Progress and Challenges with Luttinger-Ward Approaches for Going Beyond DFT

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The well-known and well-used Density Functional Theory (DFT) is a variational theory for the ground-state. There are no guarantees that it delivers good results for excited state properties such as quasiparticle energies or wave function. All that is guaranteed is that the total energy is exact, the chemical potential is correct, and that the effective electronic states (Kohn-Sham states) generate the right electron density at the variational minimum.

Luttinger-Ward approaches to electronic structure are attractive as beyond-DFT schemes since, in principle, they offer a variational functional of the one-electron Green's function that yields both the correct total energy and all one-particle properties at the variational extremum. However, compared to DFT, these methods face a number of additional challenges beyond the familiar problem of choosing an exchange-correlation functional: (a) they have a much greater computational cost compared to DFT, (b) one must choose some set of trial Green's functions, and (c) one must locate an extremum (not necessarily a minimum).

This talk aims both to be pedagogical and to provide a summary of our most recent work in this area. We focus mainly on the random-phase approximation (RPA) for the correlation functional which yields the GW self-energy for the Green's function. We will describe efficient approaches for computing the RPA correlation energy; how various types of approximations to the correlation energy create a ladder of approximate self-energy operators and what type of physics is included in these approximations (exchange, screening, Hubbard U, etc.); and how the extremization is in fact highly problematic. We will end with some ideas for making practical progress with the extremization and their relation to the successful Quasiparticle Self-consistent GW (QSGW) scheme [1].

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[1] M. van Schilfgaarde, T. Kotani, and S. Faleev, Phys. Rev. Lett. **96**, 226402 (2006); Phys. Rev. B **76**, 165106 (2007).

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