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Fast RPA and GW calculations: cubic system size scaling

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The random phase approximation (RPA) to the correlation energy and the related GW approximation are among the most promising methods to obtain accurate correlation energy differences and QP energies from diagrammatic perturbation theory at reasonable computational cost. The calculations are, however, usually one to two orders of magnitude more demanding than conventional density functional theory calculations. Here, we show that a cubic system size scaling can be readily obtained reducing the computation time by one to two orders of magnitude for large systems. Furthermore, the scaling with respect to the number of k points used to sample the Brillouin zone can be reduced to linear order. In combination, this allows accurate and very well-converged single-point RPA and GW calculations, with a time complexity that is roughly on par or better than for self-consistent Hartree-Fock and hybrid-functional calculations [1-2]. Furthermore, the talk discusses the relation between the RPA correlation energy and the GW approximation: the self-energy is the derivative of the RPA correlation energy with respect to the Green's function. The calculated self-energy can be used to compute QP-energies in the GW approximation, any first derivative of the total energy, as well as corrections to the correlation energy from the changes of the charge density when switching from DFT to a many-body body description (GW singles energy contribution) [3]. [1] Merzuk Kaltak, Jiří Klimeš, and Georg Kresse, J. Chem. Theory Comput., 10, 2498–2507 (2014).
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