Beyond the GW approximation: Combining correlation channels

Pina Romaniello,[1,2,4] Friedhelm Bechstedt,[3,4] and Lucia Reining[2,4]

[1]*Laboratoire de Physique Théorique-IRSAMC, CNRS, Université Paul Sabatier, F-31062 Toulouse Cedex, France*

[2]*Laboratoire des Solides Irradiés UMR 7642, CNRS-CEA/DSM, École Polytechnique, F-91128 Palaiseau, France*

[3]*Institut für Festkörpertheorie und-Optik, Friedrich-Schiller-Universität, Max-Wien-Platz 1, 07743 Jena, Germany*

[4]*European Theoretical Spectroscopy Facility (ETSF)*

(Received 17 June 2011; revised manuscript received 16 February 2012; published 19 April 2012)

In many-body perturbation theory (MBPT) the self-energy $\Sigma = iGW\Gamma$ plays a key role since it contains all the many-body effects of the system. The exact self-energy is not known; as a first approximation one can set the vertex function Γ to unity which leads to the GW approximation. The latter properly describes the high-density regime, where screening is important; in the low-density regime, instead, other approximations are proposed, such as the T matrix, which describes multiple scattering between two particles. Here we combine the two approaches. Starting from the fundamental equations of MBPT, we show how one can derive the T-matrix approximation to the self-energy in a common framework with GW. This allows us to elucidate several aspects of this formulation, including the origin of, and link between, the electron-hole and the particle-particle T matrix, the derivation of a screened T matrix, and the conversion of the T matrix into a vertex correction. The exactly solvable Hubbard molecule is used for illustration.

DOI: 10.1103/PhysRevB.85.155131 PACS number(s): 71.10.−w, 71.45.Gm

I. INTRODUCTION

The GW approximation (GWA) to the electron self-energy Σ[1] is nowadays the method of choice for band-structure[2,3] and photoemission calculations (see, e.g., Refs. 4–7). In the general expression $\Sigma = iGW\Gamma$, it approximates the vertex function $\Gamma \approx 1$ and keeps only the one-particle Green's function G and the screened Coulomb interaction W. In the high-density regime, where screening is important, the GWA works reasonably well; in the low-density limit, instead, where the quantum nature of the system dominates, GW shows some failures.[8–13] One, hence, needs to go beyond GW. Iterating Hedin's equations further seems the obvious thing to do, but this is technically difficult and there is no guarantee that results will quickly improve. To overcome the problems of finite-order corrections to the self-energy, one might then use the strategy of creating an infinite number of diagrams via a Dyson equation for the Green's function. This is what is done in GW, where the Green's function is determined to infinite order in W using a Dyson equation with a kernel (the self-energy) that is only linear in W. A similar strategy can be used for the self-energy itself by introducing the scattering T matrix[14–17] that yields the self-energy as $\Sigma = GT$. In the so-called Bethe-Goldstone approximation, originally introduced in the nuclear many-body problem[18] for the two-particle Green's function, T describes multiple scattering between two particles (two electrons or two holes) or an electron and a hole. The approximation is justified in the limit of low density of electrons or holes, i.e., close to completely filled or completely empty bands. T-matrix approaches have been extensively used in the context of Hubbard models[19–23] and the results have confirmed that this approximation is very good at low-electron density, precisely where GW fails, but is not superior to the GWA at half filling where the correlation gap is not well reproduced.[22] However, in general, none of the three possibilities (GWA, particle-particle, or electron-hole T matrix) will give an exhaustive description. This reflects the dilemma of how to decide which two-particle correlation to favor in the description of a (at least) three-particle problem. It suggests working with combinations. There are several ways to combine different correlation channels, and care must be taken to prevent double counting of low-order terms.[24,25] The "fluctuating exchange" (FLEX) approximation by Bickers *et al.*[26,27] starts from the second Born self-energy, i.e., the exact self-energy to second order in the Coulomb potential, and then sums all contributions, starting from the third order, in each channel separately (i.e., there are no mixed diagrams). It contains, hence, the GWA and its exchange counterpart to all orders, plus, starting from third order, all T-matrix particle-particle diagrams and all T-matrix electron-hole diagrams. In particular for the Hubbard model with its local interaction, where the exchange contribution simply leads to a spin dependence of the interaction, calculations remain quite efficient. The Bethe-Goldstone T-matrix and GW approximations can be regarded as an approximation to FLEX where only one channel is taken into account. Beyond the summation of independent channels two-step FLEX approaches have been proposed, where one channel enters the calculation of a second channel through an effective screening.[28–30] One can also couple particle-particle and electron-hole channels on an equal footing, which then leads to the rather involved parquet theory.[24,31] In the same spirit, in Ref. 32 a variational functional of the Green's function and the two-particle scattering vertex (which is a T matrix as defined in Ref. 33) has been proposed. Its systematic construction yields the particle-particle T-matrix approach as simple approximation and adds electron-hole diagrams at a higher level of perturbation theory. In this work we propose an alternative way to derive the coupling of GW and T-matrix channels on an equal footing starting from exact many-body equations. Attempts to go beyond GW by summing the GW self-energy to screened versions of the T-matrix self-energy are found in the literature.[12,34–39] However, only putting the different approximations on the same footing one can get unambiguous corrections to GW from the T

matrix. These screened T matrices indeed require appropriate double counting corrections to keep the second-order terms exact and to avoid negative spectral functions. Therefore, in the following we present a unified framework that links GW, $GW\Gamma$, and T matrix. This allows us to address several questions, in particular, *What is the origin of, and link between, the particle-particle and the electron-hole contributions to the T matrix? How do we get a screened version of the T matrix? How do we translate the physical content of the T matrix into a vertex correction?* These questions will be answered in Sec. II. In Sec. III we will then apply the T matrix to the Hubbard molecule at 1/4 and 1/2 filling. This system allows us to compare the T matrix, GW, and the exact results, and, hence, to illustrate the performances of the different approximations. Conclusions are given in Sec. IV.

II. A UNIFIED FRAMEWORK

In order to use a common language for $GW\Gamma$ and T matrix, we start from the following exact expression for the self-energy:

$$\Sigma(11') = -iv_c(1^+2)G_2(12;32^+)G^{-1}(31'), \tag{1}$$

where $(1) = (r_1,\sigma_1,t_1)$, $(1^+) = (r_1,\sigma_1,t_1^+)$ with $t_1^+ = t_1 + \delta$ ($\delta \to 0^+$) describe space, spin, and time coordinates, and integration over indices not present on the left is implicit throughout the paper. By adding a perturbing potential $U_{\rm ext}$ and using the relation $G_2(12;32^+;[U_{\rm ext}])|_{U_{\rm ext}=0} = G(13)G(22^+) - \frac{\delta G(13)}{\delta U_{\rm ext}(2)}|_{U_{\rm ext}=0}$,[40] Eq. (1) can be written as

$$\Sigma(11') = v_H(1)\delta(11') - iv_c(1^+2)G(13)\left.\frac{\delta G^{-1}(31')}{\delta U_{\rm ext}(2)}\right|_{U_{\rm ext}=0}, \tag{2}$$

where $\frac{\delta G}{\delta U_{\rm ext}} = -G\frac{\delta G^{-1}}{\delta U_{\rm ext}}G$ is used. Here $v_H(1) = -iv(1^+2)G(22^+)$ is the Hartree potential and the second term on the right-hand side defines the exchange-correlation contribution to the self-energy, Σ_{xc}. With the help of the Dyson equation for G, Eq. (2) can be further rearranged as

$$\Sigma(11') = v_H(1)\delta(11') + \Sigma_x(11') + iv_c(1^+2) \times G(13)\Xi(35;1'4)L(42;52^+), \tag{3}$$

with $\Sigma_x(11') = iv(1^+1')G(11')$, $\Xi(35;1'4) = \frac{\delta\Sigma(31')}{\delta G(45)}$ the effective interaction, and $L(42;52) = \frac{\delta G(45)}{\delta U_{\rm ext}(2)}|_{U_{\rm ext}=0}$ the time-ordered "response" of the system to an external perturbation $U_{\rm ext}$. This way of writing the self-energy directly displays the physics behind it, i.e., the description of a particle interacting with the system: The particle can scatter against the density of the system (Hartree term), it can exchange with another particle of the system (exchange term), and it can do something to the system (last term), i.e., it can have an effective interaction with the system (Ξ), the system responds (L), and the particle feels this response through the Coulomb interaction (v_c).

There are two essential ingredients in Eq. (3): The effective interaction $\Xi(35;1'4)$ and the response of the system $L(42;52)$. Combining approximations to Ξ and to L, various approximations to the self-energy can be created. In situations where the screening is important, one should make an effort to obtain a good L, whereas in situations where the quantum nature of the interaction is important,[41] one would concentrate on Ξ, although L and Ξ are, of course, in principle, linked through the Bethe-Salpeter equation[33] and one might wish to keep them approximately consistent.

A. How to get GW

Neglecting the variation of Σ_{xc} in Ξ, i.e., keeping only the classical interaction v_c, one obtains $\Sigma_{xc}(11') = \Sigma_x + iv_c(12)G(11')v_c(1'4)\chi(42)$, with $\chi(42) = -iL(42;42)$ the time-ordered response function. Hence, one gets a screening contribution with respect to Σ_x: This is the GW form, with $W = v_c + v_c\chi v_c$. At this stage it has not been specified yet how to calculate the screening: Different approximations to the screening will give the various GW flavors (e.g., $GW^{\rm RPA}$, with W within the random-phase approximation, and beyond).[42] If one keeps an approximate Σ_{xc} in Ξ one goes beyond GW and includes vertex corrections. For example, approximating Σ_{xc} by the exchange-correlation potential of DFT, v_{xc}, one gets $\Sigma_{xc}(11') = \Sigma_x + iv_c(12)G(11')[v_c(1'4) + f_{xc}(1'4)]\chi(42)$, where $f_{xc} = \frac{\delta v_{xc}}{\delta\rho}$; this leads to $\Sigma_{xc} = iGW\Gamma$ with an approximate vertex function $\Gamma = 1 + f_{xc}P$, where $P = iGG\Gamma$ is the irreducible polarizability and we used $\chi = P + Pv_c\chi$.[43]

B. How to get the T matrix

One could also use the rough approximation $L(42;52) = -G(47)\frac{\delta G^{-1}(78)}{\delta U_{\rm ext}(2)}G(85) \approx G(42)G(25)$ but concentrate on a clever approximation for Ξ. This modifies the exact self-energy (3) as

$$\Sigma(11') \approx v_H(1)\delta(11') + \Sigma_x(11') + iv_c(12) \times G(13)\left[\frac{\delta\Sigma(31')}{\delta G(45)}G(42)G(25)\right]. \tag{4}$$

1. An effective four-point interaction O

An appropriate approximation for the functional derivative on the right-hand side of Eq. (4) still remains to be found. One can introduce an effective four-point interaction O such that, similarly to GW,

$$\Sigma(11') = G(42)O(12;1'4). \tag{5}$$

Note that Eq. (5) is closely related to the expression of the self-energy within the T-matrix approximation as given, e.g., by Kadanoff and Baym [see Eq. (56) in Ref. 17], which is the goal of this derivation. However, at this stage, O is not yet the T matrix. Since $G(42)O(12;1'4)$ cannot be inverted to find O, several choices of O make the correct Σ.[44] First, note that in Eq. (4) there are direct and exchange terms. Therefore, it is convenient to divide the self-energy as $\Sigma = \Sigma_1 + \Sigma_2$ and, consequently, $O = O_1 + O_2$ with

$$O_1(12;1'4) = -iv_c(12)\delta(11')\delta(42) + iv_c(12) \times G(13)\left[\frac{\delta\Sigma_1(31')}{\delta G(45)}G(25)\right], \tag{6}$$

$$O_2(12;1'4) = iv_c(12)\delta(21')\delta(41) + iv_c(12) \times G(13)\left[\frac{\delta\Sigma_2(31')}{\delta G(45)}G(25)\right]. \tag{7}$$

This decomposition of O allows us to find two interaction channels as in the T-matrix self-energy with a direct term (here given by O_1) and an exchange term (here given by O_2) [see, e.g., Eq. (13.23) of Ref. 45].

