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Approximations for many-body Green's functions: insights from the fundamental equations

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Abstract. Several widely used methods for the calculation of band structures and photo emission spectra, such as the GW approximation, rely on many-body perturbation theory. They can be obtained by iterating a set of functional differential equations (DEs) relating the one-particle Green's function (GF) to its functional derivative with respect to an external perturbing potential. In this work, we apply a linear response expansion in order to obtain insights into various approximations for GF calculations. The expansion leads to an effective screening while keeping the effects of the interaction to all orders. In order to study various aspects of the resulting equations, we discretize them and retain only one point in space, spin and time for all variables. Within this one-point model we obtain an explicit solution for the GF, which allows us to explore the structure of the general family of solutions and to determine the specific solution that corresponds to the physical one. Moreover, we analyze the performances of established approaches like GW over the whole range of interaction strength, and we explore alternative approximations. Finally, we link certain approximations for the exact solution to the corresponding manipulations of the DE which produces them. This link is crucial in view of a generalization of our findings to the real (multidimensional functional) case where only the DE is known.

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Contents

1. Introduction

The one-particle Green's function (GF) [1–3] is a powerful quantity since it contains a wealth of information about a physical system, such as the expectation value of any single-particle operator over the ground state, the ground-state total energy and the spectral function. In order to access this quantity, one can start from its equation of motion [4–6]:

$$\left[\mathrm{i}\frac{\partial}{\partial t_1} - h(r_1)\right] G(1,2) + \mathrm{i}\int d3\, v(1^+,3) G_2(1,3;2,3^+) = \delta(1,2), \tag{1}$$

where $h(r_1)$ is the one-electron part of the many-body Hamiltonian, $G_2(1,3;2,3^+)$ is the two-body GF and $v(1^+,3)$ is the Coulomb potential. The space, spin and time variables are all combined in $(1) = (r_1, \sigma_1, t_1)$ and $(1^+) = (r_1, \sigma_1, t_1^+)$ with $t_1^+ = t_1 + \delta$ $(\delta \to 0^+)$.

Equation (1) can be manipulated in order to get a more practical expression by introducing the non-interacting GF G_0 with

$$\left[\mathrm{i}\frac{\partial}{\partial t_1} - h(r_1)\right] G_0(1,2) = \delta(1,2), \tag{2}$$

which reinserted in equation (1) gives

$$G(1,2) = G_0(1,2) - \mathrm{i}\int d3d4 G_0(1,3) v(3^+,4) G_2(3,4;2,4^+). \tag{3}$$

In (3), G_0 determines the appropriate initial condition in time; note that the solutions of (1) and (2) are not unique. Moreover, in order to calculate G, knowledge of G_2 is required (which

in turn requires knowledge of G_3 and so on) [4, 6]. In order to obtain a closed expression one can generalize $G(1,2)$ to $G(1,2;[\varphi])$, where an external fictitious time-dependent potential φ is applied to the system. This allows one to express G_2 as [7]

$$G_2(3,4;2,4^+;[\varphi]) = G(3,2;[\varphi])G(4,4^+;[\varphi]) - \frac{\delta G(3,2;[\varphi])}{\delta\varphi(4)}. \tag{4}$$

Note that in (4) all GFs are generalized to non-equilibrium since they depend on the perturbing potential. The equilibria G and G_2 in (3) are then obtained by taking $\varphi = 0$. Inserting (4) into (3) yields a set of functional differential equations (DEs) [4] for the unknown G

$$G(1,2;[\varphi]) = G_0(1,2) + \int d3\, G_0(1,3)V_{\mathrm{H}}(3;[\varphi])G(3,2;[\varphi]) + \int d3\, G_0(1,3)\varphi(3)G(3,2;[\varphi])$$
$$+ \mathrm{i}\int d4d3\, G_0(1,3)v(3^+,4)\frac{\delta G(3,2;[\varphi])}{\delta\varphi(4)}, \tag{5}$$

where $V_{\mathrm{H}}(3) = -\mathrm{i}\int d4\, v(3,4)G(4,4^+;[\varphi])$ is the Hartree potential. Since the Hartree potential contains the GF, this term makes the equations nonlinear. We are interested in the solution of equation (5) for $\varphi = 0$. Its calculation would, hence, require the solution of a set of coupled, nonlinear, first-order DEs, which is clearly a non-trivial task. Moreover, one would need a new initial condition to completely define the desired solution of this DE, since the derivative $\frac{\delta G}{\delta\varphi}$ has been introduced. Therefore, usually another route is taken: one includes the functional derivative in (5) in the definition of a self-energy [4]

$$\Sigma(1,3) = \mathrm{i}\int d4d2\, v(1^+,4)\frac{\delta G(1,2;[\varphi])}{\delta\varphi(4)}\bigg|_{\varphi=0} G^{-1}(2,3), \tag{6}$$

which, inserted into equation (5) for $\varphi = 0$, gives

$$G(1,2) = G_0(1,2) + \int d3\, G_0(1,3)V_{\mathrm{H}}(3)G(3,2) + \int d4d3\, G_0(1,3)\Sigma(3,4)G(4,2). \tag{7}$$

This is the Dyson equation for G, where Σ contains all the many-body effects (beyond the Hartree contribution) present in the system. Of course, $\frac{\delta G}{\delta\varphi}$ and therefore Σ are still not known and, in practice, Σ has to be approximated. A good starting point is obtained by reformulating the problem in terms of a coupled set of equations containing the one-particle GF, the polarizability P, the self-energy Σ, the screened Coulomb interaction W and the vertex Γ. These equations are most often solved within the so-called GW approximation (GWA) [8], where the vertex Γ is set to unity, resulting in $\Sigma \approx \mathrm{i}GW$. Over the last two decades, the GW method has become the tool of choice for calculations of quasi-particle band structures ([9] and references therein; [10] and references therein) of many materials and direct and inverse photo emission spectra (see, e.g., [11–14]) improving substantially on the results provided by static mean-field electronic structure methods.

However, the GWA suffers from some fundamental shortcomings (see, e.g., [15–18]) and, with Σ being of first order in W, is not expected to describe strong correlation. Higher orders in W could be added by iterating the equations, but this is technically difficult, and there is no guarantee that results will quickly improve. It is therefore necessary to find guidelines.

In the present work we go back to equation (5). Our aim is, firstly, to obtain new insights into standard approximations by relating them more directly to the original equations. Secondly, we want to use equation (5) to explore alternative approximations. Finally, it might be interesting to concentrate directly on the set of coupled, nonlinear, first-order functional DEs for G, equation (5), although it has been acknowledged that no 'practical technique for solving such functional differential equation exactly' [4] is available. However, one may still hope that with new algorithms and the increase in computer power, numerical solutions might become accessible. The present work is hence also meant to explore strategies for, and possible problems of, such a route.

In the following we resort to two approximations. Firstly, we linearize the set of equations by expanding V_{H} in terms of φ. Secondly, we discretize equation (5) and consider in the first instance only one point for each space, spin and time variable: we will call this latter approximation the 'one-point model', as opposed to the full functional problem. The strategy underlying this procedure is the following: for the one-point model, we can derive the exact explicit solution of the now algebraic DE, and solve the initial value problem. One can, hence, explore approximations to the full solution, which yields valuable insights into the performance of current approaches and suggestions for alternative ones. By determining which manipulations of the DE produce such approximate solutions, one obtains suggestions for analogous manipulations on the DE for the full functional problem, which opens the way to translate our model findings into realistic calculations.

This paper is structured as follows. In section 2, we present the linearized differential equation which can be solved exactly within the one-point framework. We discuss in particular the initial value problem and how it can be overcome. In section 3, we examine, in the one-point framework, various common approximations to the solution of the DE: the iteration of equation (5) and approximations based on a Dyson equation, in particular different GW flavors. In section 4, we explore other routes to manipulate the initial DE and obtain approximate solutions. We, finally, give our conclusions and perspectives on future work in section 5.

2. The screened equation in a one-point framework

Our first goal is to simplify the equations such that the main physics is retained, but manipulations become more straightforward. To this end, we linearize the DE with an expansion of the Hartree potential to first order in the external potential φ,

$$V_{\mathrm{H}}(3;[\varphi]) \approx -\mathrm{i}\int d4v(3^+,4)G(4,4^+;[\varphi])\Big|_{\varphi=0} - \mathrm{i}\int d4\,d5\,v(3^+,4)\frac{\delta G(4,4^+;[\varphi])}{\delta\varphi(5)}\Big|_{\varphi=0}\varphi(5)+o(\varphi^2). \tag{8}$$

Equation (5) hence becomes

$$G(1,2;[\bar{\varphi}]) = G^0_{\mathrm{H}}(1,2)+\int d3G^0_{\mathrm{H}}(1,3)\bar{\varphi}(3)G(3,2;[\bar{\varphi}]) + \mathrm{i}\int d3d5G^0_{\mathrm{H}}(1,3)W(3^+,5)\frac{\delta G(3,2;[\bar{\varphi}])}{\delta\bar{\varphi}(5)}, \tag{9}$$

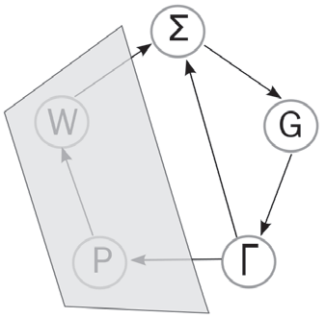

Figure 1. Hedin's pentagon when W is fixed: one iterates only three equations, namely the ones for G, Σ, Γ, rather than the full set. Note that fixing W also implies fixing the polarizability P.

where G_{H}^0 is a Hartree GF containing the Hartree potential at vanishing φ, $\bar{\varphi} = \epsilon^{-1}\varphi$ is the renormalized external potential and $W = \epsilon^{-1}v$ is the screened Coulomb potential with ϵ the dielectric function at $\varphi = 0$.[4]

Concerning equation (9), three important remarks should be made: firstly, through the linearization the screened interaction W becomes the central quantity of the equation. This is justified by the physics of extended systems, where screening and plasmons are key concepts.

