Self-consistent Green function equations and the hierarchy of approximations for the four-point propagator

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The equation of motion for the Green function is combined with the Bethe-Salpeter equation for the scattering amplitude yielding a concise and formally closed system of three equations that encapsulates the essence of Green function theory. Two of the three equations formally resemble a Dyson-like relation. We prove that this formally simple set is exactly equivalent to Hedin's equations. Our derivation therefore constitutes an alternative to Hedin's derivation which is based on functional derivatives. Furthermore, we briefly discuss how approximations can be introduced as a hierarchy of approximations to the four-point Green function.

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I. INTRODUCTION

Many-body Green function theory is a widespread method in *ab initio* electronic structure theory. Conceptually, Green function theory results from the application of quantum-field-theoretical methods to the electronic many-body problem.[1] The Green functions form an infinite hierarchy but already the simplest Green function, the two-point Green function, allows for the calculation of all expectation values of one-particle operators, of the total ground-state energy, and of the excitation spectrum.[2] From a practical point of view, the main problem with the Green function approach lies in the impossibility of writing down a closed, tractable equation allowing for the determination of the Green function. In practice, Green function perturbation theory is a standard approach.[2,3] Even superior to simple perturbation theory are self-consistent diagrammatic methods that are capable of summing infinitely many subsets of Feynman diagrams. For these, for the past 40 years or so, the universal starting point has been Hedin's set of equations.[4,5] For Hedin's equations a number of approximation schemes have been developed as, for example, the widespread GW approximation.[6–8] The implementation of such approximations[9–13] makes the Green function theory a well-established practice in electronic structure theory.[14]

The main purpose of this paper is to derive a self-consistent set of equations for the Green function starting directly from the equation-of-motion (EOM) theory and combining it with the Bethe-Salpeter equation (BSE). We begin with a short review of the equation-of-motion theory and Green function approach including its connection to the Hartree-Fock approximation. We then shortly review Hedin's equations and the Bethe-Salpeter equation. The central results of the paper are stated in Eqs. (32)–(34). As emphasized before, they are derived directly from the EOM and the BSE, without further approximations, and are in fact not much more than a recast of those equations. As a matter of fact, these equations can be derived also starting either from Hedin's equations[4,5] or from Baym and Kadanoff's work,[15,16] but this rather clouds their underlying physical principle. In fact, we found it more convenient to rederive Hedin's equations from the three equations.

II. OVERVIEW

A. Green function theory

Ultimately, the goal of many-body physics is to extract information about a system described by a Hamiltonian $\hat{H} = \hat{H}_0 + \hat{V}$ acting on a many-body Hilbert space $\mathcal{H}^N = \wedge^N \mathcal{H}$. States in such a Hilbert space are antisymmetrized functions of N (compound) variables, say $(\mathbf{x}\sigma)$. This makes any direct approach through the Schrödinger equation $i\hbar\partial_t \Psi = \hat{H}\Psi$ completely intractable for realistic N. Within the Green function approach, this problem is overcome by the introduction of the two-point propagator

$$i\hbar G(\mathbf{x}t,\mathbf{x}'t') = \langle \Psi_0 | \mathcal{T}\hat{\psi}(\mathbf{x}t)\hat{\psi}^\dagger(\mathbf{x}'t')|\Psi_0\rangle, \tag{1}$$

where Ψ_0 denotes the N-particle ground state of $\hat{H}$ (supposed to be nondegenerate). Explicit spin indices have been omitted. The spin can always be reinstalled by reinterpreting $\mathbf{x}$ as a compound variable consisting of position and spin. Although G is a function (actually a distribution) of only two arguments, no matter how big N is it suffices to evaluate all one-particle operators, the total ground-state energy through the Galitskii-Migdal formula, and the quasiparticle excitation spectrum through the Lehmann representation. The drawback, however, is that it is far from obvious how G can be calculated. Here, two seemingly different *Ansätze* come into play: perturbation theory and equation of motion theory.[17] As the name suggests, equation-of-motion theory starts from the time derivative with respect to the time t of the Green function which by linearity is pulled under the expectation value $\langle\Psi_0||\Psi_0\rangle$ where it acts on the field operator $\hat{\psi}(\mathbf{x}t)$. For the field operator one then uses the Heisenberg equation of motion $i\hbar\partial_t\hat{\psi}(\mathbf{x}t) = [\hat{\psi}(\mathbf{x}t), \hat{H}]$. For a standard Hamiltonian consisting of a kinetic term, an external potential and the Coulomb interaction $v(\mathbf{x}-\mathbf{x}')$, the Heisenberg equation of motion yields

$$i\hbar\partial_t\hat{\psi}(\mathbf{x}t) = -\frac{\hbar^2}{2m}\Delta\hat{\psi}(\mathbf{x}t) + v_{\text{ext}}(\mathbf{x})\hat{\psi}(\mathbf{x}t) + \int d\mathbf{x}'\, v(\mathbf{x}'-\mathbf{x})\hat{\psi}^\dagger(\mathbf{x}'t)\hat{\psi}(\mathbf{x}'t)\hat{\psi}(\mathbf{x}t).$$

This leads to the equation of motion[1,17] for the Green function

$$\left(i\hbar\partial_t + \frac{\hbar^2}{2m}\Delta_{\mathbf{x}} - v_{\text{ext}}(\mathbf{x})\right)G(\mathbf{x}t,\mathbf{x}'t') = \delta(t-t')\delta(\mathbf{x}-\mathbf{x}') + \frac{1}{i\hbar}\langle\mathcal{T}[\hat{\psi}(\mathbf{x}t),\hat{V}]\hat{\psi}^\dagger(\mathbf{x}'t')\rangle, \quad (2)$$

where the last term can be rewritten as

$$-i\hbar\int d\mathbf{x}''\, v(\mathbf{x}-\mathbf{x}'')G^4(\mathbf{x}''t,\mathbf{x}t,\mathbf{x}''t,\mathbf{x}'t'). \quad (3)$$

Here $G^4(\mathbf{x}''t,\mathbf{x}t,\mathbf{x}''t,\mathbf{x}'t')$ is to be understood as the equal-time limit

$$\lim_{t_5\to t^-}\lim_{t_3\to t^+}\lim_{t_4\to t_3^+} G^4(\mathbf{x}''t_3,\mathbf{x}t_5,\mathbf{x}''t_4,\mathbf{x}'t') \quad (4)$$

of the four-point (= two-particle) Green function

$$(i\hbar)^2 G^4(\mathbf{x}_1t_1,\mathbf{x}_2t_2,\mathbf{x}_3t_3,\mathbf{x}_4t_4) = \langle\Psi_0|\mathcal{T}\hat{\psi}(\mathbf{x}_1t_1)\hat{\psi}(\mathbf{x}_2t_2)\hat{\psi}^\dagger(\mathbf{x}_4t_4)\hat{\psi}^\dagger(\mathbf{x}_3t_3)|\Psi_0\rangle.$$

This shows that the Green functions form an infinite hierarchy (the time-dependent generalization to the Bogoliubov-Born-Green-Kirkwood-Yvon hierarchy for the density matrices): due to the Heisenberg equation of motion for the field operator, every equation of motion for the Green function involves a Green function of higher order.

