Abstract Submitted
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New expressions for the correlation energy functional within the GW-RPA approximation[1] SOHRAB ISMAIL-BEIGI, Yale University — Approaches such as the Luttinger-Ward formalism allow one, in principle, to compute both total energies and quasiparticle excitations (i.e., electron and hole energies and wave functions) simultaneously from first principles by working with total energy functionals of the one-particle Green's function. We briefly review our recent results on exact and approximate expressions for the GW-RPA correlation energy. We then provide some numerical results on atoms assessing the quality and superior convergence properties of these new expressions. We end by discussing our finding that unconstrained optimization of the total energy functional over non-interacting Green's functions or equivalently over non-local exchange correlation potentials leads to unphysical results: This shows that when using such approaches, one must place constraints on the Green's function or exchange-correlation potential.

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