The solutions (6) and (7) are not unique; one could equally have written

$$\begin{aligned}\Sigma(11') &= G(25)O(15;1'2)\\ &:= G(25)[O_1(15;1'2)+O_2(15;1'2)]\\ &:= \Sigma_1(11')+\Sigma_2(11'),\end{aligned} \tag{8}$$

with

$$\begin{aligned}O_1(15;1'2) &= -iv_c(1'2)\delta(11')\delta(52)+iv_c(12)\\ &\quad\times G(13)\left[\frac{\delta\Sigma_1(31')}{\delta G(45)}G(42)\right],\end{aligned} \tag{9}$$

$$\begin{aligned}O_2(15;1'2) &= iv_c(1'2)\delta(12)\delta(51')+iv_c(12)\\ &\quad\times G(13)\left[\frac{\delta\Sigma_2(31')}{\delta G(45)}G(42)\right].\end{aligned} \tag{10}$$

These two decompositions of the self-energy are equivalent, i.e., they give the same self-energy if the exact Σ is used.

2. *A Dyson equation for O: The particle-particle and electron-hole T matrix*

At this level we do not have yet a closed expression for O, but Eq. (5) suggests an approximation to the functional derivative, analogously with what one usually does in the framework of Bethe-Salpeter calculations based on GW:[46–49]

$$\frac{\delta\Sigma_i(31')}{\delta G(45)}\approx O_i(35;1'4). \tag{11}$$

Note that, with Eqs. (4) and (11), O is only an approximation to the total interaction Ξ. Note also that approximation (11), together with Eq. (5) and Ref. 44, is along the same line of the approximations based on the Ward identity used, e.g., in Refs. 50–53.

This approximation used in Eqs. (6) and (7) allows one to determine O from an integral equation

$$\begin{aligned}O_1^{\rm pp}(12;1'4) &= -iv_c(12)\delta(11')\delta(42)+iv_c(12)\\ &\quad\times G(13)G(25)O_1^{\rm pp}(35;1'4),\end{aligned} \tag{12}$$

$$\begin{aligned}O_2^{\rm pp}(12;1'4) &= iv_c(12)\delta(21')\delta(41)+iv_c(12)\\ &\quad\times G(13)G(25)O_2^{\rm pp}(35;1'4).\end{aligned} \tag{13}$$

Here the subscript pp indicates the particle-particle nature of the interaction O that comes from the time ordering of the kernel GG (see Appendix A). Note that the zeroth-order term in Eq. (13) has simply a minus sign and the indices 4 and $1'$, which, moreover, are external indices in $O_i^{\rm pp}$, exchanged with respect to Eq. (12) for $O_1^{\rm pp}$; therefore, one can relate $O_2^{\rm pp}$ to $O_1^{\rm pp}$ as

$$O_2^{\rm pp}(12;1'4) = -O_1^{\rm pp}(12;41'). \tag{14}$$

$O^{\rm pp}=O_1^{\rm pp}+O_2^{\rm pp}$ with $O_1^{\rm pp}$ and $O_2^{\rm pp}$ given by Eqs. (12) and (13) can be identified with the *particle-particle* T matrix.[14,45] Using Eq. (14), one can verify that the pp T matrix meets the cross relation $O^{\rm pp}(12;1'4)=-O^{\rm pp}(12;41')$ arising from the Pauli principle. Moreover, one can also verify that $O^{\rm pp}(12;1'4)=O^{\rm pp}(1'4;12)$, i.e., the T matrix remains the same for a scattering process reversed.

Equivalently, using the approximation of Eq. (11) for O in Eqs. (9) and (10), one also obtains Bethe-Salpeter-like equations

$$\begin{aligned}O_1^{\rm eh}(15;1'2) &= -iv_c(1'2)\delta(11')\delta(52)+iv_c(12)\\ &\quad\times G(13)G(42)O_1^{\rm eh}(35;1'4),\end{aligned} \tag{15}$$

$$\begin{aligned}O_2^{\rm eh}(15;1'2) &= iv_c(1'2)\delta(12)\delta(51')+iv_c(12)\\ &\quad\times G(13)G(42)O_2^{\rm eh}(35;1'4),\end{aligned} \tag{16}$$

where the subscript eh indicates the *electron-hole* nature of the T matrix. Note that, similarly to the particle-particle T matrix, the zeroth-order term in $O_2^{\rm eh}$ has simply a minus sign and the indices 1 and 5 exchanged with respect to $O_1^{\rm eh}$. However, the fact that 1 and 5 are not external indices prevents from relating $O_2^{\rm pp}$ to $O_1^{\rm pp}$, unlike in the case of the pp T matrix.[54] This is because the Pauli principle does not apply. The symmetry with respect to a reversed scattering process, instead, holds.

Because of the approximation of Eq. (11), the pp T matrix and the eh T matrix do not, in general, give the same self-energy anymore. In the first iteration of Eqs. (12) and (13) and Eqs. (15) and (16) the equality still holds, with

$$\begin{aligned}\Sigma^{\rm pp,(1)}(11') &= \Sigma^{\rm eh,(1)}(11')\\ &= T_0(11') = v_H(1)\delta(11')+\Sigma_x(11')\\ &\quad+v_c(12)v_c(1'5)G(11')G(52)G(25)\\ &\quad-v_c(12)v_c(1'5)G(21')G(52)G(15),\end{aligned} \tag{17}$$

which is the second Born approximation. With the second iteration differences appear (see Fig. 1). Indeed, one obtains

$$\Sigma^{\rm pp,(2)}(11') = T_0(11')+T_1(11'), \tag{18}$$

$$\Sigma^{\rm eh,(2)}(11') = T_0(11')+T_2(11'), \tag{19}$$

with

$$\begin{aligned}T_1(11') &= iv_c(12)v_c(35)v_c(1'4)G(13)G(31')G(54)G(42)G(25)\\ &\quad-iv_c(12)v_c(35)v_c(1'4)G(13)G(34)G(51')\\ &\quad\times G(42)G(25),\end{aligned} \tag{20}$$

$$\begin{aligned}T_2(11') &= iv_c(12)v_c(34)v_c(1'5)G(13)G(31')G(54)G(42)G(25)\\ &\quad-iv_c(12)v_c(34)v_c(1'5)G(13)G(35)G(54)\\ &\quad\times G(42)G(21').\end{aligned} \tag{21}$$

If one considers also the term $\delta O/\delta G$ in the iteration [in Eqs. (6) and (7) or Eqs. (9) and (10)], then the equality of the self-energy via a pp or a eh channel is re-established, i.e.,

$$\begin{aligned}\Sigma^{\rm pp,(2)}_{\rm full}(11') &= \Sigma^{\rm eh,(2)}_{\rm full}(11') = T_0(11')+T_1(11')\\ &\quad+T_2(11')+T_3(11')\end{aligned} \tag{22}$$

with

$$\begin{aligned}T_3(11') &= iv_c(12)v_c(35)v_c(1'4)G(13)G(32)G(21')G(45)G(54)\\ &\quad-iv_c(12)v_c(35)v_c(1'4)G(13)G(32)G(24)\\ &\quad\times G(45)G(51').\end{aligned} \tag{23}$$

Therefore, in the case of the pp T matrix, the two terms T_2 and T_3 come from the functional derivative $\delta O^{\rm pp,(1)}/\delta G$, whereas, in the case of the eh T matrix, the two terms T_1 and T_3 are the

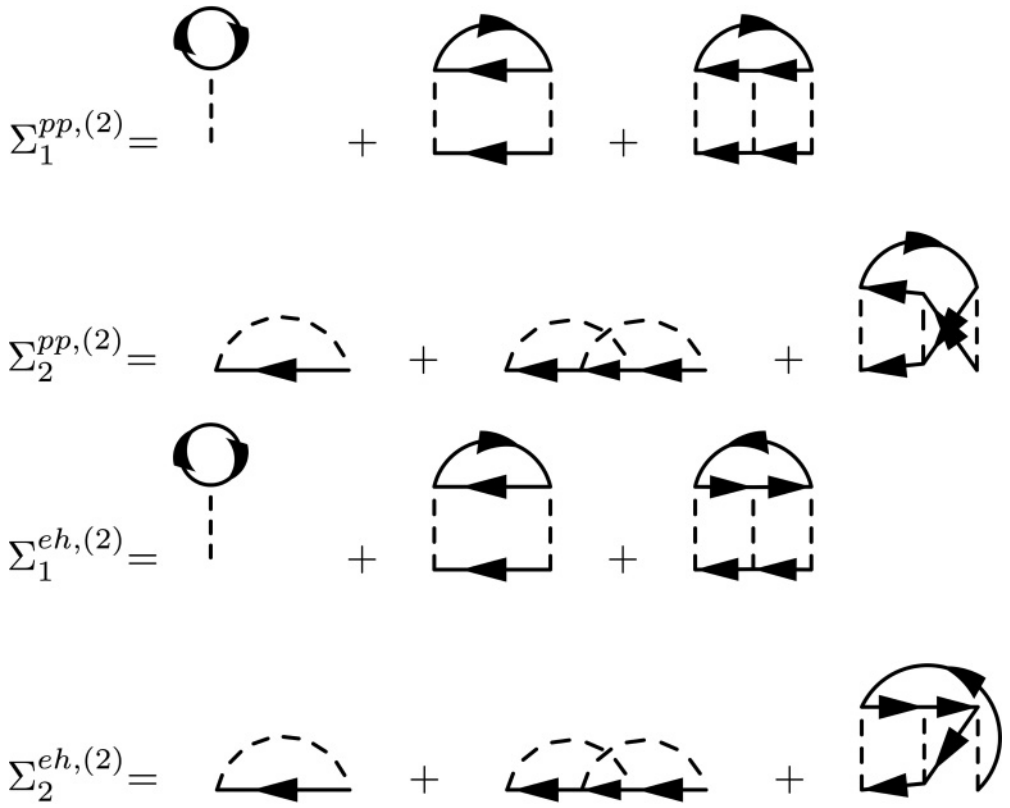

FIG. 1. Diagrams corresponding to the self-energy obtained with the second iteration of the particle-particle T matrix ($\Sigma_1^{\mathrm{pp},(2)}$ and $\Sigma_2^{\mathrm{pp},(2)}$) and electron-hole T matrix ($\Sigma_1^{\mathrm{eh},(2)}$ and $\Sigma_2^{\mathrm{eh},(2)}$).

ones that are due to $\delta O^{\mathrm{eh},(1)}/\delta G$. We also note that $\delta O^{(0)}/\delta G = 0$, i.e., the functional derivative does not contribute to the first iteration, which explains why the pp and eh self-energy are the same after the first iteration. One can also rewrite Eq. (22) as

$$\Sigma_{\mathrm{full}}^{(2)} = (\Sigma^{\mathrm{pp},(2)} + \Sigma^{\mathrm{eh},(2)}) - T_0 + T_3, \tag{24}$$

or, alternatively, for example, as

$$\Sigma_{\mathrm{full}}^{(2)} = \tfrac{1}{2}(\Sigma^{\mathrm{pp},(2)} + \Sigma^{\mathrm{eh},(2)}) + \tfrac{1}{2}(T_1 + T_2) + T_3. \tag{25}$$

This shows that one might try to sum the pp and eh self-energies to account for some terms of the functional derivatives $\delta O/\delta G$, but such a sum is not obvious. For example, *would it be worse to neglect (besides T_3) the term $-T_0$ or $(T_1 + T_2)/2$?* We will discuss this issue in Sec. III.

Based on Eq. (3), we can now directly compare the different approximations: In GW or an approximate $GW\Gamma$, one fixes an approximation for the functional derivative of the self-energy to a low-order approximation, but one tries to treat L well. In the T-matrix approximation the latter is treated quite badly, whereas the former is kept, though approximatively, to infinite order in v_c thanks to the Dyson-like equation for the effective interaction. Both approximations allow one to describe physical processes involving three particles: The particle that is added to the system and the electron-hole pair that it creates. Ideally, one would propagate the three particles together, which is not numerically affordable. Therefore, one chooses to propagate a pair and to treat the third particle in a kind of mean field of the other two. This is illustrated in Fig. 2: In GW one propagates together the electron-hole pair created by the additional particle, whereas in the T matrix one propagates together the additional electron (additional hole) and the excited electron (hole left behind) (pp T matrix) or the additional electron (additional hole) and the hole left behind in the electron excitation (excited electron) (eh T matrix). The choice is not obvious; therefore, it is desirable to go beyond the simple scheme and to include terms coming from both the approaches. Before we have discussed pp and eh T matrices. Now we go toward a scheme that combines T matrix and GW. In order to do so, we can see wether a Dyson equation for the T matrix can also be obtained with an improved approximation for L.

