

Many-Body Approximation Scheme beyond GW

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We explore the combination of the extended dynamical mean field theory (EDMFT) with the GW approximation (GWA); the former sums the local contributions to the self-energies to infinite order in closed form and the latter handles the nonlocal ones to lowest order. We investigate the different levels of self-consistency that can be implemented within this method by comparing to the exact quantum Monte Carlo solution of a finite-size model Hamiltonian. We find that using the EDMFT solution for the local self-energies as input to the GWA for the nonlocal self-energies gives the best result.

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Introduction.—The GW approximation (GWA) [1] is one of the most successful methods to describe electronic structure of weakly correlated materials. It includes the lowest order perturbative corrections in the screened Coulomb interaction to the electron self-energy. In real space time, the electron self-energy is given by the product “GW,” where “G” represents the electron Green’s function and “W” represents the random-phase approximation (RPA) screened Coulomb interaction. The GWA has been successfully applied to the calculations of quasiparticle spectra of semiconductors and insulators [2]. (For recent reviews, see Ref. [3].) It describes well the experimentally observed energy gaps in semiconductors [3–8].

The GWA self-energies were first calculated as a one-shot perturbation by using the unperturbed local-density approximation (LDA) Green’s functions [2]. However, as we will show in this Letter, the one-shot GWA breaks down as soon as the correlations are moderately strong, as expected for a non-self-consistent leading order approximation. The problem should be solved by including higher order corrections to extend the scope of the method. This is the main motivation of our work. The Baym-Kadanoff formulation [9] of the GWA, which makes the method automatically conserving, requires one to evaluate the self-energy, the polarization bubble, and the Green’s function self-consistently [1]. While this has been successfully implemented [10] and shows improvement on the values of the total energy, the self-consistent GWA brings up a debate over whether the full self-consistency improves the spectra [6–8,11–14]. This is due to the fact that the vertex correction, which is omitted in GWA, shows a tendency to cancel the self-energy insertion when the full Green’s function is used in calculating the exchange self-energy [15–17]. As a result, the one-shot GWA or partial-self-consistent ones (in which, e.g., one fixes the W obtained from the LDA input while solving G self-consistently) are favored sometimes [11–13]. This issue entails the usage of higher order self-energy diagrams and provides us a second motivation for improving systematically the approximation beyond the leading order.

In this Letter, we extend the GWA by using the extended dynamical mean field theory (EDMFT) [18–21], which treats all the local polarization, self-energy, and vertex corrections in closed form, following the ideas proposed in Refs. [20,21,22]. According to these approaches, the local polarization and self-energy should be solved by EDMFT nonperturbatively, while the nonlocal ones should be solved via GWA. The cancellation of the self-energy insertion and the vertex correction is carried out *locally* to infinite order within EDMFT. However, the same ambiguity of implementation (with or without self-consistency) remains in the nonlocal GWA part. This question can not be addressed without benchmarking the different schemes.

Main Results.—We compared and contrasted the different implementations of combining EDMFT with GWA. Our numerical calculation suggests that the schemes using the EDMFT solution of the local self-energies as input to the GWA for the nonlocal self-energies give the best result. In other words, it is favorable *not* to allow the feedback of the nonlocal GWA on the local EDMFT self-energies due to the different nature of the two methods, GWA being perturbative and EDMFT nonperturbative. On the other hand, when using the EDMFT result as input, it makes little difference whether one performs GWA with a single shot or partial self-consistency (it is partial because the local polarization and self-energy from EDMFT are fixed). This supports the picture [21,22] that, in a correlated phase far away from a phase transition, the temporal correlations reflected through the local polarization and self-energy are dominant and should be treated nonperturbatively, while the spatial correlations are weaker and can be handled perturbatively.

