Full self-consistency versus quasiparticle self-consistency in diagrammatic approaches: exactly solvable two-site Hubbard model

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Abstract
Self-consistent solutions of Hedin’s equations (HE) for the two-site Hubbard model (HM) have been studied. They have been found for three-point vertices of increasing complexity (Γ = 1 (GW approximation), Γ₃ from the first-order perturbation theory, and the exact vertex Γ₃ₑ). Comparison is made between the cases when an additional quasiparticle (QP) approximation for Green’s functions is applied during the self-consistent iterative solving of HE and when QP approximation is not applied. The results obtained with the exact vertex are directly related to the present open question—which approximation is more advantageous for future implementations, GW + DMFT or QPGW + DMFT. It is shown that in a regime of strong correlations only the originally proposed GW + DMFT scheme is able to provide reliable results. Vertex corrections based on perturbation theory (PT) systematically improve the GW results when full self-consistency is applied. The application of QP self-consistency combined with PT vertex corrections shows similar problems to the case when the exact vertex is applied combined with QP sc. An analysis of Ward Identity violation is performed for all studied in this work’s approximations and its relation to the general accuracy of the schemes used is provided.

Keywords: GW + DMFT, Hubbard model, strongly correlated systems

1. Introduction
One of the challenges for computational theorists working in the solid-state electronic structure field is the robust implementation of the so-called GW + DMFT method (a combination of GW approximation (G—Green’s function, W—screened interaction) and dynamical mean-field theory). The scheme was originally proposed by Sun and Kotliar [1] and in a slightly different (but probably more commonly known) form by Biermann et al [2] The basic idea of the approach is to separate all of the active space of the basis set into a ‘weakly correlated’ part, for which GW approximation is supposed to work well, and a ‘strongly correlated’ part, for which one sums up many diagrams (up to an infinite order if one uses a non-perturbative DMFT solver, for example, the quantum Monte Carlo—QMC). In order to have a well defined method, everything should be done till full self-consistency (sc), including the iterations of the GW part itself and the ‘internal’ iterations of the DMFT part, to ensure that the solution to the impurity problem reproduces the same G and W in a strongly correlated subspace as the ones projected from the GW part onto the same subspace.

Despite its obvious appeal, GW + DMFT has made only slow progress in more than a decade since its first appearance in the above-mentioned papers. The reason was not just because scGW is quite demanding computationally but mostly because one has to satisfy the impurity sc condition not only for the G (as in the LDA + DMFT method—a combination of
local density approximation in density functional theory and DMFT) but also for the W, which seems to be not an easy task. Recently, the implementation of GW + DMFT for the two-dimensional Hubbard model was published [3]. It provided a few important new insights into the physics of the model. However, to the best of my knowledge there were only ‘one-shot’ type calculations for real materials [4], where GW iterations were neglected altogether and DMFT self-consistency was imposed only on G, whereas W was fixed at the LDA level and correspondingly the U was considered as an external parameter (calculated in constrained random phase approximation—cRPA). Such an implementation, of course, is a definite step towards a full GW + DMFT scheme, but still one cannot say that there was a summation of all the ‘correlated’ graphs in it, which would require that the W in the GW part and W_{imp} in the impurity (DMFT) part be the same. Instead they were totally decoupled, which makes it unclear what kind of diagrams from the DMFT part was actually added to the GW part. Nevertheless, together with the development of QMC solvers capable of handling dynamical interactions, [5, 6] hope is growing that a full GW + DMFT scheme will eventually be implemented.

There are some subtleties about the GW part as well. In its full sc implementation the method is very time consuming, which in part has prevented its applications for real materials. However, a few works have been published regarding the application of scGW to atoms and molecules [7–12]. Recently an efficient implementation of scGW for solids has been achieved [13], where the most computationally demanding parts (the calculation of polarizability P and self-energy Σ) are performed in real space and Matsubara’s time. As a result, it became possible to successfully apply scGW to the actinides Pu and Am and (earlier) to simple sp-materials [14]. However for the majority of solids, scGW produces worse spectra than fast ‘one-shot’ GW and this is the other reason why scGW is not popular. The reason for the failure of scGW with spectra may be traced to an extremely non-symmetrical ‘dressing’ of the ‘initial’ Green’s function with self-energy insertions of GW-only forms in the course of self-consistency iterations and the neglecting of vertex corrections.

The origin of the problem with the scGW method can also be formulated in terms of the absence of Z-factor cancelation [15], which again happens because we neglect vertex corrections. To resolve this problem, Kotani and Schilfgaarde [15] devised the beautiful trick of doing yet another approximation. They used the quasiparticle (QP) part of a Green’s function G_QP (instead of a full Green’s function G calculated from Dyson’s equation (DE)) to calculate P and Σ on every iteration till self-consistency. The trick is that the errors from the above two approximations (using G_QP instead of full G and neglecting vertex corrections) mostly cancel each other out and as a result the QPscGW (self-consistent quasiparticle GW) method usually gives much better spectra than full scGW. The important fact is that QPscGW not just slightly improves the one-shot GW description of sp-materials (which are good enough already in one-shot GW), but often gives reasonable results for materials with d- or f-electrons too [16], and the method doesn’t rely on a particular starting point. It is totally self-consistent.

Considerable support for using quasiparticle approximation comes from the recent work by Ismail-Beigi [17], where it has been shown that quasiparticle approximation similar to the one introduced in [15] minimizes error when one wants to approximate the true Green’s function by a non-interacting one. It has been demonstrated in [17] that the result is general and applies to any self-energy operator, not only to its GW form.

Quite naturally, the success of QPscGW with spectral properties (as compared to full scGW) has ignited ideas to formulate another approach, QPscGW + DMFT [18, 19], where one supposedly adds DMFT corrections to P and Σ as in GW + DMFT but uses QPscGW for ‘big’ iterations in the ‘weakly correlated’ part.