3. Screened T matrix I

Equations (12) and (13) and Eqs. (15) and (16) define the equations for the T matrix. One can go beyond this approximation and include the Hartree potential or even a local part of the exchange-correlation self-energy $\Sigma_{xc}^{\mathrm{loc}}$ in the variation $\delta G^{-1}/\delta U_{\mathrm{ext}}$. This yields $L(42;52) \approx G(47)\epsilon^{-1}(72)G(75)$, where ϵ^{-1} is a test charge-test charge screening function $\epsilon^{-1} = 1 + v\chi$ if only the Hartree part is included, otherwise at least a partially test charge-test electron screening $\epsilon^{-1} = 1 + [v + \frac{\delta\Sigma_{xc}^{\mathrm{loc}}}{\delta\rho}]\chi$.[55] This makes the expression much more, though not fully, consistent: Now ϵ^{-1} contains a large part of the derivative of the self-energy, which is also considered in the effective interaction, and L contains the screening of the formerly independent propagators GG, which is itself based on the two-particle correlation function. Equation (3) then

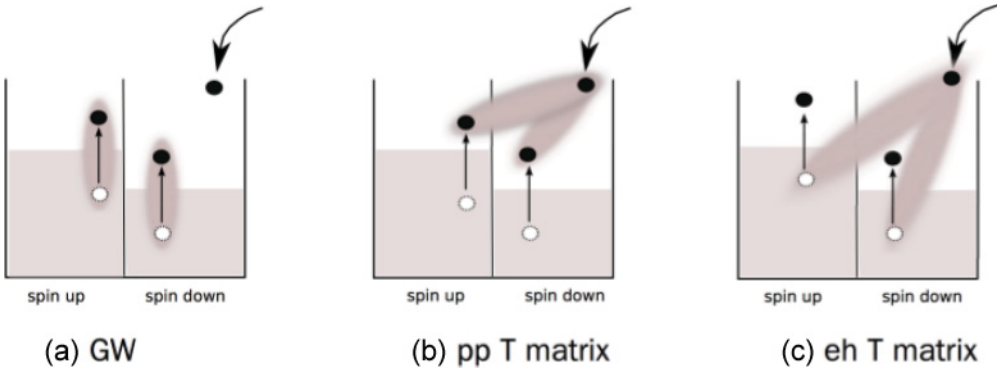

FIG. 2. (Color online) Schematic representation of the physical contents of GW (a), pp T matrix (b), and eh T matrix for particles with collinear spins.

becomes

$$\Sigma(11') \approx v_H + \Sigma_x + iv_c(12)\epsilon^{-1}(72)G(13) \times \left[\frac{\delta\Sigma(31')}{\delta G(45)}G(47)G(75)\right]. \quad (26)$$

Note that this is the same equation as Eq. (4), but now with $W = \epsilon^{-1}v_c$ replacing the bare Coulomb interaction under the integral. This leads to a screened matrix O: $\Sigma(11') = G(42)O_s^{\rm pp}(12;1'4)$, with $O_s^{\rm pp} = O_{s,1}^{\rm pp} + O_{s,2}^{\rm pp}$ and

$$O_{s,1}^{\rm pp}(12;1'4) = -iv_c(12)\delta(11')\delta(42) + iW(12)G(13)G(25)O_{s,1}^{\rm pp}(35;1'4), \quad (27)$$

$$O_{s,2}^{\rm pp}(12;1'4) = iv_c(12)\delta(14)\delta(1'2) + iW(12)G(13)G(25)O_{s,2}^{\rm pp}(35;1'4). \quad (28)$$

In principle, one could include also a nonlocal part of the exchange-correlation self-energy, but the equations become more involved.

As for the T matrix, also for the screened version one has $O_{s,2}^{\rm pp}(12;1'4) = -O_{s,1}^{\rm pp}(12;41')$. Similarly, one can derive the electron-hole screened T matrix, which looks like Eqs. (9) and (10) with W replacing the bare Coulomb potential in the last term on the right-hand side. When $\epsilon^{-1} = 1$, and, hence, $W = v_c$, this version of the screened T matrix reduces to the one of Refs. 17 and 56. Note that the Hartree and exchange parts remain unscreened, which is in net contrast with other versions of the screened T matrix reported in the literature.[12,34–39]

It is interesting to take the screened T-matrix equation in its first iteration: In this case, the self-energy (particle-particle version) becomes

$$\Sigma_{s,1}^{\rm pp,(1)}(11') = \delta(11')v_H(1) + iW(12)G(11')v_c(1'4)L_0(24), \quad (29)$$

$$\Sigma_{s,2}^{\rm pp,(1)}(11') = \Sigma_x(11') - W(12)G(14)v_c(41')G(21')G(42), \quad (30)$$

with $L_0(24) = -iG(24)G(42)$. The electron-hole screened T matrix produces the same self-energy as the particle-particle screened T matrix in its first iteration, as in the case of the T-matrix approximation. Moreover, the resulting self-energy is exact to second order in the Coulomb interaction.

In the RPA, $W(12)v_c(1'4)L_0(24) = [v_c + v_cL_0v_c/(1 - L_0)v_c]L_0v_c = W - v_c$. The sum of Σ_1 and Σ_2 yields, hence, GW, plus the last term of Σ_2. In Fig. 3 we report the diagrammatic representation of this self-energy: The first two diagrams represent the Hartree and GW contributions, respectively, whereas the last one is a term corresponding to the second-order screened exchange (SOSEX). The latter contribution is becoming popular as correction to RPA in order to produce accurate results in the description of electronic correlation in atoms and solids.[57]

We, hence, can conclude that GW is contained in this screened T-matrix approach, which, moreover, contains promising higher-order terms. In literature other versions of the screened T matrix[12,34–39] are proposed which are combined with the GW approximation to get the total self-energy. However, since some of the terms in the T matrix are already contained in the GW approximation, care must be taken to avoid double counting. In our formulation, instead, the screened T matrix naturally contains GW; there is, hence, no need to add *ad hoc* corrections.

Because of the appearance of both v_c and W, the screened T-matrix approximation of Eqs. (27) and (28) does not fulfill some symmetry conditions to be fully conserving, unlike self-consistent GW and (unscreened) T matrix.[17] For example, the momentum conservation law is violated.

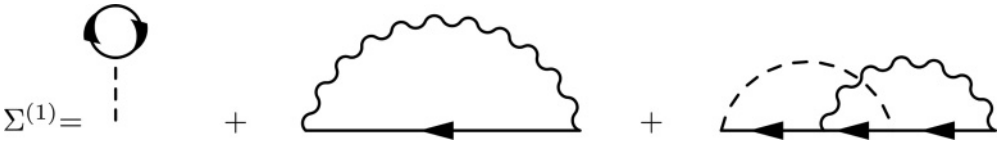

FIG. 3. Diagrams corresponding to the self-energy obtained with the first iteration of the screened T matrix I. The diagrams, from left to right, represent the Hartree, GW, and second-order screened exchange (SOSEX) terms, respectively. Note that in the GW term we collapsed the two terms that for $\epsilon^{-1} = 1$, i.e., $W = v_c$, reduce to the second and first diagrams of $\Sigma_1^{\rm pp/eh}$ and $\Sigma_2^{\rm pp/eh}$, respectively, of Fig. 1.

4. Screened T matrix II

Starting from Eq. (3), one can also write

$$\Sigma_{xc}(11') = \Sigma_x(11') + iv_c(12)G(13)\left[\frac{\delta v_H(3)\delta(31')}{\delta G(45)}L(42;52) + \frac{\delta\Sigma_{xc}(31')}{\delta G(45)}L(42;52)\right] = \Sigma_{GW} + iv_c(12)G(13)\frac{\delta\Sigma_{xc}(31')}{\delta G(45)}L(42;52). \quad (31)$$

Using again the approximation $L(42;52) \approx G(47)\epsilon^{-1}(72)G(75)$ one obtains

$$\Sigma_{xc}(11') \approx \Sigma_{GW} + iW(17)G(13)\frac{\delta\Sigma_{xc}(31')}{\delta G(45)}G(47)G(75). \quad (32)$$

Note that here only the exchange-correlation part of the self-energy appears. The ansatz will now use a screened exchange-correlation matrix O: $\Sigma_{xc}(11') = G(42)O^{\rm pp}_{\rm sxc}(12;1'4)$ [or, equivalently, $\Sigma_{xc}(11') = G(25)O^{\rm eh}_{\rm sxc}(15;1'2)$]; the structure of the resulting equation

$$O^{\rm pp}_{\rm sxc}(12;1'4) = iW(12)\delta(21')\delta(41) + iW(12) \times G(13)\left[O^{\rm pp}_{\rm sxc}(35;1'4)G(25)\right] \quad (33)$$

is equal to the one determining the screened $O^{\rm pp}_{s,2}$, Eq. (28), which for $\epsilon^{-1} = 1$ reduces to $O^{\rm pp}_2$. Similarly, the structure of the electron-hole T matrix $O^{\rm eh}_{\rm sxc}(15;1'2)$ is equal to the one determining the screened $O^{\rm eh}_{s,2}$, which for $\epsilon^{-1} = 1$ reduces to $O^{\rm eh}_2$. Note that this screened T matrix yields a self-energy corresponding to the exchange term only of Refs. 12 and 35, where a screened T matrix is also used.

Iterating this equation for $O^{\rm pp}_{\rm sxc}$ once, one gets the $GW\Gamma^{(1)}$[1,58] approximation, namely

$$O^{{\rm pp},(1)}_{\rm sxc}(12;1'4) \approx iW(12)\delta(21')\delta(41) - W(12)G(14)W(41')G(21'), \quad (34)$$

from which $\Sigma_{xc}(11') = \Sigma^{GW}_{xc} - G(42)W(12)G(14)W(41')G(21')$. One can verify that the electron-hole screened T matrix produces the same self-energy as the particle-particle screened T matrix in its first iteration, as in the case of the T-matrix approximation. It is, not surprisingly, also what one obtains by iterating Hedin's equations[1]: Starting from $\Sigma_{xc} = iGW$ the equation for the irreducible vertex function reads

$$\Gamma(12;3) = \delta(12)\delta(13) + iW(21)G(16)G(72)\Gamma(67;3). \quad (35)$$

To first order one gets, hence, $\Gamma(12;3) = \delta(12)\delta(13) + iW(21)G(13)G(32)$ and

$$\Sigma_{xc}(11') = iG(14)\Gamma(41';2)W(21) \approx \Sigma^{GW}_{xc} - G(14)W(1'4)G(42)G(21')W(21), \quad (36)$$

which is exactly the exchange-correlation self-energy obtained using Eq. (34). There is, instead, no equivalent to Eq. (27) or its eh counterpart. However, in this second version of the screened T matrix, Hartree and exchange are not treated on the same level, since the latter is included in the definition of the T matrix and the former not. This also explains why, for $\epsilon^{-1} = 1$, this screened T matrix does not reduce to the T matrix; in fact, it reduces to only a part of it, i.e., to O_2. In Sec. III we will show that this unbalance prevents this version of the screened T matrix to give the exact result for one electron in the atomic limit, unlike the screened T matrix given by Eqs. (27) and (28).