Lattice Model.—In comparing different GW approaches, many of which apply to realistic materials, one always encounters the problem that there are as many important differences in the implementations as in the GWA methodologies themselves. These include the implementations of GWA in imaginary time or frequency space, the choice and construction of the local

basis set, and the further approximations like the plasmon-pole approximation [3]. In order to compare the many-body schemes without additional complications, it is desired to employ simple model systems on the lattice [11,23]. Following the same strategy, we study the following generalized Hubbard model:

$$\hat{H} = -\frac{1}{2} \sum_{ij,\sigma} t_{ij} (\hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma} + \hat{c}_{j\sigma}^\dagger \hat{c}_{i\sigma}) + \frac{1}{2} \sum_{ij} \hat{n}_i v_{ij} \hat{n}_j, \quad (1)$$

where $\hat{c}_{i\sigma}$ ($\hat{c}_{i\sigma}^\dagger$) annihilates (creates) an electron of spin σ ($=\uparrow, \downarrow$) at the lattice site i . \hat{n}_i is the electron density. We consider only the paramagnetic phase.

Approximation Schemes.—The self-consistent schemes are summarized in Fig. 1. [We use $(\dots)_{\text{SC}}$ for a self-consistent (SC) loop and $(\dots)_{\text{PSC}}$ for a partially SC loop.] The full functional in Fig. 1 can be separated into local and nonlocal parts, which are functionals of the local and nonlocal Green's functions, respectively: $\Phi = \Phi_{\text{EDMFT}}(G_{\text{Local}}, D_{\text{Local}}) + \Phi_{\text{Nonlocal GW}}(G_{\text{Nonlocal}}, D_{\text{Nonlocal}})$. The local (nonlocal) self-energies, which are obtained from the functional derivatives of Φ_{EDMFT} ($\Phi_{\text{Nonlocal GW}}$), are functions of the local (nonlocal) parts of the Green's functions only: $\Sigma_{\text{EDMFT}} = \Sigma_{\text{EDMFT}}(G_{\text{Local}}, D_{\text{Local}})$ and $\Sigma_{\text{Nonlocal GW}} = \Sigma_{\text{Nonlocal GW}}(G_{\text{Nonlocal}}, D_{\text{Nonlocal}})$ for the electron, $\Pi_{\text{EDMFT}} = \Pi_{\text{EDMFT}}(G_{\text{Local}}, D_{\text{Local}})$ and $\Pi_{\text{Nonlocal GW}} = \Pi_{\text{Nonlocal GW}}(G_{\text{Nonlocal}}, D_{\text{Nonlocal}})$ for the boson.

The approximation schemes we tested in combining EDMFT with GW are (i) the fully self-consistent $(\text{EDMFT} + \text{GW})_{\text{SC}}$ solves the full Dyson equations for $G = G_{\text{Local}} + G_{\text{Nonlocal}}$ and $D = D_{\text{Local}} + D_{\text{Nonlocal}}$: $G = (G_0^{-1} - \Sigma_{\text{EDMFT}} - \Sigma_{\text{Nonlocal GW}})^{-1}$ and $D = (D_0^{-1} - \Pi_{\text{EDMFT}} - \Pi_{\text{Nonlocal GW}})^{-1}$, with G_0 and D_0 the free electron and boson Green's functions on the lattice. The non-self-consistent schemes begin with the solution of the EDMFT, which solves $G_{\text{Local}} = (G_0^{-1} - \Sigma_{\text{EDMFT}})_{\text{Local}}^{-1}$ and $D_{\text{Local}} = (D_0^{-1} - \Pi_{\text{EDMFT}})_{\text{Local}}^{-1}$.

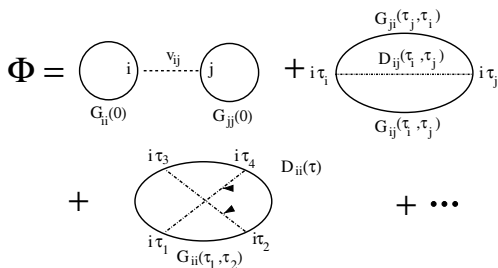


FIG. 1. The potential Φ of the Baym-Kadanoff functional [9,19] for $(\text{EDMFT} + \text{GW})_{\text{SC}}$. $(\text{EDMFT})_{\text{SC}}$ is obtained by restricting the exchange diagram (the second on the right-hand side) to be local in space, $i = j$. The first line by itself represents the standard $(\text{GW})_{\text{SC}}$ scheme. In this formulation, the boson Green's function D describes the screened interaction. The boson self-energy plays a similar role as the electron-hole bubble in GWA.

