

## A 22: Charged ions and their applications

Time: Thursday 10:30–12:30

Location: A-H1

## Invited Talk

**Optimizing large atomic structure calculations with machine learning** — ●PAVLO BILOUS<sup>1</sup>, ADRIANA PÁLFFY<sup>2</sup>, and FLORIAN MARQUARDT<sup>1</sup> — <sup>1</sup>Max-Planck-Institut für die Physik des Lichts, D-91058 Erlangen, Germany — <sup>2</sup>Department of Physics, Friedrich-Alexander-Universität Erlangen-Nürnberg, D-91058 Erlangen, Germany

Atomic structure calculations for heavy atoms and ions are computationally demanding due to the presence of strong electronic correlations. These corrections account for admixture of electronic configurations with excitations to unoccupied (virtual) or partially occupied orbitals. For systems with many electrons the number of such additional configurations becomes exponentially large. In this work, we make an attempt to employ a neural network to select which configurations do influence the physical quantity of interest (e.g. a transition energy or a hyperfine structure constant), and which can be omitted without significant loss of precision. As an example, we consider a highly charged Th<sup>35+</sup> ion with the electronic configuration  $4f^9$ . This case allows for an electronic bridge scheme [1] relevant for a nuclear clock based on the 8 eV nuclear <sup>229</sup>Th isomeric state. In this approach, accurate electronic transition energies are required. The latter were obtained recently in Ref. [2] under usage of massive computational resources. We discuss how the required resources can be reduced by carrying out neural-network-assisted calculations instead.

[1] P. V. Bilous et al., Phys. Rev. Lett. 124, 192502 (2020).

[2] S. G. Porsev et al., Quantum Sci. Technol. 6(3), 034014 (2021).

**First storage of highly charged ions in an ultralow-noise superconducting radio-frequency ion trap** — ●CHRISTIAN WARNECKE<sup>1,2</sup>, ELWIN A. DIJCK<sup>1</sup>, MALTE WEHRHEIM<sup>1</sup>, JULIA EFF<sup>1</sup>, ALVARO GARMENDIA<sup>1</sup>, ANDREA GRAF<sup>1</sup>, RUBEN HENNINGER<sup>1</sup>, CLAUDIA VOLK<sup>1</sup>, MORTEN WILL<sup>1</sup>, LAKSHMI PRIYA KOZHIPARAMBIL SAJITH<sup>4</sup>, KOSTAS GEORGIU<sup>3</sup>, CHRISTOPHER MAYO<sup>3</sup>, THOMAS PFEIFER<sup>1</sup>, and JOSÉ RAMON CRESPO LÓPEZ-URRUTIA<sup>1</sup> — <sup>1</sup>Max-Planck-Institute for Nuclear Physics, Saupfercheckweg 1 69117 Heidelberg Germany — <sup>2</sup>Heidelberg Graduate School for Physics, Im Neuenheimer Feld 226 69120 Heidelberg Germany — <sup>3</sup>School of Physics and Astronomy, University of Birmingham, Edgbaston, Birmingham, B15 2TT, UK — <sup>4</sup>Deutsches Elektronen-Synchrotron (DESY), Humboldt Universität zu Berlin

To provide an environment free of noise induced by external alternating electromagnetic fields, we developed a quasi-monolithic, superconducting quadrupole resonator combined with a Paul trap reaching a very high Q-factor up to  $2 \times 10^5$  at the working frequency of about 34 MHz. Such a high quality factor filters the radio-frequency trap drive noise significantly. Thus, heating rates of the radial modes are reduced. The cavity is a promising step to increase coherence times for quantum logic spectroscopy experiments, which will lead the way to future spectroscopy measurements with highly charged ions (HCI) in the Lamb-Dicke regime. Recently, first HCI have been successfully re-trapped and sympathetically cooled with a single Be<sup>+</sup> ion. We present the recent development of our setup and first characterizations.

