Random numbers enable large scale electronic structure computations

Roi Baer

Fritz Haber Center for Molecular Dynamics, Institute of Chemistry, The Hebrew University of Jerusalem, Jerusalem 91904, Israel

Eran Rabani

School of Chemistry, The Sackler Faculty of Exact Sciences, Tel Aviv University, Tel Aviv 69978, Israel

Daniel Neuhauser

Department of Chemistry, University of California at Los Angeles, CA-90095 USA

Abstract

Accurate prediction of electronic properties of materials on the nanoscale is a considerable challenge for theoretical chemistry and solid state physics. In many cases of practical importance theoretical developments produce techniques that require computer resources scaling only polynomially with system size. Despite these great achievements the polynomial exponent (typically 3 or 4) prevents application of the methods to experimentally relevant systems of nanoscale sizes. We present here new concepts and techniques, relying on the use of stochastic orbitals, that reduce the numerical effort to sub-linear scaling in a broad range of materials and system sizes. I discuss briefly some of the new paradigms we introduced and then present encouraging results showing that it endows density functional and many-body perturbation theory an ability to treat large systems having thousands of electrons with linear or sublinear-scaling numerical effort. See recent references [1–6].

[1] Roi Baer and Daniel Neuhauser. Communication: Monte Carlo calculation of the exchange energy. *J. Chem. Phys.*, 137(5):051103–4, 2012.

[2] R. Baer and E. Rabani. Expeditious stochastic calculation of multiexciton generation rates in semiconductor nanocrystals. *Nano Lett.*, 12:2123, 2012.

[3] Roi Baer, Daniel Neuhauser, and Eran Rabani. Self-averaging stochastic kohn-sham density-functional theory. *Phys. Rev. Lett.*, 111:106402, Sep 2013.

[4] Roi Baer and Eran Rabani. Communication: Biexciton generation rates in cdse nanorods are length independent. *J. Chem. Phys.*, 138(5):051102–4, 2013.

[5] Daniel Neuhauser, Eran Rabani, and Roi Baer. Expeditious stochastic approach for mp2 energies in large electronic systems. *J. Chem. Theory Comput.*, 9(1):24–27, 2013.

[6] Daniel Neuhauser, Eran Rabani, and Roi Baer. Expeditious stochastic calculation of random-phase approximation energies for thousands of electrons in three dimensions. *J. Phys. Chem. Lett.*, 4(7):1172–1176, 2013.