(ii) $(\text{EDMFT})_{\text{SC}} + \text{GW}$ uses the local EDMFT self-energies to calculate the nonlocal Green's functions, $G_{\text{EDMFT, Nonlocal}} = (G_0^{-1} - \Sigma_{\text{EDMFT}})_{\text{Nonlocal}}^{-1}$ and $D_{\text{EDMFT, Nonlocal}} = (D_0^{-1} - \Pi_{\text{EDMFT}})_{\text{Nonlocal}}^{-1}$. It obtains in one-shot the estimation for $\Sigma_{\text{Nonlocal GW}} = \Sigma_{\text{Nonlocal GW}}(G_{\text{EDMFT, Nonlocal}}, D_{\text{EDMFT, Nonlocal}})$ and $\Pi_{\text{Nonlocal GW}} = \Pi_{\text{Nonlocal GW}}(G_{\text{EDMFT, Nonlocal}})$. (iii) $(\text{EDMFT})_{\text{SC}} + (\text{GW})_{\text{PSC}}$ solves for G_{Nonlocal} and D_{Nonlocal} self-consistently from $G_{\text{Nonlocal}} = (G_0^{-1} - \Sigma_{\text{EDMFT}} - \Sigma_{\text{Nonlocal GW}})_{\text{Nonlocal}}^{-1}$ and $D_{\text{Nonlocal}} = (D_0^{-1} - \Pi_{\text{EDMFT}} - \Pi_{\text{Nonlocal GW}})_{\text{Nonlocal}}^{-1}$, with Σ_{EDMFT} and Π_{EDMFT} fixed.

Benchmark.—To compare and contrast the approximation schemes, we perform a benchmark calculation using the model (1) on a 4×4 , 2D square lattice with periodic boundary condition. We use, for the free electron dispersion, $\epsilon_{\vec{k}} = -(1/2)[\cos(k_x) + \cos(k_y)]$. The half-bandwidth is taken as the energy unity. The interaction is given by $v_{\vec{k}} = U + 2V[\cos(k_x) + \cos(k_y)]$. We study the half-filling case, where the strongest correlation shows up. We fix the inverse temperature $\beta = 8.0$ and the ratio $V/U = 0.25$. We vary U from 0.0 to 3.0 for the approximation schemes. We benchmark the calculation at $U = 0.5, 1.0, 1.5$ by using direct quantum Monte Carlo (QMC) calculation via the Hirsch-Fye algorithm [24]. In all the results we are going to present, the major error of the calculation comes from the QMC part, in both the exact solution and the EDMFT impurity solver. In the latter we solve the EDMFT electron-boson impurity problem by a hybridized Monte Carlo method [21,25–27], which employs an additional continuous auxiliary field [28].

At the given $V-U$ ratio, a charge density wave instability at wave vector (π, π) is present in the one-shot GW. The breakdown is shown in Fig. 2. In the exact solution, however, no charge or spin instability is observed up to $U = 1.5$. To compare the different schemes on the same footing, we restrict ourselves to the paramagnetic phase. Depending on the different schemes, this may mean

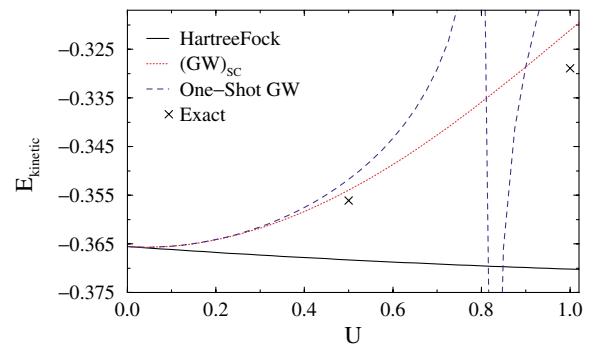


FIG. 2 (color online). In our model system, the one-shot GWA, using the Hartree-Fock result as input, breaks down at $U \approx 0.825$. This is an instability against the formation of a charge density wave at (π, π) [27]. The other results are plotted as references.

