A 26: Poster: Atomic systems in external fields

Time: Wednesday 16:30–19:00 Location: Poster.V

A 26.1 Wed 16:30 Poster.V

Dynamics of laser-cooled Ca^+ ions in a Penning trap with a rotating wall — •Manuel Vogel[1], Shailen Bharadia[2], Richard Thompson[2], and Danny Segal[2] — [1]TU Darmstadt and GSI Darmstadt — [2]Imperial College London, UK

We have performed systematic measurements of the dynamics of laser-cooled $^{40}Ca^+$ ions confined in a Penning trap and driven by a rotating dipole field ("rotating wall"). The size and shape of the ion cloud has been monitored using a CCD camera to image the fluorescence light resulting from excitation by the cooling laser. We have systamatically varied the experimental conditions such as amplitude and frequency of the rotating wall drive as well as the trapping parameters. The rotating wall has been used for a more than 10-fold radial compression of the ion cloud thus increasing the ion density in the trap. We have also observed plasma mode excitations in agreement with theoretical expectations. This work will allow to define the optimum parameters for high compression of ions as needed for precision spectroscopy of forbidden transitions as in the SPECTRAP experiment at the HITRAP facility at GSI Darmstadt.

A 26.2 Wed 16:30 Poster.V

Parity Violation in Hydrogen — •Martin-Isbjörn Trappe, Thomas Gasenzer, and Otto Nachtmann — Institute for Theoretical Physics, University of Heidelberg

We discuss the propagation of hydrogen atoms in static electric and magnetic fields in a longitudinal atomic beam spin echo (lABSE) Interferometer. The atoms acquire geometric (Berry) phases that exhibit a manifestation of parity-(P-)violation effects arising from electroweak Z-boson exchange between electron and nucleus. We provide analytical as well as numerical calculations of the behaviour of the metastable n=2 states of hydrogen. We are able to systematically search for Berry phases with tailored properties. Besides maximizing P-violating geometric phases emerging for the respective states we also find the possibility to modify their decay rates, nearly at the order of a percent, solely through P-conserving geometric phases.

A 26.3 Wed 16:30 Poster.V

Dominant interaction Hamiltonians — •Carlos Zagoya[1], Martin Gerlach[1], Jan-Michael Rost[1], and Frank Grossmann[2] — [1]Max Planck Institute for the Physics of Complex Systems, D-01187 Dresden — [2]Institut für Theoretische Physik, Technische Universität Dresden, D-01062 Dresden

We introduce the concept of dominant interaction Hamiltonians (DIH) in order to disentangle non-separable dynamics by splitting it into spatial regions where the dominant potential is taken as the only interaction. Firstly, by applying the DIH concept we obtain an integrable approximation to the dynamics of an electron exposed to a strong laser field and an atomic potential. The high harmonic generation spectrum obtained by using the semiclassical Herman-Kluk propagator (HK) [1] is in excellent agreement with the full quantum mechanical result [2]. Secondly, we apply the DIH scheme to the classical two electron dynamics of electron-ion scattering. We find that the energy sharing deflection function and energy sharing cross-section obtained by the DIH approximation show the essential features present in the full dynamics [3].

[1] M. F. Herman and E. Kluk, Chem. Phys. **91**, 27 (1984)
[2] G. van de Sand and J.-M. Rost, Phys. Rev. Lett. **83**, 524 (1999)
[3] M. Gerlach et al., preprint, arXiv:1110.1545

This work was partly supported by the DFG through grant GR 1210/4-2 (FG).

A 26.4 Wed 16:30 Poster.V

Fingerprints of exceptional points in the survival probability of resonances in atomic spectra — •Holger Cartarius[1,2], Günter Wunner[1], Jörg Main[1], and Nimrod Moiseyev[3] — [1]1. Institut für Theoretische Physik, Universität Stuttgart — [2]Chemical Physics Department, Weizmann Institute of Science, Rehovot, Israel — [3]Department of Physics and Minerva Center for Nonlinear Physics of Complex Systems, Technion, Haifa, Israel

Exceptional points, i.e. branch point singularities in non-Hermitian physical systems, where two complex eigenvalues degenerate and the corresponding eigenstates coalesce, have shown to exhibit prominent effects not observable in their absence. They appear in quantum resonance spectra and have been found for decaying unbound states of the hydrogen atom in crossed electric and magnetic fields [1].

