptography with chocolate balls
 Am. J. Phys., 74/9 (2006), 800 - 803.
- P. van Nieuwenhuizen, A. Rebhan, D.V. Vassilevich, R. Wimmer
Boundary terms in supergravity and supersymmetry
 International Journal of Modern Physics D, 15 (2006), 1643 - 1658.
- M. Wickenhauser, J. Burgdörfer, F. Krausz, M. Drescher
Attosecond streaking of overlapping Fano resonances
 Journal of Modern Optics, 53/1-2 (2006), 247 - 257.
- M. Wickenhauser, X.-M. Tong, D. Arbó, J. Burgdörfer, C.-D. Lin
Signatures of tunneling and multiphoton ionization in the electron-momentum distributions of atoms by intense few-cycle laser pulses
 Physical Review A, 74 (2006), 041402-1 - 041402-4.
- S. Yoshida, C. O. Reinhold, J. Burgdörfer, W. Zhao, J.J. Mestayer, J. Lancaster, F.B. Dunning
Influence of a dc offset field on kicked quasi-one-dimensional Rydberg atoms: Stabilization and frustrated field ionization
 Physical Review A, 73 (2006), 033411-1 - 033411-7.
- W. Zhao, J.J. Mestayer, J. Lancaster, F.B. Dunning, C. O. Reinhold, S. Yoshida, J. Burgdörfer
Bidirectionally kicked Rydberg atoms: Population trapping near the continuum
 Physical Review A, 73 (2006), 015401-1 - 015401-4.
- W. Zhao, J.J. Mestayer, J. Lancaster, F.B. Dunning, C. O. Reinhold, S. Yoshida, J. Burgdörfer
Navigating localized wave packets in phase space
 Physical Review Letters, 97 (2006), 253003-1 - 253003-4.

C.2 Articles in Conference Proceedings

- D. Blaschke, M. Schweda, F. Gieres, O. Piguet
A vector supersymmetry killing the infrared singularity of gauge theories in noncommutative space
 in: "5th International Conference on Mathematical Methods in Physics", Proceedings of Science, Trieste, 2006, PoS(IC2006)005, 1 - 10.
- J. Burgdörfer, C. Lemell, K.-M. Schiessl, B. Solleder, C. O. Reinhold, K. Tökési, L. Wirtz
Collisions of slow highly charged ions with surfaces
 in: "Photonic, Electronic and Atomic Collisions - Proceedings of the XXIV International Conference", World Scientific, 2006, 16 - 45 .
- C. Deiss, N. Rohringer, J. Burgdörfer
Interaction of ultra-short laser pulses with clusters: short-time dynamics of a nano-plasma
 in: "The physics of ionized gases", AIP Conference Proceedings 876 (2006) 143 - 153.
- C. Deiss, N. Rohringer, J. Burgdörfer, E. Lamour, C. Prigent, J. Rozet, D. Vernhet
X-ray generation by laser-cluster interaction
 in: "8e Colloque sur les Sources Cohérentes et Incohérentes UV, VUV et X (UVX 2006)", J. Phys. IV France 138 (2006) 55 - 62.
- A. Gerhold, A. Ipp, A. Rebhan
Thermodynamics of QCD at large quark chemical potential
 in: "29th Johns Hopkins Workshop on current problems in particle theory: strong matter in the heavens", (eds.) Jonathan Bagger, Gabor Domokos, David E. Kaplan, Susan Kovesi-Domokos, Raman Sundrum; Proceedings of Science, Trieste, 2006, Paper-Nr. PoS(JHW2005)013, 19 S.
- 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
 in: "Lecture Notes in Computer Science: Large-Scale Scientific Computing: 5th International Conference, LSSC 2005, Sozopol, Bulgaria", I. Lirkov, S. Margenov, J. Wasniewski (eds.); Springer-Verlag, Berlin/Heidelberg, 2006, 586 -593.
- K. Svozil
Aesthetics and scarcity
 in: "On transient realities and their generators"
 FOAM, Brussels, Belgium, 2006, 152 - 167.
- K. Svozil
Characterization of quantum computable decision problems by state discrimination
 in: "Quantum Theory - Reconsideration of Foundations - 3", G. Adenier, A. Khrennikov, T.M. Nieuwenhuizen (eds.); AIP Conference Proceedings 810 (2006), 271 - 279.