**Bound Electron  $g$  Factor Measurements of Highly Charged Tin** — ●JONATHAN MORGNER<sup>1</sup>, CHARLOTTE M. KÖNIG<sup>1</sup>, TIM SAILER<sup>1</sup>, FABIAN HEISSE<sup>1</sup>, BINGSHENG TU<sup>3</sup>, VLADIMIR A. YEROKHIN<sup>2</sup>, BASTIAN SIKORA<sup>1</sup>, ZOLTÁN HARMAN<sup>1</sup>, JOSÉ R. CRESPO LÓPEZ-URRUTIA<sup>1</sup>, CHRISTOPH H. KEITEL<sup>1</sup>, SVEN STURM<sup>1</sup>, and KLAUS BLAUM<sup>1</sup> — <sup>1</sup>Max-Planck Institut für Kernphysik, Heidelberg — <sup>2</sup>Center for Advanced Studies, St. Petersburg — <sup>3</sup>Institute of Modern Physics, Shanghai

Highly charged ions are a great platform to test fundamental physics in strong electric fields. The field-strength experienced by a single electron bound to a high  $Z$  nucleus reaches strengths exceeding  $10^{16}$  V/cm. Perturbed by the strong field, the  $g$  factor of a bound electron is a sensitive tool that can be both calculated and measured to high accuracy. In the recent past,  $g$ -factor measurements of low  $Z$  ions reached precisions of low  $10^{-11}$ . Following this, the ALPHATRAP Penning-trap setup is dedicated to precisely measure bound-electron  $g$  factors of the heaviest highly-charged ions.

In this contribution, our recent measurement of bound-electron  $g$  factors in highly charged <sup>118</sup>Sn will be presented. Over the course of several months,  $g$  factors for three different charge states have been measured, each allowing a unique test of QED in a heavy highly charged ion, probing different  $g$ -factor contributions. Furthermore, progress on a new EBIT setup is presented. This will eventually allow ALPHATRAP to inject and measure even heavier highly charged systems beyond hydrogenlike lead (Pb<sup>81+</sup>).

**From single-particle picture to many electron QED** — ●ROMAIN SOGUEL<sup>1</sup> and ANDREY VOLOTKA<sup>2</sup> — <sup>1</sup>Helmholtz-Institut Jena, Jena, 07743, Germany — <sup>2</sup>ITMO University, St. Petersburg, 197101, Russia

The redefined vacuum approach, which is frequently employed in the many-body perturbation theory, proved to be a powerful tool for formula derivation. Here, we elaborate this approach within the bound-state QED perturbation theory. In addition to general formulation, we consider the particular example of a single particle (electron or vacancy) excitation with respect to the redefined vacuum. Starting with simple one-electron QED diagrams, we deduce first- and second-order many-electron contributions: screened self-energy, screened vacuum polarization, one-photon exchange, and two-photon exchange. The redefined vacuum approach provides a straightforward and streamlined derivation and facilitates its application to any electronic configuration. Moreover, based on the gauge invariance of the one-electron diagrams, we can identify various gauge-invariant subsets within derived many-electron QED contributions.

The employment of the redefined vacuum approach allowed us to identify the gauge-invariant subsets, within the two-photon-exchange diagrams, at two- and three-electron diagrams and separate between the direct and exchange contributions at two-electron graphs. The gauge invariance of found subsets is demonstrated both analytically (for an arbitrary state) as well as numerically for 2s, 2p<sub>1/2</sub>, and 2p<sub>3/2</sub> valence electron in Li-like ions.

**Dynamics of a trapped ion in a quantum gas: Effects of particle statistics** — ●LORENZO OGHITTO<sup>1</sup>, MELF JOHANNSEN<sup>1</sup>, ANTONIO NEGRETTI<sup>1</sup>, and RENE GERRITSMAN<sup>2</sup> — <sup>1</sup>Zentrum für Optische Quantentechnologien, Universität Hamburg, Luruper Chaussee 149, 22761 Hamburg, Germany — <sup>2</sup>Van der Waals Zeeman Institute, Institute of Physics, University of Amsterdam, Science Park 904, 1098 XH Amsterdam, The Netherlands