For the decay of two resonances exactly at the exceptional point parameters a unique time signature is expected. We show that indeed the survival probability $S(t) = |\langle\psi(0)|\psi(t)\rangle|^2$ decays exactly as $|1 - at|^2 e^{-\Gamma_{EP} t/\hbar}$ where Γ_{EP} is associated with the decay rate at the exceptional point and a is a complex constant depending solely on the initial wave packet that populates exclusively the two almost degenerate states of the non-Hermitian Hamiltonian [2]. This may open the possibility for a first experimental detection of exceptional points in a quantum system.

[1] H. Cartarius, J. Main, G. Wunner, Phys. Rev. Lett. 99, 173003 (2007)
[2] H. Cartarius, N. Moiseyev, Phys. Rev. A 84, 013419 (2011)

A 26.5 Wed 16:30 Poster.V

Treatment of spatially inhomogeneous, finite systems with the Generalized Kadanoff–Baym Ansatz — •Sebastian Hermanns, Karsten Balzer, and Michael Bonitz — Institut für Theoretische Physik und Astrophysik, CAU Kiel, Leibnizstraße 15, 24098 Kiel

For the description of many–particle systems the Green's function method has become widely used in the last decades. In this formalism the Kadanoff–Baym equation is solved using an appropriate self–energy. Additionaly the Generalized Kadanoff–Baym ansatz[1] (GKBA) is introduced to reconstruct the double–time single–particle Green's function from its time–diagonal value: $G(t_1, t_2) = F_{GKBA}[G(t_1 = t_2)]$. This approximation is well tested for large, homogeneous systems.

In this contribution, we apply the proposed scheme to *finite* model systems with *strong spatial inhomogeneities*: a Hubbard model, a 4–electron quantum dot[2] and a one–dimensional helium model. By comparing with results obtained from exact diagonalization, solutions of the time–dependent Schrödinger equation[3], Hartree–Fock– and full double–time Green's function calculations[4], we test the validity of the approximation used.

[1] P. Lipavsky, V. Spicka, and B.Velicky, Phys. Rev. B **34**, 6933–6942 (1986), [2] for comparison see poster by K. Balzer, [3] K. Balzer, S. Bauch, and M. Bonitz, Phys. Rev. A **81**, 022510 (2010), [4] K. Balzer, S. Bauch, and M. Bonitz, Phys. Rev. A **82**, 033427 (2010)

A 26.6 Wed 16:30 Poster.V

Double excitations from the solution of the Kadanoff–Baym equations — •Karsten Balzer and Michael Bonitz — Institut für Theoretische Physik und Astrophysik, CAU Kiel, Leibnizstraße 15, 24098 Kiel

In a quantum many–body system, the population of states of double excitation character (doubly excited states) is a clear indicator for correlations importantly contributing to the nonequilibrium dynamics.

In this contribution, we analyze such correlation-induced transitions, being absent in a mean–field Hartree–Fock (HF) treatment, on the basis of the nonequilibrium Green function solving the Kadanoff–Baym equations by direct time–propagation [1]. As test system, we consider a four–electron quantum dot at zero temperature in the regime of moderate–to–strong coupling (see also poster by S. Hermanns [3]). The approximate (HF and second-order Born) absorption spectra are compared to exact diagonalization results where singly, doubly and other multiply excited states are identified by means of the approximate excitation level [2].

[1] K. Balzer, S. Bauch and M. Bonitz, Phys. Rev. A 81, 022510 (2010); ibid. 82, 033427 (2010). [2] J.F. Stanton and R.J. Bartlett, J. Chem. Phys. 98, 7029 (1993). [3] This contribution focuses on the generalized Kadanoff–Baym ansatz.