Secondly, in principle, W is the exact screened interaction, which of course is not known. One can, however, adopt two strategies: either W is considered to be an *externally* given quantity, obtained within a good approximation, e.g. from a time-dependent density functional theory (TDDFT) calculation [19]; or one could also recalculate W from $G[\bar{\varphi}]$ (see in the next section). In this work, we will adopt the first strategy, which is illustrated in figure 1. Such a philosophy is rigorously justified. In particular, in the framework of the theory of functionals it is possible to pass from the Luttinger–Ward functional (given as functional of G, although indeed one should add the bare Coulomb interaction v as argument) to the so-called Ψ-functional, where v_{c} is replaced by W [20]. This explains, for example, why self-consistency in G only (and not in W) is sufficient to have a conserving GWA. Moreover, in practice this is the most current way of proceeding, corresponding, e.g., in a GW calculation to the 'best G, best W' approach: while the non-interacting G is taken, e.g., to be the Kohn–Sham GF, W is calculated as accurately as possible, e.g. in the adiabatic local density approximation to TDDFT. Thirdly, by approximating the functional derivative $\frac{\delta G}{\delta \bar{\varphi}} = -G\frac{\delta G^{-1}}{\delta \bar{\varphi}}G \approx GG$ (which supposes the self-energy to be independent of $\bar{\varphi}$) one obtains the Dyson equation for the one-particle GF in the GWA to the self-energy. The proof is given in appendix A. This result shows that, even though the linearization procedure is an approximation, equation (9) is still a promising starting point to analyze the different flavors of the GWA and to go beyond.

After linearizing, the next step consists in *discretizing* equation (9) and then in considering only one value for the space, spin and time variables, respectively (or equivalently concerning space and spin, in considering all GFs to be diagonal in a given basis): this is the one-point model employed throughout the whole paper. The one-point framework has already been used by other authors: in [21, 22], Hedin's equations are combined in a single algebraic DE which

[4] For simplicity we use the same symbol for $G[\bar{\varphi}]$ and $G[\varphi]$; of course it is understood that the corresponding functional is taken.

is solved as a series expansion. This allows the authors to enumerate the diagrams for a certain order of expansion. Several expansion parameters are examined, for example, vG_{H}^2, with v being the bare Coulomb potential and G_{H} the Hartree GF, vG^2, with G being the exact GF, WG^2, with W being the screened Coulomb potential, etc, which shows how at various orders of expansion the number of diagrams decreases by increasing the degree of renormalization. This is also the spirit behind the linearized equation (9), in which the natural expansion parameter would be WG_{H}^2, where W is treated as an externally given interaction. The advantage of using the one-point framework is that the equations become algebraic and thus the enumeration of diagrams is facilitated.

In [23], a similar strategy as that in [21, 22] is used to enumerate diagrams, focusing in particular on the asymptotic behavior of the counting numbers. Moreover, Hedin's equations are transformed into a single first-order DE for the GF as a function of an interaction parameter and an implicit solution is obtained. In order to fix the particular solution of this DE, the initial condition $G_{(v=0)} = G_0$ is used.

Instead, here we concentrate on (5), or better its linearized form (9), which is *another* DE for G, as a functional of an external potential. This choice allows us to (i) emphasize the essential physics contained in the screened Coulomb interaction W, (ii) discuss various aspects of the many-body problem in a clear and simple way and (iii) obtain an exact solution of the approximate equation that can be used as a benchmark. Moreover, we believe that the one-point version of equation (9) can be a natural starting point for a generalization to the full functional problem. While the equations are easier to manipulate, physical information is of course lost in the one-point framework. In particular, no poles (addition/removal energies) of the GF appear. However, the various aspects that will be explored in the following are intrinsically related to the structure of the equations and hence exportable also to the full functional problem, in the same spirit as in [21–23].

2.1. One-point differential equation (DE)

In the one-point model equation (5) reduces to an algebraic, nonlinear, first-order DE

$$y(z) = y_0 + vy_0y^2(z) + y_0zy(z) - vy_0\frac{\mathrm{d}\,y(z)}{\mathrm{d}z}, \tag{10}$$

where $\varphi \to z$, $G(1,2;[\varphi]) \to y(z)$ and $G_0(1,2) \to y_0$. Moreover, $\mathrm{i}v(3^+,4) \to -v$: this change of prefactor compensates for the time or frequency integrations that have been dropped in the one-point model and corresponds to a standard procedure in this context [21, 23]. We can now linearize equation (10) in the same way as we did starting with equation (5) and obtaining equation (9). This yields

$$y_u(x) = y_{\mathrm{H}}^0 + y_{\mathrm{H}}^0 x y_u(x) - u y_{\mathrm{H}}^0 \frac{\mathrm{d}\,y_u(x)}{\mathrm{d}x}. \tag{11}$$

Hence with respect to equation (9), $\bar{\varphi} \to x$, $G_{\mathrm{H}}^0(1,2) \to y_0^{\mathrm{H}}$ and $\mathrm{i}W(3^+,5) \to -u$; the subscript u in y_u highlights its u dependence. In the following, for simplicity of notation, we denote y_{H}^0 by y_0 unless stated differently. In appendix B, we sketch the main steps to solve equation (11), based on the general ansatz $y_u(x) = A(x)\cdot\mathcal{I}(x)$. With the choice

$$A(x) = \exp\left(\frac{x^2}{2u} - \frac{x}{uy_0}\right), \tag{12}$$

one obtains the equation

$$\frac{\mathrm{d}\mathcal{I}(x)}{\mathrm{d}x} = \frac{1}{u}\exp\left[-\left(\frac{x^2}{2u} - \frac{x}{uy_0}\right)\right] \tag{13}$$

and the general solution $y_u(x)$ reads

$$y_u(x) = \sqrt{\frac{\pi}{2u}}\exp\left(\frac{x^2}{2u} - \frac{x}{uy_0} + \frac{1}{2uy_0^2}\right)\left\{\mathrm{erf}\left[\left(x - \frac{1}{y_0}\right)\sqrt{\frac{1}{2u}}\right] - C(y_0, u)\right\}, \tag{14}$$

where $C(y_0, u)$ is to be set by an initial condition. In the limit $x \to 0$, which is the equilibrium solution we are looking for, equation (14) becomes

$$y_u = -\sqrt{\frac{\pi}{2u}}\exp\left(\frac{1}{2uy_0^2}\right)\left\{\mathrm{erf}\left(\sqrt{\frac{1}{2uy_0^2}}\right) + C(y_0, u)\right\}. \tag{15}$$

Note that a similar ansatz can also be used for the full functional problem, namely $G(1,2) = \int d3\, A(1,3)\cdot\mathcal{I}(3,2)$, in order to get a set of DEs that are less complicated to manipulate than the original one.

2.2. *The initial value problem*

In general, in order to set $C(y_0, u)$, $y_u(x)$ has to be known for a given potential x_β (i.e. $y_u(x_\beta) = y_u^\beta$). However, it is far from obvious to formulate such a condition in the realistic full functional case; this would indeed require the knowledge of the full interacting G for some given potential φ. Therefore the question is whether one can reformulate the condition in a simpler way in order to set C.

To answer this question we expand the exact solution for small values of u, obtaining

$$y_u \approx -\sqrt{\frac{\pi}{2u}}\exp\left(\frac{1}{2uy_0^2}\right)\left(1 + C(u, y_0)\right) + \left\{y_0 - uy_0^3 + 3u^2y_0^5 - 15u^3y_0^7 + o(u^4)\right\}. \tag{16}$$

When $u \to 0$ the one-body GF G has to reduce to the non-interacting G_0; in our framework this translates into $y_u|_{u\to 0} \equiv y_0$. Imposing this condition on equation (16) gives

$$\sqrt{\frac{\pi}{2u}}\exp\left(\frac{1}{2y_0^2u}\right)\left(1 + C(u, y_0)\right) = 0, \quad u \to 0, \tag{17}$$

which is satisfied if

$$C(u, y_0) = -1, \quad u \to 0. \tag{18}$$

This result for C holds also for $u \neq 0$. Indeed, it guarantees a non-divergent result for any non-vanishing potential x in (14). Moreover, it reproduces the perturbative result, which is obtained by iterating equation (11); for example, the sixth iteration yields

$$y_u^{(6)} = y_0 - uy_0^3 + 3u^2y_0^5 - 15u^3y_0^7. \tag{19}$$

This is precisely the same series as the one appearing in equation (16) when $C(u, y_0)$ is set to -1.