C.3 Invited Talks

- J. Burgdörfer
Atomic dynamics on the attosecond scale
 37th Meeting of the Division of Atomic, Molecular and Optical Physics (DAMOP) of the American Physical Society, Knoxville, TN, USA 16.05.2006 - 20.05.2006.
- J. Burgdörfer
Highly charged ions interacting with surfaces
 Workshop on Ion-Beam Science - Solved and Unsolved Problems (ION06), Copenhagen, Denmark, 30.04.2006 - 05.05.2006.
- J. Burgdörfer
Interaction of ultrashort pulses with clusters: Short-time dynamics of a nano plasma
 23rd Summer School and International Symposium on the Physics of Ionized Gases, Kopaonik, Serbia, 28.08.2006 - 01.09.2006.
- C. Deiss, N. Rohringer, J. Burgdörfer, E. Lamour, C. Prigent, J. Rozet, D. Vernhet
Emission X générée par interaction laser-agrégats
 8ème Colloque National sur les Sources Cohérentes et Incohérentes UV, VUV et X: Applications et Développements Récents, Colleville sur Mer, France 06.07.2006 - 09.07.2006.
- G. Kahl
Freezing transitions in soft condensed matter
 ODICS Seminar University of Vienna, Vienna, Austria, 28.06.2006.
- C. Lemell, J. Burgdörfer
Light-phase-sensitive photoemission
 International Conference on Laser Probing, Vienna, Austria, 12.09.2006.
- C. Lemell, K.-M. Schiessl, J. Burgdörfer
Simulation of heavy-ion guiding in insulators
 International Conference on Atomic Collisions in Solids (ICACS 2006), Berlin, Germany, 21.07.2006 - 26.07.2006.
- F. Libisch, S. Rotter, J. Burgdörfer
"Chladni figures" in Andreev billiards
 Chladni Workshop, Wittenberg, Germany 24.07.2006 - 28.07.2006.
- B. Mladek
Clustering transition in soft matter systems
 TAM 2006, Barcelona, Spain, 14.06.2006 - 16.06.2006.
- B. Mladek, D. Gottwald, G. Kahl, M. Neumann, C.N. Likos
Formation of polymorphic cluster phases for purely repulsive soft systems
 Seventh Liblice Conference on the Statistical Mechanics of Liquids, Lednice, Czech Republic, 11.06.2006 - 16.06.2006.

- A. Rebhan
Weak coupling expansions in deconfined QCD at small and large quark chemical potential
ECT* International Workshop on QCD at finite density, Trento, Italien, 24.03.2006.
- S. Rotter
Shot noise in the quantum-to-classical crossover regime
Condensed Matter Seminar, Yale, USA 30.03.2006.
- S. Rotter, F. Aigner, J. Burgdörfer
Mesoscopic transport and shot noise in the quantum-to-classical crossover Department of Applied Physics Yale, Yale, USA, 23.10.2006.
- S. Rotter, F. Aigner, J. Feist, J. Burgdörfer
Suppression of shot noise and divergence of localization lengths in the quantum-to-classical crossover
Group Seminar, Prof. Eric Heller, Harvard University, Cambridge, USA, 14.12.2006.
- K. Svozil
The constructive side of Gleason's theorem
Foundations of Probability and Physics 2006, Växjö, Sweden, 04.06.2006 - 09.06.2006.
- C. Tutschka
Theorie thermodynamischer Phasen
Institut für Statistik und Wahrscheinlichkeitstheorie, TU Vienna, Austria, 20.10.2006.
- S. Yoshida
Enhanced recombination rate in ion storage rings
37th Meeting of the Division of Atomic, Molecular and Optical Physics (DAMOP) of the American Physical Society, Knoxville, TN, USA 16.05.2006 - 20.05.2006.

