Correlated wavefunction methods for inelastic atomic collisions

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Abstract

Inelastic ionic or atomic collisions with matter probe the response of many-electron systems ranging from linear response in the perturbative limit to the strong-field non-linear response in the non-perturbative regime at low projectile velocities. The characteristic energy loss or stopping power, one central theme of Peter Sigmund's research, represents one important observable quantifying this response. Recent progress in methods for solving the time-dependent many-electron problem and the increased availability of computational power has now opened up opportunities for ab-initio simulations of the many-electron response. We will review recent applications of correlated wavefunction (CW) methods to inelastic ion-matter collisions. We will illustrate progress and current challenges with the help of two prototypical cases: antiproton collisions with helium and with LiF. While for simple atomic targets a numerically exact solution for the correlated wavefunction is meanwhile in reach, for the wide band-gap insulators such as LiF progress towards an accurate description has been made by employing advanced quantum-chemistry inspired CW methods within the framework of an embedded cluster approach (ECA) for the extended system.

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