A 26: Atomic systems in external fields

Time: Wednesday 16:15–18:15   Location: S Fobau Physik

A 26.1   Wed 16:15   S Fobau Physik

Influence of nuclear motion on two-center photoionization — •Fiona Grüll, Alexander B. Voitkiv, and Carsten Müller — Institut für Theoretische Physik I, Heinrich-Heine-Universität Düsseldorf, Deutschland

Photoionization of an atom A can be strongly enhanced in the presence of a neighboring atom B due to two-center electron correlations. For certain resonant photon energies, atom B can first be excited and afterwards transfer the excitation energy radiationlessly via dipole-dipole interactions to atom A, leading to its ionization. This indirect ionization pathway can dominate over the direct photoionization by several orders of magnitude, as was predicted some years ago assuming a fixed internuclear distance [1]. A related experiment observed enhanced photoionization in heteroatomic dimers, though at substantially reduced scale [2]. In light of this, we analytically study how two-center photoionization is influenced by the nuclear motion in a molecule when considering Li-He dimers as an example. Shifts of the atomic energy levels in the presence of a neighboring atom are calculated as a function of the internuclear distance. Besides, the internuclear motion is accounted for by considering the relevant vibrational states in the molecule.

[1] B. Najjari, A. B. Voitkiv and C. Müller, Phys. Rev. Lett. 105, 153002 (2010)
[2] F. Trinter et al., Phys. Rev. Lett. 111, 233004 (2013)

A 26.2   Wed 16:15   S Fobau Physik

QPROP 3.0: an improved t-SURFF 2.0 algorithm for a trusted Schrödinger solver — •Vasily Tulsky and Dieter Bauer — University of Rostock, Rostock, Germany

Solving the time-dependent Schrödinger equation (TDSE) for an atom in a strong laser field is often a delicate problem and requires numerical methods to obtain accurate results. In the particular case of calculating photoelectron spectra (PES) the t-SURFF method [1] is efficiently applied, allowing to significantly reduce the size of the numerical grid. This poster is devoted to our TDSE solver named QPROP [2-3] and the fresh improvement to its t-SURFF part.

Once the ionizing laser pulse is over, the propagation of the wavefunction is determined by a time-independent Hamiltonian. This allows to analytically obtain the contribution to the surface flux after the pulse [4], covering the infinite time interval in a single step, significantly speeding up the calculation of the PES and allowing to exactly reproduce even its low-energy domain.

[1] L. Tao, A. Scrinzi, New Journal of Physics **14**, 013021 (2012).
[2] D. Bauer, P. Koval, Computer Physics Communications **174**, 396 (2006).
[3] V. Mosert and D. Bauer, Computer Physics Communications **207**, 452 (2016).
[4] F. Morales, T. Bredtmann, S. Patchkovskii, J. Phys. B **49**, 245001 (2016).

A 26.3   Wed 16:15   S Fobau Physik

A rydberg-atom based detector for terahertz radiation — •Lara Torralbo-Campo[1], Manuel Kaiser[1], Raphael Wieland[1], Fabian Rudau[1], Jens Grimmel[1], Xiang Lue[2], Lutz Schrottke[2], Holger Grahn[2], Reinhold Kleiner[1], and Jozsef Fortagh[1] — [1]Universität Tübingen, Physikalisches Institut, Auf der Morgenstelle 14, 72076 Tübingen — [2]Paul-Drude-Institut fuer Festkoerperelektronik, Leibniz-Institut im Forschungsverbund Berlin e.V

Rydberg atoms have proven to be an excellent sensitive probe to electromagnetic fields. Here, we present our ongoing development of a Rydberg atom-detector using a four atomic level scheme based on electromagnetically induced transparency (EIT) in a hot atomic vapour. This detector is used to characterize different types of terahertz (THz) source emitters such as superconductors emitters and quantum cascade lasers.

Besides, THz induced single atom transitions and subsequent single atom counting in an ultracold atomic cloud, making the detector suitable for the measurement of photon statistics of the THz emitters.

This detector will enhance the technological development of new THz sources and detectors.