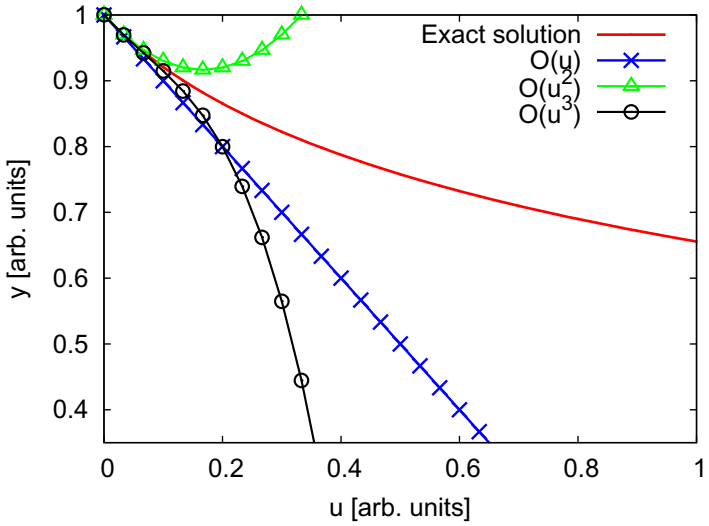

Figure 2. Comparison between the exact solution (red plain line, equation (15)) and the iterative solution for $x = 0$ of (equation (20)). The blue crosses represent the first-order expansion (equation (21)), while the green triangles and black circles are, respectively, the second (equation (22)) and third order (equation (19)). All three orders are close to the exact solution for small u values, whereas when a given order of the series starts to diverge, the lower orders of the expansion reproduce the exact results better. For each curve $C(u, y_0) = -1$, and we arbitrarily set $y_0 = 1$.

3. Analysis of common methods for calculating the one-body *G*

In the following, we will analyze various established approximations for the calculation of the one particle G, using knowledge of the exact solution.

3.1. Iteration of the DE

Let us first iterate equation (11) starting from $y_u^{(0)}(x) = y_0$, according to

$$y_u^{(n+1)}(x) = y_0 + y_u^{(n)} x y_0 - u y_0 \frac{\mathrm{d}y_u^{(n)}(x)}{\mathrm{d}x}. \tag{20}$$

For $x = 0$ the first two orders in u read

$$y_u^{(2)} = y_0 - u y_0^3, \tag{21}$$

$$y_u^{(4)} = y_0 - u y_0^3 + 3u^2 y_0^5, \tag{22}$$

and equation (19) for the third order. Results as a function of u are depicted in figure 2 together with the exact solution. Two observations can be made: (i) very few terms are needed to obtain a good approximation to the exact solution in the small u regime; (ii) for a given $u = u_n$, the expansion diverges starting from an order n. The larger the u_n, the smaller the n, which limits the precision that can be obtained. As mentioned previously, the iteration coincides with the expansion for small u of the exact solution. Since the small u expansion is *de facto* the asymptotic expansion of the error function times an exponential (as can be seen in (16)) the

divergent behavior of the iteration in (20) is not surprising. Divergences of higher orders have been found in perturbation expansions for realistic systems, e.g. for orders higher than 3 in the Møeller–Plesset scheme [24, 25].

3.2. Self-energy-based approximations

In this section, the introduction of a self-energy Σ will be discussed along with its most common approximations.

The Dyson-like form for equation (11), which is the equivalent of equation (7), reads

$$y_u(x) = y_0 + y_0 x y_u(x) + y_0 \Sigma_u [y_u(x)]\, y_u(x), \tag{23}$$

where a self-energy kernel has been defined as

$$\Sigma_u [y_u(x)] = -u \frac{\mathrm{d}y_u(x)}{\mathrm{d}x} \frac{1}{y_u(x)}. \tag{24}$$

With $\frac{\mathrm{d}y_u(x)}{\mathrm{d}x} = -y_u^2(x) \frac{\mathrm{d}y_u^{-1}(x)}{\mathrm{d}x}$ and the definition $\Gamma_u [y_u(x)] = -\frac{\mathrm{d}y_u^{-1}(x)}{\mathrm{d}x}$ for the vertex function, the self-energy reads

$$\Sigma_u [y_u(x)] = -u y_u(x) \Gamma_u [y_u(x)], \tag{25}$$

which is the equivalent of $\Sigma = \mathrm{i}\, GW\Gamma$ [8]. The Bethe–Salpeter equation for the vertex function Γ is then derived from (23)

$$\begin{aligned} \frac{\mathrm{d}y_u^{-1}(x)}{\mathrm{d}x} &= -1 - \frac{\mathrm{d}\Sigma_u [y_u(x)]}{\mathrm{d}x} \\ &= -1 - \frac{\mathrm{d}\Sigma_u [y_u(x)]}{\mathrm{d}y_u(x)} \frac{\mathrm{d}y_u(x)}{\mathrm{d}x}, \end{aligned} \tag{26}$$

from which for $x \to 0$

$$\Gamma_u(y_u) = 1 + \frac{\mathrm{d}\Sigma_u(y_u)}{\mathrm{d}y_u} \Gamma_u(y_u) y_u^2, \tag{27}$$

where $y_u = y_u(x \to 0)$. For $x = 0$ equations (23), (25) and (27) correspond to a subset of the so-called Hedin's equations [8], obtained by fixing W. A pictorial representation of this subset for a given W is given in figure 1. In the following, we will approximate the equations and the results will be compared to the exact solution of the DE, in order to obtain greater insight into these self-energy-based techniques. From now on, all quantities will hence be understood to be taken at $x = 0$.

3.2.1. G_0W_0 and self-consistency. Let us first look at different flavors of the GWA [8]. Setting $\Gamma_u(y_u)$ to unity, it follows that $\Sigma_u(y_u) = -u y_u$. Within the initial guess $y_u^{(0)} = y_0$, one obtains a so-called G_0W_0 self-energy $\Sigma_u = -u y_0$.[5] This is then employed in the Dyson equation (23) in order to get an improved $y_u^{(1)}$. To go beyond this first approximation one can iterate further within the GWA, i.e. keeping $\Gamma_u = 1$. This corresponds to an iteration towards a GW_0 result, since G is iterated towards self-consistency but u, which represents the screened interaction,

[5] In realistic calculations, G_0 is often taken to be a Kohn–Sham GF; here, to be consistent, it corresponds to the Hartree GF G_{H}^0.

is fixed. We report here the expressions obtained for G_0W_0, i.e. the first solution of the Dyson equation, and for three successive loops

$$y_u^{(1)} = y_u^{G_0W_0} = \frac{y_0}{1+uy_0^2}, \tag{28}$$

$$y_u^{(2)} = y_0 \frac{1+uy_0^2}{1+2uy_0^2}, \tag{29}$$

$$y_u^{(3)} = y_0 \frac{1+2uy_0^2}{1+3uy_0^2+u^2y_0^4}, \tag{30}$$

$$y_u^{(4)} = y_0 \frac{1+3uy_0^2+u^2y_0^4}{1+4uy_0^2+3u^2y_0^4}. \tag{31}$$

We call this procedure the *iterative self-consistent* scheme, in contrast with the *direct self-consistent* scheme where one solves directly the Dyson equation (23), for $x = 0$, with $\Sigma_u = -uy_u$. In this latter case, one gets a second-order equation with two solutions

$$y_u = \frac{\pm\sqrt{1+4uy_0^2}-1}{2uy_0}. \tag{32}$$

Note that for the full functional problem one would find even more solutions, since a second-order equation has to be solved for each matrix element of G.

In order to choose the physical solution, we Taylor expand the square root around $u = 0$, which leads to

$$y_u \approx \pm\left(y_0 + \frac{1}{2uy_0}\right) - \frac{1}{2uy_0}. \tag{33}$$

Since for $u = 0$ one has to obtain $y_u = y_0$, the physical solution is $y_u = \frac{\sqrt{1+4uy_0^2}-1}{2uy_0}$. In figure 3, we can appreciate how well these GW-based methods are performing against the exact solution in a wide u range.

Interestingly, *odd* iterations quickly converge to the *physical* solution of the direct sc-GW_0, while *even* iterations do also converge but at a slower pace: it can be shown that for $u \to \infty$ their limit forms the sequence of rational numbers $\left\{\frac{1}{2}; \frac{1}{3}; \frac{1}{4}; \frac{1}{5}; \frac{1}{6}; \cdots\right\}$ which ultimately converges to 0. All the *odd* iterations have instead the exact large u limit (namely $y_u = 0$ when $u \to \infty$). One might use this property to improve the convergence of the series.