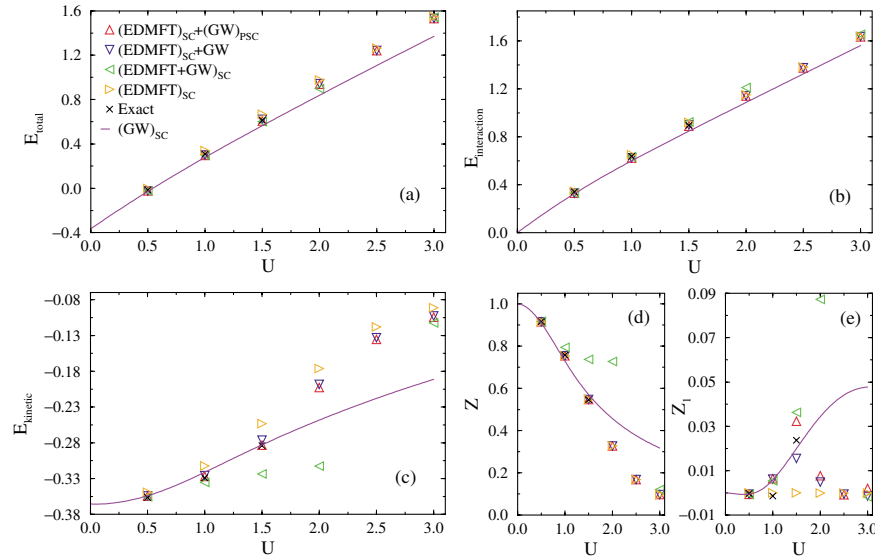


FIG. 3 (color online). The energies, the quasiparticle residue (Z), and the nonlocal contribution to the self-energy (Z_1) as defined in the text. The same symbol scheme defined in (a) applies to all the diagrams. Z is the same for $(\text{EDMFT})_{\text{SC}} + (\text{GW})_{\text{PSC}}$, $(\text{EDMFT})_{\text{SC}} + \text{GW}$, and $(\text{EDMFT})_{\text{SC}}$, since the same local self-energy is used. For Z_1 , which reflects the spatial extension of the self-energy, we are comparing numbers at least one order smaller than those for other quantities.

studying a paramagnetic metastable solution when the possible instability appears. We find it allowed for $(\text{GW})_{\text{SC}}$ up to the largest U ($= 3.0$) that we studied and the same for the EDMFT related schemes we described, except for $(\text{EDMFT} + \text{GW})_{\text{SC}}$ in which the self-consistent solution does not exist at $U = 2.5$.

Our main results are presented in Figs. 3 and 4, in which the results from the exact QMC and the $(\text{GW})_{\text{SC}}$ are also plotted. The definitions of the plotted quantities are as follows: The E_{kinetic} and $E_{\text{interaction}}$ are the hopping and interaction energies per site, calculated via the Galitskii-Migdal formula [29]. $E_{\text{total}} = E_{\text{kinetic}} + E_{\text{interaction}}$. The local electron self-energy of $(\text{EDMFT})_{\text{SC}}$ is obtained directly from the EDMFT solution, while for those with spatial extension, $\Sigma^{\text{local}}(ip_n) = (1/N)\sum_{\vec{k}}\Sigma(\vec{k}, ip_n)$, with $N = 4 \times 4$. The local Green's function $G^{\text{local}}(ip_n) = (1/N)\sum_{\vec{k}}\{[G_0(\vec{k}, ip_n)]^{-1} - \Sigma(\vec{k}, ip_n)\}^{-1}$. The quasiparticle residue $Z = [1 - \text{Im}\Sigma^{\text{local}}(ip_0)/p_0]^{-1}$. We measure the spatial extension of the electron-self-energy by $Z_1 = (1/N)\sum_{\vec{k}}\text{Im}\{[\Sigma(\vec{k}, ip_1) - \Sigma(\vec{k}, ip_0)]/(p_1 - p_0)\}\text{cos}k_x$.