A 26.7 Wed 16:30 Poster.V

Two-photon transitions of high-Z few electron ions in strong laser fields — •Thorsten Jahrsetz[1,2] and Andrey Surzhykov[1,2] — [1]Physikalisches Institut University of Heidelberg — [2]GSI Helmholtzzentrum für Schwerionenforschung GmbH, D-64291 Darmstadt, German

During the last decades, two-photon transitions in highly charged heavy ions have attracted much attention as a promising tool for studying atomic parity-violation (PV) effects [1]. For example, the $1s_{1/2}2s_{1/2} : J = 0 \rightarrow 1s_{1/2}2p_{1/2} : J = 0$ transition of helium-like uranium, when induced by polarized light, should proceed via the PV electric-dipole 2E1 channel and provide an accurate probe of parity non-conservation. Theoretical predictions for this transition clearly indicate the need for high-intensity lasers in order to make the parity-violating transitions visible [2]. However, such intense laser fields also may lead to sizable Stark shift and mixing of different ionic levels even in the high-Z regime. In this contribution, therefore, we apply the Green's function approach and relativistic Dirac theory in order to investigate the influence of Stark effects on the total as well as differential two-photon rates. Special emphasis in our analysis is placed on the (laser-dressed) $2p_{1/2} \rightarrow 1s_{1/2}$ and $1s_{1/2}2p_{1/2} : J = 0 \rightarrow 1s^2_{1/2} : J = 0$ transitions in hydrogen-and helium-like heavy ions.

[1]A Schäfer et al. PRA 40,12(1989)

[2] A. Surzhykov et al., Phys. Rev. A 84, 022511 (2011)

This work was supported by the Helmholtz Gemeinschaft (Nachwuchsgruppe VH-NG-421).

A 26.8 Wed 16:30 Poster.V

Numerical simulations of the pump-probe ionization of Lithium — •David Hochstuhl and Michael Bonitz — Universität Kiel

In this contribution we study the IR-XUV pump-probe ionization of Lithium. The basic scenario is [1]: (i) the XUV photon ionizes an 1s electron. (ii) the 2s electron becomes excited through a shake-up process. (iii) depending on the frequency and intensity of the IR field, the 2s electron is excited above the threshold and gets ionized by the IR field. In existing models, this process is described using certain approximations to the XUV ionization step (like the strong field approximation), as well as to the subsequent inner-electronic processes (like a sudden switching to the ion). To overcome these limitations, we directly solve the time-dependent Schrödinger equation in a restricted, problem-adapted subspace of the three-particle Hilbert space.

[1] A.K. Kazansky, N.M. Kabachnik, J. Phys. B 41 135601

A 26.9 Wed 16:30 Poster.V

Quantum Breathing Mode of Interacting Particles in a Harmonic Trap — •Jan Willem Abraham, David Hochstuhl, Karsten Balzer, and Michael Bonitz — Institut für theoretische Physik und Astrophysik, CAU Kiel

Time-dependent properties of interacting, harmonically confined quantum systems are of growing interest in many areas, including correlated electrons in metal clusters or quantum dots and ultracold Bose and Fermi gases in traps or optical lattices. Among these properties the behaviour of the breathing mode (BM)—the [uniform] radial expansion and contraction of the system—attracts special interest as it is easily excited experimentally, and turns out to give information of the system's dimensionality, spin statistics, as well as the form and strength of the pair interaction potential. Extending our previous work, we deepen the understanding of the BM during the transition from the ideal quantum to the strongly coupled classical regime, where the breathing frequency depends on the pair interaction strength. We present time-dependent Hartree-Fock simulations for 2 to 20 fermions with Coulomb interaction which yield the dependency of the quantum BM on the particle number.