5. Vertex corrections from the T matrix

Above we have shown that the pp screened T matrix of Eqs. (27) and (28) (as well as the eh screened T matrix) contains GW plus extra terms beyond GW. We can therefore use the T matrix to formulate vertex corrections beyond GW. Starting from the self-energy $\Sigma = GO^{\rm pp}_s = G[O^{\rm pp}_{s,1} + O^{\rm pp}_{s,2}]$ with $O^{\rm pp}_{s,1}$ and $O^{\rm pp}_{s,2}$ given by Eqs. (27) and (28),

$$\Sigma(11') \approx v_H + iG(13)\left[v_c(13)\delta(1'3) + W(12)O^{\rm pp}_s(35;1'4) \times G(42)G(25)\right]. \quad (37)$$

Using $v_c(13) = W(13) - W(12)P(25)v_c(53)$ we can rewrite Eq. (37) as

$$\Sigma(11') \approx v_H + iG(13)\left[W(12)\delta(1'3)\delta(23) - W(12)P(25)v_c(53)\delta(1'3) + W(12)O^{\rm pp}_s(35;1'4)G(42)G(25)\right] = v_H + iG(13)W(12)\Gamma(31';2), \quad (38)$$

where

$$\Gamma(31';2) = \delta(31')\delta(21') - P(25)v_c(53)\delta(31') + O^{\rm pp}_s(35;1'4)G(42)G(25). \quad (39)$$

This is an approximate vertex function that will generate the same self-energy as the pp screened T matrix. In an analogous way, one can obtain an approximate vertex function that will yield the same self-energy as the eh screened T matrix: The equation will be the same as Eq. (39) with $O^{\rm eh}_s$ replacing $O^{\rm pp}_s$ on the right-hand side. It is interesting to compare this vertex function with the exact expression derived by Bruneval *et al.*[55] that reads

$$\Gamma(31';2) = \delta(31')\delta(21') + \frac{\delta\Sigma_{xc}(31')}{\delta\rho(5)}P(52). \quad (40)$$

One can approximate the second term on the right-hand side of Eqs. (40) as

$$\frac{\delta\Sigma_{xc}(31')}{\delta\rho(5)}P(52) = \frac{\delta[\Sigma(31') - v_H(3)\delta(31')]}{\delta\rho(5)}P(52) = \frac{\delta\Sigma(31')}{\delta G(45)}\frac{\delta G(45)}{\delta V_{\rm tot}(2)} - P(25)v_c(53)\delta(31') \approx O_s(35;1'4)G(42)G(25) - P(25)v_c(53)\delta(31') \quad (41)$$

with $V_{\rm tot} = U_{\rm ext} + v_H$ as the total classical potential. The last line is an approximation obtained with $\frac{\delta\Sigma}{\delta G} \approx O_s$, where O_s is either the pp or eh screened T matrix and $\frac{\delta G}{\delta V_{\rm tot}} \approx GG$. Equation (41) with Eq. (40) yields Eq. (39). It then becomes clear that the term $-Pv_c$ in Eq. (39), which is created by the induced Hartree potential felt by a classical particle, needs to be subtracted since it is already described by the GW approximation for $\Gamma = 1$, whereas the remaining part is responsible for the induced exchange-correlation potentials

felt by a fermion. We also note that the term Pv_c, which comes out in a natural way in our derivation, gives rise to the correlation part of the GW self-energy, $\Sigma_c^{GW} = iGv_cPW = iG(W - v_c)$. It equals the correction done *a posteriori* in the other existent formulations of the screened T matrix to avoid double counting.[12,35,59]

III. APPLICATION TO THE HUBBARD MOLECULE

In the following the performance of the T matrix as well as the screened T matrix I, and, hence, of the approximate vertex function [Eq. (39)], is illustrated using the exactly solvable Hubbard molecule at 1/4 and 1/2 filling[60,61] discussed, e.g., in Ref. 13. The Hubbard model is traditionally used to model strongly correlated systems; these are precisely the systems for which GW shows failures. This, together with an exact analytical solution at hand, represents a powerful tool to test the improvements over GW due to the inclusion of pp and eh correlation for low-density systems.

The Hamiltonian of the Hubbard molecule reads,

$$H = -t \sum_{\substack{i,j=1,2 \\ i\neq j}} \sum_{\sigma} c_{i\sigma}^{\dagger} c_{j\sigma} + \frac{U}{2} \sum_{i=1,2} \sum_{\sigma\sigma'} c_{i\sigma}^{\dagger} c_{i\sigma'}^{\dagger} c_{i\sigma'} c_{i\sigma} + \epsilon_0 \sum_{\sigma,i=1,2} n_{i\sigma} + V_0. \tag{42}$$

Here $n_{i\sigma} = c_{i\sigma}^{\dagger} c_{i\sigma}$, where $c_{i\sigma}^{\dagger}$ and $c_{i\sigma}$ are the creation and annihilation operators for an electron at site i with spin σ, U is the on-site (spin-independent) interaction, $-t$ is the hopping kinetic energy, and ϵ_0 is the orbital energy. Further, the Hamiltonian contains a potential V_0 that can be chosen to fix the zero-energy scale. The physics of the Hubbard model arises from the competition between the hopping term, which prefers to delocalize electrons, and the on-site interaction, which favors localization. The ratio U/t is a measure for the relative contribution of both terms and is the intrinsic, dimensionless coupling constant of the Hubbard model, which will be used in the following.

Projected onto the (orthonormal) site basis of the Hubbard model the T matrix of Eqs. (12) and (13) and Eqs. (15) and (16) becomes

$$O_{ilkj}^{\sigma_1\sigma_2}(\omega) = -i\delta_{il}\delta_{jk}\left[\bar{O}_{1,ij}^{\sigma_1\sigma_2}(\omega) - \delta_{\sigma_1\sigma_2}\bar{O}_{1,ij}^{\sigma_1\sigma_1}(\omega)\right], \tag{43}$$

with $\bar{O}_1^{\sigma_1\sigma_2}(\omega) = [1 + UL_0^{\sigma_1\sigma_2}(\omega)]^{-1}U$, from which

$$\Sigma_{ij}^{\sigma_1}(\omega) = -i\int \frac{d\nu}{2\pi} G_{ji}^{\bar{\sigma}_1}(\nu)\bar{O}_{ij}^{\sigma_1\bar{\sigma}_1}(\omega \pm \nu). \tag{44}$$

Here $\bar{\sigma}$ indicates a spin opposite to σ, the $+$ sign refers to the particle-particle contribution for which $L_{0,ij}^{\sigma_1\sigma_2,\mathrm{pp}}(\omega) = -i\int \frac{d\omega'}{2\pi} G_{ij}^{\sigma_1}(\omega')G_{ij}^{\sigma_2}(\omega - \omega')$, and the $-$ sign refers to the electron-hole contribution for which $L_{0,ij}^{\sigma_1\sigma_2,\mathrm{eh}}(\omega) = -i\int \frac{d\omega'}{2\pi} G_{ij}^{\sigma_1}(\omega')G_{ij}^{\sigma_2}(\omega' - \omega)$. More details on the spin structure of the T matrix can be found in Appendix B.

The equations for the screened T matrix are more involved: Because the screened Coulomb interaction W is nonlocal in space and frequency dependent (see Ref. 13 and (C7)), where a RPA W is given), one has to solve a four-point equation similar to the dynamical Bethe-Salpeter equation for electron-hole excitations.[47,62,63] This is beyond the scope of this paper and of the majority of the applications. Moreover, we observe that when there is no screening in the system (which is the case in the atomic limit $t \to 0$ for the model used here) the screened T matrix reduces to the T matrix, and one, hence, retrieves the same results as those obtained with the latter. For a finite t we assume that for the model used here the major contribution to the T matrix arises from the on-site screened interaction. This is dominated by the bare interaction U, which justifies taking the screened interaction in its static ($\omega = 0$) limit. In this case, the structure of the screened T matrix is the same as for the T matrix with the on-site screened Coulomb interaction $W = U - \frac{(1+\delta_{N=2})U^2t}{h^2}$, with $h^2 = 4t^2 + 2Ut(1 + \delta_{N=2})$ and N the total number of electrons in the system [see Ref. 13 and (C7)], replacing U. We notice that with this approximation, in particular assuming a static W, the screened T matrix will no longer reduce to the T matrix in the atomic limit. This is because in the atomic limit the frequency-dependent part of the screened interaction, i.e., $\frac{(1+\delta_{N=2})U^2t}{(\omega^2-h^2)}$, vanishes if $\omega \neq 0$ but will reduce to $-\frac{U}{2}$ if $\omega = 0$.

Another simplification that will be adopted in the following is the neglect of self-consistency. In principle, the T-matrix approximation requires self-consistency in order to be conserving. The various levels of self-consistency in the T matrix have been addressed by several authors, in particular, in model systems (see, e.g., Refs. 21–23,64–66). When the quantity of interest is the spectral function, as in our case, self-consistency was found to deteriorate spectra.[21–23,67–69] In practice, as in the case of the GWA, a non-self-consistent "best G" strategy is adopted.

A. Hubbard molecule, 1/4 filling

We, first, consider the Hubbard model with only one electron in the ground state; the ground state is $|\Psi_0\rangle = 1/\sqrt{2}\,(|\uparrow\ 0\rangle + |0\uparrow\rangle)$, where the electron has spin up (equivalently, the spin-down situation could be chosen).

1. T matrix

Using the noninteracting Green's function for 1/4 filling of Ref. 13 [Eqs. (16) and (18)] and Eq. (44), the particle-particle contribution to the T matrix yields the exact self-energy, which reads

$$\Sigma_{ij}^{\mathrm{pp},\uparrow} = 0 \tag{45}$$

$$\Sigma_{ij}^{\mathrm{pp},\downarrow} = \frac{U}{2}\delta_{ij} + \frac{U^2}{8}\left[\frac{1}{\omega - \epsilon_0 - \frac{U}{2} - 3t + i\eta} + \frac{(-1)^{(i-j)}}{\omega - \epsilon_0 - \frac{U}{2} - t + i\eta}\right]. \tag{46}$$

This self-energy gives rise to the exact one-particle Green's function and spectral function.

The eh T matrix also yields the exact result for the spin-up self-energy, but a spin-down self-energy with poles that are

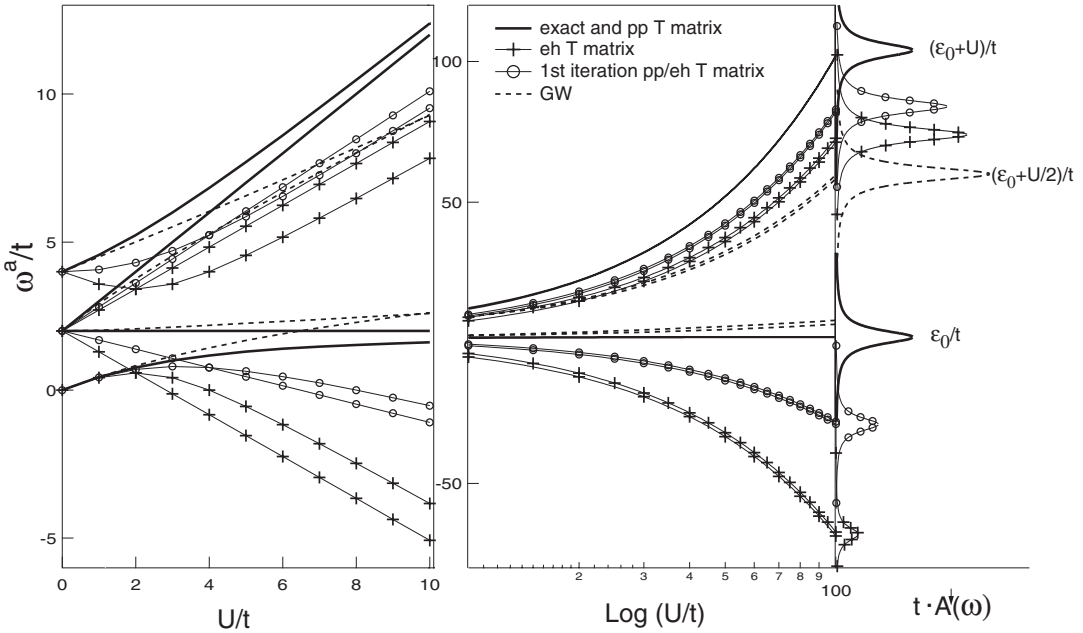

FIG. 4. Two-site Hubbard model at 1/4 filling: Comparison between the exact spin-down renormalized addition energies ω^a/t (solid lines) as a function of U/t (left panel) and log(U/t) (right panel) and the results obtained from GW (dashes), particle-particle (solid lines, equal to the exact result), electron-hole (crosses), and first-iteration T matrix (circles). In the atomic limit, the spectral function, i.e., the peak positions and weights, is illustrated on the right-hand side, on multiplying by t and taking the $t \to 0$ limit.

shifted by U from the exact ones:

$$\Sigma_{ij}^{\mathrm{eh},\uparrow} = 0 \tag{47}$$

$$\Sigma_{ij}^{\mathrm{eh},\downarrow} = \frac{U}{2}\delta_{ij} + \frac{U^2}{8}\left[\frac{1}{\omega - \epsilon_0 + \frac{U}{2} - 3t + i\eta} + \frac{(-1)^{(i-j)}}{\omega - \epsilon_0 - t + \frac{U}{2} + i\eta}\right]. \tag{48}$$

The poles of this spin-down self-energy give addition and removal energies that are, overall, in bad agreement with the exact result, as shown in Fig. 4, where exact, T-matrix, and GW renormalized addition energies ω^a/t for the spin-down channel are reported versus U/t. Particularly interesting is the spectral function at $U/t \to \infty$: As discussed in Ref. 13, when $t \to 0$ (atomic limit), the electron is localized either on one site or the other with the same probability. Therefore, two electron peaks, with the same weight 1/2, appear in the spectral function (see Fig. 4), one corresponding to the addition of the second electron on the empty site (peak at ϵ_0) and the other corresponding to the addition on the filled site (peak at $\epsilon_0 + U$). The GWA produces only one peak at $\epsilon_0 + U/2$ with spectral weight 1. This is due to the interpretation of the charge density as an average charge distribution rather than a probability. The T matrix, instead, "sees" where the electron is, although only the pp T matrix "sees" well. Indeed, the eh T matrix yields two peaks with the correct spectral weight, but at the wrong position, namely $\epsilon_0 + U\sqrt{2}/2$ and $\epsilon_0 - U\sqrt{2}/2$. Therefore, it is clear that in the case of the Hubbard molecule with one electron, the particle-particle contribution to the T matrix describes the essential physics.