As it appears, now we have two schemes proposed: GW + DMFT and QPGW + DMFT. In this work I am making an attempt to ‘estimate’ what to expect from a future implementation of the schemes. To be more specific, I will assume that GW + DMFT is defined by equations (6)–(12) of [2]. I also assume that QPGW + DMFT is defined by the same equations; only equation (11), which essentially is based on Dyson’s equation, is replaced with QP approximation for the Green’s function. Further analysis strongly depends on the ‘separability’ of the weakly and strongly correlated parts. I will assume here that they are perfectly separable and the correlations in the GW part are really weak. In this case, the Z-factor in the GW part is close to 1, so that this part is equally well described in both the GW and QPGW approximations. The difference correspondingly comes only from the DMFT (strongly correlated) part. For this part I assume that we are able to solve it exactly (i.e. solve exactly the problem with action (6) of [2]). Next, I assume that both the self-consistency conditions for G and W (equations (11) and (12) in [2]) are satisfied. For GW + DMFT, it means G = G_{imp}, W = W_{imp}, and for QPGW + DMFT, it means G_QP = G_{imp}, W_QP = W_{imp}. The exact solution of the action and the satisfaction of both sc conditions guarantee that all ‘strongly correlated’ diagrams constructed from G and W have been summed up. This fact together with the above assumption that for the ‘weakly correlated part’ GW is already good enough means that the self-energy for the whole system can be written in its diagrammatic form: Σ_{GW+DMFT} = − G_{W} or Σ_{QPGW+DMFT} = − G_{QPGW} W_{QPGW}, with Γ (Γ_QP) being the three-point vertex function from the impurity problem, which is solved exactly. It is clear that with the above assumptions the GW + DMFT approach provides us with the exact self-energy, whereas the self-energy in QPGW + DMFT is approximate. Essentially, the question is whether Σ_{QPGW+DMFT} is better than Σ_{QPGW} or not. Following the arguments of [15], we have for the Q Green’s function G_QP ≈ 4

But, following again the arguments from [15], it becomes clear that in the QPGW + DMFT case, i.e. when we include the exact vertex and continue to apply QP approximation for G, we will have a problem, because the factor 1/2 appears from the vertex and it doesn’t cancel the Z-factor from G, as happens in GW + DMFT. Basically it means the violation of the Ward Identity (WI) in the QPGW + DMFT scheme.
Thus, from this point of view, QPGW + DMFT is highly problematic and its difficulties should increase when the correlation strength improves, because the 1/Z-factor increases.

The arguments above have been given for the schemes where vertex corrections are provided by DMFT, which is considered as one of the most promising approaches for strongly correlated materials nowadays. But it is clear that the problem is quite general and the above arguments are valid for any vertex-corrected schemes. What is missing is a numerical evidence. It is natural to provide it first using exactly solvable models. In this work I present some results related to the above problem for the exactly solvable two-site Hubbard model. Different aspects of the two-site Hubbard model have been studied before [20–22]. For this model I exactly calculate the three-point vertex function and use it to self-consistently calculate the Green’s functions $G$ and $G_{QP}$ following two slightly different sc schemes (the scheme on the left side is basically Hedin’s sc equations [23] but with the 3-point vertex precalculated exactly):

$$P = G_t^{\text{Exact}}G, \quad P_{QP} = G_{QP}G_t^{\text{Exact}}G_{QP}$$

$$W = U + UPW, \quad W_{QP} = U + UP_{QP}W_{QP}$$

$$\Sigma = -G_t^{\text{Exact}}W, \quad \Sigma_{QP} = -G_{QP}G_t^{\text{Exact}}W_{QP}$$

$$G = G_0 + G_0\Sigma G, \quad G_{QP} = \frac{G_0}{1 - G_0\Sigma_{QP}}, \quad (1)$$

where $U$ is the bare interaction in the Hubbard model and $G_0$ is the Green’s function in Hartree approximation. In (1), for the QP case (the right column), I formally represent the quasiparticle approximation for $G$ by simply dividing the full Green’s function from Dyson’s equation by the Z-factor. This is for brevity. In fact I use the algorithm described in [13] to construct $G_{QP}$.

It is obvious that at self-consistency the scheme on the left side (I will call it $G_t^{\text{Exact}}W$) is equivalent by construction to the exact solution to the problem at hand. In this work I use $G_t^{\text{Exact}}W$ to check the numerical accuracy of 3-point vertex evaluation. The scheme on the right-hand side (I will call it QPGW$G_t^{\text{Exact}}W$) is designed to mimic the solution to the problem when we are able to sum up all diagrams, but instead of the exact solution of DE we impose QP approximation. The important assumption here is that the sum of all the diagrams constructed from $G_{QP}$ and $W_{QP}$ provides a vertex function which has approximately the same value of 1/Z in the longwave limit as does $G_t^{\text{Exact}}$. The QPGW$G_t^{\text{Exact}}W$ scheme is approximate and below I will explore its accuracy in different regimes of correlation strength for the 2-site Hubbard model. Also I will directly relate the problems of the QPGW$G_t^{\text{Exact}}W$ scheme with the degree of WI violation. The Ward Identity has been used in conjunction with scGW calculations of homogeneous electron gas before [24–26] but in a different aspect—as a constraint on the vertex function which ensures that the calculated self-energy satisfies the WI.

Another goal of the present work is to explore the possibility of combining the GW and QPGW methods with the perturbative calculation of the 3-point vertex function. To this end I will again use schemes similar to equation (1) but with $\Gamma$ expanded to the first order in $W (\Gamma)$ instead of exact $\Gamma$. I also will show how the two corresponding perturbation theory based schemes ($G_t^{\text{Exact}}W$ and QPGW$G_t^{\text{Exact}}W$) behave in different regimes of parameters of the Hubbard model. This part of the present study is directly relevant to the research performed by Ismail-Beigi [17]. Namely, even if quasiparticle approximation is in a certain sense the best approximation for $G$ among all non-interacting Green’s functions, the question remains: does improvement in self-energy (by adding more diagrams) necessarily improve the quality of quasiparticle $G$ or not? Besides, vertex-corrected GW calculations are still scarce in the literature [27–31] and, correspondingly, are interesting in themselves irrespective of what self-consistency is imposed.

This paper begins with the formal presentation of the two-site Hubbard model and the formulae used in the calculations (section 2). In section 3 the results are presented and discussed. Finally in section 4 conclusions are given and future plans are outlined.

2. Two-site Hubbard model

The Hamiltonian of the two-site Hubbard model as it is used in this work is as follows:

$$H = -t \sum_{i\neq j,\sigma} c_{i\sigma}^c c_{j\sigma}^+ + \frac{U}{2} \sum_i \sum_{\sigma\sigma'} c_{i\sigma}^c c_{i\sigma'}^+ c_{i\sigma} c_{i\sigma'}, \quad (2)$$

where $t$ and $U$ are the standard parameters of the Hubbard model, $c$ and $c^+$ are the destruction and creation operators, respectively, indices $i$ and $j$ belong to the sites (1 or 2), and $\sigma, \sigma'$ are spin indices.