In perturbation theory, one takes a different approach. The famous Gellmann-Low theorem[2] in combination with the cancellation (or linked cluster) theorem expresses the Green function $i\hbar G(\mathbf{x}t,\mathbf{x}'t')$ as a sum $\sum_{n=0}^{\infty}(-\frac{i}{\hbar})^n\frac{\lambda^n}{n!}$ over integrals

$$\int_{-\infty}^{\infty} dt_1\cdots dt_n\langle\Phi_0|\mathcal{T}\hat{H}_{\text{I}}(t_1)\cdots\hat{H}_{\text{I}}(t_n)\hat{\psi}(\mathbf{x}t)\hat{\psi}^\dagger(\mathbf{x}'t')|\Phi_0\rangle_{\text{c}}$$

where Φ_0 is the noninteracting ground state and the time dependence of the field operators is induced by the free Hamiltonian. $\hat{H}_{\text{I}}(t)$ is the two-particle perturbation (here the Coulomb potential) in the interaction picture. By the Wick theorem such an expectation value over field operators can be decomposed into products of two-point Green functions. The cancellation theorem restricts the respective contributions to the so-called connected graphs. The upshot of this is that we have a perturbative expansion of the Green function into expressions of the free Green function G_0 and the Coulomb potential. If one defines the (reducible) self-energy Σ to be the sum over all contributions with external free propagator lines amputated, then trivially $G = G_0 + G_0\Sigma G_0$. The irreducible or proper self-energy $\tilde{\Sigma}$ (sometimes self-energy tout court) is defined as the subsum of Σ consisting of graphs which cannot be put into two pieces by removing a single G_0 line. One shows easily that this implies[2]

$$\Sigma = \tilde{\Sigma} + \tilde{\Sigma}G_0\Sigma, \quad (5)$$

$$G = G_0 + G_0\tilde{\Sigma}G. \quad (6)$$

The last equation is the so-called Dyson equation. Identifying G_0 as the inverse of $i\hbar\partial_t - \hat{H}_0$ and multiplying Eq. (6) from the left with $i\hbar\partial_t - \hat{H}_0$, one sees that the Dyson equation is equivalent to an equation of motion for the Green function of the form $(i\hbar\partial_t - \hat{H}_0)G = 1 + \tilde{\Sigma}G$ [cf. Eq. (2)].

B. Hartree-Fock equations

It is now tempting to simply evaluate $\tilde{\Sigma}$ order by order, e.g., up to first order $\tilde{\Sigma}_1[G_0]$, and calculate $G = G_0 + G_0\tilde{\Sigma}_1[G_0]G$. The first-order self-energy in terms of the Hartree propagator is explicitly given by

$$\Sigma_1[G_0] = i\hbar v(1,3^+)G_0(1,3). \quad (7)$$

We now shortly review how the replacement of the first-order perturbation theory given by $\Sigma_1[G_0]$ with the self-consistent self-energy $\Sigma_1[G]$ leads to the well-known Hartree-Fock approximation.[2] On the one hand, one discovers through iteration that the replacement of $G = G_0 + G_0\tilde{\Sigma}_1[G_0]G$ with the self-consistent equation

$$G = G_0 + G_0\tilde{\Sigma}_1[G]G \quad (8)$$

corresponds to an infinite summation of graphs of arbitrary order which result from the first-order self-energy graphs by all kinds of mutual insertions. On the other hand, by inserting a complete set of $(N\pm1)$-particle eigenstates into the defining equation one shows that the Green function has a so-called Lehmann representation which reads in the frequency domain

$$G(\mathbf{x},\mathbf{x}';\omega) = \sum_{s;N\pm1}\frac{f_s(\mathbf{x})f_s^*(\mathbf{x}')}{\hbar\omega - e_s + \text{sg}(e_s-\mu)i\eta}, \quad (9)$$

where the equation of motion (2) for G implies for the Lehmann amplitudes the quasiparticle equation

$$\left(-\frac{\hbar^2}{2m}\Delta + v_{\text{ext}}(\mathbf{x})\right)f_s^\pm(\mathbf{x}) + \int d\mathbf{x}'\,\tilde{\Sigma}(\mathbf{x},\mathbf{x}';e_s)f_s^\pm(\mathbf{x}') = e_s f_s^\pm(\mathbf{x}),$$

with $\varepsilon_s^\pm = E_s^{N\pm1} - E_0^N$, $f_s^+(\mathbf{x}) = \langle\Psi_0^N|\hat{\psi}(\mathbf{x})|\Psi_s^{N+1}\rangle$, $f_s^-(\mathbf{x}) = \langle\Psi_s^{N-1}|\hat{\psi}(\mathbf{x})|\Psi_0^N\rangle$, and $e_s = \pm\varepsilon_s^\pm$. The decisive point is that the equation $G = G_0 + G_0\tilde{\Sigma}_1[G]G$ implies that the corresponding Lehmann amplitudes fulfill the Hartree-Fock equations.[2] This is a typical example for the generation of a certain approximation by a self-consistent Green function approach. It corresponds to a summation of a subset of infinitely many diagrams.

