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MODERN OPTICS

Theoretical Atomic, Molecular, and Optical Physics

The research group *Modern Optics* investigates a variety of different topics in the field of theoretical atomic, molecular, and optical physics. This ranges from the behaviour of atoms and molecules in ultra-short, ultra-intense laser pulses, over coherent control of (chemical) reactions and the physics of ultra-cold atomic and molecular gases to the interaction of matter with antimatter. The research mainly aims for the understanding of fundamental processes in mostly small molecular systems under extreme or very unusual conditions.

The complete understanding of the behaviour of atoms and molecules exposed to ultra-short and ultra-intense laser pulses is difficult to achieve for a number of reasons. First, the intensity that can be achieved in present days lasers is comparable or even larger than the binding forces within atoms and molecules. Second, the laser pulse length can be on the time scale or even faster than that of nuclear motion. In fact, depending on the laser pulse length, three different time scales (the one of the electrons, nuclei, and the field variation) have to be considered. Third, besides the competition between purely electronic or nuclear excitation (including ionization and dissociation, respectively) a combination of these effects can occur. Finally, depending on the laser parameters very different interaction mechanisms can be observed. In a simplified picture, it is possible to distinguish four regimes of laser-atom interaction depending on the peak intensity of the laser and the photon frequency (see Fig. 1): the so-called quasi-static regime (itself divided into the tunnelling and over-the-barrier ionization regimes) and the multi-photon regime (again divided into the perturbative and non-perturbative regimes where in the former lowest-order perturbation theory (LOPT) is applicable). While simple tunnelling formulas exist for predicting the tunnel ionization of hydrogen-like (one-electron) atoms, neither their validity for multi-electron atoms or molecules nor their extension to the over-the-barrier ionization regime is known. Also the calculation of LOPT cross-sections is a non-trivial task, since it requires an (in principle infinite) summation over matrix elements between field-free states, including the corresponding continua. Again, a relatively well-known solution to this computational task exists only for hydrogen-like one-electron atoms. The most challenging regime from the theoretical viewpoint is, however, the non-perturbative multi-photon regime that fills the gap between the LOPT and the quasi-static regimes whose exact border-line of validity is in fact

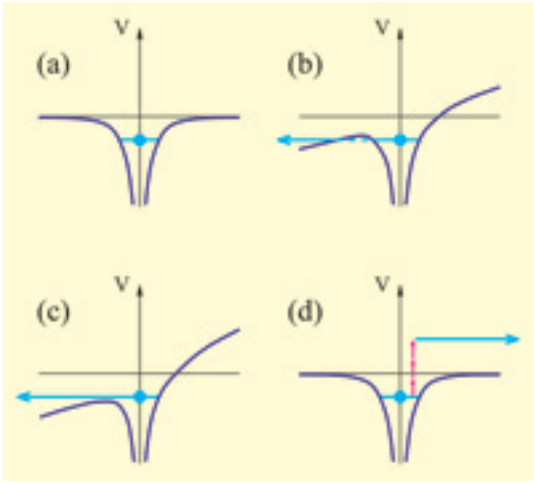

Fig. 1
In a strong electric or slowly varying laser field (quasi-static regime) the atomic Coulomb potential (a) is distorted and the electron can undergo tunnel ionization through the distorted barrier (b). In even stronger fields the barrier can be so strongly distorted that the electron can escape over the lowered barrier leading to over-the-barrier ionization (c). If the field variation is fast on the electronic time scale (high photon frequency, multiphoton regime), the electron has no time to tunnel through the field-distorted barrier, but it can escape via multi-photon absorption (d).

