Time: Monday 16:00–18:30

# Location: P1

## A 7.1 Mon 16:00 P1 Parity-Violation in Hydrogen: Precision Enhancement through Many-Particle Squeezing — •Martin-Isbjörn Trappe, THOMAS GASENZER, and OTTO NACHTMANN — Institut für Theoretische Physik, Heidelberg

We discuss the propagation of hydrogen atoms in static electric and magnetic fields in a longitudinal atomic beam spin echo (IABSE) 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 IABSE experiments require a high precision for detecting atoms in specific states. We investigate possibilities to enhance the precision of IABSE experiments beyond the standard quantum limit using squeezed many-particle hydrogen states.

## A 7.2 Mon 16:00 P1

Hartree-Fock calculations of the photoionization of light to medium atoms and ions in neutron star magnetic fields — PE-TER DIEMAND, THORSTEN KERSTING, •DAMIR ZAJEC, and GÜNTER WUNNER — 1. Institut für Theoretische Physik, Universität Stuttgart Using the method described in the talk by Diemand et al., we determine the photoionization cross section in dipole approximation for light to medium atoms and ions in neutron star magnetic field strengths. Continuum states are treated in adiabatic approximation in a selfconsistent 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 with regard to chemical composition, magnetic field strength, temperature and redshift.

A 7.3 Mon 16:00 P1

Hartree-Fock calculations for the photoionization of heavy atoms and ions in neutron star magnetic fields — PETER DIE-MAND, •THORSTEN KERSTING, DAMIR ZAJEC, and GÜNTER WUNNER — 1. Institut für Theoretische Physik, Universität Stuttgart

Using the method described in the talk by Diemand et al., we determine the photoionization cross section in dipole approximation for heavy atoms and ions in neutron star magnetic field strengths. Continuum states are treated in adiabatic approximation in a selfconsistent 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 with regard to chemical composition, magnetic field strength, temperature and redshift.

### A 7.4 Mon 16:00 P1

Correlation function quantum Monte Carlo calculations for ground and excited states of many-electron atoms and ions in neutron star magnetic fields — •SEBASTIAN BOBLEST, DIRK MEYER, and GÜNTER WUNNER — 1. Institut für Theoretische Physik, Universität Stuttgart

We apply the correlation function quantum Monte Carlo method to the calculation of atomic data of medium-heavy atoms and ions in neutron star magnetic fields. This method allows for the calculation of both ground and excited states, as well as transition rates.

We use basis sets which account for the growing dominance of the cylindrical symmetry as the magnetic field is increased. These basis sets are computed using the Hartree-Fock-Roothaan method.

The atomic data obtained in these calculations are of relevance to the analysis of features discovered in the thermal emission spectra of isolated neutron stars.

A 7.5 Mon 16:00 P1 Recent Improvements in Transport and Application of Hyperpolarized Xe-129 — •Maricel Repetto<sup>1</sup>, Mathis Düwel<sup>2</sup>, Werner Heil<sup>1</sup>, Hans W. Spiess<sup>2</sup>, Peter Blümler<sup>1</sup>, and KerSTIN MÜNNEMANN<sup>2</sup> — <sup>1</sup>Johannes Gutenberg University, Institute of Physics, Mainz, Germany. — <sup>2</sup>Max Planck Institute for Polymer Research, Mainz, Germany.

Hyperpolarized (HP) Xe-129 has numerous applications in medicine and fundamental physics. For separating HP Xe-129 from other gases used in the hyperpolarization process, it can be accumulated at 77K. The conditions of this process must be carefully evaluated in order to minimize polarization losses. Different devices and results for this separation process are presented. Additionally, HP Xe-129 must be transported to other sites (e.g. clinics). Therefore, the relaxation time, T1, must be kept as long as possible. Different strategies (e.g. admixing of gases and low-field storage) to achieve this goal are presented together with suitable home-build instrumentation to determine T1. Finally, the application to the patient must be realized in a rapid and biocompatible way. Here we found a very elegant solution by using oxygenation membranes, which dissolve Xe instantaneously and without foaming in any suitable carrier liquid or even blood.