C. Hedin's equations

As shown by the Hartree-Fock example, self-consistent Green function methods are superior to simple perturbation theory because they imply the summation over infinite subclasses of Feynman graphs. It is therefore desirable to have a self-consistent set of equations which starts from the Dyson equation (6), is in principal exact (in the sense that in its exact version it includes all graphs), and which through the expansion of a certain quantity automatically generates all relevant approximations. This problem has been solved by the introduction of Hedin's equations[4,5]

$$G(1,2) = G_0(1,2) + \int d(3,4)G_0(1,3)\tilde{\Sigma}_{\text{xc}}(3,4)G(4,2), \quad (10)$$

$$\tilde{\Sigma}_{\text{xc}}(1,2) = i\hbar\int d(3,4)G(1,4)W(1,3)\tilde{\Lambda}(4,2;3), \quad (11)$$

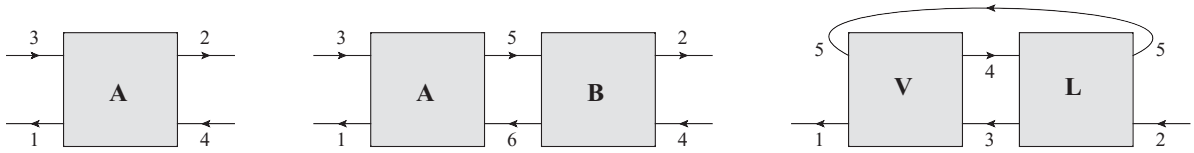

FIG. 1. Four-point formalism.

$$\tilde{P}(1,2) = -i\hbar \int d(5,6)G(1,6)G(5,1^+)\tilde{\Lambda}(6,5;2),$$

$$W(1,2) = v(1,2) + \int d(3,4)v(1,3)\tilde{P}(3,4)W(4,2), \quad (12)$$

$$\tilde{\Lambda}(1,3;2) = \delta(1,2)\delta(2,3) + i\hbar \int d(5,6,7,8)\tilde{I}(1,5,3,6) \times G(6,7)G(8,5)\tilde{\Lambda}(7,8;2),$$

where $\tilde{\Sigma}_{\rm xc}$ is the nonlocal part of the self-energy (the local part being the self-consistent Hartree-type potential) and G_0 is now the inverse of the Hartree operator $i\hbar\partial_t - \hat{H}_0 - v_{\rm H}$, i.e.,

$$[i\hbar\partial_t - \hat{H}_0(1) - v_{\rm H}(1)]G_0(1,2) = \delta(1,2), \quad (13)$$

the density in $v_{\rm H}$ being given by $-i\hbar G(1,1^+) = n(1)$. $\tilde{I}$ is the irreducible scattering amplitude. This is the quantity whose perturbative expansion $\tilde{I}[G,V,W]$ generates all approximations. The standard derivation of Hedin's equations works by complicated formal functional derivatives, the calculation of which is based on the Gellmann-Low formula. Our main purpose in the following is to give a direct rederivation of Hedin's equations from the equation of motion without the use of functional derivatives. To this end, the Bethe-Salpeter equation will be required as well.

D. Bethe-Salpeter equation

The Wick theorem for the free $2n$-point Green functions implies for the free four-point propagator

$$G_0^4(1,2,3,4) = G_0(1,3)G_0(2,4) - G_0(1,4)G_0(2,3). \quad (14)$$

For the full four-point propagator, one therefore makes the *Ansatz*[3]

$$G^4(1,2,3,4) = G(1,3)G(2,4) - G(1,4)G(2,3) - i\hbar \int d(5,6,7,8)G(1,5)G(2,6) \times \Gamma(5,6,7,8)G(7,3)G(8,4), \quad (15)$$

where the so-called scattering amplitude Γ is implicitly defined by this *Ansatz*. A Feynman graph analysis shows that the scattering amplitude Γ is the sum over all amputated graphs which can be put between two electron-hole pairs. If one defines a subsum I which corresponds to all graphs which are irreducible in the electron-hole channel, then one necessarily has

$$\Gamma = I + (i\hbar)IGGI + (i\hbar)^2 IGGIGGI + \cdots$$

implying

$$\Gamma(1,2,3,4) = I(1,2,3,4) + i\hbar \int d(5,6,7,8)I(1,5,3,6) \times G(6,7)G(8,5)\Gamma(7,2,8,4).$$

This is the well-known Bethe-Salpeter equation.[3] We now want to combine the Bethe-Salpeter equation with the equation-of-motion theory into a self-consistent set of equations.

III. SELF-CONSISTENT SET OF EQUATIONS

First, we introduce a consistent notation. We define the following matrix products of four-point quantities:

$$(AB)(1,2,3,4) \stackrel{\rm def}{=} \int d(5,6)A(1,5,3,6)B(6,2,5,4), \quad (16)$$

$$(A \cdot B)(1,2) \stackrel{\rm def}{=} \int d(3,4,5)A(1,4,5,3)B(3,5,4,2). \quad (17)$$

Matrix products of two-point functions are defined in the standard way:

$$(AB)(1,2) \stackrel{\rm def}{=} \int {\rm d}3A(1,3)B(3,2). \quad (18)$$

The matrix multiplication rules can be easily represented graphically (see Fig. 1).

Furthermore, we define a left and a right Dirac distribution via

$$\delta^{\pm}[f] = \int dt\, f(t)\delta(t^{\pm}) = \lim_{t\to 0^{\pm}} f(t). \quad (19)$$

We can think of $\delta^{\pm}$ as acting on an extended space of test functions that are continuous up to countably many jumps. For two-point quantities we introduce the notation $\delta(1,2^+) = \delta(1^-,2)$ with $\delta(1,2^+) = \delta(\mathbf{x}_1 - \mathbf{x}_2)\delta(t_1 - t_2^+)$ indicating that time limit $1 \to 2$ has to be performed such that $t_2 \geqslant t_1$ or $t_2 \to t_1^+$. So, a typical calculation is

$$\int d\,3\delta(1,3^+)F(3,2) = \lim_{t_3\to t_1^+} F(\mathbf{x}_1 t_3, \mathbf{x}_2 t_2). \quad (20)$$