In this section, all equations which are used in the analysis of the 2-site Hubbard model are collected for reference. First I provide the energies and eigenvectors of the exact many-body states of the model for different occupancies. Then, the exact expressions for the Green’s function and density–density correlation function are given. From them the exact self-energy, polarizability, dielectric function, and screened interaction can be calculated using standard formulae. Next, two subsections provide the formulae for the exact 3-point vertex function and how it is used to evaluate the corrections to the polarizability and to the self-energy in the sc scheme (1). Perturbation theory based equations for the 3-point vertex function are given next. Then I provide expressions for the Ward Identity, which are used later in this paper. Finally formulae relevant to the evaluation of the current three-point vertex function are given. For brevity, derivations of the formulae are not provided, or only a sketch of the derivation is given. In this work, the finite temperature framework is used so that in all equations below the time-frequency arguments are Matsubara’s time ($\tau$) and Matsubara’s frequencies ($\omega$) is for a fermion frequency and $\nu$ is for a boson frequency.

2.1. Many-body states

In order to represent the many-body states of the model it is convenient to introduce basis vectors $|\{abc\}|$ where all entries are equal to 0 or 1 in accordance with the occupancies of the
corresponding one-electron states. In this work the first two one-electron occupancies (a and b) correspond to the spin-up and spin-down one-electron states of the first site, and the third and fourth (c and d) correspond to those of the second site. The many-body energies and states below have two indices: the upper one corresponds to the full occupancy (0, 1, 2, 3, or 4) of the system, and the lower one distinguishes the states within the same occupancy.

For the full occupancy \( N \) equal to zero, we correspondingly have:

\[
E^0_1 = 0; \Psi^0_1 = |0000\rangle, \tag{3}
\]

for \( N = 1 \)

\[
E^1_1 = -t; \Psi^1_1 = \frac{1}{\sqrt{2}}(|1000\rangle + |0010\rangle)
\]

\[
E^1_2 = -t; \Psi^1_2 = \frac{1}{\sqrt{2}}(|0100\rangle + |0001\rangle)
\]

\[
E^1_3 = t; \Psi^1_3 = \frac{1}{\sqrt{2}}(|1000\rangle - |0010\rangle)
\]

\[
E^1_4 = t; \Psi^1_4 = \frac{1}{\sqrt{2}}(|0100\rangle - |0001\rangle), \tag{4}
\]

for \( N = 2 \)

\[
E^2_1 = \frac{U - c}{2}; \Psi^2_1 = 4t\sqrt{a(c - U)} \frac{|1001\rangle - |0110\rangle + |1100\rangle + |0011\rangle}{a}
\]

\[
E^2_2 = 0; \Psi^2_2 = |1010\rangle
\]

\[
E^2_3 = 0; \Psi^2_3 = |0101\rangle
\]

\[
E^2_4 = 0; \Psi^2_4 = \frac{1}{\sqrt{2}}(|1001\rangle + |0110\rangle)
\]

\[
E^2_5 = U; \Psi^2_5 = \frac{1}{\sqrt{2}}(|1100\rangle - |0011\rangle)
\]

\[
E^2_6 = \frac{U + c}{2}; \Psi^2_6 = 4t\sqrt{b(c + U)} \frac{|1001\rangle - |0110\rangle}{b} - \frac{|1100\rangle + |0011\rangle}{a}
\]

\[
\text{with } a = \sqrt{2 + \frac{32t^2}{(U - c)^2}}, b = \sqrt{2 + \frac{32t^2}{(U + c)^2}}, \text{ and } c = \sqrt{16t^2 + U^2}. \tag{5}
\]

For \( N = 3 \)

\[
E^3_1 = U - t; \Psi^3_1 = \frac{1}{\sqrt{2}}(|1011\rangle - |1110\rangle)
\]

\[
E^3_2 = U - t; \Psi^3_2 = \frac{1}{\sqrt{2}}(|0111\rangle - |1101\rangle)
\]

\[
E^3_3 = U + t; \Psi^3_3 = \frac{1}{\sqrt{2}}(|1011\rangle + |1110\rangle)
\]

\[
E^3_4 = U + t; \Psi^3_4 = \frac{1}{\sqrt{2}}(|0111\rangle + |1101\rangle), \tag{6}
\]

and for \( N = 4 \)

\[
E^4_1 = 2U; \Psi^4_1 = |1111\rangle. \tag{7}
\]

2.2. Partition function, Green’s function and self-energy

For convenience, first I introduce ‘shifted’ many-body energies \( E_n^N = E_n^N - \mu N \), with \( \mu \) being the chemical potential. Then I renormalize them, defying the minimal \( E_{\min}^n \) among them and subtracting it \( E_{\min}^n = E_n^N - E_{\min} \). This also factorizes the partition function:

\[
Z(\mu) = \sum_{nN} e^{-\beta E_n^N} = e^{-\beta E_{\min}^n} \sum_{nN} e^{-\beta E_n^N} = e^{-\beta E_{\min}^n} Z'(\mu), \tag{8}
\]

where \( \beta \) is the inverse temperature.

It is clear that now in every Gibbs average one can use \( E'; Z' \) instead of \( E; Z \), which is numerically more stable (big numbers have been subtracted).

For the exact Green’s function, one obtains through the standard spectral decomposition:

\[
G^0_\omega(\omega) = \frac{1}{Z} \sum_{N} \sum_{nN} \sum_{mN+1} e^{-\beta E_{nN}^m} e^{-\beta E_{nN}^m} \langle \Psi^N_{nN} | c_{mN}^+ | \Psi^N_{mN+1} \rangle \langle \Psi^N_{mN+1} | c_{mN} | \Psi^N_{mN+1} \rangle, \tag{9}
\]

The exact self-energy is obtained by inversion of the Dyson’s equation:

\[
\Sigma^0_\omega(\omega) = G_{0,ij}^{-1}(\omega) - G_{ij}^{-1}(\omega), \tag{10}
\]

where the Green’s function in Hartree approximation \( G_{0,ij}^{-1}(\omega) = (i\omega + \mu - U\rho)\delta_{ij} + (1 - \delta_{ij}) \) is used (\( \rho \) is the occupancy (‘density’) of the site \( i \)).