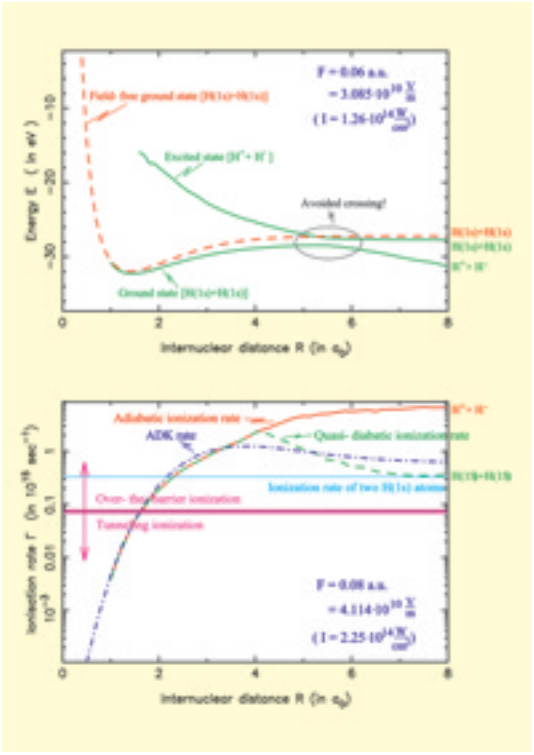

Fig. 2
Behaviour of H_2 in a static electric or quasi-static laser field. The field-free (adiabatic) ground-state potential curve is distorted, since it shows an avoided crossing with the excited state dissociating into the ion pair H^++H^- that is strongly influenced by the field (top). This distortion leads to bond softening (dissociation through or over the lowered barrier) and to enhanced ionization, i.e. *a strong increase (note the logarithmic scale) of the ionization rate at a specific inter-nuclear distance R (bottom). The* ab initio *rates are also compared to the prediction of a simple atomic tunnelling model (ADK).*

Moderne Optik: Theoretische Atom-, Molekül- und optische Physik

In der Arbeitsgruppe *Moderne Optik* werden eine Vielzahl verschiedener Themen auf dem Gebiet der theoretischen Atom-, Molekül- und optischen Physik bearbeitet. Dies reicht von dem Verhalten von Atomen und Molekülen in ultrakurzen, ultraintensiven Laserpulsen über kohärente Kontrolle von (chemischen) Reaktionen und die Physik ultrakalter atomarer und molekularer Gase bis hin zur Wechselwirkung von Materie mit Antimaterie. Die Forschung zielt dabei vornehmlich auf ein besseres Verständnis der fundamentalen Prozesse in zumeist kleinen molekularen Systemen unter extremen oder äußerst ungewöhnlichen Verhältnissen.

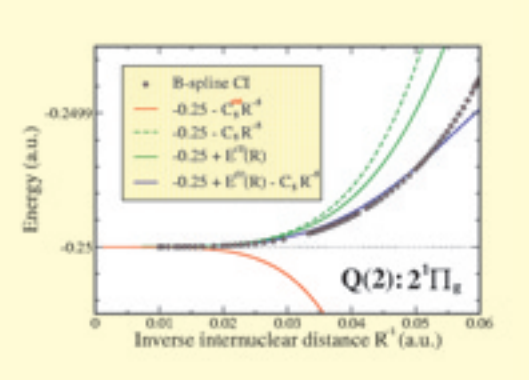

Fig. 3
The theoretical investigation of ultra-cold atomic collisions requires the extremely accurate knowledge of the corresponding molecular potential curves describing the inter-atomic interaction, up to very large inter-nuclear distances R. *Our newly developed quantum mechanical* ab initio *code (using* B *splines) allows very precise calculations also at very large inter-nuclear distances. In this way it was even possible to find errors in the van-der-Waal's coefficients predicted from perturbation theory (C_5^{old}) for the interaction of two excited hydrogen atoms, while good agreement is found with the results obtained from the corrected perturbation theory including previously neglected off-diagonal terms ($E^{(1)}$) and the newly calculated C_6 coefficients.*