We introduce a four-point Coulomb kernel by

$$V(1,2,3,4) = v(1,4^+)\delta(4,2^+)\delta(3,1^+), \quad (21)$$

with $v(1,2^+) = v(\mathbf{x}_1 - \mathbf{x}_2)\delta(t_1 - t_2^+)$. The advantage of this definition of the four-point Coulomb potential is that it automatically produces the right time order in all products involving V. For example,

$$\begin{aligned}
&\int d(3,4,5)V(1,4,5,3)G^4(3,5,4,2) \\
&= \int d(3,4,5)v(1,3^+)\delta(3,4^+)\delta(5,1^+)G^4(3,5,4,2) \\
&= \lim_{t_5\to t_1^-} \lim_{t_3\to t_1^+} \lim_{t_4\to t_3^+} \int d\mathbf{x}_3\; v(\mathbf{x}_1,\mathbf{x}_3)G^4(\mathbf{x}_3 t_3, \mathbf{x}_1 t_5, \mathbf{x}_3 t_4, \mathbf{x}_2 t_2) \\
&= -(i\hbar)^2 \int d\mathbf{x}_3 v(\mathbf{x}_1 - \mathbf{x}_3)\langle \mathcal{T}\hat{\psi}^\dagger(\mathbf{x}_3 t_1)\hat{\psi}(\mathbf{x}_3 t_1)\hat{\psi}(\mathbf{x}_1 t_1) \\
&\quad \times \hat{\psi}^\dagger(\mathbf{x}_2 t_2)\rangle,
\end{aligned}$$

where the left- and right-Dirac delta imply the limit to be taken such that $t_5 \leqslant t_1 \leqslant t_3 \leqslant t_4$. Thus, using definition (21) one does not have to fix the right equal-time limit *ex post*.

The decisive observation is now that although G^4 does not fulfill a Bethe-Salpeter equation,

$$L(1,2,3,4) = G^4(1,2,3,4) - G(1,3)G(2,4) \tag{22}$$

does. As in Hedin's equation, G_0 from now on denotes the inverse Hartree operator

$$[i\hbar\partial_t - \hat{H}_0(1) - v_{\mathrm{H}}(1)]G_0(1,2) = \delta(1,2).$$

With these definitions, one arrives at the system of equations

$$G = G_0 - i\hbar G_0 V \cdot L, \tag{23}$$

$$L = L_0 + i\hbar L_0 I L, \tag{24}$$

with $L_0(1,2,3,4) = -G(1,4)G(2,3)$. The first equation follows from reexpressing the equations of motion (2) and (3) in terms of L and multiplying with $G_0 = (i\hbar\partial_t - \hat{H}_0 - v_{\mathrm{H}})^{-1}$. In fact, the equation of motion in terms of L simply reads

$$\left(i\hbar\partial_t + \frac{\hbar^2}{2m}\Delta_{\mathbf{x}} - v_{\mathrm{ext}}(\mathbf{x}) - v_{\mathrm{H}}(\mathbf{x})\right)G(\mathbf{x}t,\mathbf{x}'t') = \delta(t-t')\delta(\mathbf{x}-\mathbf{x}') - i\hbar\int dx''\, v(x-x'')L(x'',x,x'',x'),$$

where the equal-time limits in L are to be taken as in the equation of motion in terms of G^4. The GG term in G_0VG^4 produces the Hartree potential v_{H}. Multiplying with the inverse Hartree propagator and using the four-point kernel form of the Coulomb potential then yields Eq. (23) in the form

$$G(1,2) = G_0(1,2) - i\hbar\int d(3,4,5,6)G_0(1,6)V(6,4,5,3) \times L(3,5,4,2).$$

We again stress that the Hartree-type potential v_{H} has to be calculated in terms of the self-consistent density $n(1) = -i\hbar G(1,1^+)$, not in terms of G_0. In particular, that means that $G_0 = G_0[G]$ is a functional of G and cannot simply be replaced by the Hartree propagator. An excellent and well-established approximation, however, seems to be the replacement of the self-consistent density with a fixed density stemming from a density functional theory calculation since density functional theory is supposed to yield the exact ground-state density.

Equation (24) follows from expressing L in terms of Γ as [cf. Eq. (16)]

$$L(1,2,3,4) = -G(1,4)G(2,3) - i\hbar\int d(5,6,7,8) \times G(1,5)G(2,6)\Gamma(5,6,7,8)G(7,3)G(8,4),$$

and iterating the Bethe-Salpeter equation for Γ. This equation coincides with Eq. (43) in the seminal paper of Kadanoff and Baym[15] under the identification (45). In the context of this paper, the equation has been derived by the method of functional derivatives.

The set of equations (23) and (24) is already a self-consistent set of equations which is as closed as Hedin's equations. For every desired level of accuracy one can choose a graphical expansion of $I = I[G,V]$ turning Eqs. (23) and (24) into a closed system. Recall in this context that I is the electron-hole channel irreducible scattering amplitude and the simplest contribution to I is simply V.

Inspired by Hedin's work, we introduce the four-point quantity W through

$$W \overset{\mathrm{def}}{=} V + i\hbar VLV, \tag{25}$$

which is of course the well-known screened potential commonly used in Hedin's equations. Next, we formulate an irreducible counterpart to the above self-consistent system of equations (23) and (24) via the introduction of

$$I \overset{\mathrm{def}}{=} \tilde{I} + V, \quad \tilde{L} \overset{\mathrm{def}}{=} L_0 + i\hbar L_0 \tilde{I}\tilde{L}, \quad \tilde{\Gamma} \overset{\mathrm{def}}{=} \tilde{I} + i\hbar\tilde{I}GG\tilde{\Gamma}.$$

$\tilde{I}$ will later turn out to be the same quantity which appears in Hedin's fifth equation (12), the electron-hole channel irreducible scattering amplitude with the simplest contribution V being removed. With these definitions one finds

$$L = \tilde{L} + i\hbar\tilde{L}VL. \tag{26}$$

This follows from rewriting Eq. (24) as

$$L_0^{-1} - L^{-1} = i\hbar I \tag{27}$$

and hence

$$L_0^{-1} - \tilde{L}^{-1} + \tilde{L}^{-1} - L^{-1} = i\hbar\tilde{I} + i\hbar V. \tag{28}$$

In this argument, we implicitly assumed that L can be inverted. From the definition of L, one reads off that L can certainly be inverted if L_0 can because in that case $L_0^{-1} - i\hbar I$ is the inverse of L. $L_0(1,2,3,4) = -G(1,4)G(2,3)$ in turn can be inverted if G can be inverted. Thus, the invertibility of the full Green function is crucial. This, however, is a standard assumption in any approach, although to the best of our knowledge it has never been proven. Finally, by Eq. (25) one finds

$$\tilde{L}W = \tilde{L}V + i\hbar\tilde{L}VLV = (\tilde{L} + i\hbar\tilde{L}VL)V = LV.$$