2.3. Response function, polarizability, dielectric function, and \( W \)

The exact two-point density–density correlation function is also obtained through spectral decomposition:

\[
\chi_{ij}^{dd}(\nu) = \frac{1}{Z} \sum_{N} \sum_{nN} \sum_{mN+1} e^{-\beta E_{nN}^m} e^{-\beta E_{nN}^m} \langle \Psi^N_{nN} | c_{mN}^+ c_{mN} | \Psi^N_{mN+1} \rangle \langle \Psi^N_{mN+1} | c_{mN}^+ c_{mN} | \Psi^N_{mN+1} \rangle, \tag{11}
\]

with the density operator \( \hat{c}_{\alpha} = \sum_\beta c_{\alpha}^\dagger c_{\beta} \). It is convenient to also define the density–density response function:

\[
R_{ij}^{dd}(\nu) = \beta \delta_{ij} \rho \rho_j - \chi_{ij}^{dd}(\nu). \tag{12}
\]

After that, one can find the density–density dielectric function

\[
e_{ij}^{dd}(\nu) = \delta_{ij} + UR_{ij}^{dd}(\nu), \tag{13}
\]

the density–density polarizability

\[
F_{ij}^{dd}(\nu) = \sum_k R_{ik}^{dd}(\nu) e_{kj}^{dd}(\nu), \tag{14}
\]

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and the screened interaction

\[ W_{ij}(\nu) = U\delta_{ij} + U^2 R_{ij}^{dd}(\nu). \]  

(15)

The response function, the dielectric function, the polarizability, and the screened interaction calculated using the formulae (12)–(15) from the exact correlation function are by construction exact and can be compared with the corresponding quantities obtained using PT.

2.4. Exact 3-point vertex function in density channel

To find the exact 3-point density vertex function, first I calculate the following three-point correlation function:

\[ \chi^{\sigma,d}_{ijk}(\tau, \tau') = \langle c_{\sigma\alpha}(\tau)c_{\rho\beta}^*(\tau')\delta_{\gamma}(0) \rangle \]

with \( \tau, \tau' \) being Matsubara’s time and ‘\( d \)’ meaning ‘density’. In the site-frequency domain its spectral decomposition reads as follows:

\[ \chi^{\sigma,d}_{ijk}(\omega; \nu) = \frac{1}{Z} \sum_{N} \left\{ \sum_{p \in N} \sum_{n \in N+1} \langle \Psi_{p}^{N+1} | c_{\sigma\alpha}^{+} | \Psi_{n}^{N} \rangle \frac{i}{i\omega - \nu + E_{p}^{N} - E_{n}^{N+1}} \sum_{m \in N+1} \langle \Psi_{m}^{N} | c_{\rho\beta}^{+} | \Psi_{n}^{N+1} \rangle \right. \\
- \sum_{p \in N+1} \sum_{m \in N} \langle \Psi_{p}^{N+1} | c_{\rho\beta}^{+} | \Psi_{m}^{N} \rangle \frac{i}{i\omega - \nu + E_{p}^{N+1} - E_{m}^{N}} \sum_{n \in N} \langle \Psi_{n}^{N} | c_{\sigma\alpha}^{+} | \Psi_{m}^{N+1} \rangle \\
+ \sum_{p \in N} \sum_{n \in N+1} \langle \Psi_{p}^{N} | c_{\sigma\alpha}^{+} | \Psi_{n}^{N+1} \rangle \frac{i}{i\omega - \nu + E_{p}^{N} - E_{m}^{N}} \sum_{m \in N+1} \langle \Psi_{m}^{N} | c_{\rho\beta}^{+} | \Psi_{n}^{N+1} \rangle \\
+ \sum_{p \in N+1} \sum_{m \in N} \langle \Psi_{p}^{N+1} | c_{\rho\beta}^{+} | \Psi_{m}^{N} \rangle \frac{i}{i\omega - \nu + E_{p}^{N+1} - E_{m}^{N}} \sum_{n \in N} \langle \Psi_{n}^{N} | c_{\sigma\alpha}^{+} | \Psi_{m}^{N+1} \rangle \right\}. \]  

(16)

After that the three-point density response function is calculated as

\[ R_{ijk}^{\sigma,d}(\omega; \nu) = \frac{\delta G_{ij}^{\sigma}(\omega)}{\delta \phi_k(\nu)}, \]

\[ = \beta \delta_{ik} G_{ij}^{\sigma}(\omega) \phi_k + \chi^{\sigma,d}_{ijk}(\omega; \nu), \]  

(17)

where I have indicated that the three-point response function is defined as the functional derivative of the Green’s function with respect to an external perturbing field \( \phi_k(\nu) \). The ‘screened’ 3-point density vertex function \( \Gamma^{\sigma,d}_{ijk}(\omega; \nu) \) is defined as the functional derivative of the inverse Green’s function with respect to the external perturbing field \( \phi_k(\nu) \) and correspondingly can be related to the above defined 3-point response function:

\[ \Gamma^{\sigma,d}_{ijk}(\omega; \nu) = -\frac{\delta G_{ij}^{\sigma}(\omega)}{\delta \phi_k(\nu)}, \]

\[ = \sum_{l} G_{ij}^{\sigma}(\omega) R_{ijl}^{\sigma,d}(\omega; \nu) G_{lj}^{\sigma}(\omega - \nu). \]  

(18)

Finally the three-point vertex function entering equation (1) (the ‘bare’ three-point vertex) is defined as the functional derivative of the inverse Green’s function with respect to the total field \( \Phi_{ij}(\nu) \) (perturbing external plus induced internal) and is related to the ‘screened’ vertex through the density–density dielectric matrix (this equation is the density–density part of the more general equation (41)):

\[ \Gamma_{ij}^{\sigma,d}(\omega; \nu) = -\frac{\delta G_{ij}^{\sigma}(\omega)}{\delta \Phi_k(\nu)} = \sum_{l} \Gamma_{ijl}^{\sigma,d}(\omega; \nu) \epsilon_{ikl}(\nu). \]  

(19)

2.5. Vertex-corrected polarizability and self-energy

The vertex-corrected density–density polarizability and the self-energy entering equation (1) are calculated as follows:

\[ P_{ij}^{dd}(\nu) = \frac{1}{\beta} \sum_{\omega} \sum_{\sigma} \sum_{kl} G_{ij}^{\sigma}(\omega) \Gamma_{ijl}^{\sigma,d}(\omega; \nu) G_{lj}^{\sigma}(\omega - \nu), \]  

(20)

and

\[ \Sigma_{ij}^{\sigma}(\omega) = \frac{1}{\beta} \sum_{\nu} \sum_{kl} G_{ij}^{\sigma}(\omega + \nu) \Gamma_{ijl}^{\sigma,d}(\omega + \nu; \nu) W_{kl}(\nu). \]  

(21)

The formulae (20) and (21) are used also when the three-point vertex is obtained within the perturbation theory.