A 26.10 Wed 16:30 Poster.V

Phase-controlled electron acceleration from metal clusters in few-cycle laser pulses — •Lennart Seiffert, Jörg Köhn, and Thomas Fennel — Universität Rostock, 18051 Rostock, Germany

It is well-known that the ionization of atoms and molecules in intense few-cycle laser pulses can be precisely controlled (with sub-fs resolution) by the carrier-envelope-phase [1]. Recently it has been shown that such pulses also allow to unravel and control ionization processes in more complex many particle systems, such as silica nanoparticles [2]. Here we investigate the phase controlled electron acceleration from laser driven metal clusters, where the resonant excitation of Mie-plasmons leads to extreme field enhancement. Angular- and energy resolved electron spectra are calculated for resonant jellium-like clusters using a semiclassical Vlasov approach [3]. We observe a strong phase dependence of the electron spectra, with pronounced left-right asymmetry in the energy distribution of electrons emitted parallel to the laser polarization axis. A detailed analysis of the electron trajectories allows the identification of the leading acceleration mechanisms and supports the dominant role of surface plasmon assited rescattering in clusters (SPARC) [3]. A systematic analysis of the phase effects as function of the laser pulse duration is presented.

[1] G. G. Paulus et al., Phys. Rev. Lett. 91, 253004 (2003)

[2] S. Zherebtsov et al., Nature Phys. 7, 656 (2011)

[3] Th. Fennel et al., Phys. Rev. Lett. 98, 143401 (2007)

A 26.11 Wed 16:30 Poster.V

Temporal dynamics of Coulomb correlations in atomic strong-field processes — •Maximilian Hollstein, Benjamin Baxevanis, and Daniela Pfannkuche — 1. Institut für Theoretische Physik, Universität Hamburg, Hamburg,Germany

The temporal dynamics of Coulomb correlations in atomic strong-field processes are investigated theoretically on a model system.

In order to study atomic strong-field processes various methods have been developed to solve the time-dependent Schrödinger equation as for instance the single-active-electron approach or the time-dependent configuration-interaction singles method. In contrast to these approaches which do not take into account the complete Coulomb correlations we are using a numerically exact method to study the ionization process on a model system. We are focusing on the temporal dynamics of the Coulomb correlations by considering the time evolution of pair correlation functions. By comparing the exact results with Hartree-Fock based methods we are investigating the importance of Coulomb correlations atomic strong-field processes.

A 26.12 Wed 16:30 Poster.V

Analysis of Freeman resonances in strong field ionization — •Thomas Keil and Dieter Bauer — Institut für Physik, Universität Rostock, 18051 Rostock, Germany

The interaction of atoms with a strong laser field leads to nonperturbative AC Stark shifts of atomic energy levels. Especially in the multiphoton regime these shifts affect the ionization rate. By varying the laser intensity bound states can be shifted into and out of multiphoton resonances. In the case of Rydberg states the corresponding phenomena are called Freeman resonances. These resonances are treated numerically by solving the time-dependent Schrödinger equation as well as analytically by applying perturbation theory and the strong field approximation. Floquet-results from Potvliege and Shakeshaft are reproduced numerically using trapezoidal laser pulses. Possible explanations for the ionization behavior are presented in terms of atomic levels involved in the process. The resulting line shape in the ionization rate vs intensity is discussed.

A 26.13 Wed 16:30 Poster.V

Breathing modes in harmonically confined quantum systems — •David Hochstuhl[1], Jan-Willem Abraham[1], Chris McDonald[2], Thomas Brabec[2], and Michael Bonitz[1] — [1]Christian-Albrechts-Universität Kiel — [2]University of Ottawa

The Breathing Mode (BM), collective oscillations induced by monopole excitations, constitutes a versatile tool for the characterization of many-particle systems as, e.g., Bose-Einstein condensates, nuclear matter or quantum dots. It has been thoroughly investigated in classical Coulomb systems [1], where it shows a universal, particle-number independent frequency of $\omega = \sqrt{3}$ (in units of the harmonic trap frequency). For BMs in quantum systems, due to the non-locality of the wavefunctions, a different picture arises: the classical frequency is recovered only in the Wigner-cristallization regime. On the other hand, in the ideal quantum limit of weakly interacting systems, the BM frequency approaches $\omega = 2$. These two extrema are well known and can be conveniently handled by perturbation theory.