C.4 Contributed Presentations at Conferences

- F. Aigner
Shot noise and full counting statistics in mesoscopic quantum dots
Quantum Coherence, Noise and Decoherence in Nanostructures
DECONS 06, Dresden, Germany, 15.05.2006 - 26.05.2006.
- F. Aigner
Shot noise in transport through quantum dots: Clean versus disordered samples
Intern. Workshop on Computational Electronics (IWCE-11), Vienna, Austria, 25.05.2006 - 27.05.2006.
- C. Deiss, J. Burgdörfer
Cluster-laser interaction: hot electron production by short laser pulses
27.EAS-Tagung 2006, Riezlern, 05.02.2006 - 10.02.2006
in: "EAS Arbeitsbericht 2006", (2006), 28.
- C. Deiss, N. Rohringer, J. Burgdörfer, E. Lamour, C. Prigent, J. Rozet, D. Vernhet

Laser-cluster interaction: X-ray production by short laser pulses

37th Meeting of the Division of Atomic, Molecular and Optical Physics (DAMOP) of the American Physical Society, Knoxville, TN, USA, 16.05.2006 - 20.05.2006
in: "Bull. Am. Phys. Soc.", 51 (2006), 29.

- C. Deiss, E. Lamour, C. Prigent, J. Rozet, D. Vernhet, J. Burgdörfer
X-ray generation by laser-cluster interaction
IAMPI 2006 Int. Conf. on the Interaction of Atoms, Molecules and Plasmas with Intense Ultrashort Laser Pulses, Szeged, Hungary, 01.10.2006 - 05.10.2006
in: "Book of Abstracts IAMPI 2006", (2006), 28.
- K. Dimitriou, S. Yoshida, J. Burgdörfer, H. Shimada, Y. Yamazaki
Momentum distribution of multiply charged ions ionized by intense lasers
37th Meeting of the Division of Atomic, Molecular and Optical Physics (DAMOP) of the American Physical Society, Knoxville, TN, USA; 16.05.2006 - 20.05.2006;
in: "Bull. Am. Phys. Soc", 51 (2006), 21.
- M.-J. Fernaund, G. Kahl, C.N. Likos
Structural properties of a fluid of polymers confined in a porous matrix of star polymers
International Workshop on Dynamics in Confinement (CONFIT06), Grenoble, France, 23.03.2006 - 26.03.2006.
- J. Fornleitner, D. Gottwald, G. Kahl, C.N. Likos
Genetic algorithms - an attractive new tool in (soft) matter physics
Seventh Liblice Conference on the Statistical Mechanics of Liquids, Lednice, Czech Republic, 11.06.2006 - 16.06.2006.
- E. Lamour, C. Prigent, J. Rozet, D. Vernhet, C. Deiss, N. Rohringer, J. Burgdörfer
L'émission X: une sonde de la dynamique de l'interaction laser de puissance-agrégats
4ème Colloque de la Division Physique Atomique, Moléculaire et Optique de la Société Française, Dijon, France, 05.07.2006 - 07.07.2006,
in: "Book of Abstract PAMO 2006", (2006), 91.
- C. Lemell, K.-M. Schiessl, J. Burgdörfer
Simulation of capillary guiding
Symp. on Surface Science 2006 (3S'06), St. Christoph am Arlberg, 10.03.2006,
in: "Book of Abstracts 3S'06", F. Aumayr, P. Varga (eds.), (2006), 167 - 168.
- F. Libisch, S. Rotter, J. Burgdörfer
Mathematical modelling of semiconductor - superconductor hybrid structures
MATHMOD 2006, Vienna, Austria, 07.02.2006 - 10.02.2006
- F. Libisch, S. Rotter, J. Burgdörfer
Properties of Andreev eigenstates
Quantum Coherence, Noise and Decoherence in Nanostructures
DECONS 06, Dresden, Germany, 15.05.2006 - 26.05.2006.
- F. Libisch, S. Rotter, J. Burgdörfer
Properties of Andreev eigenstates

Dynamics and Relaxation in Complex Quantum and Classical Systems and Nanostructures, COQUSY 2006, Dresden, Germany, 25.09.2006 - 01.10.2006.

