Stochastic Vector Techniques for Strongly Coupled Coulomb Systems

Roi Baer*

Fritz Haber Research Center of Molecular Dynamics, Institute of Chemistry, Edmond J. Safra Campus, The Hebrew University of Jerusalem, 9190401 Israel.

We review a suite of stochastic vector computational approaches [1] for studying the equations-of-state and electronic structure of extended condensed matter systems under high-temperature conditions. These techniques help reduce algorithmic complexity, facilitate efficient parallelization, simplify computational tasks, accelerate calculations, and diminish memory requirements. We limit our exposition to finite-temperature density functional theory (DFT) [2,3] and low order perturbation theory[4]. First, we explain how to use stochastic vectors in computations on equations of state using Langevin dynamics [5]. Next, we discuss highly effective techniques to reduce statistical errors [6]. Finally, we review the use of stochastic vector techniques for calculating Kubo-Greenwood conductivity [7] and electron correlation effects using the second-order finite temperature (GF2) approach [4].

Bibliography

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* Email: roi.baer@gmail.com