A 7.6 Mon 16:00 P1 Numerical signatures of non-selfadjointness in quantum Hamiltonians — •MATTHIAS RUF<sup>1</sup>, CARSTEN MÜLLER<sup>1</sup>, and RAINER GROBE<sup>2</sup> — <sup>1</sup>Max-Planck-Institut für Kernphysik, Saupfercheckweg 1, D-69117 Heidelberg — <sup>2</sup>Intense Laser Physics Theory Unit and Department of Physics, Illinois State University, Normal, IL 61790-4560 USA

There are quantum mechanical Hamiltonians, which may lose their self-adjointness if certain parameters exceed certain values. For example, it is well known that the Dirac Hamiltonian for the Coulomb potential V(r) = -Z/r loses its essential self-adjointness if the nuclear charge Z exceeds the critical value of  $Z_{\rm cr} = 118$  [1].

While non-selfadjoint quantum mechanical operators do not necessarily possess eigenvalues, finite  $N \times N$  matrix representations of these, however, may be hermitian and therefore have a finite set of N real eigenvalues. Using the momentum operator, the kinetic energy operator, and the relativistic Hamiltonian of the Coulomb problem for the Klein-Gordon equation as examples, we examine analytically and numerically the properties of the spectrum and eigenvectors in finite dimensional Hilbert spaces. We study the limit of  $N \to \infty$  for which some eigenvalues cease to exist as the corresponding operators are not selfadjoint.

[1] B. Thaller, The Dirac Equation, Springer (1992)

A 7.7 Mon 16:00 P1

Construction of a Compact <sup>3</sup>He Polarizing Facility for Local Usage — •Christian Mrozik, Oliver Endner, Christopher Hauke, Werner Heil, Sergei Karpuk, Jan Klemmer, and Ernst Otten — Johannes Gutenberg-Universität Mainz

Since a decade hyperpolarized  ${}^{3}$ He, used in fundamental research as well as in medical imaging, 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. At these parameters the process requires the magnetic field to have a relative gradient of  $\Delta B/B < 3.8 \cdot 10^{-4} \text{ cm}^{-1}$ . 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. 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. Compared to the currently used facility, a neat linear motor replaces the cumbersome hydraulical drive of the piston, which compresses the gas without polarization-losses from 1 mbar up to 5 bar. The design of the compact apparatus aims to reach a flux of hyperpolarized  $^3\mathrm{He}$  at P>65% of several standard liters per hour.

A 7.8 Mon 16:00 P1 Ultracold long-range giant dipole molecules in crossed electric and magnetic fields — •MARKUS KUR2<sup>1</sup>, MICHAEL MAYLE<sup>2</sup>, and PETER SCHMELCHER<sup>1</sup> — <sup>1</sup>Zentrum für Optische Quantentechnologien, Universität Hamburg, Luruper Chaussee 149, 22761 Hamburg, Germany —  $^2 \rm JILA,$  NIST and University of Colorado, Boulder, Colorado 80309-0440, USA

Giant dipole atoms in crossed electric and magnetic fields have been proven to exhibit extraordinary properties such as a strongly decentered wave function and a huge dipole moment ([1,2]).

Here we explore the existence of ultracold long-range giant dipole molecules by binding a neutral ground state atom to the decentered electronic wave function of the giant dipole atom. It is shown that the adiabatic potential surfaces emerging from the interaction of the ground state atom with the giant dipole electron posses a rich topology depending on the degree of electronic excitation. Binding energies and the vibrational motion in these surfaces are analyzed. Beyond this, we demonstrate the existence of intersection manifolds of excited electronic states potentially to a fast vibrational decay of the ground state atom dynamics [3].

[1] O. Dippel, Phys. Rev. A 49, 4415 (1994)

[2] V. Averbukh, Phys. Rev. A, 59, 3695 (1999)

[3] M. Kurz, in preparation

A 7.9 Mon 16:00 P1

Building mathematical foundations for time-dependent density functional theory — •MARKUS PENZ<sup>1</sup> and MICHAEL RUGGENTHALER<sup>2</sup> — <sup>1</sup>Institut für Theoretische Physik, Universität Innsbruck, 6020 Innsbruck, Austria — <sup>2</sup>Department of Physics, Nanoscience Center, University of Jyväskylä, 40014 Jyväskylä, Finland

In this presentation we study the essential mathematical structures for a rigorous foundation of time-dependent density functional theory, a reformulation of many-body quantum mechanics where the wave function as a fundamental variable is replaced by the electronic density. We introduce a new fixed-point proof of the fundamental one-to-one correspondence between densities and external potentials. Our approach not only sharpens the Theorems of Runge and Gross and van Leeuwen, as no additional time regularity is needed, but also yields interesting restrictions on the density and leads to a problem-adapted set of external potentials.