A 26.4   Wed 16:15   S Fobau Physik

A laser system for imaging of rubidium at high magnetic fields — •Jennifer Koch[1], Daniel Adam[1], Quentin Bouton[1], Daniel Mayer[1], Jens Nettersheim[1], Felix Schmidt[1], and Artur Widera[1,2] — [1]Departmet of Physics and State Research Center OPTIMAS, University of Kaiserslautern, Erwin-Schrödinger-Str. 46, 67663 Kaiserslautern, Germany — [2]Graduate School Materials Science in Mainz, Erwin-Schrödinger-Str. 46, 67663 Kaiserslautern, Germany

Impurities in quantum systems are the origin of many fascinating phenomena such as polarons or the Kondo system, for example. Our approach to realize such a system immerses cold single cesium atoms as impurities into an ultracold quantum gas of rubidium. The interaction between the two species can be tuned by magnetic Feshbach resonances at magnetic fields of up to 350 G. In order to characterize our impurity-BEC system, absorption imaging for rubidium and fluorescence imaging for cesium is employed, where resonant light is required in both cases.

In order to allow imaging of or removing the rubidium cloud from the system at high magnetic field, we have constructed a diode-based laser system. At field strengths above 200 G, transition frequencies are shifted by the order of some GHz due to the magnetic field. The stabilization of the linear interference-filter lasers used is based on a flexible frequency offset locking scheme. We present characterization of the system and current status of the project. The system will allow high-field and in-situ imaging of cesium impurities and the rubidium BEC.

A 26.5   Wed 16:15   S Fobau Physik

"Selection rules" for atomic excitation by twisted light — •Yuxiong Duan[1,2], Robert Müller[1,2], and Andrey Surzhykov[1,2] — [1]Physikalisch–Technische Bundesanstalt, D–38116 Braunschweig, Germany — [2]Technische Universität Braunschweig, D–38106 Braunschweig, Germany

Atomic excitation by twisted light has attracted much attention recently [1,2]. Here we present a thorough theoretical analysis of the selection rules for this process. We show that these rules originate from the complex interplay between the structure of the atomic target and of the incident light beam. Since the twisted light has very complex internal structure, where the multipole components of the beam vary significantly within the wave front, the selection rules depend on both the position of the target atom and beam parameters. In order to investigate this dependence, we present detailed calculations for the twisted-light-induced transition $4s\,^2S_{1/2} \to 3d\,^2D_{5/2}$ of a Ca^+ ion.

[1]C. T. Schmiegelow et al., Nat. Commun. **7**, 12998 (2016).
[2]A. Afanasev et al., New J. Phys. **20**, 023032 (2018).

A 26.6   Wed 16:15   S Fobau Physik

Mass defect of electronic transitions in atoms and ions — Simon Eilers, •Víctor J. Martínez-Lahuerta, Marius Schulte, and Klemens Hammerer — Institute for Theoretical Physics and Institute for Gravitational Physics (Albert-Einstein-Institute), Leibniz University Hannover, Appelstrasse 2, 30167 Hannover, Germany

In this work we will present a low-order relativistic correction to the multipolar atom-light Hamiltonian for two bound particles corresponding to a simple model for Hydrogen-like atoms and ions. From this result we can systematically predict frequency shifts in atomic clocks based on trapped ions due to the mass defect and the quadrupole effect caused by external fields, as recently discussed by V. Yudin and A. V. Taichenachev (Laser Phys. Lett. 15, 035703, 2018).

A 26.7   Wed 16:15   S Fobau Physik

Understanding Correlation Effects in Photoelectron Circular Dichroism — •Manel Mondelo-Martell, Christiane Koch, and Daniel Reich — Institüt für Physik, Universität Kassel, Germany

Chirality is a fundamental symmetry breaking, defined by the impossibility to superpose the mirror images of a given object, highly relevant in the fields of AMO and chemistry. Current experimental techniques based on chiral radiation–matter interactions, such as Photoelectron Circular Dichroism (PECD)[1], provide detailed information about such systems, but theoretical models are crucial for its interpretation. Accurate numerical simulation of the photoionization process is limited to ~three electron systems, and studies pursuing a time–resolved solution of the process for larger systems generally need to rely on a simplified

ansatz to become numerically affordable, which usually leads to a poor description of electronic correlation and thus only qualitative results.

We present a time–resolved simulation of photoelectron spectra in chiral environments using the MCTDHF[2] approach. This algorithm allows for a numerically efficient representation of the wave function through the use of time–dependent basis sets, and includes electronic correlation due to its multiconfigurational character. To study the suitability of this technique for the study of chiral effects in correlated many-electron systems, the photoionization of a He atom embedded in a chiral potential will be simulated. Comparison with the TDHF approach and possible improvements will be discussed.

References [1] I. Powis, in Adv. Chem. Phys. (2008), pp. 267-329. [2] D. Hochstuhl and M. Bonitz, J. Chem. Phys. 134, 084106 (2011).