Our focus here is on the intermediate region. Therefore, we solve the Schrödinger equation for systems consisting up to 12 particles, trapped in a two-dimensional parabolic potential, and determine their BM frequencies with respect to the particle interaction strength. For the solution, we apply the Multiconfigurational time-depedent Hartree-Fock method as well as a restricted active-space variant of the Configuration Interaction method.

[1] C. Henning, et al., Phys. Rev. Lett. 101 045002 (2008) [2] S. Bauch, et al., Phys. Rev. B 80 054515 (2009)

A 26.14 Wed 16:30 Poster.V

Monte-Carlo Simulation of Atomic and Molecular Fragmentation Processes in Reaction Microscopes. — •Philipp Cörlin, Arne Senftleben, Alexander Sperl, Michael Schönwald, Andreas Fischer, Robert Moshammer, and Joachim Ullrich — Max-Planck-Institut für Kernphysik, 69117 Heidelberg, Deutschland

By reconstructing the trajectories of electrons and (molecular) ions in an electric and a magnetic field, reaction microscopes are used to measure the three dimensional momenta of the ionization products. In combination with ultra short laser pulses this allows one to image ultra-fast molecular dynamics.

In this work laser-induced ionization of atoms and Coulomb explosion of small molecules are simulated in order to determine appropriate operating parameters for reaction microscopes. This is done by analyzing simulated time-of-flight spectra as well as hit positions on the detectors for different sets of parameters.

Furthermore, characteristic time-of-flight spectra of Coulomb exploding polyatomic molecules are created in order to simplify the interpretation of experimental data.

A 26.15 Wed 16:30 Poster.V

New Compact Magnetically Shielded ^{3}He MEOP Polarizing Facility — •Christian Mrozik, Werner Heil, Sergei Karpuk, and Ernst Otten — Institut für Physik, Johannes Gutenberg-Universität Mainz

Applications of hyperpolarized ^{3}He exist in fundamental research as well as in medical studies. Since a decade ^{3}He is polarized in a central facility, located at the University of Mainz and shipped to the users. The gas is polarized via metastability exchange optical pumping (MEOP) at a pressure of approximately 1 mbar inside a magnetic field of 1 mT. The process requires a magnetic field with a relative gradient of $\Delta B/B < 3.8 \cdot 10^{-4}\,\mathrm{cm}^{-1}$. To construct a compact facility for local gas-polarization it is imperative to create a sufficiently homogeneous magnetic field all over a solenoid's volume in order to be able to use its complete volume for the MEOP assembly. Our concept of a spacious homogenization of a solenoid's magnetic field consists of enclosing it into a shielding of soft magnetic material, providing a high magnetic permeability [1]. In addition to the homogenization of the magnetic field a new concept for the optics, used for the optical pumping has been developed, to fit into the new compact facility. The design of the compact apparatus aims to reach a flux of hyperpolarized ^{3}He at $P > 65\%$ of several standard liters per hour. First experimental results, gained from the new compact polarizing apparatus, will be presented.

[1] C. Mrozik *et al.* Journal of Physics: Conference Series **294** (2011)

A 26.16 Wed 16:30 Poster.V

Nonequilibrium Green's functions approach to the pair distribution function of quantum many-body systems — •Kay Kobusch, Karsten Balzer, Lasse Rosenthal, Alexei Filinov, and Michael Bonitz — Institut für Theoretische Physik und Astrophysik, Universität Kiel, D-24098 Germany

The pair distribution function (PDF) is a key quantity for analyzing correlation effects of quantum systems both in and far from equilibrium. We derive an expression for the PDF in terms of single particle Green's functions - the solutions of the Keldysh-Kadanoff-Baym equations in the two-time plane. The result includes initial correlations and generalizes previous density matrix expressions from single-time quantum kinetic theory. As an illustration we present numerical results for the PDF of electrons and holes in a strongly correlated electron-hole bilayer. These are calculated in different many-body approximations and then compared with Path integral Monte Carlo results.