Time-dependent Density Functional Theory determination of stopping-power and conductivity in warm, dense matter environments

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ABSTRACT

We have explored a variety of warm dense matter (WDM) and hot plasma systems with a quantum molecular dynamics (QMD) approach. In the QMD, we solve the many-body Schrodinger equation for a large, representative sample of atoms, periodically replicated through space to effect the characteristics of a fluid, which may include a mix of atoms, molecules, ions, and free electrons. For the electrons, we employ density-functional theory (DFT) in two guises: an orbital-based in the Kohn-Sham (KS) form and an orbital-free (OF), usually in a Thomas-Fermi-Dirac approximation. This dual capability permits thorough coverage of these extreme conditions and provides a set of consistent static, dynamic, and optical properties such as equation of state (EOS), mass transport (viscosity/diffusion), opacity, and conductivity (thermal/electrical).

We have also developed time-dependent (TD) versions of both the KS and OF approaches in order to treat primarily electron conductivities and stopping power. The advantages of the time-independent KS for the perturbative determination of these properties quickly vanishes with rising temperatures due to the large numbers of required eigenstates. The nonperturbative TD schemes offer a more viable path into the upper ranges of the WDM regime. They also permit the examination of the interaction of intense laser pulses with a plasma, as well as other nonlinear and nonequilibrium interactions.

We have investigated the electron stopping power for proton stopping in deuterium and beryllium and alpha particles in deuterium-tritium mixtures. The computational efficiency of Orbital-Free TD-DFT allows for the large simulation sizes. This is required for the direct calculation of stopping power for MeV projectiles, relevant to ICF plasma heating. We have compared OF and KS stopping powers, showing excellent agreement for high velocities, and derived a current-dependent kinetic energy functional that improves agreement with the KS results at low velocities while significantly improving propagation stability.

REFERENCES

[1] Y.H. Ding, A.J.White, O. Certik, S.X. Hu, and L.A. Collins, ”Ab initio Studies of Stopping Power in Warm Dense Matter using Tine-Dependent Density Functional Theory,” Phys. Rev. Lett. (to be submitted).