From the *overall* features of the results, we see that (i) the $(\text{EDMFT})_{\text{SC}} + (\text{GW})_{\text{PSC}}$ gives the best results up to the largest benchmarked U at 1.5 times the half-bandwidth. (ii) The difference between $(\text{EDMFT})_{\text{SC}} + (\text{GW})_{\text{PSC}}$ and $(\text{EDMFT})_{\text{SC}} + \text{GW}$ is small quantitatively, since the local self-energies from $(\text{EDMFT})_{\text{SC}}$ is dominant. (iii) $(\text{EDMFT} + \text{GW})_{\text{SC}}$ is not a good scheme in the sense that it sees an artificial charge density instability around $U \sim 2.5$, where no self-consistent solution is found. Even before reaching that regime, the $(\text{EDMFT} + \text{GW})_{\text{SC}}$ shows significant deviations from the exact solution. (iv) From the plottings of Z and Z_1 in Fig. 3, we see that $(\text{GW})_{\text{SC}}$ misses the crossover to localization at large U , while the EDMFT based calculations correctly capture this feature. Actually, all the EDMFT related schemes give results close to each other at $U = 3.0$ since the spatial extensions of the self-energies are no longer important. Our results show that, with moderate and strong correlations, one needs to include higher order contributions beyond GWA. The schemes,

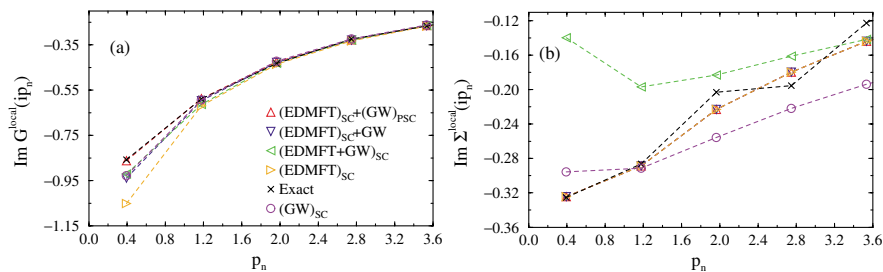


FIG. 4 (color online). The local electron Green's function and self-energy at $U = 1.5$. The same symbol scheme defined in (a) applies to (b). The lines connecting the points are guides to the eye. The fermion Matsubara frequency $p_n = (\pi/\beta)(2n + 1)$.

(EDMFT)_{SC} + (GW)_{PSC} and (EDMFT)_{SC} + GW, offer a reliable solution towards this direction.

Conclusion.—To summarize, we presented a many-body scheme that handles the local self-energies non-perturbatively via EDMFT and the nonlocal ones perturbatively via GWA. As an improvement over the leading order GWA, the new scheme better captures the effects of correlation. We described several implementations, which perform self-consistency at different levels, and benchmarked them by comparing with the exact solution of a finite-size model system. We found that (EDMFT)_{SC} + (GW)_{PSC} and (EDMFT)_{SC} + GW gave very close results. For the model we studied, (EDMFT)_{SC} + (GW)_{PSC} gave the best result.

Finally, we should point out that, similar to the self-consistent GWA [13,16], our scheme has the problem that the polarization does not have the proper asymptotic behavior in the long wave length limit [$\lim_{k \rightarrow 0} P(k, \omega) \propto (k/\omega)^2$]. Since the schemes combining EDMFT with GWA include local vertex corrections nonperturbatively, this violation is less severe than that in GWA [27,30].

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