A 16: Atomic systems in external fields I

Time: Wednesday 14:00–16:00 Location: BAR 106

A 16.1 Wed 14:00 BAR 106

Parity-Violation in Hydrogen: Precision Enhancement through Many-Particle Squeezing — •Martin-Isbjörn Trappe, Thomas Gasenzer, and Otto Nachtmann — Institut für Theoretische Physik, Philosophenweg 16, 69120 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. Possible measurements of P-violating geometric phases in lABSE experiments require a high precision for detecting atoms in specific states. We investigate possibilities to enhance the precision of lABSE experiments beyond the standard quantum limit using squeezed many-particle hydrogen states.

A 16.2 Wed 14:15 BAR 106

On the applicability of the Floquet theorem to TDDFT — •Varun Kapoor and Dieter Bauer — Institut für Physik, Universität Rostock, 18051 Rostock, Germany

We investigate the applicability of the Floquet ansatz to time-dependent density functional theory (TDDFT). We find that the periodicity of the TDDFT-Hamiltonian with just the laser period, as required by the Floquet ansatz, is conditional. We obtain the exact Hartree-exchange-correlation potential for exactly solvable model systems and Fourier transform it to check for periodicity of the TDDFT-Hamiltonian. We find that only if the ground state evolves adiabatically in the laser field and the laser frequency is non-resonant, Floquet-TDDFT states exist and the Floquet ansatz is applicable. We use the novel Floquet analysis we developed to obtain the populated Floquet states which qualitatively agree with the populated Floquet states obtained by solving the Schrödinger equation. A comparison is also made between Floquet-TDDFT states obtained by exact and Hartree-exchange-only TDDFT.

A 16.3 Wed 14:30 BAR 106

Resonance wave functions located at the Stark saddle point — •Holger Cartarius[1], Jörg Main[2], Thorsten Losch[2], and Günther Wunner[2] — [1]Chemical Physics Department, Weizmann Institute of Science, 76100 Rehovot, Israel — [2]1. Institut für Theoretische Physik, Universität Stuttgart , 70550 Stuttgart, Germany

The hydrogen atom in crossed static electric and magnetic fields is an important example for a quantum system accessible both in experiments and numerical calculations. Adding external fields to the Coulomb potential of the hydrogen atom opens the possibility for wave functions to be localized far away from the nucleus. In particular, the existence of resonances localized in the vicinity of the Stark saddle point predicted by simple expansions of the potential around the saddle [1] has been unclear for a long time.

We calculate quantum mechanically exact wave functions of resonances in spectra of the hydrogen atom in crossed external fields and prove the existence of the long-lived decaying quantum states localized at the Stark saddle point [2]. A spectrum of ground and excited states reproducing the nodal patterns expected from simple quadratic and cubic expansions of the potential in the vicinity of the saddle can be identified.

[1] C. W. Clark, E. Korevaar, and M. G. Littman, Phys. Rev. Lett. **54**, 320 (1985)
[2] H. Cartarius, J. Main, T. Losch, and G. Wunner, Phys. Rev. A **81**, 063414 (2010)

A 16.4 Wed 14:45 BAR 106

Classical approaches to quantum dynamical systems — •Heiko Bauke and Christoph H. Keitel — Max-Planck-Institut für Kernphysik, Saupfercheckweg 1, 69117 Heidelberg

Quantum dynamical systems are often investigated by classical or semi-classical approaches. Classical methods are applied when a full quantum mechanical treatment is not feasible. They allow to work in the framework of familiar classical concepts and to investigate the quantum-to-classical transition [1]. However, the limits of classical approaches to quantum dynamical systems are often not very well understood.

In our contribution, we investigate the validity and the limits of the classical trajectory Monte Carlo method [2] by comparing the dynamics of non-interacting classical particles under the evolution of the Liouville equation with the quantum dynamics in phase space under the quantum Liouville equation. Our results allow us to estimate in which setups quantum effects become non-negligible. We show that a modified classical trajectory Monte Carlo method becomes equivalent to the actual quantum dynamics in the limit that all forces are harmonic. This method allows us to study timde-dependent processes in driven many particle quantum systems with harmonic interactions.

