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Quasiparticle spectra obtained through stochastic many-body methods VOJTECH VLCEK, Department of Chemistry and Biochemistry, University of California, Los Angeles, USA, ROI BAER, Fritz Haber Center for Molecular Dynamics, Institute of Chemistry, The Hebrew University of Jerusalem, Jerusalem, Israel, ERAN RABANI, Department of Chemistry, University of California and Materials Science Division, Lawrence Berkeley National Laboratory, Berkeley, USA, DANIEL NEUHAUSER, Department of Chemistry and Biochemistry, University of California, Los Angeles, USA — We present the linearly scaling stochastic approach to many-body perturbation theory and to calculations of quasiparticle energies in G_0W_0 approximation and beyond. Our approach overcomes the steep scaling of conventional deterministic schemes. Further, it allows a simple incorporation of higher order interactions (vertex corrections). Exemplifying on covalently bonded systems (nanocrystals and polymer chains), we show practical calculations of quasiparticle spectra, and self-energies for large systems with thousands of electrons. The linear scaling is fundamental nature of our approach, which does not rely on a particular character of the electronic structure (e.g., there is no need for sparsity of the density matrices). The scaling prefactor is small so the stochastic G_0W_0 method is thus a method of choice for all systems from few tens to thousands – and in the near horizon hundreds of thousands – of electrons.

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