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Systematic method to improve first principle calculations of materials under extreme conditions[1] JUSTIN SMITH, KIERON BURKE, University of California, Irvine — We develop an exact method for calculating the density and free energy of electronic systems at high temperatures that is used in conjunction with existing computational approaches. This method defines an effective thermal potential (ETP) that is used in an accurate hot temperature solver to get the properties at a colder temperature. In practical calculations, the ETP must be approximated using thermal DFT at the cold and hot temperature which is then fed into a quantum Monte Carlo calculation at the hot temperature to yield better results than thermal DFT alone at the colder temperature of interest. In this work we lay out the formalism of the scheme and provide a proof-of-principle calculation using the asymmetric Hubbard dimer. We show that our method improves the calculations of approximate densities and maintains the accuracy of the free energy.

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