- F. Libisch, S. Rotter, J. Burgdörfer
Andreev billiards
IVth Billiard Workshop 2006, Marburg, Germany, 05.10.2006.
- W. Meissl, M. Simon, HP. Winter, F. Aumayr, B. Solleder, C. Lemell, J. Burgdörfer, J.R. Crespo López-Urrutia, H. Tawara, J. Ullrich
Electron emission from insulator surfaces induced by impact of slow highly charged ions
16th Intern. Workshop on Inelastic Ion-Surface Collisions (IISC-16), Hernstein/NÖ, 21.09.2006,
in: "Book of Abstracts, 16th Intern. Workshop on Inelastic Ion-Surface Collisions (IISC-16)", F. Aumayr, C. Lemell (eds.), (2006), 105.
- J.J. Mestayer, W. Zhao, J. Lancaster, F.B. Dunning, C.O. Reinhold, S. Yoshida, J. Burgdörfer
First application of engineered very -high-n polarized Rydberg states
37th Meeting of the Division of Atomic, Molecular and Optical Physics (DAMOP) of the American Physical Society, Knoxville, TN, USA, 16.05.2006 - 20.05.2006,
in: "Bull. Am. Phys. Soc.", 51 (2006), 101.
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Hyperstructures formed by clusters in purely repulsive soft matter systems
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Computational materials design: searching for macromolecules that cluster
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Generation of attosecond half-cycle pulses: Inclusion of propagation effects
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- A. Rebhan
Weibel instabilities in anisotropically expanding quark-gluon plasma
Int. Workshop on Non-Equilibrium Quark-Gluon Plasma, Washington University, Seattle, USA, 27.09.2006.
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Hard-Expanding-Loop Dynamics of Plasma Instabilities
Strong and Electroweak Matter 2006, Brookhaven National Laboratory, Upton, New York, 11.05.2006.
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Interplay between the mesoscopic Stoner and Kondo effects
Dynamics and Relaxation in the Complex Quantum and Classical Systems and Nanostructures, Dresden, Germany, 01.08.2006.
- K.-M. Schiessl, E. Persson, A. Scrinzi, J. Burgdörfer
Resonant two-color driving in high harmonic generation: Single-atom and pulse propagation
27. EAS-Tagung 2006, Riezlern, Austria, 06.02.2006.
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Electron emission during scattering of N^{6+} ions from a magnetized iron surface
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- K. Svozil
Staging quantum cryptography with chocolate balls
 Lange Nacht der Forschung, TU Wien, Vienna, Austria, 17.02.2006.
- H.E. Türeci, Y. Alhassid, A.D. Stone, S. Rotter
Spin-orbit interaction in the eigenbasis of the universal Hamiltonian
 APS Spring Meeting 2006, Baltimore, USA, 14.03.2006.
- HP. Winter, C. Lemell, J. Burgdörfer, S. Lederer, H. Winter
Below threshold kinetic electron emission
 Symp. on Surface Science 2006 (3S'06), St. Christoph am Arlberg, 09.03.2006
 in: "Proc. 3S'06", F. Aumayr, P. Varga (Hrg.), (2006), 149 - 150.
- S. Yoshida, J. Burgdörfer, C. O. Reinhold, W. Zhao, J.J. Mestayer, J. Lancaster, F.B. Dunning
Noise induced decoherence of Rydberg atoms in a DC field
 37th Meeting of the Division of Atomic, Molecular and Optical Physics (DAMOP) of the American Physical Society, Knoxville, TN, USA, 16.05.2006 - 20.05.2006
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- W. Zhao, J.J. Mestayer, J. Lancaster, F.B. Dunning, C.O. Reinhold, S. Yoshida, J. Burgdörfer
Navigating in phase space
 37th Meeting of the Division of Atomic, Molecular and Optical Physics (DAMOP) of the American Physical Society, Knoxville, TN, USA, 16.05.2006 - 20.05.2006
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Appendix D

Graduates

Master Degree

- M. Attems
Gauge independence of infrared singularities in Slavnov modified noncommutative $U(1)$ theory
Supervisor: M. Schweda
- J. Feist
Transport through quantum wires with surface disorder
Supervisor: J. Burgdörfer, S. Rotter
- C. Mayrhofer
Quantisation of supersymmetric CP^1 solitons
Supervisor: A. Rebhan
- M. Ortner
Canonical quantization of Slavnov modified noncommutative $U(1)$ gauge field
Supervisor: M. Schweda
- B.C. Pirvu
IR renormalization of Hawking radiation from Black Holes
Supervisor: W. Kummer
- S. Stricker
 θ -expanded QED as weak field gravity
Supervisor: M. Schweda