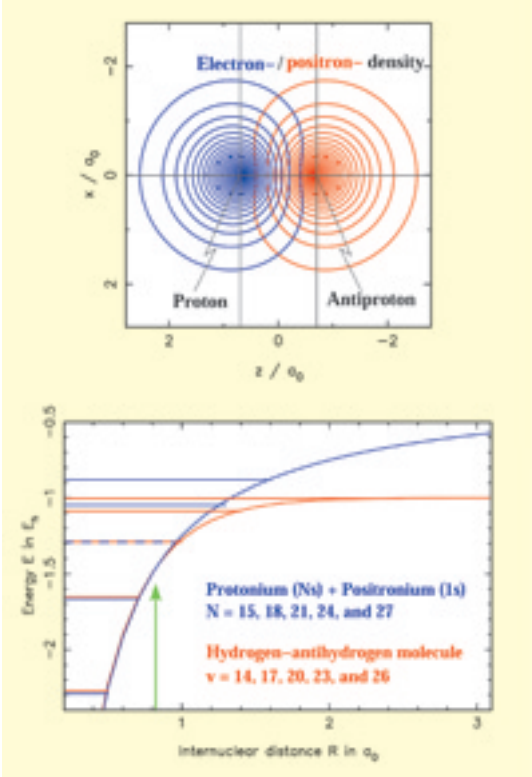

Fig. 4
Ground-state densities of the hydrogen-antihydrogen system (top). While the electron is attracted by the proton and repelled by the antiproton and the opposite is true for the positron, the electron and positron try to maximize their mutual overlap. The hydrogen-antihydrogen »molecule« is vibrationally (»chemically«) bound, but meta-stable with respect to annihilation and (for inter-nuclear distances below the critical distance R_c *indicated by the green arrow) with respect to a rearrangement into protonium and positronium, since below* R_c *the protonium/positronium curves lies below the one of hydrogen/antihydrogen (bottom). In contrast to the infinite series of »vibrational« protonium states (*Ns, N=1 to ∞*) hydrogen-antihydrogen possesses only a finite number of vibrational states* ν.

unknown. The theoretical treatment of this regime requires a full solution of the time-dependent Schrödinger equation describing the atomic or molecular system in a laser field. The main question we would like to answer in the field of laser-matter interaction is the following: is it possible, at least for the smallest »multi-electron« »multi-atom« molecule (H_2) to fully understand its interaction with strong laser fields? If this should be the case, what can we learn for larger molecules?

As a starting point for the investigation of the quasi-static regime a new method was developed and applied that allowed the first fully correlated three-dimensional calculation of the behaviour of H_2 in a static electric field (for both ground and excited states). As a surprise, it was found that a forty-year old prediction was wrong. In contrast to general believe, two molecular strong-field effects that were assumed to be present only in odd-numbered (diatomic) molecules or molecular ions and to be absent in covalently bound molecules with an even number of electrons (as in H_2) were showed to be present in H_2 [1]. These are the field-induced distortion of the molecular ground-state potential curve leading to bond softening and a strong peak in the ionization rate at a specific inter-nuclear distance (enhanced ionization) (see Fig. 2). It was even possible to find a simple quantum-mechanical explanation for the occurrence of these effects that allows to predict their universality. Also the validity and break-down of simple atomic tunnel-ionization models when applied to H_2 was investigated for the first time. Based on the calculated electric-field induced distortions of the potential curves and ionization rates it was very recently possible to develop a time-averaged quasi-static model that allowed to predict the vibrational distribution of H_2^+ that is formed after strong-laser-field ionization of H_2 [2]. The predicted distribution differs substantially from the Franck-Condon distribution that was so far almost exclusively used in the interpretation of experimental data, but compares very favourably with an experiment that for the first time was able to directly measure this vibrational distribution. Also in the opposite limit, the LOPT regime, the first fully correlated three-dimensional calculations for H_2 have been performed in our group [3]. Presently, the first results are obtained for the full three-dimensional solution of the time-dependent Schrödinger equation describing H_2 in an ultra-short laser pulse. Hopefully, this will allow to bridge the different simplified regimes (quasi-static and perturbative multi-photon regime) and to finally provide a complete understanding of the behaviour of H_2 in strong laser pulses. This would form the basis to extend this understanding to more complicated molecules.

Another interesting aspect of the laser-matter interaction is based on the use of the coherence of laser light. This has lead to the field of coherent control of (chemical) reactions. Different coherent-control schemes have been proposed and were successfully realized. The basic idea behind these schemes is the use of quantum interferences between different paths leading to the same final state. This can be used to either enhance the yield of wanted transitions or to suppress unwanted ones. While the recently developed method of laser-pulse shaping in combination with self-learning algorithms has lead to a tremendous progress in this field, the theoretical understanding is lagging behind. Using simple molecular systems like H_2 or alkali dimers that allow a rather complete theoretical treatment we try to improve the understanding of these coherent-control schemes [4].