An important question now is: does the result of the self-consistent procedure depend on the starting point of the iteration? Here we have naturally chosen $y_u^{(0)} = y_0$, but one might fear that this choice is simply lucky. Let us therefore look at the general iterative scheme which is obtained by solving the Dyson equation (23) for $x = 0$

$$y_u = \frac{y_0}{1+y_0uy_u}. \tag{34}$$

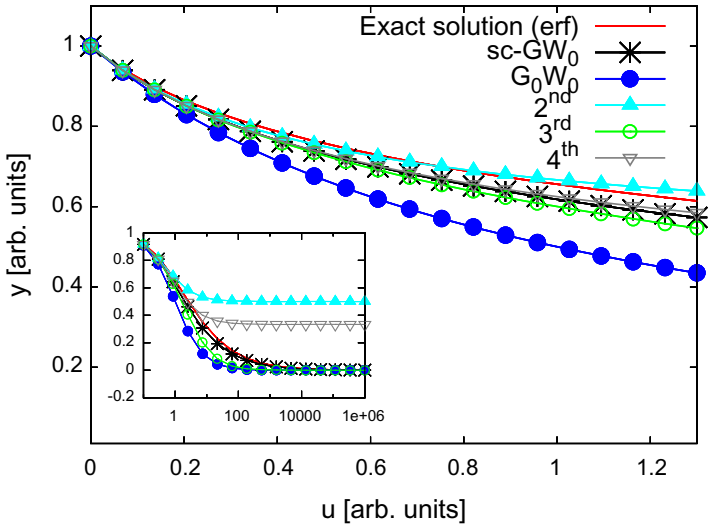

Figure 3. Comparison between the exact solution (red plain line, equation (15)) and different flavors of the GWA. In general, the self-energy-based approximations perform better than iteration of the DE shown in figure 2. In the main panel, the sc-GW_0 (black stars, equation (32)) is the best approximation to the exact result. Iterations starting from $G = G_0$ converge towards the self-consistent result (the second iteration is represented by light blue triangles, the third with green circles and the fourth with gray empty triangles). However, analyzing a larger u range (inset), one observes that odd iterations approach the exact $u = \infty$ limit, while the even ones do not seem to. It can be shown that they also do, but, in a very slow fashion and according to the following sequence: $y^{(2n)}_{u\to\infty} = \{1/2, 1/3, 1/4, 1/5, 1/6, \ldots\}$.

By starting the iteration with a guess for y_u on the right side, one obtains

$$y_u^{(n+1)} = \frac{y_0}{1 + y_0 u y_u^{(n)}}. \tag{35}$$

For $y_u^{(0)} = y^s$, one has, e.g., after the third iteration

$$y_u^{(3)} = \frac{y_0}{1 + \dfrac{uy_0^2}{1+\dfrac{uy_0^2}{1+y_0uy^s}}}. \tag{36}$$

This contains nothing else but the continued fraction representation for the square root

$$\sqrt{1+z} = 1 + \frac{z/2}{1 + \dfrac{z/4}{1+\dfrac{z/4}{1+\dfrac{z/4}{1+\cdots}}}}, \tag{37}$$

corresponding to the physical solution $y_u = \frac{\sqrt{1+z}-1}{2uy_0}$ where $z = 4uy_0^2$. It converges for all values of the terminator y^s. Therefore, *this iteration will always converge to the physical solution.* Does this mean that there is no risk of running into the unphysical solution? The answer is that it depends on the iterative scheme that is used, and *not* on the starting point. Look at the following

way to rewrite the Dyson equation (23): $-uy_u = \frac{1}{y_0} - \frac{1}{y_u}$ (in other words, $\Sigma = G_0^{-1} - G^{-1}$). If we iterate this equation by starting with some $y_u^{(0)} = y^s$ on the rhs, we obtain

$$y_u^{(n+1)} = -\frac{1}{uy_0} + \frac{1}{uy_u^{(n)}}, \tag{38}$$

hence

$$2uy_0 y = -2 - \cfrac{2uy_0^2}{1 + \cfrac{uy_0^2}{1 + \cfrac{uy_0^2}{1 + \cfrac{uy_0^2}{\ddots}}}}, \tag{39}$$

which, with equation (37), is just the continued fraction representation for the unphysical solution $y_u = (-\sqrt{1+4uy_0^2} - 1)/2uy_0$. In a way, this is good news: usually the iterative scheme adopted in the context of GW calculations is rather the first, safe one. Indeed it has been found empirically that such a scheme leads to self-consistent results independent of the starting point and in reasonably good agreement with experiments (see, e.g., [26–28]). However, when one goes beyond GW, higher-order equations appear, as we will see in the following. There are hence more and more solutions, and more and more ways of iterating the equations. In other words, *there will be increased danger of running into the wrong solution*. One should keep this in mind when trying to add vertex corrections beyond GW.

3.2.2. Vertex corrections—first-order Γ. We will now analyze the effects of a first-order vertex correction which is obtained employing $\Sigma_u = -uy_u$ in equation (27) [8, 29]. Solving for Γ_u gives

$$\Gamma_u^{(1)}(y_u) = \frac{1}{1+uy_u^2}. \tag{40}$$

Employing this vertex, the self-energy (25) becomes

$$\Sigma_u^{(1)}(y_u) = -uy_u\left[\frac{1}{1+uy_u^2}\right]. \tag{41}$$

Now two routes can be taken and either a $G_0W_0\Gamma^{(1)}(y_0)$ or a self-consistent $GW_0\Gamma^{(1)}(y_u)$ calculation can be performed. The first of the two is once more based on the initial guess for the GF $y^{(0)} = y_0$, and consequently the vertex and the self-energy in (40) and (41) read, respectively, $\Gamma_u^{(1)}(y_0) = \frac{1}{1+uy_0^2}$ and $\Sigma_u^{(1)}(y_0) = -uy_0\left[\frac{1}{1+uy_0^2}\right]$. Solving the Dyson equation with the above ingredients yields

$$y_u^{G_0W_0\Gamma} = \frac{y_0\left(1+uy_0^2\right)}{1+2uy_0^2}. \tag{42}$$

Instead, solving the Dyson equation in a self-consistent fashion, with the expressions (40) and (41), yields

$$y_u^{GW_0\Gamma} = \sqrt[3]{\frac{y_0}{2u} + \sqrt{\frac{1}{27u^3} + \frac{1}{4u^2}}} - \sqrt[3]{\frac{y_0}{2u} - \sqrt{\frac{1}{27u^3} + \frac{1}{4u^2}}}. \tag{43}$$

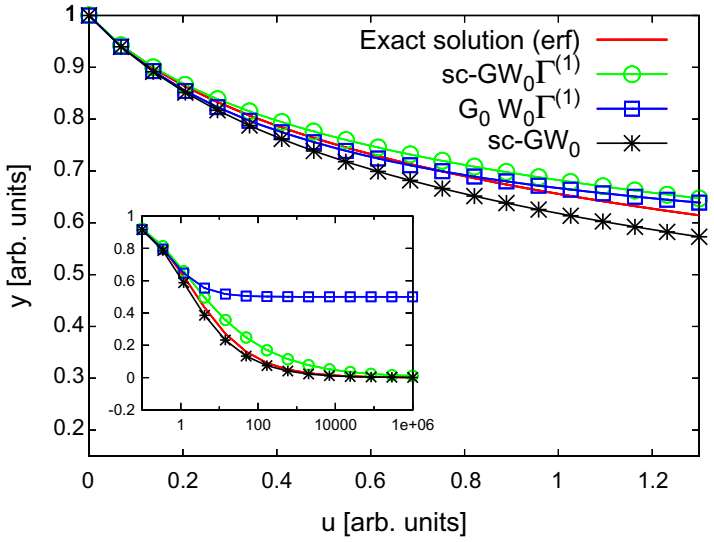

Figure 4. In the main panel, a comparison between the DE's exact solution (red plain line, equation (15)), $G_0W_0\Gamma^{(1)}$ (blue squares, equation (42)), $GW_0\Gamma^{(1)}$ (green empty circles, equation (43)) and sc-GW_0 (black stars, equation (32)) is shown. In this range of u, adding a vertex correction, no matter if within a self-consistent scheme or not, improves over the simpler sc-GW_0. However, analyzing a wide u range (inset, semi-logarithmic plot) gives a different perspective: the first iteration of $G_0W_0\Gamma^{(1)}$ clearly exhibits the wrong $u \to \infty$ limit and the sc-GW_0 scheme becomes the closest approximation to the exact result.

As can be noticed from the result, a cubic equation for the unknown y_u had to be solved within this more sophisticated approach. Again the limit of vanishing interaction has been used to pick the physical solution. In figure 4, we can directly compare the two types of vertex corrections. For small u values their performance is similar; however, in a wider u range (see inset), the $G_0W_0\Gamma^{(1)}$ scheme diverges from the exact solution and has the wrong asymptotic limit $u \to \infty$: it hence behaves as the first iteration of the sc-GW_0 approach, which also exhibits the wrong large u limit. Figure 4 also shows how the $GW_0\Gamma^{(1)}$ scheme, for small u values, slightly improves over the sc-GW_0. However, given the augmented complexity already at this first order of the correction (one could very well iterate further the equations for Γ and Σ and get higher-order corrections), the benefits of employing vertex corrections are not obvious. Also note that, interestingly, on the scale from $u = 0$ to $u \to \infty$, the closest curve to the exact one is the sc-GW_0 one.

4. Exploring other approximations for *G*

In this section, we will explore alternative approximations to the exact solution of the one-point DE and the corresponding manipulations of the initial DE producing them. Here, we will report, in particular, approximations that might be eventually transposed to the full functional framework.

