CFEL SCIENCE

SEMINAR

18th October 2017 - 2:00 p.m.

CFEL-bldg. 99, seminar room IV

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Electron-Nuclear Dynamics in atomic and molecular collisions: From charge transfer to energy loss

The treatment of the electron and nuclei dynamics in time-dependent processes is fundamental to the understanding of matter-interaction in atomic and molecular physics. By using the time-dependent variational principle, the wave function for electrons and nuclei is evolved in time and a system of coupled, first-order, nonlinear differential equations is obtained for a general molecular system. The equations form a classical Hamiltonian system within a generalized phase space that allows a systematic time-dependent study of atomic and molecular processes. The approach is general and provides a computational framework for a variety of properties such as transition and excitation probabilities in atomic and molecular collisions. The simplest approximation corresponds to the choice of a single determinantal wave function for the electrons and classical nuclei. Illustrative applications to atomic and molecular collision processes are presented with good agreement to other theoretical and experimental data. Specific examples are provided for charge transfer total and differential cross sections as well as for the energy loss and stopping cross section as well as some examples towards femtosecond laser assisted collisions.

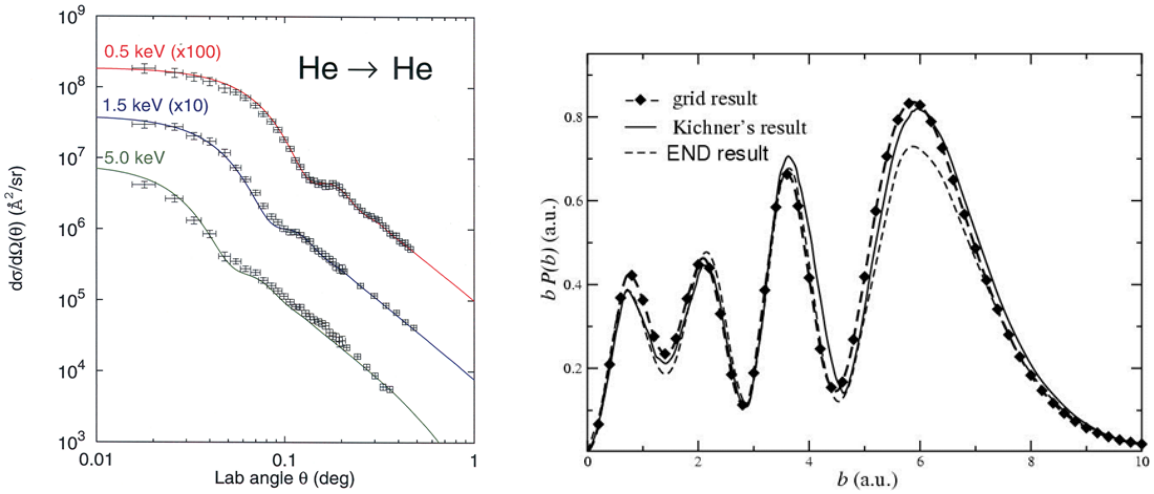

Fig. a) Direct differential cross section for He atoms colliding on He at 0.5, 1.5, and 1.5 keV. b) Impact parameter dependence of the charge transfer probability for He^{2+} colliding on atomic H at 2 keV.

Host: Robin Santra – CFEL-DESY Theory Division