

Stochastic Methods for Electronic Structure

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Abstract:

I discuss two new stochastic approaches to electronic structure and dynamics. First, a stochastic method for the equation of state of warm dense matter (WDM) using finite temperature Kohn-Sham density functional theory. The method's complexity scales as $O(NT^{-1})$, to be contrasted with the $O(N^3T^3)$ scaling of deterministic approaches, where N is the system size and T is the temperature. A stochastic method for calculating the conductivity of WDM will also be displayed. A second topic I will discuss is the development of an approximate approach, based on the Lindblad formalism and the Hubbard-Stratonovich transformation, allowing to evolve non-interacting Fermions in open quantum systems interacting with a Boson bath.