Note that the eh T matrix at first iteration performs as the pp T matrix, since $\Sigma^{\mathrm{eh},(1)} = \Sigma^{\mathrm{pp},(1)}$, as we have already shown. In the atomic limit, the T matrix at the first iteration shows two peaks in the spin-down spectral function: One located at $\omega = \epsilon_0 + U(1 - \sqrt{5})/4$ with spectral weight $(1 - 1/\sqrt{5})/2 \approx 0.28$ and the other one located at $\omega = \epsilon_0 + U(1 + \sqrt{5})/4$ with spectral weight $(1 + 1/\sqrt{5})/2 \approx 0.72$ (see Fig. 4). It, hence, contains the right physics, although the results are still poor.

2. *Screened T matrix*

As illustrated above, the pp T matrix yields the exact result for the Hubbard molecule at 1/4 filling. However, if one is interested in many-electron systems, where screening becomes important, the screened T matrix is more appropriate. It is interesting to check how well the screened T matrix performs in the one-electron limit. In order to do so we concentrate on the pp screened T matrix only. Using the on-site and instantaneous approximation $W = U - U^2 t/h^2$ (with $h^2 = 4t^2 + 2Ut$) for the screened Coulomb interaction, the screened pp T matrix yields the self-energy

$$\Sigma_{s,ij}^{\mathrm{pp},\uparrow} = 0 \tag{49}$$

$$\Sigma_{s,ij}^{\mathrm{pp},\downarrow} = \frac{U}{2}\delta_{ij} + \frac{UW}{8}\left[\frac{1}{\omega - \epsilon_0 - \frac{W}{2} - 3t + i\eta} + \frac{(-1)^{(i-j)}}{\omega - \epsilon_0 - \frac{W}{2} - t + i\eta}\right], \tag{50}$$

which gives rise to the spin-down addition energies reported in Fig. 5. The approximate screened T matrix performs, in general, much better than GW; in particular, in the atomic limit,

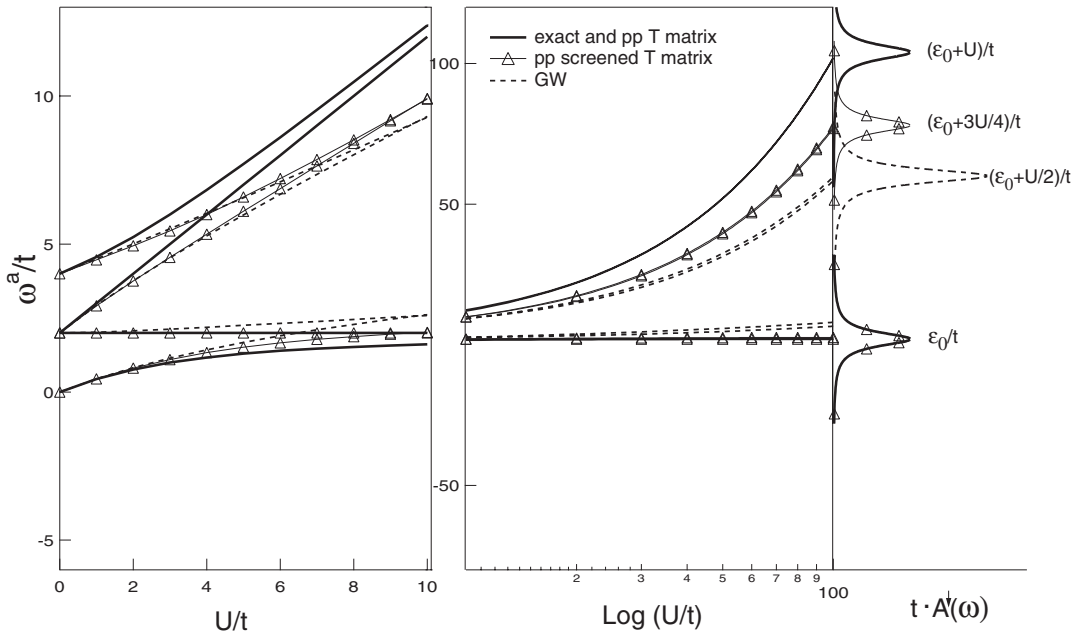

FIG. 5. Two-site Hubbard model at 1/4 filling: Comparison between the exact spin-down renormalized addition energies ω^a/t (solid lines) as a function of U/t (left panel) and log(U/t) (right panel) and the results obtained from GW (dashes) and particle-particle (solid lines, equal to the exact result) and (approximate) screened T matrix (triangles). In the atomic limit, the spectral function, i.e., the peak positions and weights, is illustrated on the right-hand side, on multiplying by t and taking the $t \to 0$ limit.

although it does not reproduce the exact result, it produces the correct number of peaks in the spectral function, unlike the GW approximations that yields only one peak. Therefore, even in this approximate version the screened T matrix I contains the essential interaction processes. Note that the dynamically screened T matrix I reproduces exactly the atomic limit for the present problem.

The screened T matrix II, instead, does not reproduce correctly the atomic limit. Indeed, with $W = v_c$, the screened T matrix II reduces to the O_2 component only of the T matrix, and this is not sufficient to capture the interactions in the atomic limit. One finds the self-energy

$$\Sigma_{ij}^{\mathrm{pp},\uparrow}(\omega) = \Sigma_{ij}^{\mathrm{eh},\uparrow}(\omega) = 0 \tag{51}$$

$$\Sigma_{ij}^{\mathrm{pp},\downarrow}(\omega) = \Sigma_{ij}^{\mathrm{eh},\downarrow}(\omega) = \frac{U}{2}\delta_{ij}, \tag{52}$$

which is the same as the one obtained within GW.

B. Hubbard molecule, 1/2 filling

We now consider the case with two electrons in the ground state. Technical details are given in Appendix C (see also Ref. 70).

1. T matrix

In this case, neither the pp nor the eh T matrix reproduce the exact result, with the self-energy reading as

$$\Sigma_{ij}^{\mathrm{pp},\sigma}(\omega) = \frac{U}{2}\delta_{ij} + \frac{U^2 t}{4\bar{h}}\left[\frac{1}{\omega - t - \bar{h} + i\eta} + \frac{(-1)^{(i-j)}}{\omega + t + \bar{h} - i\eta}\right] \tag{53}$$

with $\bar{h}^2 = 4t^2 + 2tU$, in the particle-particle T-matrix approximation, and

$$\Sigma_{ij}^{\mathrm{eh},\sigma}(\omega) = \frac{U}{2}\delta_{ij} + \frac{U^2 t}{4\bar{h}'}\left[\frac{1}{\omega - t - \bar{h}' + i\eta} + \frac{(-1)^{(i-j)}}{\omega + t + \bar{h}' - i\eta}\right], \tag{54}$$

with $\bar{h}'^2 = 4t^2 - 2tU$, in the electron-hole T-matrix approximation. The pp T matrix performs rather well over a wide U/t range as one can see in Fig. 6, where the renormalized addition and removal energies ω/t are plotted versus U/t. In particular, the satellite energies (outer energies) are better described than in GW, in line with previous findings.[12,21,22] The energies calculated using the electron-hole T matrix, instead, show divergencies. In the $U/t \to \infty$ limit, all approximations studied are rather poor.

In the atomic limit, there are no double occupancies, therefore, the two electrons, one with spin up and the other with spin down, are localized one on one site and the other on the other site with equal probability, i.e., the ground state is the singlet $|\Psi_0\rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$. The spectral function, thus, shows, for each spin, two peaks with the same spectral weight 1/2, one for the removal of an electron (peak at ϵ_0) and one for the addition of a second electron (peak at $\epsilon_0 + U$), as shown in Fig. 6. In Appendix C we show that, using the noninteracting Green's function, GW fails also in the case of 1/2 filling, producing for each spin only one kind of peak at $\epsilon_0 + U/2$ with spectral weight 1/2, both for electron removal and addition. This can again be understood considering that GW treats the charge/spin density as a classical distribution, namely a half electron with half spin up and a half electron with half spin

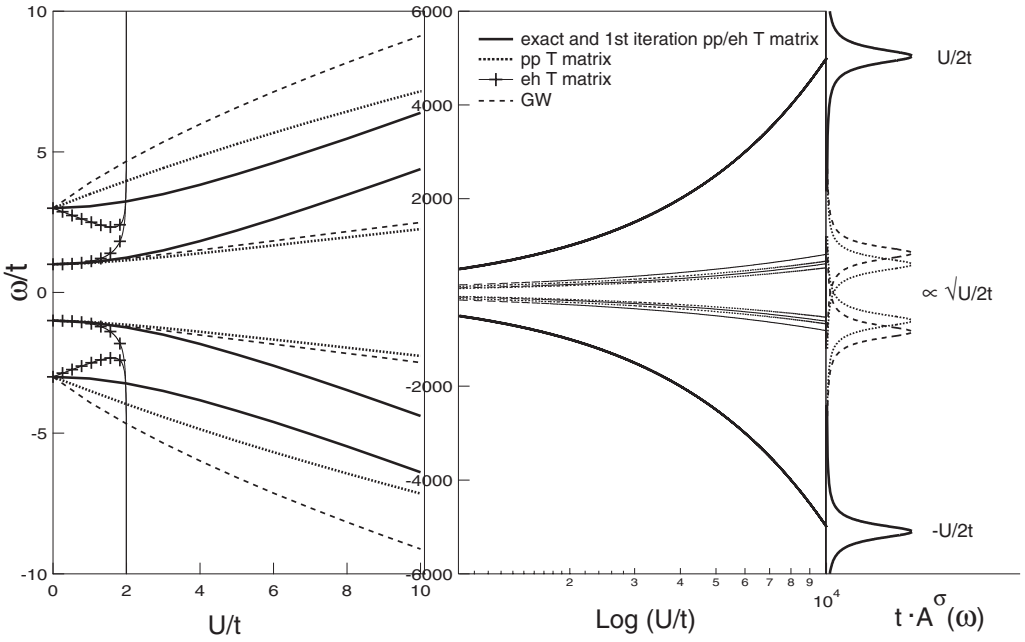

FIG. 6. Two-site Hubbard model at 1/2 filling: Comparison between the exact renormalized addition/removal energies ω/t (solid lines) as a function of U/t (left panel) and log(U/t) (right panel) and the results obtained from GW (dashes), particle-particle (dots), electron-hole (crosses), and first-iteration T matrix (solid lines, equal to the exact result). In the atomic limit, the spectral function, i.e., the peak positions and weights, is illustrated on the right-hand side, on multiplying by t and taking the $t \to 0$ limit.

down on each atom that respond to the additional electron or hole in the atomic limit. We find that the particle-particle T matrix yields the same result as GW in the atomic limit, whereas the electron-hole T matrix shows divergencies.

