Time-Dependent Close-Coupling Calculations for Ion-Impact Ionization of Atoms and Molecules

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Synopsis We summarize the application of the time-dependent close-coupling method to the study of ion-impact ionization of atoms and molecules. Ionization cross sections are presented for bare ion, antiproton, and neutron collisions with light atoms and molecules

A detailed understanding of the breakup of atomic and molecular systems remains a challenging task. Although perturbative methods do well in treating ion-impact single ionization of atoms and molecules, non-perturbative methods are needed to make accurate predictions, for instance, for ion-impact double ionization of atoms and molecules.

Only in the last decade have theoretical methods been developed that provide a complete description of the photon-impact double ionization of helium and the electron-impact ionization of hydrogen, the simplest quantal three-body Coulomb breakups. Only within the past few years has the treatment of quantal four-body Coulomb breakups become possible, thanks to the exponential growth of computational power. Insight into the full dynamics of these systems has enabled a better understanding of the photon and electron ionization of all atoms.

A variety of non-perturbative time-dependent close-coupling (TDCC) methods have been developed to exactly handle quantal three-body and four-body Coulomb breakups found in photon-impact, electron-impact, and ion-impact ionization of atoms, molecules, and their ions. For atoms and low charged atomic ions, the time-dependent Schrödinger equation (TDSE) is solved using an expansion in coupled spherical harmonics. For diatomic molecules and low charged molecular ions, the TDSE is solved using an expansion in rotational functions. In all cases the resulting time-dependent close-coupled equations for the expansion coefficients are solved on 2D, 3D, or 4D numerical lattices using massively parallel supercomputers. A large collection of additional numerical codes is used to extract observables, e.g. total and energy and angle differential cross sections, from the time-propagated numerical expansion coefficients.

Since atomic and molecular processes are present in most physical phenomena, ranging from astronomical observations of the early universe to the laboratory nanostructure engineering, a more complete understanding of the few-body dynamics of atoms and molecules can lead to a wealth of new scientific discoveries

The aim of this contribution is to review the application of the TDCC method to the study of ion-impact ionization of atoms and molecules. Ionization cross sections for bare ion, antiproton, and neutron collisions with light atoms and molecules are presented. A brief summary and future plans will also be discussed [1].

References

[1] M. S. Pindzola, *et al.*, Time-Dependent Close-Coupling Calculations for Ion-Impact Ionization of Atoms and Molecules. In: Ennio Arimondo, Chun C. Lin and Susanne F. Yelin, editors, *Advances In Atomic, Molecular, and Optical Physics*, Vol. 65, Burlington: Academic Press, 2016, pp. 291-319.

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