4.1. Continued fraction approximation

A well-known approximation for the error function is its *continued fraction* representation [30]. The exact expression for y_u (equation (15)) transforms into

$$y_u = \frac{1}{\sqrt{2u}} \cfrac{1}{\cfrac{1}{\sqrt{2uy_0^2}} + \cfrac{1/2}{\cfrac{1}{\sqrt{2uy_0^2}} + \cfrac{1}{\cfrac{1}{\sqrt{2uy_0^2}} + \cfrac{3/2}{\cfrac{1}{\sqrt{2uy_0^2}} + \cdots}}}} \tag{44}$$

$$= \cfrac{y_0}{1 + \cfrac{uy_0^2}{1 + \cfrac{2uy_0^2}{1 + \cfrac{3uy_0^2}{1 + \cdots}}}}. \tag{45}$$

We will now show how one can obtain equation (45) starting simply from the initial DE in equation (11), equivalent to (9), without any information about its exact solution. Beginning with equation (11) and taking successively higher-order derivatives of the equation, one obtains

$$\frac{\mathrm{d}y_u(x)}{\mathrm{d}x} = y_0 y_u(x) + y_0 x \frac{\mathrm{d}y_u(x)}{\mathrm{d}x} - u y_0 \frac{\mathrm{d}^2 y_u(x)}{\mathrm{d}x^2}, \tag{46}$$

$$\frac{\mathrm{d}^2 y_u(x)}{\mathrm{d}x^2} = 2y_0 \frac{\mathrm{d}y_u(x)}{\mathrm{d}x} + y_0 x \frac{\mathrm{d}^2 y_u(x)}{\mathrm{d}x^2} - u y_0 \frac{\mathrm{d}^3 y_u(x)}{\mathrm{d}x^3}, \tag{47}$$

$$\frac{\mathrm{d}^3 y_u(x)}{\mathrm{d}x^3} = 3y_0 \frac{\mathrm{d}^2 y_u(x)}{\mathrm{d}x^2} + y_0 x \frac{\mathrm{d}^3 y_u(x)}{\mathrm{d}x^3} - u y_0 \frac{\mathrm{d}^4 y_u(x)}{\mathrm{d}x^4} \tag{48}$$

and so on. Neglecting derivatives e.g. from the fourth order on and then setting $x = 0$, this *truncation* allows us to solve all the above equations, beginning with equation (48) (now an algebraic equation in the unknown $\frac{\mathrm{d}^3 y_u(x)}{\mathrm{d}x^3}$ by keeping $\frac{\mathrm{d}^2 y_u(x)}{\mathrm{d}x^2}$ as parameter); subsequently we insert the result in (47) and solve for $\frac{\mathrm{d}^2 y_u(x)}{\mathrm{d}x^2}$, (46) for $\frac{\mathrm{d}y_u(x)}{\mathrm{d}x}$ and ultimately equation (11), getting

$$y_u = \cfrac{y_0}{1 + \cfrac{uy_0^2}{1 + \cfrac{2uy_0^2}{1 + 3uy_0^2}}}, \tag{49}$$

which is precisely the result obtained by approximating the exact solution with a continued fraction expression for the error function (equation (45)). We will name this manipulation *limited order DE*. In figure 5, we compare the different orders of this approximation to the exact expression for y_u. The approximation gets rapidly closer and closer to the exact solution by including higher derivatives. However, also for this continued fraction, odd and even orders, converge towards the exact result with a different speed. In analogy with the continued fraction of equation (37), even iterations have the correct large u limit, while the odd ones do not, although they do eventually approach it for a very large number of steps. We notice that the above continued fraction converges slower than the one arising from the sc-GW_0; however, the former will eventually converge towards the exact solution, whereas the latter only to the sc-GW_0 result. It is therefore interesting to note that such a procedure can in principle be used

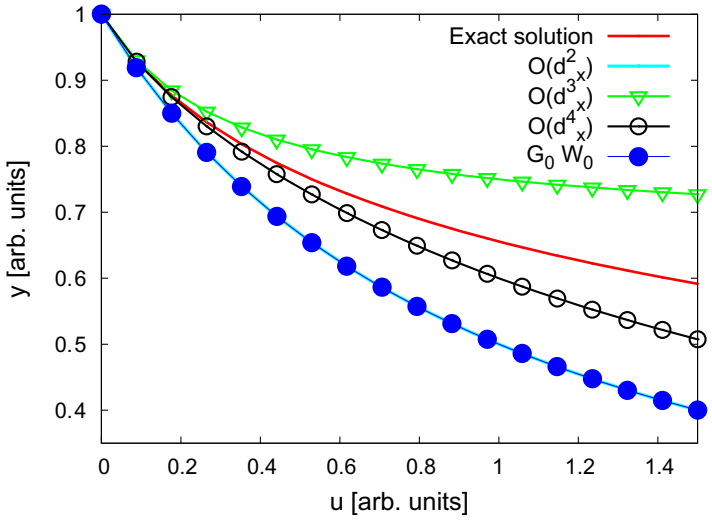

Figure 5. Comparison between the exact solution (red plain line, equation (15)) of the DE and the results obtained through the first three orders of the *limited order DE* (equation (49)). The notation $O(d_x^n)$ indicates that derivatives of order $\geqslant n$ have been neglected. As expected the result improves when more terms are included: the curve $O(d_x^2)$ (light blue line, equation (46)) is superimposed on the G_0W_0 one (dark blue dots, equation (28)) and the curve $O(d_x^4)$ (black circles, equation (48)) is close to the exact result in a small u range.

also in the full functional framework (see related manipulations, e.g., in [6, 31]), where the functional DE can be differentiated to an arbitrary order and the corresponding approximated G obtained. For example, differentiating equation (9) with respect to the external potential $\bar{\varphi}$, one obtains

$$\frac{\delta G(1,2;[\bar{\varphi}])}{\delta\bar{\varphi}(6)} = \int d3G_{\mathrm{H}}^0(1,3)\frac{\delta\bar{\varphi}(3)}{\delta\bar{\varphi}(6)}G(3,2;[\bar{\varphi}]) + \int d3G_{\mathrm{H}}^0(1,3)\bar{\varphi}(3)\frac{\delta G(3,2;[\bar{\varphi}])}{\delta\bar{\varphi}(6)}$$
$$+\mathrm{i}\int d3d5W(3^+,5)G_{\mathrm{H}}^0(1,3)\frac{\delta^2 G(3,2;[\varphi])}{\delta\bar{\varphi}(6)\delta\bar{\varphi}(5)}. \tag{50}$$

Truncating the highest-order derivative $\frac{\delta^2 G}{\delta\bar{\varphi}^2}$ and solving for $\varphi = 0$ (which means also $\bar{\varphi} = 0$) gives

$$\frac{\delta G(1,2;[\bar{\varphi}])}{\delta\bar{\varphi}(5)}\Big|_{\bar{\varphi}=0} = G_{\mathrm{H}}^0(1,5)G(5,2), \tag{51}$$

which reinserted in equation (9) yields

$$G(1,2;[\bar{\varphi}]) = G_{\mathrm{H}}^0(1,2) + \mathrm{i}\int d3d5G_{\mathrm{H}}^0(1,3)W(3^+,5)G_{\mathrm{H}}^0(3,5)G(5,2). \tag{52}$$

Like in the one-point model, this first step simply provides the one-particle GF in the $G_{\mathrm{H}}^0W_0$ approximation to the self-energy. One can go further: differentiating equation (50) with respect

to $\bar{\varphi}$ and neglecting the third-order derivative $\frac{\delta^3 G}{\delta\bar{\varphi}^3}$ yields

$$G(1,2) = G^0_{\mathrm{H}}(1,2) - \mathrm{i}\int d5d3d8d9 G^0_{\mathrm{H}}(1,3) W(3^+,5)\bar{m}^{-1}(3,5;9,8) G^0_{\mathrm{H}}(9,8) G(8,2) \tag{53}$$

with

$$\bar{m}(16;57) := -\delta(15)\delta(76) + \mathrm{i}\int d3 G^0_{\mathrm{H}}(1,3) W(3^+,5)\delta(7,6)\left[G^0_{\mathrm{H}}(3,6) + G^0_{\mathrm{H}}(3,5)\right], \tag{54}$$

which is a four-point quantity of a similar complexity as the Bethe–Salpeter equation [5]. Indeed in the full functional problem the equations become quite involved since terms like uy_0^2 correspond to large matrices. However, the approach does not require self-consistency. This might turn out to be a significant advantage, compared to vertex corrections to Σ, as we have discussed in the previous subsection concerning self-consistency. More details of the derivation are given in appendix C.

4.2. Large u expansions

Perturbation theory usually deals with weak interactions, hence the small u limit. However, it is also very interesting to examine the *large u* limit for several reasons: (i) this is the regime of *strong correlation*, where current approximations exhibit failures; (ii) the large u expansion of the exact solution gives a convergent series (being a product of two convergent Taylor expansions, one for the exponential and the other one for the error function) and one can, for instance, obtain a better approximation to the exact solution by adding higher-order terms (which instead does not improve the result for the small u expansion of the solution); (iii) excellent approximations for the exact solution are *Padé approximants* [32], which have to be constructed using both the small and the large u limit. In this subsection, we will present two possible routes to approach this limit: the first is a straightforward large u expansion of the exact solution for y_u, while the second combines the latter with the large u expansion for the Dyson equation.