Using this and the symmetry properties

$$L(1,2,3,4) = L(2,1,4,3), \tag{29}$$

$$\tilde{L}(1,2,3,4) = \tilde{L}(2,1,4,3), \tag{30}$$

one can show (see Appendix A) that

$$V \cdot L = W \cdot \tilde{L}. \tag{31}$$

On the other hand,

$$W = V + i\hbar VLV = V + i\hbar V\tilde{L}V + (i\hbar)^2 V\tilde{L}VLV = V + i\hbar V\tilde{L}(V + i\hbar VLV) = V + i\hbar V\tilde{L}W.$$

Combining Eqs, (23), (31), and (26), one arrives at the system of equations

$$G = G_0 - i\hbar G_0 W \cdot \tilde{L}, \tag{32}$$

$$\tilde{L} = L_0 + i\hbar L_0\tilde{I}\tilde{L}, \tag{33}$$

$$W = V + i\hbar V\tilde{L}W, \tag{34}$$

where G_0 is given by Eq. (13). In fact, this set of equations—which is the central result of this paper— encapsulates the whole Green function theory and is equivalent to Hedin's equations as shown below.

IV. HEDIN'S EQUATIONS RECONSIDERED

Finally, we come to the question of how the above set of equations is related to Hedin's equations. In order to derive Hedin's equations, one needs to introduce an auxiliary vertex function $\tilde{\Xi}$ through

$$\tilde{\Xi}(1,2,3,4) = \delta(1,4)\delta(2,3) + i\hbar \int d(5,6)\tilde{\Gamma}(1,5,3,6) \times G(6,4)G(2,5), \tag{35}$$

where $\tilde{\Gamma}$ is defined by the Bethe-Salpeter equation $\tilde{\Gamma} = \tilde{I} + i\hbar \tilde{I} G G \tilde{\Gamma}$. With this definition, one shows easily that the auxiliary vertex function obeys a Bethe-Salpeter equation of the form

$$\tilde{\Xi}(1,2,3,4) = \delta(1,4)\delta(2,3) + i\hbar \int d(5,6,7,8)\tilde{I}(1,5,3,6) \times G(6,7)G(8,5)\tilde{\Xi}(7,2,8,4). \tag{36}$$

Furthermore, the exchange-correlation self-energy operator needs to be defined through

$$(i\hbar)^{-1}\tilde{\Sigma}_{\mathrm{xc}}(1,2) \stackrel{\mathrm{def}}{=} \int d(3,4,5,6)G(5,6)W(1,4,5,3)\tilde{\Xi}(6,3,2,4).$$

A straightforward but lengthy calculation (see Appendix B) then shows that

$$-W \cdot \tilde{L} = (i\hbar)^{-1}\tilde{\Sigma}_{\mathrm{xc}} G. \tag{37}$$

One can now rewrite the self-consistent set of equations as

$$G(1,2) = G_0(1,2) + \int d(3,4)G_0(1,3)\tilde{\Sigma}_{\mathrm{xc}}(3,4)G(4,2), \tag{38}$$

$$\tilde{\Sigma}_{\mathrm{xc}}(1,2) = i\hbar \int d(3,4,5,6)G(5,6)W(1,4,5,3)\tilde{\Xi}(3,6,4,2), \tag{39}$$

$$\tilde{L}(1,2,3,4) = -\int d(5,6)G(1,6)G(5,3)\tilde{\Xi}(6,2,5,4), \tag{40}$$

$$W(1,2,3,4) = V(1,2,3,4) + i\hbar \int d(5,6,7,8)V(1,7,3,5)\tilde{L}(5,6,7,8) \times W(8,2,6,4), \tag{41}$$

$$\tilde{\Xi}(1,2,3,4) = \delta(1,4)\delta(2,3) + i\hbar \int d(5,6,7,8)\tilde{I}(1,5,3,6) \times G(6,7)G(8,5)\tilde{\Xi}(7,2,8,4). \tag{42}$$

Here, Eq. (38) follows from inserting Eq. (37) into Eq. (32). Equation (39) is the defining equation for $\tilde{\Sigma}_{\mathrm{xc}}$. Equation (40) follows from multiplying Eq. (35) with GG and comparing with Eqs. (15) and (22). Equation (41) is the defining equation for W and Eq. (42) equals Eq. (36).

In fact, we have derived Hedin's equations if not in their standard form but in their unitarily covariant form. That means that the above equations automatically carry over to an arbitrary orthonormal basis in the one-particle Hilbert space through a simple reinterpretation of the spatial arguments as, e.g., orbital indices. In such a basis, a generic quantity such as $\tilde{L}$ is given by a time-dependent matrix $\tilde{L}^{ij}_{kl}(t_1,t_2,t_3,t_4)$, where the first arguments were written as upper and the last arguments as lower indices. This indicates the different transformation behavior. Under a change of basis $U : \mathcal{H} \to \mathcal{H}$ in the one-particle Hilbert space, the lower indices transform with U^i_j, whereas the upper indices transform with the complex conjugate matrix. This is analogous to the relativistic quantum field theory, where with the fundamental representation of the Lorentz group (or rather the special linear group in two dimensions), one has a complex conjugate representation which transforms with the complex conjugate matrix. (In this field, the respective indices are dotted.) As long as the indices refer to spatial points, we do not have to differentiate between upper and lower indices because a coordinate transformation in real space in the sense of a renumbering of the spatial lattice is implemented by a real valued matrix. Note that in principle, also the time variables group into "covariant" and "contravariant" variables in that under a Fourier transform, they behave as

$$L(\omega_1,\ldots,\omega_4) = \int dt_1 \ldots dt_4 \mathrm{e}^{i(\omega_1 t_1 + \omega_2 t_2)} L(t_1,t_2,t_3,t_4) \mathrm{e}^{-i(\omega_3 t_3 + \omega_4 t_4)}$$

Finally, it should be borne in mind that the above form of Hedin's equations is not invariant under arbitrary basis changes, i.e., they change their form if one goes to a nonorthonormal basis. This is not due to a failure of this formalism but to the definition of the matrix elements of the respective quantities in terms of the scalar product. For example, for the Coulomb potential

$$V^{ij}_{kl} = \int d\mathbf{x}\, d\mathbf{x}'\, \varphi^*_i(\mathbf{x})\varphi^*_j(\mathbf{x}')v(\mathbf{x},\mathbf{x}')\varphi_k(\mathbf{x})\varphi_l(\mathbf{x}')$$

or

$$V^{ij}_{kl} = \langle \varphi_i \varphi_j | \hat{V} | \varphi_k \varphi_l \rangle. \tag{43}$$

This corresponds to a definition of the dual basis as $\varphi^i = \langle \varphi_i | \cdot \rangle$ implying that for arbitrary (i.e., nonunitary) transformations, we do not have $\varphi^i(\varphi_j) = \delta^i_j$. In order to have general form invariance of matrix products in a vector space, one has to introduce a dual basis by $e^i(e_j) = \delta^i_j$ implying that dual vectors transform with the contragredient matrix. This definition of the dual basis and the "quantum mechanical" definition coincide as long as the respective transformation leaves the standard scalar product invariant. *Per definitionem*, this holds true for unitrary transformations. For these, the complex conjugate matrix *is* the contragredient matrix.