2.6. 3-point vertex function from perturbation theory in density channel

The first-order (in \( W \)) term of the perturbation theory for the three-point density vertex function is

\[ \Gamma_{ij}^{\sigma,d}(\tau; \tau') = -W_{ij}(\tau - \tau') G_{ij}^{\sigma}(\tau) G_{ij}^{\sigma}(\tau'). \]  

(22)

In frequency representation it can be conveniently evaluated as follows:
\[
\Gamma^\sigma_{\alpha k}(\omega, \nu) = -\int \! d\tau e^{i\omega \tau} W_{\alpha}(\tau) \times \frac{1}{\hbar} \sum_{\sigma'} e^{-i\nu \sigma'} G_{\alpha}^{\sigma}(\omega') G_{\beta}^{\sigma'}(\omega' - \nu). \tag{23}
\]

2.7. Ward Identities

In order to write down the Ward Identities one needs to specify the current operator. It is convenient to introduce it through a substitution in the kinetic part of the Hamiltonian:

\[
H' = -i \sum_{\alpha r} c^\dagger_{\alpha r}(A_t - A_r)c_{\alpha r} + \frac{U}{2} \sum_{\alpha} \sum_{\sigma} c^\dagger_{\alpha \sigma} c_{\alpha \sigma} c_{\alpha \sigma} c^\dagger_{\alpha \sigma}, \tag{24}
\]

where \(A_t\) is the vector potential and the following convention for the sites was adopted: \(1 = 2, \xi = 1\). With the above definition the current operator for the model reads as follows:

\[
\hat{J}_i = -\frac{\delta H'}{\delta A_t} = i \sum_{\alpha} \{ c^\dagger_{\alpha \sigma} c_{\alpha \sigma} - c_{\alpha \sigma} c^\dagger_{\alpha \sigma} \}, \tag{25}
\]

with \(\hat{J}_i = -\hat{J}_i\). From the equation of motion for the density operator, one calculates

\[
\frac{\delta \hat{J}_i}{\delta \tau} = -i\hat{J}_i, \tag{26}
\]

which is the continuity equation for the model. Relating the ‘screened’ 3-point current vertex function to the corresponding 3-point response function (similarly to the density case and in space-time coordinates for brevity; ‘c’ goes for ‘current’)

\[
G^\sigma(14)\gamma^{\sigma, c}(453)G^\sigma(52) = G^\sigma(12)J(3) + \langle c_{\sigma}(1)c^\dagger_{\sigma}(2)J(3) \rangle, \tag{27}
\]

one explicitly calculates the time derivatives and, also using the continuity equation (26), one obtains

\[
G^\sigma(14)\left\{ \frac{\partial}{\partial \tau} \gamma^{\sigma, d}(453) + iy^{\sigma, c}(453) \right\}G^\sigma(52) = \frac{\partial}{\partial \tau} (c_{\sigma}(1)c^\dagger_{\sigma}(2)\hat{J}(3)) + i(c_{\sigma}(1)c^\dagger_{\sigma}(2)\hat{J}(3)) = G^\sigma(12)\{\delta(13) - \delta(23)\}, \tag{28}
\]

which is equivalent to

\[
\frac{\partial}{\partial \tau} \gamma^{\sigma, d}(123) + iy^{\sigma, c}(123) = G^{-1}\gamma^{\sigma, d}(12)\{\delta(23) - \delta(13)\}. \tag{29}
\]

In site-frequency representation, (29) reads as follows:

\[
i\{\gamma^{\sigma, d}_{\alpha k}(\omega; \nu) + y^{\sigma, c}_{\alpha k}(\omega; \nu)\} = G^{-1}_{\alpha k}(\omega - \nu) \delta_{\nu k} - G^{-1}_{\alpha k}(\omega) \delta_{\nu k}. \tag{30}
\]

Equation (30) can be simplified by removing the Hartree–Fock contribution on both sides of it. For the vertices, one obtains in the Hartree–Fock approximation

\[
\gamma^{\sigma, d}_{\alpha k}(\omega; \nu) = \delta_{\nu} \delta_{\nu k}. \tag{31}
\]

and

\[
y^{\sigma, c}_{\alpha k}(\omega; \nu) = it\{\delta_{\nu} - \delta_{\nu k}\}. \tag{32}
\]

For the schemes with full sc (without QP approximation), removing the Hartree–Fock contribution on the right side of (30) through Dyson’s equation gives

\[
i\{\nu \Delta \gamma^{\sigma, d}_{\alpha k}(\omega; \nu) + \Delta y^{\sigma, c}_{\alpha k}(\omega; \nu)\} = \Sigma_{\alpha k}^{\sigma}(\omega - \nu) \delta_{\nu k} - \Sigma_{\alpha k}^{\sigma}(\omega) \delta_{\nu k}, \tag{33}
\]

where \(\Delta \gamma\) means the ‘screened’ vertex part beyond the Hartree–Fock approximation, and \(\Sigma\) is the correlation (frequency-dependent) part of the self-energy. For the QP-based schemes the Dyson equation is not satisfied and instead of (33) one has

\[
i\{\nu \Delta \gamma^{\sigma, d}_{\alpha k}(\omega; \nu) + \Delta y^{\sigma, c}_{\alpha k}(\omega; \nu)\} = \{H_{\alpha k}^{HF} - H_{\alpha k}^{OP}\}[\delta_{\nu k} - \delta_{\nu k}], \tag{34}
\]

where the static effective Hamiltonians \(H_{\alpha k}^{HF}\) and \(H_{\alpha k}^{OP}\) (correspondingly in the Hartree–Fock and QP approximations) were introduced:

\[
H_{\alpha k}^{OP} = -t(1 - \delta_{\nu k}) + \delta_{\nu k}(V_{\nu}^H + \Sigma_{\nu}^{\alpha}), \tag{35}
\]

with \(V_{\nu}^H\) and \(\Sigma_{\nu}^{\alpha}\) being the Hartree potential and the exchange part of the self-energy, respectively, and

\[
H_{\alpha k}^{HF} = \mu[\delta_{\nu k} - Z_{\nu}] + \sum_{kl} Z_{\nu}^{1/2}[H_{kl}^{HF} + \Sigma_{\nu}(0)]Z_{\nu}^{1/2}. \tag{36}
\]

where \(Z_{\nu}\) is the renormalization factor, whereas \(\Sigma_{\nu}(0)\) stands for the correlation part of the self-energy at zero frequency. When the effect of the correlations is neglected the renormalization factor becomes equal to 1, and the correlation part of the self-energy becomes zero, which means that in this case \(H^{OP} = H^{HF}\).