[1] *Quantum-Classical Correspondence*, Josef Bolitschek, Springer, 2004
[2] Proceedings of the Physical Society, **88**:861, 1966; Proceedings of the Physical Society, **88**:873, 1966

A 16.5 Wed 15:00 BAR 106

Alignment of atomic inner-shell vacancies following nuclear α decay — •Sean McConnell[1,2] and Andrey Surzhykov[1,2] — [1]Physikalisches Institut der Universität Heidelberg — [2]GSI Helmholtzzentrum für Schwerionenforschung GmbH, Darmstadt

The alpha decay of Polonium has the potential to induce the ionisation of any of the electrons initially bound to the nucleus. Should this process involve the ionisation of an electron from the L_3 sub-shell, the remaining hole may appear to be aligned. In order to estimate such an alignment, theoretical calculations were performed in Ref. [1] based, however, on solutions of the non-relativistic Schrödinger equation. Moreover, that work did not account for shake–off or recoil effects that may significantly influence the inner-shell ionisation process. In this contribution, we present a fully-relativistic description of the inner-shell ionisation with a special emphasis on the alignment of the residual atom. Our theoretical treatment includes not only nuclear shake-off effects and compensation for the realistic motion of the α particle as it escapes from the daughter Lead nucleus, but also accounts for electron screening effects. To understand better the role of these effects on the alignment of the $2p_{3/2}$ vacancy, detailed calculations are performed for a wide range of common α particle energies and have been compared with previous data. We can demonstrate through our calculations, that as well as the aforementioned disregard of shake-off and recoil corrections among other important factors, non-negligible inaccuracies have surfaced in previous estimations of alignment.

[1] N M Kabachnik, J. Phys. B: At., Mol., Phys. **18(13)** (1985) L423

A 16.6 Wed 15:15 BAR 106

Global fixed point proof for time-dependent density functional theory — •Michael Ruggenthaler and Robert van Leeuwen — Department of Physics, Nanoscience Center, University of Jyväskylä, 40014 Jyväskylä, Finland

Time-dependent density-functional theory is the extension of the highly successful ground-state density-functional theory to time-dependent phenomena. The basic theorem by Runge and Gross [1] shows under the assumption of Taylor-expandable external potentials that every observable is in principle uniquely defined by the one-particle density of the quantum system. The van Leeuwen theorem [2] provides under similar restrictions, that there is an auxiliary system of noninteracting particles generating the exact density of the interacting system. This so-called Kohn-Sham construction makes an ab initio solution for big quantum systems feasible. By rewriting the question whether a system is uniquely defined by its density as a fixed point question, we can proof both theorems without assumptions on the time-dependence of the potentials. We discuss implications and applications of this novel approach to fundamental questions of many-body physics.

[1] E. Runge and E.K.U. Gross, Phys. Rev. Lett. **52**, 997 (1984).
[2] R. van Leeuwen, Phys. Rev. Lett. **82**, 3863 (1999).

A 16.7 Wed 15:30 BAR 106

Ultra-fast calculation of bound atomic states and transitions in neutron star atmospheres with very strong magnetic fields — •Christoph Schimeczek and Günter Wunner — 1. Institut für Theoretische Physik, Universität Stuttgart

X-ray absorption spectra of neutron stars contain broad line features

which still defy interpretation but are most likely due to electromagnetic transitions of atoms and ions contained in the hot thin atmosphere covering the neutron stars. The presence of a very strong magnetic field with about 10^8T distorts all atomic structures and creates totally new spectral behaviour. We developed an ultra-fast Hartree-Fock-Roothaan code to calculate atomic states and transition rates under such abnormal conditions with high precision and set up a database of up to now a hundred thousand unique atomic states. This data can serve as input for quantitative model atmosphere calculations, which will ultimately clarify the physical properties of the atmosphere.

A 16.8 Wed 15:45 BAR 106

Hartree-Fock calculations for the photoionization of atoms and ions from hydrogen to iron in neutron star magnetic fields — •Peter Diemand, Thorsten Kersting, Damir Zajec, and Günter Wunner — 1. Institut für theoretische Physik, Universität Stuttgart

We derive the photoionization cross section in dipole approximation for many-electron atoms and ions in neutron star magnetic field strengths. Continuum states are treated in adiabatic approximation in a self-consistent way. Bound states are calculated by solving the Hartree-Fock-Roothaan equations using finite-element and B-spline techniques. The data are of importance for the quantitative interpretation of observed X-ray spectra that originate from the thermal emission of isolated neutron stars. They can serve as input for modelling neutron star atmospheres as regards chemical composition, magnetic field strength, temperature, and redshift. We demonstrate example results for astrophysically relevant atoms and ions in the range Z=1,...26.