Doctorates

- M. Nigsch
Studies of multiple scattering in low-dimensional systems
Supervisor: P. Kasperkovitz
- M. Wickenhauser
Ionization dynamics of atoms in femto- and attosecond pulses
Supervisor: J. Burgdörfer, C.-D. Lin

Habilitation

- C. Lemell
Response of solid surfaces interacting with particles and laser pulses
Supervisor: J. Burgdörfer

Appendix E

Projects

E.1 Projects started in 2006

- Joachim Burgdörfer
Interaction of ultrashort electromagnetic pulses with matter-theory
Fonds zur Förderung der wissenschaftlichen Forschung (FWF)
Project-Nr.: F1610
Amount: EUR 366.380,00
01.04.2006 - 31.03.2010
- Joachim Burgdörfer
ADLIS - Advanced light sources
Fonds zur Förderung der wissenschaftlichen Forschung (FWF)
Project-Nr.: F1601
Amount: EUR 419.680,00
01.04.2006 - 31.03.2010
- Joachim Burgdörfer
Optimal control theory for propagation effects in high-harmonics generation
Max-Planck-Institut
Project-Nr.: –
Amount: EUR 30.000,00
01.07.2007 - 30.06.2008
- Joachim Burgdörfer
Ion technology and spectroscopy at low energy ion beam facilities (ITS-LEIF)
(theory part of joint project with HP. Winter and F. Aumayr) European Commission (EC)
Project-Nr.: JRA6
Amount: EUR 66.000,00
01.01.2006 - 31.12.2009
- Maximilian Kreuzer
General geometries of effective actions
Fonds zur Förderung der wissenschaftlichen Forschung (FWF)
Project-Nr.: P19051-N16

Amount: EUR 239.442,00
01.10.2006 - 30.09.2008

- Maximilian Kreuzer

Nonperturbative effects in string compactifications
Fonds zur Förderung der wissenschaftlichen Forschung (FWF)
Project-Nr.: P18679-N16
Amount: EUR 171.612,00
01.10.2006 - 30.09.2008

- Maximilian Kreuzer

Geometric construction in string theory
ÖAD
Project-Nr.: –
Amount: EUR 33.780,00
04.07.2006 - 03.07.2009

- Anton Rebhan

Gravity, Chern-Simons extensions, topology and solid-state physics applications
Fonds zur Förderung der wissenschaftlichen Forschung (FWF)
Project-Nr.: MOIF-CT-2006-021421
Amount: EUR 262.360,00
01.8.2006 - 31.07.2009

- Anton Rebhan

Thermodynamics and non-equilibrium dynamics of the quark gluon plasma
Fonds zur Förderung der wissenschaftlichen Forschung (FWF)
Project-Nr.: P19526-N16
Amount: EUR 208.813,50
01.8.2006 - 31.07.2009

E.2 Current projects and projects completed in 2006

- 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
10.05.2002 - 31.12.2006

- 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, 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
- 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
- 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
- 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, Rainer Dirl
Computational Material Science
Fonds zur Förderung der wissenschaftlichen Forschung (FWF)
Project-Nr.: WK004
Amount: EUR 288.060,00
30.04.2006 - 01.05.2008
- Gerhard Kahl
Atomic-scale computational materials science
European Commission (EC)
Project-Nr.: IHP-MCHT-01-1
Amount: EUR 66.000,00
06.08.2001 - 30.06.2007
- Gerhard Kahl
Phase transitions in colloids
Jubiläumsfonds der Stadt Wien (JSW)
Project-Nr.: H-1080/2002
Amount: EUR 4.000,00
17.10.2002 - 31.12.2006

- Wolfgang Kummer
Hawking flux
Fonds zur Förderung der wissenschaftlichen Forschung (FWF)
Project-Nr.: P17938-N08
Amount: EUR 52.524,00
01.01.2005 - 28.02.2006
- 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
- 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
- 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
11.03.2002 - 30.09.2006
- 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