Equations (33) and (34) are used in this work to evaluate deviations from the full Ward Identity in the different approximate methods. Two reduced forms of the WI can also be useful: the long-wave limit and the long-wave + static limit of the WI. The long-wave limit of the WI for the two-site Hubbard model consists of the summation over the index \(k\) in equations (33) and (34), which correspondingly become (the current vertex disappears after the summation)

\[
i\nu \sum_{k} \Delta \gamma^{\sigma, d}_{\alpha k}(\omega; \nu) = \Sigma_{\nu}^{\sigma}(\omega - \nu) - \Sigma_{\nu}^{\sigma}(\omega), \tag{37}
\]

and

\[
i\nu \sum_{k} \Delta y^{\sigma, c}_{\alpha k}(\omega; \nu) = 0. \tag{38}
\]

From (38) one can see that in order to satisfy the long-wave limit of the WI in the QP-based approximations one has to neglect vertex corrections altogether.

The long-wave + static limit of the WI consists in taking the limit \((\nu \rightarrow 0)\) in equations (37) and (38):

\[
\sum_{k} \Delta \gamma^{\sigma, d}_{\alpha k}(\omega; \nu = 0) = \lim_{\nu \rightarrow 0} \frac{\Sigma_{\nu}^{\sigma}(\omega - \nu) - \Sigma_{\nu}^{\sigma}(\omega)}{i\nu}. \tag{39}
\]
The arguments supporting quasiparticle approximation in [15] are based on the long-wave limit of the Ward Identity. It is clear from the above consideration that in QPGW approximation (without vertex corrections) the corresponding limit of the WI is satisfied exactly.

2.8. 3-point current vertex function

In order to use the full WI, one needs the ‘screened’ current vertex function $\gamma_{jk}^{\sigma} (\omega; \nu)$. In this work both the exact and the PT-based vertex functions are used. The exact one is evaluated following formulae (16)–(18) with the replacement ($\hat{\rho} \rightarrow \hat{J}$) in equation (16). The PT-based vertices are calculated according to the scheme outlined below.

‘Bare’ vertex functions are related to the ‘screened’ ones through the full (density-current) dielectric function:

$$\gamma_{jk}^{\sigma d} (\omega; \nu) = \sum_{\nu} \sum_{l} \Gamma_{ij}^{\sigma d} (\omega; \nu) \epsilon_{\nu}^{ij} (\nu),$$

where both $I$ and $J$ now run over the indices $d$ (density) and $c$ (current). The non-perpertubated Hamiltonian has no vector potentials, so that the full dielectric matrix has the following form (considering the first index as the density, and the second as the current):

$$\epsilon = \begin{pmatrix} \epsilon_{dd} & \epsilon_{dc} \\ 0 & 1 \end{pmatrix}.$$  

and correspondingly its inverse

$$\epsilon^{-1} = \begin{pmatrix} \epsilon_{dd} & -\epsilon_{dc} \\ 0 & 1 \end{pmatrix}.$$  

Thus, the bare current vertex can be evaluated as follows:

$$
\gamma_{jk}^{\sigma c} (\omega; \nu) = \Gamma_{ij}^{\sigma c} (\omega; \nu) - \sum_{lm} \epsilon_{ij}^{lm} (\nu) \epsilon_{ml}^{dc} (\nu),
$$

Subtraction of the Hartree–Fock contribution (32) leaves us with the expression

$$\Delta \Gamma_{jk}^{\sigma c} (\omega; \nu) = \Delta \Gamma_{ij}^{\sigma c} (\omega; \nu) - \sum_{lm} [\delta_{ji}^{lm} + \Delta \Gamma_{ij}^{\sigma d} (\omega; \nu) \epsilon_{ml}^{dc} (\nu)] \epsilon_{ml}^{dc} (\nu).$$

In the above expression the missing components are the non-trivial part of the current vertex $\Delta \Gamma_{ij}^{\sigma c} (\omega; \nu)$ and the density-current dielectric matrix $\epsilon_{ml}^{dc} (\nu)$. The first one is evaluated similar to equation (23) for the density vertex:

$$\Delta \Gamma_{jk}^{\sigma c} (\omega; \nu) = -i t \int d\epsilon \epsilon \omega \omega W_j (\tau) \frac{1}{\beta} \sum_{\alpha} e^{-i\omega \tau} \times \left\{ G_{ij}^{\sigma} (\omega') G_{jl}^{\sigma} (\omega' - \nu) - G_{ij}^{\sigma} (\omega) G_{jl}^{\sigma} (\omega') \right\}.$$  

The second is defined by the density-current polarizability $\rho_{\sigma d c}$

$$\epsilon_{ij}^{dc} (\nu) = -U \rho_{\sigma d c} (\nu),$$

which in turn is evaluated using the current vertex (46):

$$P_{\sigma c} (\nu) = \int \frac{d\omega}{2\pi} \sum_{\alpha} \left\{ G_{ij}^{\sigma} (\omega) G_{jl}^{\sigma} (\omega' - \nu) - G_{ij}^{\sigma} (\omega') G_{jl}^{\sigma} (\omega) \right\} + \frac{1}{\beta} \sum_{\alpha} \sum_{kl} \left\{ G_{ij}^{\sigma} (\omega) \Delta \Gamma_{kl}^{\sigma c} (\omega; \nu) G_{kl}^{\sigma} (\omega - \nu) \right\}.  \tag{48}
$$

2.9. Internal energy

Exact internal energy is evaluated directly as the average value of the Hamiltonian. In spectral representation it reads

$$E = \frac{1}{Z} \sum_{nN} E_n^{\alpha} e^{-\beta E_n^{\alpha}}.$$  

To evaluate internal energy in the perturbation theory based methods it is convenient to express the average value of the Hamiltonian through Green’s functions. First, one expresses it using equal time correlation functions:

$$E = - t \sum_{i \neq j, \sigma} \langle c_{i \sigma} c_{j \sigma} \rangle + U \sum_{i} \sum_{\sigma \sigma'} \langle c_{i \sigma} c_{i \sigma'} c_{i \sigma} c_{i \sigma'} \rangle.$$  

