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Variational Perturbation Theory Path Integral Monte Carlo (VPT-PIMC): Trial Path Optimization Approach for Warm Dense Matter[1] JONATHAN BELOF, JONATHAN DUBOIS, Lawrence Livermore National Laboratory — Warm dense matter (WDM), the regime of degenerate and strongly coupled Coulomb systems, is of great interest due to it's importance in understanding astrophysical processes and high energy density laboratory experiments. Path Integral Monte Carlo (PIMC) presents a particularly attractive formalism for tackling outstanding questions in WDM, in that electron correlation can be calculated exactly, with the nuclear and electronic degrees of freedom on equal footing. Here we present an efficient means of solving the Feynman path integral numerically by variational optimization of a trial density matrix, a method originally proposed for simple potentials by Feynman and Kleinert [Bachmann *et al.*, *Phys. Rev. A.*, 60:3429 (1999)], and we show that this formalism provides an accurate description of warm dense matter with a number of unique advantages over other PIMC approaches. An exchange interaction term is derived for the variationally optimized path, as well as a numerically efficient scheme for dealing with long-range electrostatics. Finally, we present results for the pair correlation functions and thermodynamic observables of the spin polarized electron gas, warm dense hydrogen and all-electron warm dense carbon within the presented VPT-PIMC formalism.

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