A second research topic of our group is the understanding of the interactions in ultra-cold atomic and molec-

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ular gases. This subject is of growing interest after the first experimental realizations of Bose-Einstein condensates in dilute atomic gases (recently awarded with the Nobel prize in physics). These coherent macroscopic quantum objects possess very peculiar properties and have recently shown evidence that (together with optical lattices) they may be also of great help to investigate fundamental questions of solid-state physics, since the interaction between the particles is tunable; in contrast to the electronic interaction in solid-state physics. This tunability is achieved either by using different atoms (that will show different interaction strengths) or even by small magnetic fields and the use of Feshbach resonances. (In a Feshbach resonance, a bound vibrational state becomes resonant with the continuum state describing two colliding atoms. This leads to a sudden change of the scattering properties of the atoms.) The collision of atoms becomes increasingly sensitive to the details of the potential curves describing their interaction, if the collision energy (and thus the temperature) is reduced. The theoretical investigation of the interactions between ultra-cold atoms thus requires a very accurate determination of the inter-atomic potential curves. The determination of these potential curves (using own computer codes [5]) and the subsequent scattering calculations are one aspect of our contribution to the field (see Fig. 3). In the context of an international collaboration the theoretical description of the scattering of two excited hydrogen atoms is developed [6]. Besides being a fundamental scattering problem (including the need for considering autoionization channels) it is also of interest for the development of a Lyman-α laser and in the context of high-precision spectroscopy. Our main focus is, however, concentrated on the accurate description of alkali dimers, since most Bose-Einstein condensates that could be created so far are made from alkali atoms. Besides structural questions we are mainly concerned with the question of how ultra-cold molecules can be produced and trapped. Different photo-association schemes are investigated with respect to their experimental realizability and their possible manipulation by optical lattices/traps. Another goal of our research is the understanding of ultra-cold samples beyond the usually adopted mean-field theory. For this purpose, new codes for simulating the fully correlated motion of trapped ultra-cold atomic samples are developed.

Finally, we are investigating a number of problems related to fundamental questions in physics. This includes the investigation of molecular effects in nuclear β decay that are important for determining an upper limit to the neutrino mass using tritium neutrino-mass experiments [7]. Another project deals with the fundamental questions related to the interaction of matter with antimatter, especially antihydrogen. The latter has recently been successfully produced at CERN by two competitive collaborations in order to use it for testing fundamental symmetries as the Charge-Parity-Time (CPT) invariance and the Weak Equivalence Principle (WEP). (In simple terms these symmetries may be described by the questions whether an anti-apple would be attracted by an anti-world in the same way as Newton's apple by our ordinary world and whether an anti-apple would be attracted by the ordinary world like an ordinary one.) While these tests require cold antihydrogen atoms in their ground states, the experiments have so far only produced hot antihydrogen in very highly excited states. Within an international collaboration we have investigated the possibility to use ultra-cold hydrogen atoms for cooling and de-exciting antihydrogen [8]. Although this idea appears to be rather stupid in view of matter-antimatter annihilation, the investigation of the very interesting hydrogen-antihydrogen system (forming a metastable »chemical« molecule, (see Fig. 4) revealed that the cross-sections for both cooling and de-excitation are rather favourable compared to annihilation. However, our newest findings have disclosed additional, so far unforeseen loss channels. Presently, we are investigating alternative schemes for producing cold ground-state antihydrogen, but already now this project has revealed a lot of exciting new physics related to fundamental but non-standard physical systems.

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Literature

[1] *Saenz, A.*: Phys. Rev. A 66, 063407 (2002); ibid. 063408 (2002).
[2] *Urbain, X.* et al.: Phys. Rev. Lett. 92, 163004 (2004).
[3] *Apalategui, A./Saenz, A.*: J. Phys. B 35, 1909 (2002).
[4] *Apalategui, A./Saenz, A./Lambropoulos, P.*: Phys. Rev. Lett. 86, 5454 (2001).
[5] *Vanne, Y./Saenz, A.*: J. Phys. B 37, 4101 (2004).
[6] *Forrey, R. C. et al.*: Phys. Rev. Lett. 85, 4245 (2000).
[7] *Saenz, A./Jonsell, S./Froelich, P.*: Phys. Rev. Lett. 84, 242 (2000).
[8] *Froelich, P. et al.*: Phys. Rev. Lett. 84, 4577 (2000); *Jonsell, S. et al.*: J. Phys. B 37, 1195 (2004).