The one-particle correlation function is just the Green’s function at $\tau = \beta$: $\langle c_{i \sigma} c_{j \sigma} \rangle = G_{ij}^{\sigma} (\tau = \beta)$, whereas the two-particle correlation function can be expressed through the definition of the mass operator $M$ (the sum of the Hartree term and self-energy): $U \sum_{i} \langle c_{i \sigma} c_{i \sigma'} c_{i \sigma} c_{i \sigma'} \rangle = \int d\tau M_{ij}^{\sigma} (\tau) G_{ij}^{\sigma} (\tau = \beta)$. Explicitly separating the mass operator into the Hartree contribution, dividing the self-energy into exchange and correlation parts, and writing the convolution of $G$ and $\Sigma$ in frequency representation, one gets an alternative expression for the internal energy, which can equally be used with exact $G$ and $\Sigma$ and with approximate ones:

$$E = t \sum_{i \neq j, \sigma} G_{ij}^{\sigma} (\tau = \beta) + U \sum_{i} \sum_{\sigma \sigma'} \rho_{\sigma d c} + \frac{1}{2} \sum_{i} \sum_{\sigma} \Sigma_{i i}^{\sigma \sigma} G_{ii}^{\sigma} (\tau = \beta) - \frac{1}{2} \sum_{i} \sum_{\sigma} \Sigma_{i i}^{\sigma \sigma} G_{ii}^{\sigma} (\tau = \beta) + \frac{1}{2 \beta} \sum_{i \neq j, \sigma} \Sigma_{i j}^{\sigma \sigma} G_{ij}^{\sigma} (\tau = \beta).$$  

If the self-energy and polarizability in (1) are evaluated with the same vertex function (exact or approximate) then the convolution of the Green’s function and self-energy can be replaced with the convolution of the polarizability and screened interaction. With $W$ as the screening (dynamical) part of $W$ ($W = W - U$), $P_0$ as the polarizability without vertex correction ($P_0 = G G$), $\Delta \Gamma$ as the nontrivial part of the vertex, and $\Delta P$ as the vertex correction to the polarizability ($\Delta P = G \Delta \Gamma$), one can rewrite the correlation energy the
The two-site Hubbard model is studied here with the value of parameter $t$ fixed and equal to 1. The temperature was also fixed at $T = 0.05t$. Thus, only parameter $U$ was changed. The quarter-filling ($\langle N \rangle = 1$) and half-filling ($\langle N \rangle = 2$) cases have been studied. The results on the key physical quantities are provided for these two fillings below.

I compare the exact results with the results obtained with the $GW$, $G_{\Delta}W$, $G_{\Gamma}W$, $QPGW$, $QPQG_{\Delta}W$, and $QPQG_{\Gamma}W$ methods, where $\Gamma_{\Delta}$ and $\Gamma_{\Gamma}$ stand for the first-order (in $W$) 3-point vertex and the exact 3-point vertex, respectively. At full self-consistency $G_{\Gamma}W$ reproduces exact results, so this approach has been used basically only as a means to adjust (by comparing with the exact result) the calculational parameters (such as the number of Matsubara’s frequencies included in the internal summations and the density of the mesh on the interval $[0 : \beta]$ for $\tau$-integrations).

3.1. Structure of the many-body energy states

Before proceeding with the applications of the approximate methods, it is instructive to look at the structure of the exact many-body energy levels of the model. Figures 1 and 2 show the modified energy levels $E_{n}^{\tau}$ as functions of the $U$ parameter for the quarter- and half-filling cases, respectively. The most striking difference between the two cases is that in the half-filling case the ground state is not degenerate (singlet), whereas in the quarter-filling case it is doublet, with total spin 1/2. Thus, the case with $\langle N \rangle = 1$ is similar to a regime well known in solid-state many-body physics, the ‘local moment’ regime, which is notoriously difficult for perturbation theory based methods. Another evidence of the qualitative difference between quarter filling and half filling cases is shown on figure 3 where the exact self energy is presented. It is obvious from figure 3 that in quarter-filling case the correlation effects are much stronger (self energy shows singular behavior at small frequencies). As it will be shown below the above differences in the energy level structure and in the self energy correlate very well with applicability of $GW$-based methods, namely with the range of $U$ values, where $GW$ and its perturbation theory based extensions are valid.

3.2. Spectral functions

Figure 4 presents the calculated spectral function for quarter-filling with $U$ equal to 0.35. Spectral functions for half-filling are shown on figures 5 and 6 for $U$ equal to 2 and 5. In order to plot the spectral functions the self energy was analytically continued to the real frequency axis according to the formula (9) in [13]. After that the imaginary part of Green’s function
was calculated as a function of real frequency with small positive imaginary part (0.1i) added. Small positive imaginary shift didn’t change the positions of the peaks (which were of principal interest in this work) but made the graphs smooth (which otherwise would look as collections of the δ-functions).

In case of quarter-filling the spectral function for very small $U$ is similar to the noninteracting case and it shows two main peaks. All approximate methods studied in this work reproduce the positions of the peaks very well. However, when $U$ increases (figure 4) both peaks begin to split into doublets. As it is seen from the figure, one needs to apply non-perturbative approach ($GW$) to describe this splitting correctly. First order vertex corrected $GW$ shows some right tendencies though: the center peak is being reduced as compared to $GW$, and two small satellites appear (but at slightly misplaced positions). Important note is that exact vertex in combination with $QP$ self-consistency is not capable to reproduce the formation of doublets. Besides, for $U > 0.35$ vertex-corrected calculations with $QP$ self-consistency become unstable because of the problems with long wave limit of polarizability (see section 3.4 below for more details).

In case of half-filling for $U \leq 2$ there are two main peaks at frequencies ±1.4 which are perfectly reproduced by all approximate methods. However, two satellites at frequencies about ±3.5 which are very small when $U \leq 2$ grow in amplitude with $U$ increasing and their effect on other calculated properties becomes more pronounced. They are not reproducible within PT based methods, as it can easily be seen. Again, an application of the exact vertex together with $QP$ self-consistency cannot reproduce simultaneously the positions of the main peaks and the satellites. Only full self in combination with exact vertex ($GW$) can do that.

3.3. Errors in self energy and screened interaction

The calculated spectra presented in the previous subsection might be considered as the main result of the present work. But it is also interesting to know the accuracy of some intermediate quantities (such as self energy and screened interaction) obtained in different approximate schemes, and how the accuracy evolves with changing the parameter $U$. Figures 7 and 8 show the average error in the calculated $\Sigma$ and $W$ for quarter of filling. Figures 9 and 10 present the same quantities for half-filling case. The average error for a quantity $F$ has been calculated according to the following formula

$$\frac{\sum_\omega \sum_{ij} |F_{ij}(\omega) - F_{\text{exact}}(\omega)|}{\sum_\omega \sum_{ij} 1}.$$  \hspace{1cm} (54)

where $i,j$ are site indexes, and Matsubara’s-frequency sums are performed from $\omega = 0$ to $\omega = 20$.

