Abstract Submitted
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Systematic method for improving first principle calculations of materials under extreme conditions[1] JUSTIN SMITH, KIERON BURKE, University of California, Irvine — We develop a new exact method for calculating the density and free energy of electronic systems at moderate temperatures that is used in conjunction with existing computational approaches. This new method relies on an effective thermal potential (ETP) that can be explicitly defined. In practical calculations, a solver that is extremely accurate at very high temperatures is used in conjunction with an approximate ETP constructed from e.g. density functional theory to calculate the properties at a moderate temperature. 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 in this case that our method improves the calculations of approximate densities and maintains the accuracy of the free energy.

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