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Bypassing the malfunction junction in warm dense matter simulations[1] ATTILA CANGI, Max Planck Institute of Microstructure Physics, AURORA PRIBRAM-JONES, University of California, Irvine — Simulation of warm dense matter requires computational methods that capture both quantum and classical behavior efficiently under high-temperature and high-density conditions. The state-of-the-art approach to model electrons and ions under those conditions is density functional theory molecular dynamics, but this method's computational cost skyrockets as temperatures and densities increase. We propose finite-temperature potential functional theory as an in-principle-exact alternative that suffers no such drawback[1]. In analogy to the zero-temperature theory developed previously[2,3], we derive an orbital-free free energy approximation through a coupling-constant formalism. Our density approximation and its associated free energy approximation demonstrate the method's accuracy and efficiency.

[1] A. Cangi and A. Pribram-Jones, arXiv:**1411.1532** (2014).
[2] A. Cangi, D. Lee, P. Elliott, K. Burke, and E.K.U. Gross, PRL **106**, 236404 (2011).
[3] A. Cangi, E.K.U. Gross, and K. Burke, PRA **88**, 062505 (2013).

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