The standard form of Hedin's equations is recovered from the unitarily covariant form by introducing $\tilde{P}(1,2) = i\hbar\tilde{L}(1,2,1^+,2^+)$, $\tilde{\Lambda}(1,2;3) = \tilde{\Xi}(1,3,2,3)$. Note that the standard form is valid only in the space-time domain. (One cannot represent $\tilde{P}$ and $\tilde{\Lambda}$ in an orbital basis.) A comparison with the derivation of Hedin's equations from the self-consistent equations with the standard derivation shows, in particular, that

$$i\hbar\tilde{I}(1,2,3,4) = \frac{\delta\tilde{\Sigma}_{\mathrm{xc}}(1,3)}{\delta G(2,4)}, \tag{44}$$

$$i\hbar I(1,2,3,4) = \frac{\delta\tilde{\Sigma}(1,3)}{\delta G(2,4)}. \tag{45}$$

V. STANDARD APPROXIMATIONS

The standard approximations can be formulated very economically within the framework of the self-consistent set of equations. In fact, we see that the standard approximations fit into a hierarchy of approximations for the four-point propagator with ever-increasing accuracy. (Apparently, this has been noticed and discussed for the first time by Baym and Kadanoff.[15,16]) In this hierarchy the accuracy grows along two different directions: inclusions of further graphs by an improved description of $\tilde{I}$ and self-consistency. Therefore, every approximation comes in two different guises: in a self-consistent and in a non-self-consistent version. The self-consistent version of first-order perturbation theory (in terms of the Hartree propagator) is the Hartree-Fock approximation, the self-consistent version of the random-phase approximation (RPA) is the GW approximation, and the self-consistent version of the ladder approximation is the W approximation. The W approximation has already been written down by Hedin (Ref. 4, Appendix, p. 822). In particular, the Hartree-Fock (HF) and GW approximations are, respectively, given by

$$L(1,2,3,4) = -G(1,4)G(2,3), \tag{46}$$

$$\tilde{L}(1,2,3,4) = -G(1,4)G(2,3). \tag{47}$$

The proof is almost trivial and follows simply from plugging in these *Ansätze* in the equation of motion for G in terms of L or $\tilde{L}$, respectively. For example, for the Hartree-Fock approximation one finds

$$\begin{aligned}
&\int d(3,4,5)V(1,4,5,3)L(3,5,4,2)\\
&\quad = -\int d(3,4,5)V(1,4,5,3)G(3,2)G(5,4)\\
&\quad = -\int d(3,4,5)v(1,3^+)\delta(1,5)\delta(4,3)G(3,2)G(5,4)\\
&\quad = -\int d\,3v(1,3^+)G(1,3)G(3,2)
\end{aligned}$$

and hence

$$\tilde{\Sigma}_{\mathrm{xc}}^{\mathrm{HF}}(1,2) \equiv \tilde{\Sigma}_x(1,2) = i\hbar v(1,2^+)G(1,2). \tag{48}$$

Finally, we calculate the corresponding expression in the frequency domain. The Fourier transform $(\mathcal{F}G)(\omega) =: G(\omega)$ is as usually defined as

$$G(\omega) = \int d\tau\, e^{i\omega\tau}G(\tau), \quad G(\tau) = \int \frac{d\omega}{2\pi} e^{-i\omega\tau}G(\omega).$$

In standard treatments, one gets the ill-defined expression $\int d\omega\, G(\omega)$ which is then cured by the *ad hoc* insertion of a convergence factor $e^{i\omega\delta}$. We will see that this is automatically produced in our approach through the left- and right-Dirac deltas. Introducing the time-difference variable $\tau = t_1 - t_2$ we have

$$\tilde{\Sigma}_x(\mathbf{x}_1,\mathbf{x}_2;\tau) = v(\mathbf{x}_1,\mathbf{x}_2)\delta^-(\tau)i\hbar G(\mathbf{x}_1,\mathbf{x}_2;\tau) \tag{49}$$

and hence

$$\begin{aligned}
&\tilde{\Sigma}_x(\mathbf{x}_1,\mathbf{x}_2;\omega)\\
&\quad = v(\mathbf{x}_1,\mathbf{x}_2)\int \frac{d\omega'}{2\pi}(\mathcal{F}\delta^-)(\omega')i\hbar G(\mathbf{x}_1,\mathbf{x}_2;\omega-\omega').
\end{aligned}$$

In Appendix C, we show that

$$(\mathcal{F}\delta^{\pm})(\omega) = \lim_{t\to 0^{\pm}} e^{i\omega t} =: e^{\pm i\omega\delta}, \tag{50}$$

where δ is a positive infinitesimal. From this it can be concluded that

$$\tilde{\Sigma}_x(\mathbf{x}_1,\mathbf{x}_2;\omega) = v(\mathbf{x}_1,\mathbf{x}_2)\int \frac{d\omega'}{2\pi}e^{i\omega'\delta}i\hbar G(\mathbf{x}_1,\mathbf{x}_2;\omega'),$$

i.e., $\tilde{\Sigma}_x(\mathbf{x}_1,\mathbf{x}_2;\omega) := \tilde{\Sigma}_{\mathrm{x}}(\mathbf{x}_1,\mathbf{x}_2)$ is effectively independent of ω. In order to perform the frequency integral, we use the residue theorem (the applicability of which is guaranteed by the factor $e^{i\omega'\delta}$ stemming from the Fourier transform of the instantaneous Coulomb potential) and close the contour in the upper half-plane. This leads to the inclusion of the poles corresponding to the occupied states. Similarly, one argues for the GW approximation. By the equations $-i\hbar W\tilde{L} = \tilde{\Sigma}_{\mathrm{xc}}G$ and $VL = W\cdot L$, we see that $\tilde{L}(1,2,3,4) = -G(1,4)G(2,3)$ implies indeed $\tilde{\Sigma}_{\mathrm{xc}} = -i\hbar WG$. Table I summarizes how all standard approximations fit into a hierarchy of approximations for the four-point propagator of ever-increasing accuracy.[20]