4.2.1. Straightforward large u expansion for y_u. By expanding both the exponential prefactor and the error function appearing in equation (15)

$$\mathrm{e}^{\frac{1}{2uy_0^2}} \approx 1 + \frac{1}{2uy_0^2} + \frac{1}{8u^2y_0^4} + \cdots, \tag{55}$$

$$\mathrm{erf}\left[\sqrt{\frac{1}{2uy_0^2}}\right] \approx \frac{2}{\sqrt{\pi}}\left[\sqrt{\frac{1}{2uy_0^2}} - \frac{1}{6uy_0^2}\sqrt{\frac{1}{2uy_0^2}} + \frac{1}{40u^2y_0^5}\sqrt{\frac{1}{2uy_0^2}} + \cdots\right], \tag{56}$$

one obtains for the different orders of the full solution

$$y_u^{(-1/2)} = \sqrt{\frac{\pi}{2u}}, \tag{57}$$

$$y_u^{(-1)} = -\frac{1}{uy_0} + \sqrt{\frac{\pi}{2u}}, \tag{58}$$

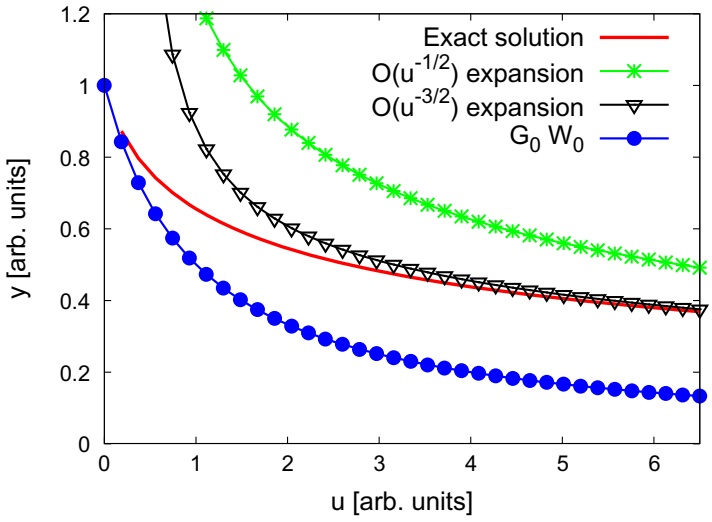

Figure 6. Comparison between the exact solution (red plain line, equation (15)) and the large u expansion for the DE. The green stars and black triangles are, respectively, $O(u^{-1/2})$ and $O(u^{-3/2})$ of the large u expansion (equations (57) and 59)). We also report the G_0W_0 result (blue dots, equation (28)) as an example of a small u expansion. Over a wide u range the large u expansions are very satisfactory.

$$y_u^{(-3/2)} = -\frac{1}{uy_0} + \frac{1}{2uy_0^2}\sqrt{\frac{\pi}{2u}} + \sqrt{\frac{\pi}{2u}}, \tag{59}$$

$$y_u^{(-2)} = -\frac{1}{uy_0} + \frac{1}{2uy_0^2}\sqrt{\frac{\pi}{2u}} - \frac{1}{6u^2y_0^3} + \sqrt{\frac{\pi}{2u}}, \tag{60}$$

$$y_u^{(-5/2)} = -\frac{1}{uy_0} + \frac{1}{2uy_0^2}\sqrt{\frac{\pi}{2u}} - \frac{1}{6u^2y_0^3} + \frac{1}{8u^2y_0^4}\sqrt{\frac{\pi}{2u}} + \sqrt{\frac{\pi}{2u}}, \tag{61}$$

$$y_u^{(-3)} = -\frac{1}{uy_0} + \frac{1}{2uy_0^2}\sqrt{\frac{\pi}{2u}} - \frac{1}{6u^2y_0^3} + \frac{1}{8u^2y_0^4}\sqrt{\frac{\pi}{2u}} + \frac{1}{10u^3y_0^5} + \sqrt{\frac{\pi}{2u}}. \tag{62}$$

Figure 6 shows how these different expansions perform versus the exact result. Overall their behavior is very good for large u and a few orders are sufficient to get a good approximation over a wide u range (which is our ultimate goal); however, for $u = 0$ they all diverge.

4.2.2. Large u expansion for y_u and for the Dyson equation. As u gets larger, Σ_u increases. This implies that, using the Dyson equation for the one-particle GF $y_u = \left(y_0^{-1} - \Sigma_u\right)^{-1}$, one could expand y_u as

$$y_u \approx -\Sigma_u^{-1}\left[1 + y_0^{-1}\Sigma_u^{-1} + y_0^{-1}\Sigma_u^{-1}y_0^{-1}\Sigma_u^{-1}\right]. \tag{63}$$

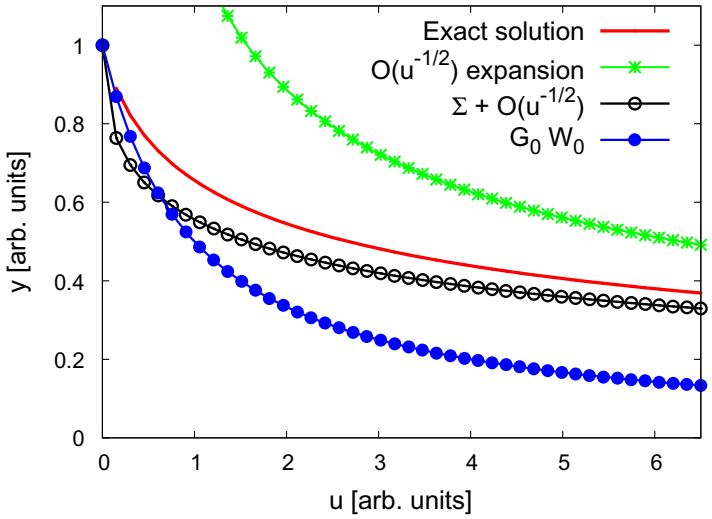

Figure 7. Comparison between the exact solution (plain red line, equation (15)), the G_0W_0 result, the order $O(u^{-1/2})$ of the DE's large u expansion (green stars, equation (57)) and the same order of the DE's large u expansion combined with the large Σ expansion (black dots, equation (66)). We observed that the latter approximation performs extremely well over the range of interactions examined, being even exact in both the large and small u limits.

Hence to lowest order $y_u \approx -\Sigma_u^{-1}$ or

$$\Sigma_u \approx -\frac{1}{y_u}. \tag{64}$$

This simple relation allows us to use the large u expansion of the exact solution for y_u to approximate Σ_u for large u; we can then use this approximate Σ_u in the Dyson equation to recalculate y_u. For example, using the lowest order of the large u expansion of the exact y_u, one gets the following self-energy:

$$\Sigma_u \approx -\left(\sqrt{\frac{\pi}{2u}}\right)^{-1}, \tag{65}$$

which reinserted in the Dyson equation $y_u = (y_0^{-1} - \Sigma_u)^{-1}$ gives

$$y_u \approx \frac{y_0}{1 + y_0\sqrt{\frac{2u}{\pi}}}. \tag{66}$$

In figure 7, the performance of this approximation for y_u is plotted against two orders of the straightforward large u expansion for the GF, G_0W_0 and the exact solution. The 'large Σ' approach shows overall good agreement (generally better than G_0W_0) with the exact solution and has the desirable property of being exact in the small and large u limits, mending the divergence of all orders of the straightforward expansion for y_u. At higher orders of the approximation this property remains true, although undesired poles appear. In conclusion the

methodology is promising and worthwhile to be explored further. The main difficulty is that in the framework of a large u expansion, without knowing the exact solution, one would not straightforwardly know how to set the constant C, i.e. how to pick the physical solution: this issue requires further analysis.

4.3. Self-consistent calculations of the Hartree Green's function and of the screened interaction

In the above discussions, we have treated the Hartree GF and the screened interaction as externally given quantities. This is justified by the fact that realistic calculations are most often following such a pragmatic ansatz. In principle, these quantities should be part of Hedin's self-consistent cycle. A fully self-consistent treatment, in the full functional framework, is out of reach today. In the one-point model, however, it is possible to go beyond this limitation and indeed, the implicit solution of Hedin's equation that has been achieved in the work of [23] contains all quantities calculated on the same footing. Also in the linearized version that is employed in this work, one can obtain the Hartree GF and the screened potential consistently from the equations, as we will discuss in the following. Let us first turn to the Hartree GF y_{H}^0. In terms of the truly non-interacting GF y_0, it reads

$$y_{\mathrm{H}}^0 = \frac{y_0}{1 - y_0 u y_u}; \tag{67}$$

in other words, it depends (through the density) on the solution y_u at vanishing external potential. In a self-consistent scheme this y_{H}^0 should then replace y_0 in the solution equation (15), which leads to an implicit equation for y_u. For a self-consistent treatment of the screened interaction, we can use the fact that the one-point DE can be solved for $\frac{\mathrm{d}y_u}{\mathrm{d}x}$, and insert the result into the expression for the screened interaction u in terms of the bare v, which reads $u = v + v\frac{\mathrm{d}y_u}{\mathrm{d}x}v$. Two routes can be taken. The first one is based on the linearized equation (11) where the interaction is already screened from the very beginning. This leads to a quadratic equation for u, with two solutions,

$$u = \frac{v}{2} \pm \sqrt{\frac{v^2}{4} + v^2 \left\{1 - \frac{y_u}{y_0} + v y_u^2\right\}}. \tag{68}$$

The physical solution is the one of the positive square root, since it approaches the bare v in the limit of vanishing interaction, hence vanishing screening. The second route consists in calculating $\frac{\mathrm{d}y_u}{\mathrm{d}x}$ from the initial equation (10), where the bare y_0 and the interaction v appear. This yields

$$u = v\left(2 - \frac{y_u}{y_0} + v y_u^2\right). \tag{69}$$

In both cases, the solution for u should be used in equation (15), which again makes the expression for the GF implicit. One may argue about which of the two ways of calculating u self-consistently is more adequate. In a realistic calculation one would probably use the former approach in an iterative way: after calculating the GF as a functional of the external potential for a given initial interaction in the linearized DE, one would recalculate the W from the functional derivative and so on. Whatever choice is made, it does not influence the main conclusions that can be drawn from the above considerations. Specifically: (i) a self-consistent calculation leads to an implicit solution (like in the work [23]), which, however, would not be identical to

theirs because of our linearization procedure; (ii) the behavior for the small interaction limit is unchanged by the self-consistent treatment, as one can verify from equations (67)–(69); this means in particular that the constant C is chosen in the same way as before. (iii) Finally, also the discussion about the limit of large interaction remains unchanged: by making the ansatz that to lowest order $y_u \propto \frac{1}{\sqrt{u}}$ one finds consistency.