A 7.10 Mon 16:00 P1

Complex dilation for time-dependent phenomena in driven helium — •FELIX JÖRDER, PIERRE LUGAN, VERA NEIMANNS, KLAUS ZIMMERMANN, and ANDREAS BUCHLEITNER — Physikalisches Institut, Albert-Ludwigs-Universität Freiburg i.Br., Deutschland

The electromagnetically driven helium atom defines a paradigmatic scenario of a fragmenting quantum system, characterized by high spectral densities and decay channels into multiple continua. A powerful tool to access the spectral structure underlying the field-induced excitation and fragmentation process is provided by complex dilation of the Hamiltonian, which uncovers the pole structure of the resolvent operator. We summarize the current status of applications of complex dilation techniques in this specific physical context, and discuss novel perspective, such as the impact of the interelectronic repulsion on dynamical localization effects in the excitation process.

A 7.11 Mon 16:00 P1 Strong-field laser atom interaction: dynamic resonances and laser-induced states — •THOMAS KEIL and DIETER BAUER — Institut für Physik, Universität Rostock, 18051 Rostock, Germany

During the interaction of strong laser fields with atoms, energy levels undergo pronounced nonperturbative AC Stark shifts. It is known, for instance, that Rydberg levels may be brought into multiphoton resonances for particular laser field intensities (Freeman resonances). Such resonances give rise to a nonmonotonic behavior of the ionization rate as a function of the laser intensity. The laser field may also induce bound states that are absent without laser field. If populated, lightinduced states are useful for the understanding of unexpected observations such as even harmonics from systems with inversion symmetry. We present photoelectron spectra obtained from the ab initio solution of the time-dependent Schrödinger equation and identify effects of Freeman resonances on them. Light-induced states are investigated via a spectral analysis of the ab initio wavefunction.

A 7.12 Mon 16:00 P1 High-Order Harmonic Generation in the Presence of a Resonance — •MARIA TUDOROVSKAYA<sup>1,2</sup> and MANFRED LEIN<sup>1</sup> — <sup>1</sup>Leibniz Universitaet Hannover, Hannover, Germany — <sup>2</sup>Institut fuer Physik, Universitaet Kassel, Kassel, Germany

High-order harmonic generation is a nonlinear process occuring in the intense laser field affecting on atomic or molecular targets. We investigate high-order harmonic generation from laser-irradiated atoms with a potential that supports a shape resonance. Although the process leads to emittion of photons with very high energy, its effitiency is not very high. Certain harmonics is enhanced due to the presence of the resonance. From the numerical solution of the time-dependent Schroedinger equation, we calculate the harmonic spectra and make time-frequency analysis, revealing the separate contribution of the short and long trajectories as well as the resonance. Using potentials with different shape, we show how parameters of the potential barrier can affect the resonance in the spectrum. We show that significant resonance in the spectrum can be achieved from the pulse length being equal to just a few optical periods of the laser. We simulate the phase matching in a gas medium by coherent summation over intensities. It is shown that the contribution of the long trajectories becomes negligible, but the signature of the resonance is still significant.

#### A 7.13 Mon 16:00 P1

Engineering the Coherences at the Single-Atom Level — •ANDREA ALBERTI, MICHAL KARSKI, LEONID FÖRSTER, ANDREAS STEFFEN, NOOMEN BELMECHRI, WOLFGANG ALT, ARTUR WIDERA, and DIETER MESCHEDE — Institut für angewandte Physik, Universität Bonn

We demonstrate the capability to coherently steer individual neutral cesium atoms with single lattice-site resolution in a spin-dependent optical lattice. Following the so-called \*bottom-up\* approach, we engineer a few-body quantum system building it up atom by atom. This has recently enabled us to experimentally investigate 1D quantum walks in real space, which form an ideal model system to investigate transport phenomena dominated by quantum interference. Furthermore, it offers us a direct handle on the boundary between classical and quantum world. The entanglement between internal and external degrees of freedom is increased with the number of steps along the walk. At the moment we preserve quantum coherences over more than 10 steps. We are currently exploring single atom interferometry to get a deeper grasp of the phase evolution of a spatially delocalized atom in a spin-dependent optical lattice.