VI. SUMMARY AND CONCLUSIONS

We have shown that the equation-of-motion theory for the Green functions can be combined with the Bethe-Salpeter equation to the self-consistent set of equations (32)–(34),

$$\begin{aligned}
&G = G_0 - i\hbar G_0 W\cdot\tilde{L}, \quad \tilde{L} = L_0 + i\hbar L_0\tilde{I}\tilde{L},\\
&W = V + i\hbar V\tilde{L}W,
\end{aligned}$$

which, as a matter of fact, turns out to be fully equivalent to Hedin's equations thereby providing an alternative proof for them. The first of these equations is somewhere in the middle between the equation of motion for G and the Dyson equation. Multiplying with $G_0^{-1} = i\hbar\partial_t - \hat{H}_0$ would give us back the equation of motion with a Hartree term absorbed in the free Hamiltonian. Factoring out a G from the right in $\tilde{L}$ would give us back the Dyson equation if the factors between G_0 and G are lumped into a new quantity, namely, $\tilde{\Sigma}_{\mathrm{xc}}$. The second equation is essentially the Bethe-Salpeter equation but pulled back on the level of the propagators (instead of scattering amplitudes). It corresponds to Eq. (43) in Ref. 15 but reformulated for the corresponding irreducible quantity $\tilde{L}$ (instead of L). The third equation is the usual equation for the screened potential rewritten as an equation for four-point quantities. This allows for the usage of $\tilde{L}$ as the integral kernel (instead of $\tilde{P}$) which gives the set of equations its compactness.

Other important aspects of this work are a concise four-point notation, and the introduction of a time-ordered Coulomb kernel. The four-point notation allows one to represent all quantities in either a spatial basis, a plane-wave basis, or an orbital basis. Changing the basis only involves unitary transformations between the basis sets. The Green function is then simply a rank two "tensor," whereas $\tilde{L}$ and W are tensors of rank 4 (neglecting the additional time dependencies). This makes implementation in standard quantum chemistry codes, which commonly rely on four-point representations of the Coulomb integrals, fairly easy and concise. Similar approaches are commonly used when the Bethe-Salpeter equation is solved.[19] They have been also applied in the context of

TABLE I. Hierarchy of approximations.

Approximation	L	$\tilde{L}$	L_0	I	$\tilde{I}$
Hartree approximation	0	0	0	0	0
First-order perturbation theory	$\tilde{L}$	L_0	$-G_0G_0$	0	0
Hartree-Fock approximation	$\tilde{L}$	L_0	$-GG$	0	0
Random-phase approximation	$\tilde{L}+i\hbar\tilde{L}VL$	L_0	$-G_0G_0$	V	0
GW approximation	$\tilde{L}+i\hbar\tilde{L}VL$	L_0	$-GG$	V	0
Ladder approximation	$\tilde{L}+i\hbar\tilde{L}VL$	$L_0+i\hbar L_0\tilde{I}\tilde{L}$	$-G_0G_0$	$V+\tilde{I}$	$-\bar{V}$
W approximation	$\tilde{L}+i\hbar\tilde{L}VL$	$L_0+i\hbar L_0\tilde{I}\tilde{L}$	$-GG$	$V+\tilde{I}$	$-\bar{W}$
Beyond	$\tilde{L}+i\hbar\tilde{L}VL$	$L_0+i\hbar L_0\tilde{I}\tilde{L}$	$-GG$	$V+\tilde{I}$	$\tilde{I}[G,V,W]$

GW calculations,[18] but never quite on that fundamental level. A final important contribution of the present work is the introduction of a time-ordered Coulomb interaction. This automatically yields the correct time order in all equations. Furthermore, it leads to a formulation of the fundamental equations which is completely independent of the concrete form of the electron-electron interaction. For example, a general interaction could be of the form $\hat{V}=\int d(1,2,3,4)v(1,2,3,4)\hat{\psi}^\dagger(1)\hat{\psi}^\dagger(2)\hat{\psi}(4)\hat{\psi}(3)$, where $v(1,2,3,4)$ does not partially diagonalize. This interaction would lead to the same fundamental set of self-consistent propagator equations (32)–(34), whereas Hedin's equations for this kind of interaction would not be so obvious.

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APPENDIX A: DOT PRODUCT OF FOUR-POINT QUANTITIES

In this Appendix, we prove that $V\cdot L=W\cdot\tilde{L}$, that $W\cdot\tilde{L}=-(i\hbar)^{-1}\tilde{\Sigma}_{\rm xc}G$ and we explicitly calculate the Fourier transform of the left- and right-Dirac delta as well as the Hartree-Fock approximation in the frequency domain.

We define

$$V'(1,2,3,4)=v(2,3^+)\delta(3,1^+)\delta(4,2^+),$$
$$W'(1,2,3,4)=w(2,3)\delta(3,1^+)\delta(4,2^+).$$

Consequently,

$$V(1,2,3,4)=V'(2,1,4,3), \tag{A1}$$
$$W(1,2,3,4)=W'(2,1,4,3), \tag{A2}$$

i.e., $V^t=V'$ and $W^t=W'$ with the transpose four-point quantity $A^t(1,2,3,4)=A(2,1,4,3)$. From

$$\begin{aligned}&\int d(5,6,7,8)V(1,5,3,6)L(6,7,5,8)V(8,2,7,4)\\&=\int d(5,6,7,8)v(1,6^+)\delta(6,5^+)\delta(3,1^+)\\&\quad\times L(6,7,5,8)v(8,4^+)\delta(4,2^+)\delta(7,8^+)\\&=\delta(3,1^+)\delta(4,2^+)\int d(6,8)v(1,6)L(6,8,6^+,8^+)v(8,4)\end{aligned}$$