Altogether, this shows that the linearization of the equations does not imply necessarily that one has to treat the Hartree GF and the screened interaction as externally given quantities. It also shows that a more refined, self-consistent treatment does not change the overall behavior of the solution.

5. Conclusions and outlook

In this paper, we explore several aspects of the set of first-order nonlinear coupled DEs which are conventionally solved perturbatively in order to calculate the one-particle GF. After the linearization of the Hartree potential with respect to the external one, we employ a one-point model where the set of—now linear—DEs reduces to a first-order algebraic DE, which can be solved exactly. This provides insights into the structure of the general family of solutions and how to determine which of them corresponds to the physical one. Within the model, we study the performance of established approaches over the whole range of interaction strengths: we find that iterations towards self-consistency in the GW scheme sensibly improve on the one-shot (G_0W_0) calculation and that including first-order vertex corrections improves the sc-GW_0 results only slightly and only for small u. We also find that in the case of sc-GW_0 two solutions are possible, of which only one is physical. We show that the standard iterative scheme will always converge to the physical solution, although other schemes may yield different results. This is an important finding: when going beyond GW both the number of possible solutions for the GF and the number of possible ways of iterating the equations increase, resulting in a danger of running into the wrong solution. Finally, we explore other approximations to the exact solution that might be transposed to the full functional framework, namely a continued fraction approximation and the expansion for large interaction, and we relate these approximations to the corresponding manipulations of the DE that produce them. These links are crucial for preparing a generalization of the approach to the full functional framework.

Acknowledgments

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Appendix A. Approximation for the Hartree term

Due to the Hartree potential $V_{\mathrm{H}} = -\mathrm{i}\, vG$ the set of DEs (5) is nonlinear. In order to simplify this problem, we first assume that V_{H} is Taylor expandable in terms of the external potential φ:

$$V_{\mathrm{H}}(3;[\varphi]) \approx -\mathrm{i}\int d4v(3^+,4)G(4,4^+;[\varphi])\Big|_{\varphi=0} - \mathrm{i}\int d4d5v(3^+,4)\,\frac{\delta G(4,4^+;[\varphi])}{\delta\varphi(5)}\Big|_{\varphi=0}\varphi(5)+o(\varphi^2). \tag{A.1}$$

The second step is to introduce $G^0_{\rm H}$ defined through

$$G^0_{\rm H}(1,2) = G_0(1,2) + \int d3 G_0(1,3) V^0_{\rm H}(3) G^0_{\rm H}(3,2), \tag{A.2}$$

with $V^0_{\rm H}(3) := -{\rm i}\int d4 v(3^+,4) G(4,4^+;[\varphi])\Big|_{\varphi=0}$. Inserting $V_{\rm H}$ in equation (5) one obtains

$$G(1,2;[\varphi]) = G^0_{\rm H}(1,2) + \int d3 d5 G^0_{\rm H}(1,3)\Big[-{\rm i}\int d4 d5 v(3^+,4)\frac{\delta G(4,4^+;[\varphi])}{\delta\varphi(5)}\Big|_{\varphi=0} + \delta(3,5)\Big]\varphi(5) G(3,2;[\varphi]) + {\rm i}\int d3 d4 G^0_{\rm H}(1,3) v(3^+,4)\frac{\delta G(3,2;[\varphi])}{\delta\varphi(4)}. \tag{A.3}$$

Since $\frac{\delta G}{\delta\varphi}$ in the second term on the rhs of equation (A.3) is a contraction of the two-particle correlation function, it yields the inverse dielectric function

$$-{\rm i}\int d4 v(3^+,4)\frac{\delta G(4,4^+;[\varphi])}{\delta\varphi(5)}\Big|_{\varphi=0} + \delta(3,5) = \epsilon^{-1}(3,5), \tag{A.4}$$

and one gets

$$G(1,2;[\varphi]) = G^0_{\rm H}(1,2) + \int d3 d5 G^0_{\rm H}(1,3)\epsilon^{-1}(3,5)\varphi(5) G(3,2;[\varphi]) + i\int d3 d4 G^0_{\rm H}(1,3) \times v(3^+,4)\frac{\delta G(3,2;[\varphi])}{\delta\varphi(4)}. \tag{A.5}$$

Now a *rescaled* perturbing potential can be introduced:

$$\bar\varphi(3) := \int d5 \epsilon^{-1}(3,5)\varphi(5), \tag{A.6}$$

and using the chain rule $\frac{\delta G}{\delta\varphi} = \frac{\delta G}{\delta\bar\varphi}\frac{\delta\bar\varphi}{\delta\varphi}$ in the last term of the rhs of equation (A.5), we obtain

$$G(1,2;[\bar\varphi]) = G^0_{\rm H}(1,2) + \int d3 d5 G^0_{\rm H}(1,3)\bar\varphi(3) G(3,2;[\bar\varphi]) + {\rm i}\int d3 d5 G^0_{\rm H}(1,3) \times W(3^+,5)\frac{\delta G(3,2;[\bar\varphi])}{\delta\bar\varphi(5)}, \tag{A.7}$$

which is precisely equation (9). Here $W = \epsilon^{-1} v$ is the screened Coulomb potential at vanishing φ. If one approximates the functional derivative $\frac{\delta G}{\delta\bar\varphi} = -G\frac{\delta G^{-1}}{\delta\bar\varphi}G \approx GG$, which comes from assuming the self-energy in the Dyson equation $G^{-1} = G_0^{-1} - v^0_{\rm H} - \Sigma - \bar\varphi$ to be independent of $\bar\varphi$, equation (A.7) becomes

$$G(1,2;[\bar\varphi]) = G^0_{\rm H}(1,2) + \int d3 d5 G^0_{\rm H}(1,3)\bar\varphi(3) G(3,2;[\bar\varphi]) + \int d3 d5 G^0_{\rm H}(1,3) \times \Sigma_{GW}(3,5;[\bar\varphi]) G(5,2;[\bar\varphi]) \tag{A.8}$$

with $\Sigma_{GW}(3,5;[\bar{\varphi}]) = \mathrm{i}\,G(3,5;[\bar{\varphi}])W(3^+,5)$. For $\varphi = 0$, equation (A.8) becomes the Dyson equation for the one-particle GF in the GWA to the self-energy[6]. This confirms that the linearization of V_{H} is a reasonable starting point for further developments.

Appendix B. Solving the DE

Equation (11) can be solved by using standard textbook methods [33, 34]. Here we choose a route that yields precious information for our final aim of generalizing to the full functional problem. A general ansatz for the structure of $y_u(x)$ is

$$y_u(x) = A(x)\cdot\mathcal{I}(x), \tag{B.1}$$

where the only restriction is that A and $\mathcal{I}$ are not zero. Substituting the ansatz in the DE (11) gives

$$A(x)\mathcal{I}(x) = y_0 + y_0 x\,A(x)\mathcal{I}(x) - uy_0\frac{\mathrm{d}A(x)}{\mathrm{d}x}\mathcal{I}(x) - uy_0A(x)\frac{\mathrm{d}\mathcal{I}(x)}{\mathrm{d}x}. \tag{B.2}$$

The idea is now to solve two separate, simpler with respect to the initial one, DEs for $A(x)$ and $\mathcal{I}(x)$. Putting together the lhs and the second and third terms of the rhs of equation (B.2), one obtains

$$A(x)\mathcal{I}(x) = y_0 x\,A(x)\mathcal{I}(x) - uy_0\frac{\mathrm{d}A(x)}{\mathrm{d}x}\mathcal{I}(x). \tag{B.3}$$

We can choose the solution

$$A(x) = \exp\left(\frac{x^2}{2u} - \frac{x}{uy_0}\right), \tag{B.4}$$

which will then determine $\mathcal{I}(x)$. One is now left with the equation for $\mathcal{I}(x)$ reading

$$y_0 - uy_0A(x)\frac{\mathrm{d}\mathcal{I}(x)}{\mathrm{d}x} = 0. \tag{B.5}$$

Plugging in the expression for $A(x)$ previously obtained and integrating on both sides, one obtains

$$\mathcal{I}(x) = \frac{1}{u}\int^x \mathrm{d}t\ \exp\left(\frac{-t^2}{2u} + \frac{t}{uy_0}\right). \tag{B.6}$$