One can see that for the methods satisfying the Dyson equation the increasing in accuracy of the vertex ($1 \rightarrow \Gamma_{\text{G}} \rightarrow \Gamma_{\text{QG}}$) consistently improves the accuracy of $\Sigma$ and $W$, finally making them exact when the exact vertex is applied.

Opposite to that, in the $QP$-based methods the situation is more complicated. First of all, it is important for the present study to mention that vertex corrected approaches with $QP$ self-consistency become unstable when $U > 0.35$ (quarter filling) and $U > 5$ (half filling). The reason for that will be explained in section 3.4 below.

At very small $U$’s vertex corrected $QP$ calculations show certain improvements as compared to the $QP$ approximation
itself, but their accuracy deteriorates quickly with \( U \) increasing and they become less accurate than QP well before their instability region.

As it is clear from the figures above, QP \( /\!\!/\Gamma_W \) method doesn’t show any noticeable improvement as compared to other approximate methods studied. Opposite to that—at half-filling it quickly becomes the worst of the methods considered.

3.4. Long wave limit of polarizability

As it was said before the problems with vertex-corrected QP calculations related to the wrong long wave limit of polarizability obtained with the corresponding approaches. In case of Hubbard dimer the long wave (LW) limit of polarizability is just the sum of on-site and off-site terms:

\[
P_{\mathrm{LW}}(\nu) = P_{11}(\nu) + P_{21}(\nu).
\]

Figures 11 and 12 show the corresponding functions for quarter filling (\( U = 0.3 \)) and for half-filling (\( U = 5 \)). Proper long wave limit of the polarizability should be zero for all frequencies in insulator case (half-filling). In metallic case (quarter-filling) it should be zero for all positive Matsubara’s frequencies (beginning with \( \nu \approx 0.3 \) in figure 11).

As one can see from the figures, the vertex correction to the long wave polarizability always has positive sign. But if in the \( GW \) case it improves the situation (\( P \) remains negative but smaller in amplitude), in QPGW case we start from exact
limit (no vertex corrections) and go in the positive region if vertex corrections are applied. Positive polarizability can easily produce poles in $W$ as it is clear from the equation for it ($W = \frac{U}{1 - U P}$), which essentially is the reason for the above mentioned problems.

3.5. Internal energy and Ward Identity

The internal energy as a function of $U$ is presented in the figures 13 and 14. Equations (51) and (53) have been used to evaluate it with essentially identical results.

In addition to the principal physical quantities discussed above, the analysis of the Ward Identities fulfillment has been performed and was used as an indicator of the accuracy of the approximations. The figures 15 and 16 show the relative violation of full WI (equations (33) and (34)) in different approximate methods as a function of $U$. The following form of the average deviation from the identity has been used

$$\frac{\sum_{\alpha, \mu} \sum_{ik} |(\text{LHS})_{\alpha \mu}(\alpha; \nu) - (\text{RHS})_{\alpha \mu}(\alpha; \nu)|}{\sum_{\alpha, \mu} \sum_{ik} 1},$$

where (LHS) and (RHS) are the left- and the right-hand sides in (33) and (34) correspondingly. The 3-point vertex pertinent
to the specific approximation (i.e. for instance the vertex $\Delta \gamma$ is zero in $GW$ and in QPGW) was used to evaluate the deviation from the WI in all approximate schemes, and the exact vertex was used in $G_{\gamma}W$ and QPGT$_{\gamma}W$. The summations over the frequencies $\omega$ and $\nu$ in (55) were performed for $|\omega| < 20$ and $0 \leq \nu < 20$.

It is clear from the above figures that the tendencies (with increasing $U$) in the accuracy of internal energy and in the degree of fulfillment of WI are very similar to the tendencies observed earlier in other quantities. Namely, for very small $U$'s (especially well it is seen for quarter filling) vertex corrections allow us to improve the accuracy of scQPGW approach in calculated internal energy and in the degree of WI fulfillment. However, when $U$ increases, the things become worse and it becomes obvious that QP self-consistency should not be combined with vertex corrections.

The $GW$-based (without QP approximation) methods give numerically exact internal energy till $U \approx 0.2$ (quarter filling) and $U \approx 2$ (half filling) which is not very surprising because they are conserving (in Baym–Kadanoff sense [32]) and in the weakly correlated regime should produce accurate total energies.

4. Conclusions

In this work the Hedin’s equations [23] for the two-site Hubbard model have been solved self-consistently with and without applying the quasiparticle approximation for the Green function. The study has been performed both when the exact three-point vertex function was used as an input and when the perturbative theory (in its zero and first orders in $W$) was used to evaluate the corresponding vertices self-consistently. The results of this work obtained with the exact vertex have an impact on what one can expect from the future implementation of $sc\ GW + \ DMFT$ and $sc\ QPGW + \ DMFT$ schemes. As it has been shown here, only $sc\ GW + \ DMFT$ approach can be considered as useful approximation. However, as it has been said in the Introduction, this work is directly related to an ideal situation, where the $GW$ part and the DMFT part are perfectly separable and the subspace where $GW$ is used is very weakly correlated (so that $GW$ and QPGW give identical results for the weakly correlated subspace). In practice, it is not always the case. The correlations in the ‘$GW$’ subspace might be noticeable. In such situation, QPGW might be superior (with respect to $GW$) for the subspace not included in the DMFT part. The conclusions about the DMFT part obviously remain as before—one should not impose the QP approximation on $G$ in the DMFT part. As it seems, in such circumstances the preference should be given to the approach ($GW$-based or QPGW-based) depending on which subspace (the ‘weakly’ or the ‘strongly’ correlated) is more important for the problem under consideration. However, on the fundamental level, such a situation should be resolved either by increasing the subspace covered by the DMFT part or (which seems to be easier practically) by including more diagrams beyond $GW$ for the ‘weakly’ correlated subspace.

It has been shown, that methods with PT-based vertices (when they are applicable) reveal similar tendencies (for example if one chooses between the QP self-consistency and the full sc) as the methods based on the exact vertices. Namely, when the correlation strength increases, both the PT-based and the exact vertices-based schemes begin to fail if one uses the QP self-consistency. Also of practical importance is the finding that the violation of the WI in any particular method correlates well with the general applicability of the given method. This can be an useful information if one sees to apply the schemes with vertex corrections to the real materials where the exact solutions are not available to serve as a judgement.

The results of this work are of the methodological importance. Of course the two-site HM doesn’t cover all possible regimes of correlations which may happen in realistic materials. In order to cover a little bit more of the possible regimes of correlations, similar work on the homogeneous electron gas is now being performed (with the three-point vertex functions calculated within the PT only).

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