Abstract Submitted
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Direct calculation of the one particle Green's function: an alternative to the self-energy GIOVANNA LANI, PINA ROMANIELLO, LUCIA REINING, Laboratoire des Solides Irradiés , Ecole Polytechnique, France and European Theoretical Spectroscopy Facility (ETSF) — Calculations of quasi-particle band structures and photo- emission spectra of materials rely more and more on perturbative many-body techniques like the GW approximation. In this approach the one-body Green's function (G) is determined from a Dyson equation containing a *self-energy* kernel Σ which is approximated as a product of G and the screened Coulomb interaction W. To go beyond the first order in W, iterative schemes of Hedin's equations [1] have been proposed. While generally successful, GW is known to fail for strongly correlated systems and it is far from obvious that one could improve on this through further iterations of Hedin's equations. In the present work we explore an alternative route: in place of approximating Σ, we reformulate the problem in terms of a set of coupled first order differential equations for the unknown G. We benchmark this approach on small Hubbard clusters, for which one can calculate the exact one-body G.

[1]Hedin, L., Phys. Rev. 139, (1965) A796

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