Why is the pp T matrix exact for one electron in the atomic limit and not for two electrons? To derive the T matrix we used the approximation $\frac{\delta G}{\delta U_{\rm ext}} \approx GG$. In the case of one electron, this is not an approximation, but it is the exact time-ordered response, and, therefore, the (pp) T matrix yields the exact result for one electron. This is not the case for two electrons for which $\frac{\delta G}{\delta U_{\rm ext}} \approx GG$ is a rough approximation, and one needs to include some screening. The screened T matrix I indeed improves over the T matrix for two electrons, even with an approximate RPA screening, as is shown in the next section. Such an approximate screening is, instead, dramatic for one electron, and a more accurate screening is needed (as pointed out above, the exact screening would yield the T matrix and, hence, an exact result for one electron). *One should, hence, use a screened T matrix with a screened interaction adapted to the system.*

Interestingly, the first iteration for both the particle-particle and electron-hole contributions to the T matrix gives the exact results for all t. Indeed, after the first iteration the T matrix reads

$$\bar{O}_{ij}^{\sigma_1\bar{\sigma}_1,(1)}(\omega) = \left[U\delta_{ij} - U^2 L_{0,ij}^{\sigma_1\bar{\sigma}_1}(\omega)\right] \tag{55}$$

with L_0 being

$$L_{0,ij}^{\sigma_1\bar{\sigma}_1,\rm pp}(\omega) = \frac{-1}{4}\left[\frac{1}{\omega - 2t + i\eta} - \frac{1}{\omega + 2t - i\eta}\right], \tag{56}$$

$$L_{0,ij}^{\sigma_1\bar{\sigma}_1,\rm eh}(\omega) = \frac{(-1)^{(i-j)}}{4}\left[\frac{1}{\omega - 2t + i\eta} - \frac{1}{\omega + 2t - i\eta}\right], \tag{57}$$

for the particle-particle and electron-hole contribution, respectively. The self-energy, hence, becomes

$$\Sigma_{ij}^{\rm pp,\sigma_1,(1)}(\omega) = \Sigma_{ij}^{\rm eh,\sigma_1,(1)}(\omega) = \Sigma_{ij}^{\sigma_1,(1)}(\omega) = \delta_{ij}\frac{U}{2} + \frac{U^2}{8}\left[\frac{1}{\omega - 3t + i\eta} + \frac{(-1)^{(i-j)}}{\omega + 3t - i\eta}\right], \tag{58}$$

which is the exact one. This result, however, is peculiar for the Hubbard molecule. Indeed, the first iteration of the T matrix corresponds to the second Born approximation, which has already been explored on bigger Hubbard clusters for different fillings and interactions.[21,22] Indeed, it does not generate the exact result and, in general, the T matrix is the most accurate at low densities; only at half-filling is the T matrix not superior to the second Born approximation, and this is in line with our findings. Within the GW approximation, if one considers W at first iteration $[W_{ij}^{(1)}(\omega) = U\delta_{ij} + U^2\sum_\sigma L_{0,ij}^{\sigma\sigma,\rm eh}(\omega)]$, the resulting self-energy is not exact but very close to the exact one, differing only in the prefactor of the frequency-dependent part that is $U^2/4$ instead of $U^2/8$. The addition and removal energies are, thus, improved with respect to GW, although the agreement with the exact result worsens with increasing U. It is worth noticing that if one considers also the exchange counterpart in GW, i.e., if one includes not only the Hartree potential but also the exchange self-energy in the self-energy variation $\delta\Sigma/\delta G$ in Eq. (3), then one obtains a GW-like self-energy with a modified spin-dependent screened interaction, $\tilde{W}_{ij}^{\sigma_1}(\omega) = U\delta_{ij} + U\sum_{r,\sigma_r} L_{0,ir}^{\sigma_r}(\omega)(1 - \delta_{\sigma_r\sigma_i})W_{rj}(\omega)$, that at second order in U produces the exact self-energy. Indeed, this is the second Born approximation.

The exact result obtained with the T matrix at first iteration, however, deteriorates with the second iteration; in this case,

the T matrix reads,

$$\bar{O}_{ij}^{\sigma_1\bar{\sigma}_1,(2)}(\omega) = \bar{O}_{ij}^{\sigma_1\bar{\sigma}_1,(1)}(\omega) + U^3 \sum_n L_{0,in}^{\sigma_1\bar{\sigma}_1}(\omega) L_{0,nj}^{\sigma_1\bar{\sigma}_1}(\omega), \quad (59)$$

and the two self-energies become

$$\Sigma_{ij}^{\mathrm{pp},\sigma_1,(2)}(\omega) = \Sigma_{ij}^{\sigma_1,(1)}(\omega) + \frac{U^3}{16}\left\{\frac{1}{(\omega-3t+i\eta)^2} - \frac{(-1)^{(i-j)}}{(\omega+3t-i\eta)^2} - \frac{1}{2t}\left[\frac{1}{\omega-3t+i\eta} + \frac{(-1)^{(i-j)}}{\omega+3t-i\eta}\right]\right\}, \quad (60)$$

$$\Sigma_{ij}^{\mathrm{eh},\sigma_1\,(2)}(\omega) = \Sigma_{ij}^{\sigma_1,(1)}(\omega) - \frac{U^3}{16}\left\{\frac{1}{(\omega-3t+i\eta)^2} - \frac{(-1)^{(i-j)}}{(\omega+3t-i\eta)^2} - \frac{1}{2t}\left[\frac{1}{\omega-3t+i\eta} + \frac{(-1)^{(i-j)}}{\omega+3t-i\eta}\right]\right\}. \quad (61)$$

Combining the two interaction channels by adding Eqs. (60) and (61), the second terms on the right-hand side of the two equations cancel each other, thus restoring the exact result if $\frac{1}{2}(\Sigma^{\mathrm{pp},(2)} + \Sigma^{\mathrm{eh},(2)})$ is taken. We have already shown in Eq. (25) that the sum $\frac{1}{2}(\Sigma^{\mathrm{pp},(2)} + \Sigma^{\mathrm{eh},(2)})$ takes into account some of the terms that would appear in the self-energy if also the functional derivative $\delta O/\delta G$ were considered. This might justify the exact result that is obtained by taking $\frac{1}{2}(\Sigma^{\mathrm{pp},(2)} + \Sigma^{\mathrm{eh},(2)})$. Also the sum $(\Sigma^{\mathrm{pp},(2)} + \Sigma^{\mathrm{eh},(2)})$ takes into account some of the terms arising from the functional derivative [see Eq. (25)]; however, it does not give the exact result. In other words it seems more important to take into account the term $-T_0$ than $(T_1 + T_2)/2$ [see Eqs. (24) and (25)] at least in the present problem. However, with the third iteration, the fourth-order terms in the pp and eh T-matrix self-energies are the same and they would not cancel each other if the sum $\frac{1}{2}(\Sigma^{\mathrm{pp},(2)} + \Sigma^{\mathrm{eh},(2)})$ is taken. Instead, with the fourth iteration, the fifth-order terms in the pp and eh T-matrix self-energies would cancel each other. In general, for the present problem, the pp and eh T-matrix self-energies show, starting from second order, the same even-order terms and opposite odd-order terms, as one can verify Taylor expanding the frequency-dependent part of the pp and eh self-energies [Eqs. (53) and (54)] for small U. The same holds for the Hubbard model at 1/4 filling. Therefore, summing the two contributions will not give the exact result. Even adding the GW self-energy terms and its exchange counterparts, in the spirit of the FLEX approximation, will not produce the exact result. These findings show that there is no an ultimate way to combine diagrams, and this is of clear relevance for realistic studies where several attempts to combine pp and eh channels have been done (see, e.g., Refs. 28–30 and 35). A possibility is to use the screened T matrix we introduced in Sec. II B 3, which produces, at least for the studied problem, results that are overall better than those from the GW and T matrix, as shown in the following.

2. *Screened T matrix*

The pp screened T matrix with the approximate on-site static Coulomb interaction $W = U - 2U^2t/h^2$ (with $h^2 = 4t^2 + 4Ut$) leads to the self-energy

$$\Sigma_{s,ij}^{\mathrm{pp},\sigma}(\omega) = \frac{U}{2}\delta_{ij} + \frac{UWt}{4\tilde{h}}\left[\frac{1}{\omega - t - \tilde{h} + i\eta} + \frac{(-1)^{(i-j)}}{\omega + t + \tilde{h} - i\eta}\right] \quad (62)$$

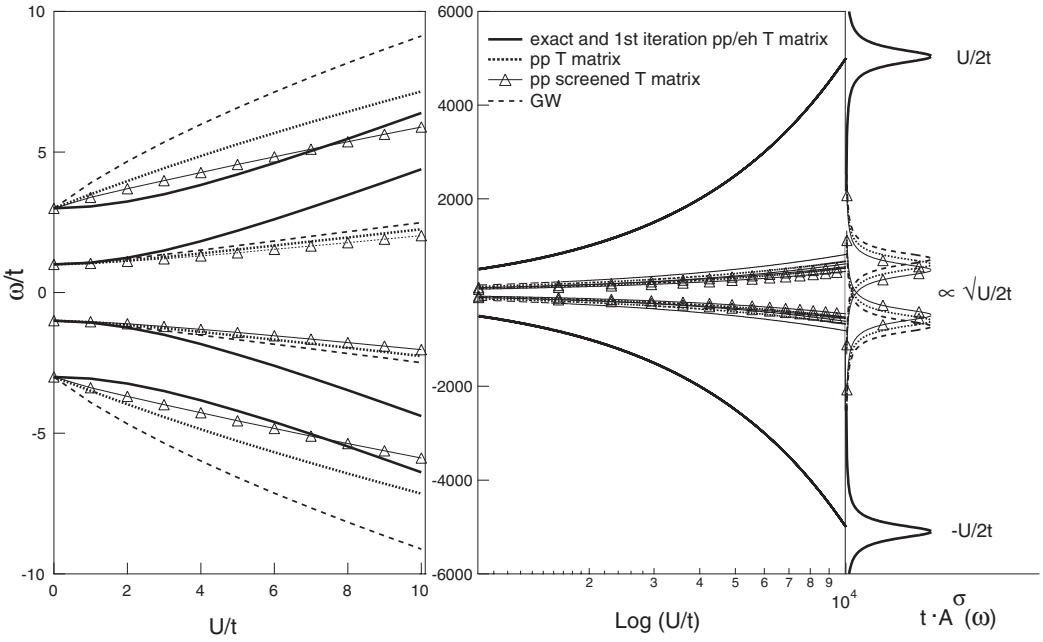

FIG. 7. Two-site Hubbard model at 1/2 filling: Comparison between the exact renormalized addition/removal energies ω/t (solid lines) as a function of U/t (left panel) and log(U/t) (right panel) and the results obtained from GW (dashes) and particle-particle (dots) and screened T matrix (triangles). In the atomic limit, the spectral function, i.e., the peak positions and weights, is illustrated on the right-hand side, on multiplying by t and taking the $t \to 0$ limit.

with $\tilde{h}^2 = 4t^2 + 2tW$. The resulting renormalized addition and removal energies ω/t are plotted in Fig. 7 versus U/t and compared with the exact, pp T matrix, and GW results. This approximate pp screened T matrix is, overall, superior to the GW and the T matrix in the selected U/t range in the left panel of Fig. 7. In the limit $U/t \to \infty$ the results get corrupted. As a consequence, the screened T matrix performs as poorly as GW and the T matrix.

Our findings suggest that the screened T-matrix approximation (or, equivalently, $GW\Gamma$, with Γ obtained from the screened T matrix) is expected to describe properly also larger, more dense, systems. This is in agreement with the idea behind the screened T matrix to combine T matrix and GW and to take advantage of the strength of both approaches. For short-range interactions, where screening is not important, the screened T matrix reduces to the T matrix, which is suitable for treating short-range correlations. For long-range interactions, where, instead, screening is important, we find that the screened T matrix behaves more like GW (in its first iteration, indeed, it gives GW and SOSEX, which is actually already used to improve GW), which is capable of taking into account long-range correlations. Therefore, the screened T matrix is able to capture the physics of systems with effective short-range interactions as well as of systems with effective long-range interactions.

For practical calculations the equations become very involved. However, the Dyson equation for the T matrix is similar to the Bethe-Salpeter equation for the eh excitations; therefore, one might use similar strategies to solve it. For example, one may consider the static approximation to the screened Coulomb interaction, as usually used for the BSE and as adopted for the screened T matrix of Ref. 12. For short-range interactions one can consider, together with the static approximation for W, also a local approximation for the four-point kernel GG which was proposed in Ref. 71 for a similar screened T matrix and validated by several applications;[34,35,71] this greatly simplifies the calculation of the screened T matrix, which becomes a two-point quantity similar to the screened Coulomb potential, W, and opens the way for wide applications.

IV. CONCLUSIONS

In this paper we have provided an alternative derivation of the T-matrix approximation to the self-energy starting from exact equations. This allowed us to (i) link the T matrix to Hedin's equations, (ii) understand the origin of the electron-hole (eh) and the particle-particle (pp) T matrix, (iii) derive a screened T matrix, (iv) translate the physical content of the T matrix into a vertex correction, and (v) put the second-order screened exchange (SOSEX) on the same level as the T matrix.