We study the quantum dynamics of an ion confined in a radio-frequency trap in interaction with either a Bose or spin-polarized Fermi gas. To this end, we derive quantum optical master equations in the limit of weak coupling and the Lamb-Dicke approximations. For the bosonic bath, we also include the so-called Lamb-shift correction to the ion trap due to the coupling to the quantum gas as well as the extended Fröhlich interaction within the Bogolyubov approximation that have been not considered in previous studies. We calculate the ion kinetic energy for various atom-ion scattering lengths as well as gas temperatures by considering the intrinsic micromotion and we analyze the damping of the ion motion in the gas as a function of the gas temperature. We find that the ion's dynamics depends on the quantum statistics of the gas and that a fermionic bath enables to attain lower ionic energies.

**Water-assisted electron capture exceeds photorecombination in biological conditions** — ●AXEL MOLLE<sup>1,2</sup>, OLEG ZATSARINNY<sup>3</sup>, THOMAS JAGAU<sup>2</sup>, ALAIN DUBOIS<sup>1</sup>, and NICOLAS SISOURAT<sup>1</sup> — <sup>1</sup>Laboratoire de Chimie Physique - Matière et Rayonnement, Sorbonne Université, Paris, France — <sup>2</sup>Quantum Chemistry and Physical Chemistry, KU Leuven, Belgium — <sup>3</sup>Department of Physics and Astronomy, Drake University, Des Moines, USA

A decade ago, an electron-attachment process called *interatomic coulombic electron capture* has been predicted to be possible through energy transfer to a nearby neighbour. It has been estimated to be competitive with environment-independent photorecombination for selected examples of reaction partners. Its impact on biological systems,

however, has yet to be investigated.

Here, we evaluate therefore the capability of alkali and alkaline earth metal cations to capture a free electron by assistance from a nearby water molecule. We introduce a characteristic distance  $r_{IC}$  for this energy transfer mechanism in equivalence to the Förster radius for energy transfer between chromophores which allows to estimate the quantum efficiency. We find  $r_{IC}$  bound from above. This water-assisted electron capture dominates over photorecombination beyond the second hydration shell of each alkali and alkaline earth cation for electron energies above a threshold. It will be measurable against photorecombination in an experiment around that threshold energy.

A 22.7 Thu 12:15 A-H1

**Parity-violation studies with partially stripped ions** — •JAN RICHTER<sup>1,2</sup>, ANNA V. MAIOROVA<sup>3,4</sup>, ANNA V. VIATKINA<sup>1,2,5,6</sup>, DMITRY BUDKER<sup>5,6,7</sup>, and ANDREY SURZHYKOV<sup>1,2,8</sup> — <sup>1</sup>Physikalisch-Technische Bundesanstalt, Germany — <sup>2</sup>Technische Universität Braunschweig, Germany — <sup>3</sup>Center for Advanced Studies, Peter the Great St. Petersburg Polytechnic University, Russia — <sup>4</sup>Petersburg

Nuclear Physics Institute of NRC "Kurchatov Institute", Russia — <sup>5</sup>Helmholtz Institute Mainz, GSI Helmholtzzentrum für Schwerionenforschung, Germany — <sup>6</sup>Johannes Gutenberg University Mainz, Germany — <sup>7</sup>Department of Physics, University of California, Berkeley, USA — <sup>8</sup>Laboratory for Emerging Nanometrology Braunschweig, Germany

We present a theoretical study of photoexcitation of highly charged ions from their ground states, a process which can be realized at the Gamma Factory at CERN. Special attention is paid to the question of how the excitation rates are affected by the mixing of opposite-parity ionic levels, which is induced both by an external electric field and the weak interaction between electrons and the nucleus. In order to reinvestigate this "Stark-plus-weak-interaction" mixing, detailed calculations are performed for the  $1s_{1/2} \rightarrow 2s_{1/2}$  and  $1s^2 2s_{1/2} \rightarrow 1s^2 3s_{1/2}$  ( $M1 + \text{parity-violating-E1}$ ) transitions in hydrogen- and lithium-like ions, respectively. In particular, we focus on the difference between the excitation rates obtained for right- and left-circularly polarized incident light. This difference arises due to the parity violating mixing of ionic levels.