(the time order in v is irrelevant under the integral) and the general symmetry property

$$L(1,2,3,4)=L(2,1,4,3),$$

we read off that

$$W'=V'+i\hbar V'LV' \tag{A3}$$

and therefore,

$$\tilde{L}W=LV \tag{A4}$$

implies

$$\tilde{L}W'=LV'. \tag{A5}$$

Now consider

$$\int d(3,4,5)V(1,4,5,3)L(3,5,4,2). \tag{A6}$$

This can be written as

$$\begin{aligned}&\int d\,5\int d(3,4)V(1,4,5,3)L(3,5,4,2)=\int d\,5(VL)(1,5,5,2)\\&=\int d(5,6)\delta(5,6)(VL)(1,5,6,2).\end{aligned}$$

Using $V'^t=V$ and $L^t=L$, we find

$$\begin{aligned}(VL)(1,2,3,4)&=\int d(5,6)V(1,5,3,6)L(6,2,5,4)\\&=\int d(5,6)V'^t(1,5,3,6)L^t(6,2,5,4)\\&=\int d(5,6)V'(5,1,6,3)L(2,6,4,5)\\&=\int d(5,6)L(2,6,4,5)V'(5,1,6,3)\\&=(LV')(2,1,4,3),\end{aligned}$$

whence,

$$\begin{aligned}&\int d(5,6)\delta(5,6)(VL)(1,5,6,2)\\&=\int d(5,6)\delta(5,6)(LV')(5,1,2,6)\\&=\int d(5,6)\delta(5,6)(\tilde{L}W')(5,1,2,6)\\&=\int d(5,6)\delta(5,6)\int d(3,4)\tilde{L}(5,3,2,4)W'(4,1,3,6)\end{aligned}$$

$$= \int d(5,6)\delta(5,6) \int d(3,4)\tilde{L}(3,5,4,2)W(1,4,6,3)$$
$$= \int d(5,6)\delta(5,6) \int d(3,4)W(1,4,6,3)\tilde{L}(3,5,4,2)$$
$$= \int d(5,6)\delta(5,6)(W\tilde{L})(1,5,6,2),$$

i.e., $V \cdot L = W \cdot \tilde{L}$.

APPENDIX B: SELF-ENERGY

We now show that $-W \cdot \tilde{L} = (i\hbar)^{-1}\tilde{\Sigma}_{\rm xc}G$. We start with

$$(W \cdot \tilde{L})(1,2) = \int d(3,4,5)W(1,4,5,3)\tilde{L}(3,5,4,2)$$
$$= -\int d(3,4,5)W(1,4,5,3)\Big[G(3,2)G(5,4) + i\hbar \int d(9,6,7,8) \times G(3,9)G(5,6)\tilde{\Gamma}(9,6,7,8)G(7,4)G(8,2)\Big]$$
$$= -\int d(3,8,4,5)W(1,4,5,3)\Big[\delta(8,3)G(8,2)G(5,4) + i\hbar \int d(9,6,7)G(3,9)G(5,6)\tilde{\Gamma}(9,6,7,8)G(7,4)G(8,2)\Big],$$

where we used Eqs. (15), (22), (26) to go from the first to the second line. Introducing now the exchange-correlation self-energy $\tilde{\Sigma}_{\rm xc}$ by

$$(i\hbar)^{-1}\tilde{\Sigma}_{\rm xc}(1,8) = \int d(3,4,5)W(1,4,5,3)\Big[G(5,4)\delta(8,3) + i\hbar \int d(9,6,7)G(3,9)G(5,6) \times \tilde{\Gamma}(9,6,7,8)G(7,4)\Big]$$
$$= \int d(5,6)G(5,6) \int d(3,4)W(1,4,5,3) \times \Big[\delta(6,4)\delta(8,3) + i\hbar \int d(9,7)\tilde{\Gamma}(6,9,8,7) \times G(3,9)G(7,4)\Big]$$
$$= \int d(5,6)G(5,6) \int d(3,4) \times W(1,4,5,3)\tilde{\Xi}(6,3,8,4)$$
$$\stackrel{\rm def}{=} \int d(3,4,5,6)G(5,6)W(1,4,5,3)\tilde{\Xi}(6,3,8,4),$$

we get

$$-(W\cdot\tilde{L})(1,2) = (i\hbar)^{-1}\int d\,3\tilde{\Sigma}_{\rm xc}(1,3)G(3,2). \quad \text{(B1)}$$

APPENDIX C: FOURIER TRANSFORM OF LEFT AND RIGHT DELTA

Finally, in order to calculate the Fourier transform of $\delta^{\pm}$, we apply it to a test function and find

$$(\mathcal{F}^{-1}\delta^{\pm})[\tilde{f}] \stackrel{\rm def}{=} \delta^{\pm}[\mathcal{F}^{-1}\tilde{f}] = \delta^{\pm}\left(\int \frac{d\omega}{2\pi}e^{-i\omega t}\tilde{f}(\omega)\right)$$
$$= \lim_{t\to 0^{\pm}}\int \frac{d\omega}{2\pi}e^{-i\omega t}\tilde{f}(\omega)$$
$$\stackrel{!}{=} \int \frac{d\omega}{2\pi}(\mathcal{F}\delta^{\pm})(-\omega)\tilde{f}(\omega).$$

From this, we read off that

$$(\mathcal{F}\delta^{\pm})(\omega) = \lim_{t\to 0^{\pm}} e^{i\omega t} =: e^{\pm i\omega\delta},$$

where δ is a positive infinitesimal in the distributional sense (i.e., integrate first and then perform the limit $\delta \to 0$). This implies

$$\tilde{\Sigma}_x(\mathbf{x}_1,\mathbf{x}_2;\omega) = \frac{i\hbar}{2\pi}v(\mathbf{x}_1,\mathbf{x}_2)\int d\omega'\, e^{-i\omega'\delta}G(\mathbf{x}_1,\mathbf{x}_2;\omega-\omega')$$
$$= \frac{i\hbar}{2\pi}v(\mathbf{x}_1,\mathbf{x}_2)\int d\omega'\, e^{-i(\omega-\omega')\delta}G(\mathbf{x}_1,\mathbf{x}_2;\omega')$$
$$= \frac{i\hbar}{2\pi}v(\mathbf{x}_1,\mathbf{x}_2)\int d\omega'\, e^{i\omega'\delta}G(\mathbf{x}_1,\mathbf{x}_2;\omega').$$

where it has been used that the convolution is commutative: $f * g = g * f$. The resulting prefactor $e^{i\omega\delta}$ does not feel the integration and becomes unity after performing the limit $\delta \to 0$.

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