Mixed Stochastic-Deterministic Density Functional Theory For Electron Transport In Matter In The Extremes

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In quantum materials modeling, Kohn-Sham density functional theory (DFT) and its time-dependent extension (TDDFT) have emerged as powerful tools for studying the structural and dynamical properties of systems ranging from those comprising just a few molecules to much more condensed phases. I will elucidate the application of DFT methods to warm dense matter (WDM) that arises intrinsically in astrophysical systems as well as in laboratory simulations of inertial confinement fusion. A quantum mechanical description of this exotic state of matter is crucial for guiding experimental efforts into probing this regime and verifying its equation of state and other transport properties typically obtained from analytical models. The computational complexity of traditional DFT scales cubically with system size and temperature, making it computationally rather expensive. I will discuss a novel proposal for a mixed DFT (mDFT) formalism that combines the stochastic and deterministic Kohn-Sham algorithms to study matter at moderate to very high temperatures. Further, I will describe the Kubo-Greenwood formulation within the mDFT framework to compute the optical conductivity of large-N WDM systems; and show a decomposition of the spectra with contributions from electronic transitions among Kohn-Sham eigenstates and stochastic "orbitals". I will highlight how targeted physical observables including diffusivity and electronic conductivity are obtained in a computationally-efficient fashion within this formalism, for multiple testbed WDM single-component systems and binary asymmetric mixtures.

[1] Sharma, V., Collins, L.A., and White, A.J., "Stochastic and mixed density functional theory within the projector augmented wave formalism for simulation of warm dense matter," Phys. Rev. E., 2023, **108**, L023201.