We applied the T matrix to the exactly solvable Hubbard molecule at $1/4$ and $1/2$ filling and we studied its performance with an increasing ratio U/t. We found that the particle-particle T matrix gives the exact removal and addition energies for $1/4$ filling. The electron-hole T matrix, instead, performs badly.

In the case of $1/2$ filling, the pp performs, in general, better than GW, in particular, in describing the satellite position, whereas the eh T matrix shows divergencies for $U/t > 2$. In the atomic limit $t \to 0$ both GW and T matrix are very poor. In their first iteration, both the particle-particle and the electron-hole T matrix produce the exact result. This result becomes corrupted with further iterations; however, the pp and eh self-energies have the same even-order terms and opposite odd-order terms (except the first-order term, which is the same) at least in the model analyzed here. This means that one obtains the exact self-energy if the sum $\frac{1}{2}(\Sigma^{\mathrm{pp},(2)} + \Sigma^{\mathrm{eh},(2)})$ at the second iteration is taken, and one retains only the even-order terms if the eh and pp self-energies are taken at infinite order. This can be of relevance in realistic calculations where eh and pp channels are combined together for improving the results.

We have also studied the performance of the pp screened T matrix. The screened T matrix I (see text), in which Hartree and exchange terms are treated on an equal footing, reduces to the T matrix in the atomic limit when a dynamically screened interaction is used; even with an approximate W it is better than GW at $1/4$ filling, whereas at $1/2$ filling it is, overall, superior to both the pp T matrix and GW over a wide U/t range. This means that the vertex corrections derived from this version of the pp screened T matrix can visibly improve over GW. The screened T matrix II (see text), in which only exchange-like terms are included, reduces to only one part of the T matrix in the atomic limit and this is not sufficient to describe exactly this limit at $1/4$ filling. We show that this version of the screened T matrix corresponds, at first iteration, to the $GW\Gamma^{(1)}$ approximation, which, hence, is also not appropriate to treat the atomic limit. Our illustration of the different T-matrix approximations on the Hubbard molecule suggests that the screened T matrix I is a promising approximation also for realistic systems, since it combines, on an equal footing, on the one hand, the physics of the T-matrix approximation, which properly describes short-range interactions, and, on the other hand, the physics of GW, which is more appropriate for long-range interactions.

ACKNOWLEDGMENTS

We are grateful for the support by ANR (Project No. NT09-610745). Financial support from the French-German Gay-Lussac Humboldt Award and the kind hospitality of the École Polytechnique are acknowledged by F.B.

APPENDIX A: TIME STRUCTURE OF THE T MATRIX

First, we examine the time structure of the T matrix of Eqs. (12) and (13) and Eqs. (15) and (16).

1. Particle-particle T matrix

We start from Eqs. (12) and (13). In the following, the indices will refer to the time only. We can define $O_1^{\mathrm{pp}}(12;1'4) := -i\delta(12)\bar{O}_1^{\mathrm{pp}}(11;1'4)$, which leads to

$$\bar{O}_1^{\mathrm{pp}}(1-1';1-4) = v_c\delta(11')\delta(41^+) + iv_cG(1-3) \times \bar{O}_1^{\mathrm{pp}}(3-1';3-4)G(1^+-3). \tag{A1}$$

Here the correct order of the field operators is explicitly ensured by the infinitesimally larger $1^+ = 1 + \eta > 1$. The two Green's functions in the product have the same time order,

contrary to the usual electron-hole response function. This leads to a particle-particle function, $L_0^{pp}(1-3) := -iG(1-3)G(1^+-3)$. We then get, in frequency space,

$$\bar{O}_1^{\rm pp}(\omega;\omega') = v_c - v_c L_0^{\rm pp}(\omega+\omega')\bar{O}_1^{\rm pp}(\omega;\omega'), \quad \text{(A2)}$$

with $L_0^{\rm pp}(\omega) = -i\int \frac{d\omega'}{2\pi} G(\omega')G(\omega-\omega')e^{i\omega'\eta}$. This, finally, implies that $\bar{O}_1^{\rm pp}$ depends only on the sum of frequencies as follows:

$$\bar{O}_1^{\rm pp}(\omega+\omega') = v_c - v_c L_0^{\rm pp}(\omega+\omega')\bar{O}_1^{\rm pp}(\omega+\omega'). \quad \text{(A3)}$$

This is a Dyson-like equation similar to the screening equation in the GW approximation. The time structure of the self-energy becomes

$$\begin{aligned}\Sigma_1(1-1') &= G(4-2^+)O_1^{\rm pp}(12;1'4)\\ &= -iG(4-1^+)\bar{O}_1^{\rm pp}(1-1';1-4) \quad \text{(A4)}\end{aligned}$$

and, hence,

$$\begin{aligned}\Sigma_1^{\rm pp}(\omega) &= -i\int \frac{d\omega'}{2\pi} G(\omega')\bar{O}_1^{\rm pp}(\omega;\omega')e^{i\omega'\eta}\\ &= -i\int \frac{d\omega'}{2\pi} G(\omega')\bar{O}_1^{\rm pp}(\omega+\omega')e^{i\omega'\eta}. \quad \text{(A5)}\end{aligned}$$

Again, this is very close to the structure of GW; simply, one has a "particle-particle-screened" interaction, $-\bar{O}_1^{\rm pp}$. One can verify that the time structure of $O_2^{\rm pp}$ is the same as that for $O_1^{\rm pp}$.

2. Electron-hole T matrix

In the case of the electron-hole T matrix of Eqs. (15) and (16) one can do similar steps as above and arrive at

$$\begin{aligned}\bar{O}_1^{\rm eh}(1-5;1-1') &= v_c\delta(11')\delta(1^+5) - v_c L_0^{\rm eh}(1-3)\\ &\quad\times \bar{O}_1^{\rm eh}(3-5;3-1'), \quad \text{(A6)}\end{aligned}$$

where we define the electron-hole function as $L_0^{\rm eh}(1-3) := -iG(1-3)G(3-1^+)$. In Fourier space one gets

$$\bar{O}_1^{\rm eh}(\omega+\omega') = v_c - v_c L_0^{\rm eh}(\omega+\omega')\bar{O}_1^{\rm eh}(\omega+\omega'), \quad \text{(A7)}$$

with $L_0^{\rm eh}(\omega) = -i\int \frac{d\omega'}{2\pi} G(\omega')G(\omega'-\omega)e^{i\omega'\eta}$.

The time structure of the self-energy becomes

$$\begin{aligned}\Sigma_1(1-1') &= G(2-5^+)O_1^{\rm eh}(15;1'2)\\ &= -iG(1-5^+)\bar{O}_1^{\rm eh}(1-5;1-1'), \quad \text{(A8)}\end{aligned}$$

hence,

$$\begin{aligned}\Sigma_1^{\rm eh}(\omega) &= -i\int \frac{d\omega'}{2\pi} G(\omega')\bar{O}_1^{\rm eh}(\omega';\omega)e^{i\omega'\eta}\\ &= -i\int \frac{d\omega'}{2\pi} G(\omega')\bar{O}_1^{\rm eh}(\omega-\omega')e^{i\omega'\eta}. \quad \text{(A9)}\end{aligned}$$

For $O_2^{\rm eh}$ one can proceed in a similar way as above.

APPENDIX B: SPIN STRUCTURE OF THE T MATRIX

We now schematize the spin structure of the T matrix. For both the pp and eh T matrix one has, in the collinear limit, $\Sigma(\sigma) = G(\sigma_2)O(\sigma\sigma_2;\sigma\sigma_2)$, with

$$O_1(\sigma\sigma_2;\sigma\sigma_2) = -iv_c + iv_c G(\sigma)O_1(\sigma\sigma_2;\sigma\sigma_2)G(\sigma_2) \quad \text{(B1)}$$

and

$$O_2(\sigma\sigma_2;\sigma\sigma_2) = iv_c\delta_{\sigma\sigma_2} + iv_c G(\sigma)O_2(\sigma\sigma_2;\sigma\sigma_2)G(\sigma_2). \quad \text{(B2)}$$

Note that, unlike the screened interaction W used in the GW approximation, the T matrix is spin dependent.

APPENDIX C: HUBBARD MOLECULE AT 1/2 FILLING

The starting point is the following Hubbard Hamiltonian:

$$\begin{aligned}H &= -t\sum_{\substack{i,j=1,2\\ i\neq j}}\sum_\sigma c_{i\sigma}^\dagger c_{j\sigma} + \frac{U}{2}\sum_{i=1,2}\sum_{\sigma\sigma'} c_{i\sigma}^\dagger c_{i\sigma'}^\dagger c_{i\sigma'}c_{i\sigma}\\ &\quad + \epsilon_0\sum_{\sigma,i=1,2} n_{i\sigma} + V_0. \quad \text{(C1)}\end{aligned}$$

Here $n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma}$, where $c_{i\sigma}^\dagger$ and $c_{i\sigma}$ are the creation and annihilation operators for an electron at site i with spin σ, U is the on-site (spin-independent) interaction, $-t$ is the hopping kinetic energy, and ϵ_0 is the orbital energy. The Hamiltonian further contains a potential V_0 that can be chosen to fix the zero-energy scale. The eigenstates of the system will be linear combinations of Slater determinants, which are denoted by the kets $|1\ 2\rangle$, with occupations of the sites 1, 2 given by $0, \uparrow, \downarrow, \uparrow\downarrow$. We choose $\epsilon_0 = -\frac{U}{2}$ and $V_0 = \frac{U}{2}N$, where N is the total number of electrons in the system, i.e., 2 in our case. This choice is particularly convenient since the obtained Hamiltonian,

$$\begin{aligned}H &= -t\sum_{\substack{i,j=1,2\\ i\neq j}}\sum_\sigma c_{i\sigma}^\dagger c_{j\sigma} + \frac{U}{2}\sum_{i=1,2}\sum_{\sigma\sigma'} c_{i\sigma}^\dagger c_{i\sigma'}^\dagger c_{i\sigma'}c_{i\sigma}\\ &\quad - \frac{U}{2}\sum_{\sigma,i=1,2} n_{i\sigma} + U, \quad \text{(C2)}\end{aligned}$$

has high symmetry (particle-hole symmetry), as we shall see below (see also Ref. 70). Using this Hamiltonian we can calculate the exact one-particle Green's function.

1. Exact solution

The main exact quantities we are interested in are

$$\begin{aligned}G_{ij}^\sigma(\omega) &= \frac{(-1)^{(i-j)}}{2a^2}\left[\frac{\left(1+\frac{4t}{(c-U)}\right)^2}{\omega-(c/2-t)+i\eta}\right.\\ &\quad\left.+\frac{(-1)^{(i-j)}\left(1-\frac{4t}{(c-U)}\right)^2}{\omega-(c/2+t)+i\eta}\right]\\ &\quad+\frac{1}{2a^2}\left[\frac{\left(1+\frac{4t}{(c-U)}\right)^2}{\omega+(c/2-t)-i\eta}\right.\\ &\quad\left.+\frac{(-1)^{(i-j)}\left(1-\frac{4t}{(c-U)}\right)^2}{\omega+(c/2+t)-i\eta}\right], \quad \text{(C3)}\\ G_{ij}^{0,\sigma}(\omega) &= \frac{(-1)^{(i-j)}}{2}\left[\frac{1}{\omega-t+i\eta}+\frac{(-1)^{(i-j)}}{\omega+t-i\eta}\right], \quad \text{(C4)}\end{aligned}$$

$$\Sigma^{\sigma}_{ij}(\omega) = \frac{U}{2}\delta_{ij} + \frac{U^2}{8}\left[\frac{1}{\omega - 3t + i\eta} + \frac{(-1)^{(i-j)}}{\omega + 3t - i\eta}\right], \tag{C5}$$

with $c^2 = 16t^2 + U^2$ and $a^2 = 2(\frac{16t^2}{(c-U)^2} + 1)$. Note that the symmetry of the system is such that $G^{\uparrow}_{11} = G^{\downarrow}_{11} = G^{\uparrow}_{22} = G^{\downarrow}_{22}$ and $G^{\uparrow}_{12} = G^{\downarrow}_{12} = G^{\uparrow}_{21} = G^{\downarrow}_{21}$ and similarly for the self-energy.