The integral on the rhs is

$$\int^x \mathrm{d}t\ \exp\left(\frac{-t^2}{2u}+\frac{t}{uy_0}\right) = \sqrt{2u}\,\mathrm{e}^{1/2uy_0^2}\int^{\frac{x}{\sqrt{2u}}-\frac{1}{\sqrt{2uy_0^2}}}\mathrm{d}\tilde{t}\mathrm{e}^{-\tilde{t}^2} = \frac{\sqrt{2u\pi}}{2}\,\mathrm{e}^{1/2uy_0^2}\mathrm{erf}\left[\left(x-\frac{1}{y_0}\right)\frac{1}{\sqrt{2u}}\right], \tag{B.7}$$

where the change of variables $\tilde{t} = \left(\frac{t}{\sqrt{2u}} - \frac{1}{\sqrt{2uy_0^2}}\right)$ has been made, and the lower limit of the last integral has been chosen to be zero, which requires to set a constant $\bar{C}(u, y_0)$. Hence

$$\mathcal{I}(x) = \sqrt{\frac{\pi}{2u}}\mathrm{e}^{1/2uy_0^2}\mathrm{erf}\left[\left(x-\frac{1}{y_0}\right)\frac{1}{\sqrt{2u}}\right] + \bar{C}(u, y_0). \tag{B.8}$$

[6] To be precise, here it is not specified how W is obtained—it is in principle the exact W, whereas in GW the screened interaction is usually calculated in the random phase approximation.

The exact solution $y_u(x) = A(x) \cdot I(x)$ is given in equation (14), where $C(u, y_0) = -\sqrt{\frac{2u}{\pi}}\bar{C}(u, y_0)\mathrm{e}^{-1/2uy_0^2}$.

Appendix C. *N*-point continued fraction approximation

We detail here how we have obtained the result of equation (53), or the order $\mathcal{O}(d_x^3)$ of the N-point limited order DE.

The starting point is equation (50), which is differentiated with respect to the external potential, yielding

$$\frac{\delta^2 G(1,2;[\bar{\varphi}])}{\delta\varphi(6)\delta\varphi(7)} = G_{\mathrm{H}}^0(1,6)\frac{\delta G(6,2;[\bar{\varphi}])}{\delta\bar{\varphi}(7)} + G_{\mathrm{H}}^0(1,7)\frac{\delta G(7,2;[\bar{\varphi}])}{\delta\bar{\varphi}(6)} + \int d3 G_{\mathrm{H}}^0(1,3)\bar{\varphi}(3)\frac{\delta^2 G(3,2;[\bar{\varphi}])}{\delta\bar{\varphi}(6)\delta\bar{\varphi}(7)} + \mathrm{i}\int d3d5 W(3^+,5) G_{\mathrm{H}}^0(1,3)\frac{\delta^3 G(3,2;[\bar{\varphi}])}{\delta\bar{\varphi}(7)\delta\bar{\varphi}(6)\delta\bar{\varphi}(5)}. \tag{C.1}$$

Neglecting the term $\frac{\delta^3 G(3,2;[\bar{\varphi}])}{\delta\bar{\varphi}(7)\delta\bar{\varphi}(6)\delta\bar{\varphi}(5)}$ and taking the limit $\varphi = 0$ yields

$$\frac{\delta^2 G(1,2)}{\delta\varphi(7)\delta\varphi(6)} = G_{\mathrm{H}}^0(1,6)\frac{\delta G(6,2;[\bar{\varphi}])}{\delta\bar{\varphi}(7)}\Big|_{\varphi=0} + G_{\mathrm{H}}^0(1,7)\frac{\delta G(7,2;[\bar{\varphi}])}{\delta\varphi(6)}\Big|_{\varphi=0}. \tag{C.2}$$

By substituting back equation (C.2) into equation (50), we obtain

$$\frac{\delta G(1,2;[\bar{\varphi}])}{\delta\bar{\varphi}(6)}\Big|_{\varphi=0} = G_{\mathrm{H}}^0(1,6)G(6,2) + \mathrm{i}\int d3d5 G_{\mathrm{H}}^0(1,3)W(3^+,5) \times\Big[G_{\mathrm{H}}^0(3,6)\frac{\delta G(6,2;[\bar{\varphi}])}{\delta\bar{\varphi}(5)}\Big|_{\varphi=0} + G_{\mathrm{H}}^0(3,5)\frac{\delta G(5,2;[\bar{\varphi}])}{\delta\bar{\varphi}(6)}\Big|_{\varphi=0}\Big]. \tag{C.3}$$

The above equation can be recast in a compact way

$$B_{xy} = B_{xy}^0 + \sum_{qp}\gamma_{(xy)(qp)}B_{qp}, \tag{C.4}$$

namely

$$\frac{\delta G(1,2;[\bar{\varphi}])}{\delta\bar{\varphi}(6)}\Big|_{\varphi=0} = G_{\mathrm{H}}^0(1,6)G(6,2) + \mathrm{i}\int d3d5d7 G_{\mathrm{H}}^0(1,3)W(3^+,5)G_{\mathrm{H}}^0(3,6) \times\delta(7,6)\frac{\delta G(7,2;[\bar{\varphi}])}{\delta\bar{\varphi}(5)}\Big|_{\varphi=0} + \int d3d5d7 G_{\mathrm{H}}^0(1,3) \times W(3^+,5)G_{\mathrm{H}}^0(3,5)\delta(7,6)\frac{\delta G(5,2;[\bar{\varphi}])}{\delta\bar{\varphi}(7)}\Big|_{\varphi=0}. \tag{C.5}$$

In the second term on the rhs, one can exchange, under the integral symbol, the indices 5 and 7, to obtain

$$\frac{\delta G(1,2;[\bar{\varphi}])}{\delta\bar{\varphi}(6)}\Big|_{\varphi=0} = G_{\mathrm{H}}^{0}(1,6)G(6,2) + \mathrm{i}\int d3d5d7 G_{\mathrm{H}}^{0}(1,3)W(3^{+},5)G_{\mathrm{H}}^{0}(3,6)$$
$$\times\delta(7,6)\frac{\delta G(5,2;[\bar{\varphi}])}{\delta\bar{\varphi}(7)}\Big|_{\varphi=0} + \int d3d5d7 G_{\mathrm{H}}^{0}(1,3)W(3^{+},5)$$
$$\times G_{\mathrm{H}}^{0}(3,5)\delta(7,6)\frac{\delta G(5,2;[\bar{\varphi}])}{\delta\bar{\varphi}(7)}\Big|_{\varphi=0}. \tag{C.6}$$

Let us now define the following quantities:

$$\frac{\delta G(1,2;[\bar{\varphi}])}{\delta\bar{\varphi}(6)}\Big|_{\varphi=0} := g(1,6),$$

$$\frac{\delta G(5,2;[\bar{\varphi}])}{\delta\bar{\varphi}(7)}\Big|_{\varphi=0} := g(5,7),$$

$$G_{\mathrm{H}}^{0}(1,6)G(6,2) := g_{0}(1,6),$$

$$m(1,6;5,7) := \mathrm{i}\int d3 G_{\mathrm{H}}^{0}(1,3)W(3^{+},5)\delta(7,6)\left[G_{\mathrm{H}}^{0}(3,6) + G_{\mathrm{H}}^{0}(3,5)\right]. \tag{C.7}$$

Recasting equation (C.6) with the new variables yields

$$g(1,6) = g^{0}(1,6) + \int d5d7\, m(1,6;5,7)g(5,7). \tag{C.8}$$

We solve for g:

$$\int d5d7\Big[m(1,6;5,7) - \delta(1,5)\delta(7,6)\Big]g(5,7) + g_{0}(1,6) = 0. \tag{C.9}$$

Defining

$$\Big[m(1,6;5,7) - \delta(1,5)\delta(7,6)\Big] = \bar{m}(1,6;5,7), \tag{C.10}$$

inserting this expression into equation (C.9):

$$\int d5d7\bar{m}(1,6;5,7)g(5,7) + g_{0}(1,6) = 0, \tag{C.11}$$

and introducing the inverse of $\bar{m}$, one obtains

$$\int d1d6d5d7\bar{m}^{-1}(8,9;1,6)\bar{m}(1,6;5,7)g(5,7) = -\int d1d6\bar{m}^{-1}(8,9;1,6)g_{0}(1,6), \tag{C.12}$$

$$g(8,9) = -\int d1d6\bar{m}^{-1}(8,9;1,6)g_{0}(1,6). \tag{C.13}$$

Transforming back to the *original* variables gives

$$\left.\frac{\delta G(1,2;[\bar{\varphi}])}{\delta\bar{\varphi}(6)}\right|_{\varphi=0} = -\int d9d8\bar{m}^{-1}(1,6;9,8)G_{\mathrm{H}}^{0}(9,8)G(8,2) \tag{C.14}$$

and finally the GF reads

$$G(1,2) = G_{\mathrm{H}}^{0}(1,2) - \mathrm{i}\int d5d3d8d9G_{\mathrm{H}}^{0}(1,3)W(3^{+},5)\bar{m}^{-1}(3,5;9,8)G_{\mathrm{H}}^{0}(9,8)G(8,2). \tag{C.15}$$

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