2. *GW* solution

Here we give the main results,

$$P^{\sigma\sigma}_{ij}(\omega) = \frac{(-1)^{(i-j)}}{4}\left[\frac{1}{\omega - 2t + i\eta} - \frac{1}{\omega + 2t - i\eta}\right], \tag{C6}$$

$$W_{ij}(\omega) = U\delta_{ij} + (-1)^{(i-j)}\frac{U^2 t}{h}\left[\frac{1}{\omega - h + i\eta} - \frac{1}{\omega + h - i\eta}\right], \tag{C7}$$

$$\Sigma^{\sigma}_{ij}(\omega) = \frac{U}{2}\delta_{ij} + \frac{U^2 t}{2h}\left[\frac{1}{\omega - (t+h) + i\eta} + \frac{(-1)^{(i-j)}}{\omega + (t+h) - i\eta}\right], \tag{C8}$$

where $h^2 = 4t^2 + 4tU$. Note that only the component $P^{\sigma\sigma}$ is given in Eq. (C6) (and not the full $P^{\sigma\sigma'}$), since only this is needed to calculate W.

The poles of the one-particle Green's function can be calculated using

$$\det[G^{-1}] = \det\left[G_0^{-1} - \Sigma\right] = \det\begin{pmatrix} \omega - \Sigma_{11} & t - \Sigma_{12} \\ t - \Sigma_{12} & \omega - \Sigma_{11} \end{pmatrix}, \tag{C9}$$

from which we get

$$\omega = t + (\Sigma_{11} - \Sigma_{12}), \quad \omega = -t + (\Sigma_{11} + \Sigma_{12}), \tag{C10}$$

which is general, i.e., we can apply for any approximation to the self-energy. In the case of GW, we get the following poles:

$$\omega_{1,2} = \frac{\frac{U}{2} - h \pm \sqrt{\left(h + \frac{U}{2} + 2t\right)^2 + \frac{4U^2 t}{h}}}{2}, \tag{C11}$$

$$\omega_{3,4} = \frac{\frac{U}{2} + h \pm \sqrt{\left(h - \frac{U}{2} + 2t\right)^2 + \frac{4U^2 t}{h}}}{2}. \tag{C12}$$

We note that, for $U \neq 0$, the particle-hole symmetry is lost due to the lack of self-consistency using the G_0W_0 approximation.[13] This symmetry can be enforced by absorbing the static part of the self-energy $(U/2)$ into the chemical potential; this ultimately corresponds to dropping the terms U/2 in Eqs. (C11) and (C12).

[1] L. Hedin, Phys. Rev. **139**, A796 (1965).
[2] W. G. Aulbur, L. Jönsson, and J. W. Wilkins, Solid State Phys. **54**, 1 (1999), and references therein.
[3] F. Aryasetiawan and O. Gunnarsson, Rep. Prog. Phys. **61**, 237 (1998), and references therein.
[4] M. Gatti, F. Bruneval, V. Olevano, and L. Reining, Phys. Rev. Lett. **99**, 266402 (2007).
[5] E. Papalazarou, M. Gatti, M. Marsi, V. Brouet, F. Iori, L. Reining, E. Annese, I. Vobornik, F. Offi, A. Fondacaro, S. Huotari, P. Lacovig, O. Tjernberg, N. B. Brookes, M. Sacchi, P. Metcalf, and G. Panaccione, Phys. Rev. B **80**, 155115 (2009).
[6] A. N. Chantis, M. van Schilfgaarde, and T. Kotani, Phys. Rev. B **76**, 165126 (2007).
[7] S. V. Faleev, M. van Schilfgaarde, and T. Kotani, Phys. Rev. Lett. **93**, 126406 (2004).
[8] N. E. Dahlen, R. van Leeuwen, and U. von Barth, Phys. Rev. A **73**, 012511 (2006).
[9] A. Stan, N. E. Dahlen, and R. van Leeuwen, Europhys. Lett. **76**, 298 (2006).
[10] W. Nelson, P. Bokes, P. Rinke, and R. W. Godby, Phys. Rev. A **75**, 032505 (2007).
[11] F. Bruneval, Phys. Rev. Lett. **103**, 176403 (2009).
[12] M. Springer, F. Aryasetiawan, and K. Karlsson, Phys. Rev. Lett. **80**, 2389 (1998).
[13] P. Romaniello, S. Guyot, and L. Reining, J. Chem. Phys. **131**, 154111 (2009).
[14] V. M. Galitskii, Zh. Eksp. Teor. Fiz. **34**, 251 (1958) [Sov. Phys. JETP **7**, 104 (2958)].
[15] J. Kanamori, Prog. Theor. Phys. **30**, 275 (1963).
[16] A. Fetter and J. D. Walwcka, *Quantum Theory of Many-Particle Systems* (Dover, Mineola, NY, 2003).
[17] G. Baym and L. P. Kadanoff, Phys. Rev. **124**, 287 (1961).
[18] H. A. Bethe and J. Goldstone, Proc. R. Soc. London A **238**, 551 (1957); [http://rspa.royalsocietypublishing.org/content/238/1215/551.full.pdf+html].
[19] M. Cini and C. Verdozzi, Solid State Commun. **57**, 657 (1986).
[20] C. Verdozzi, R. W. Godby, and S. Holloway, Phys. Rev. Lett. **74**, 2327 (1995).
[21] M. Puig von Friesen, C. Verdozzi, and C.-O. Almbladh, Phys. Rev. Lett. **103**, 176404 (2009).
[22] M. Puig von Friesen, C. Verdozzi, and C.-O. Almbladh, Phys. Rev. B **82**, 155108 (2010).
[23] A. Schindlmayr, T. J. Pollehn, and R. W. Godby, Phys. Rev. B **58**, 12684 (1998).
[24] N. E. Bickers and S. R. White, Phys. Rev. B **43**, 8044 (1991).
[25] N. Bickers, in *Theoretical Methods for Strong Correlated Electrons*, edited by David Sénchal, André-Marie Tremblay, and Claude Bourbonnais (Springer, New York, 2004).
[26] N. E. Bickers, D. J. Scalapino, and S. R. White, Phys. Rev. Lett. **62**, 961 (1989).
[27] N. E. Bickers and D. J. Scalapino, Ann. Phys. **193**, 206 (1989).
[28] A. Liebsch, Phys. Rev. B **23**, 5203 (1981).
[29] M. I. Katsnelson and A. I. Lichtenstein, J. Phys.: Condens. Matter **11**, 1037 (1999).
[30] M. Katsnelson and A. Lichtenstein, Eur. Phys. J. B **30**, 9 (2002).
[31] R. A. Smith, Phys. Rev. A **46**, 4586 (1992).
[32] R. van Leeuwen, N. E. Dahlen, and A. Stan, Phys. Rev. B **74**, 195105 (2006).

[33]G. Strinati, Riv. Nuovo Cimento **11**, 1 (1988).
[34]V. P. Zhukov, E. V. Chulkov, and P. M. Echenique, Phys. Rev. Lett. **93**, 096401 (2004).
[35]V. P. Zhukov, E. V. Chulkov, and P. M. Echenique, Phys. Rev. B **72**, 155109 (2005).
[36]V. P. Zhukov, E. V. Chulkov, and P. M. Echenique, Phys. Rev. B **73**, 125105 (2006).
[37]I. A. Nechaev and E. V. Chulkov, Phys. Rev. B **73**, 165112 (2006).
[38]I. A. Nechaev, I. Y. Sklyadneva, V. M. Silkin, P. M. Echenique, and E. V. Chulkov, Phys. Rev. B **78**, 085113 (2008).
[39]A. Mönnich, J. Lange, M. Bauer, M. Aeschlimann, I. A. Nechaev, V. P. Zhukov, P. M. Echenique, and E. V. Chulkov, Phys. Rev. B **74**, 035102 (2006).
[40]P. Martin and J. Schwinger, Phys. Rev. **115**, 1342 (1959).
[41]The atomic limit of the Hubbard molecule is an example where the correlation part of the interaction is crucial; see in Sec. III.
[42]In this case the nature of the screening would be always test-charge-test-charge.[55]
[43]In this case one can write $\Sigma_{xc} = iG\tilde{W}$ where $\tilde{W}$ is a test charge-test electron (TC-TE) screening.[55] The f_{xc} that appears makes the one-electron case exact.[13]
[44]This means that O is only determined up to changes ΔO that fulfill the condition $\int d3d4G(34)\Delta O(14;23) = 0$.
[45]L. P. Kadanoff and G. Baym, *Quantum Statistical Mechanics* (W. A. Benjamin, New York, 1964).
[46]W. Hanke and L. J. Sham, Phys. Rev. B **21**, 4656 (1980).
[47]G. Strinati, Phys. Rev. B **29**, 5718 (1984).
[48]G. Strinati, Phys. Rev. Lett. **49**, 1519 (1982).
[49]Also in the Bethe-Salpeter equation used for the calculation of the electron-hole excitations one has to approximate the kernel $\Xi = \frac{\delta\Sigma}{\delta G}$. Using the GW approximation to the self-energy, i.e., $\Sigma^{GW} = iGW$, the kernel is approximated as $\Xi \approx W$, thus neglecting the term $\frac{\delta W}{\delta G}$ in the functional derivative of Σ^{GW}. In this respect, the approximation presented in Eq. (11) is done in the same spirit as in the GW-BSE framework.
[50]T. K. Ng and K. S. Singwi, Phys. Rev. B **34**, 7738 (1986).
[51]T. K. Ng and K. S. Singwi, Phys. Rev. B **34**, 7743 (1986).
[52]G. F. Giuliani and G. Vignale, *Quantum Theory of the Electron Liquid* (Cambridge University Press, Cambridge, 2005).
[53]R. Asgari, B. Davoudi, M. Polini, G. F. Giuliani, M. P. Tosi, and G. Vignale, Phys. Rev. B **71**, 045323 (2005).
[54]One might wonder whether the eh T matrix of Eqs. (15) and (16) is the same as the one obtained using the T matrix derived by Strinati in Ref. 33 when only ladder diagrams are used [i.e., $\frac{\delta\Sigma(11')}{\delta G(2'2)} \approx iv_c(11')\delta(12')\delta(1'2)$]. One can verify that this is not the case since there is only an exchange-like term similar to $O_2^{\rm eh}$, and a different integration of variables.
[55]F. Bruneval, F. Sottile, V. Olevano, R. Del Sole, and L. Reining, Phys. Rev. Lett. **94**, 186402 (2005).
[56]Since the screened Coulomb potential is not static, the time structure of the screened T matrix is more complicated than that of the T matrix. In particular, one no longer has a strict particle-particle or electron-hole $L_0 = -iGG$. Nevertheless, we will keep this notation in order to make a link with the T matrix.
[57]A. Grüneis, M. Marsman, J. Harl, L. Schimka, and G. Kresse, J. Chem. Phys. **131**, 154115 (2009).
[58]E. L. Shirley, Phys. Rev. B **54**, 7758 (1996).
[59]I. A. Nechaev and E. V. Chulkov, Phys. Rev. B **71**, 115104 (2005).
[60]J. Hubbard, Proc. R. Soc. A **276**, 238 (1963).
[61]J. Hubbard, Proc. R. Soc. A **277**, 237 (1964).
[62]P. Romaniello, D. Sangalli, J. A. Berger, F. Sottile, L. G. Molinari, L. Reining, and G. Onida, J. Chem. Phys. **130**, 044108 (2009).
[63]D. Sangalli, P. Romaniello, G. Onida, and A. Marini, J. Chem. Phys. **134**, 034115 (2011).
[64]V. Drchal and J. Kudrnovsky, J. Phys. F **14**, 2443 (1984) .
[65]S. Verga, R. J. Gooding, and F. Marsiglio, Phys. Rev. B **71**, 155111 (2005).
[66]P. Pisarski and R. J. Gooding, J. Phys.: Condens. Matter **23**, 205603 (2011).
[67]M. Cini and C. Verdozzi, Nuovo Cimento D **9**, 1 (1987) .
[68]C.-O. Almbladh, *Progress in Nonequilibrium Greens Functions III,* J. Phys. Conf. Ser., Vol. 35, edited by M. Bonitz and A. Filinov (Institute of Physics, Bristol, 2006).
[69]B. Holm and U. von Barth, Phys. Rev. B **57**, 2108 (1998).
[70]J. M. Tomczak, Ph.D. thesis, École Polytechnique, 2007.
[71]K. Karlsson and F. Aryasetiawan, Phys. Rev. B **62**, 3006 (2000).