L16: Many-Body Perturbation Theory via Functional Derivatives

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Contents

1 Introduction and Motivation

These notes review key aspects of many-body perturbation theory (MBPT) and the functional-derivative framework for the one-body Green's function. They cover the background needed to understand how one writes the *equation of motion* for the Green's function, how two-particle correlation functions emerge, and how one can organize an approximation strategy in terms of self-energies and functional derivatives.

Chapter 10 in the book serves as essential preparation for studying the RPA (random phase approximation) and the GW approximation for the self-energy.

2 Equation of Motion for the One-Body Green's Function

2.1 Definitions and Background

The one-body Green's function, denoted by G, can be defined (for zero temperature, time-ordered version) as

$$G(1,1') \;=\; -\,i\,\langle 0|\,T\big[\hat{\psi}(1)\,\hat{\psi}^{\dagger}(1')\big]\,|0\rangle, \tag{1}$$

where we use short-hand notation $(1) \equiv (x_1, t_1)$ to specify spatial and spin variables $x_1 = (\mathbf{r}_1, \sigma_1)$, plus time t_1. The operator $\hat{\psi}(1)$ annihilates an electron at $(\mathbf{r}_1, \sigma_1, t_1)$, and $\hat{\psi}^{\dagger}(1')$ creates an electron at $(\mathbf{r}_{1'}, \sigma_{1'}, t_{1'})$. The symbol T denotes time ordering. At finite temperature, similar definitions exist with Matsubara imaginary-time operators or contour-ordered operators.

From the Heisenberg equations of motion for the field operators, one obtains an equation of motion for G. For a standard many-body Hamiltonian,

$$\hat{H} \;=\; \int dx\,\hat{\psi}^{\dagger}(x)\,h(x)\,\hat{\psi}(x) \;+\; \frac{1}{2}\iint dx\,dx'\,\hat{\psi}^{\dagger}(x)\,\hat{\psi}^{\dagger}(x')\,v_c(x,x')\,\hat{\psi}(x')\,\hat{\psi}(x), \tag{2}$$

where $h(x) = -\frac{1}{2}\nabla^2 + v_{\text{ext}}(x)$ is the single-particle (kinetic plus external) part, and v_c is the instantaneous Coulomb interaction, the resulting equation is:

$$\Big[i\,\partial_{t_1} \;-\; h(x_1)\Big]\,G(1,1') \;+\; i\int dx_2\,v_c(x_1,x_2)\,G_2(1,2;\,1',2^+) \;=\; \delta(1,1'), \tag{3}$$

where G_2 is the two-particle Green's function, and (2^+) indicates an infinitesimal time shift to maintain proper time ordering.

The presence of G_2 shows that the one-body equation is not closed; it references two-particle correlations. Proceeding to write the equation of motion for G_2 brings in a three-particle Green's function, etc.–leading to the intractable Martin–Schwinger hierarchy.

2.2 Introducing the Two-Particle Correlation Function L

A convenient step is to separate a product of one-body Green's functions out of G_2. Specifically, define the two-particle correlation function L by

$$G_2(1,2;\,1',2') \;=\; -\,L(1,2;\,1',2') \;+\; G(1,1')\,G(2,2'). \tag{4}$$

In a non-interacting or uncorrelated system, one would have $G_2 \equiv G \times G$, so L would vanish. For an interacting system, the difference from the product piece is precisely the "excess correlation" part.

When we insert Eq. (4) back into the equation of motion (3), one obtains an equation for G in terms of L. In fact, one can isolate the simpler product $G \times G$ from the more complicated correlations. Concretely:

$$G(1,1') \;=\; G_0(1,1') \;+\; G_0(1,2)\,\big[v_H(2)\big]\,G(2,1') \;+\; i\,G_0(1,2)\,v_c(2,3)\,L\big(2,3^+;\,1',3^{++}\big). \tag{5}$$

Here G_0 is the non-interacting Green's function, and v_H the Hartree potential. The correlation piece is now carried by L. However, we still need to determine L.

3 Functional-Derivative Approach

Rather than writing a higher-order chain of equations for $G_2, G_3, G_4, \ldots$, an elegant *functional-derivative* method rewrites the two-particle Green's function as a variation of G with respect to an artificial external potential. This yields a single (though complicated) integral–differential equation for G, avoiding direct references to G_2.

3.1 Key Identities with External Perturbation u

Central trick: add a small, fictitious external potential $u(3)$ to the Hamiltonian, so that it couples to the electron density at point (3),

$$\hat{H} \;\to\; \hat{H} + \int d3\, u(3)\, \hat{n}(3).$$

Denote the resulting one-body Green's function by G_u. Then one shows that

$$\frac{\delta G_u(2,1')}{\delta u(3)} \;=\; L_u(2,3;\, 1',3^+). \tag{6}$$

Hence the two-particle correlation function emerges as a functional derivative of G_u. In the end, we take $u \to 0$; that is, the external potential is *purely formal.* But this derivative at $u = 0$ encodes exactly the same correlation effects that would appear as G_2.

Replacing $\mathbf{G_2} \mapsto \boldsymbol{\delta G/\delta u}$. In the single-particle equation of motion, the term involving G_2 can now be replaced by a term involving $\delta G_u/\delta u$. Thus:

$$G_u(1,1') \;=\; G_0(1,1') \;+\; G_0(1,2)\left[u(2) + v_H(2)\right] G_u(2,1') \;+\; i\, G_0(1,2)\, v_c(2,3)\, \frac{\delta G_u(2,1')}{\delta u(3^+)}. \tag{7}$$

At the end, we set $u \to 0$. The result is a (nonlinear) functional-differential-integral equation in terms of *one unknown function* G, rather than infinite coupled $G, G_2, G_3, \ldots$.

Physical Meaning of Turning Off u→ 0

We do not physically apply this external field. Instead, the field is a "mathematical probe"—we see how G changes if we add an infinitesimal potential at (3), i.e. how the system responds. After performing the derivative, we revert to $u = 0$. This approach is in the same spirit as adding an infinitesimal source $J(\phi)$ in quantum field theory to generate correlation functions by $\delta/\delta J$, or adding a small potential in linear-response Kubo formulas $\chi = \delta n/\delta v$.

4 Dyson Equations

Motivation. Previous sections introduced how the one-body Green's function G can be expressed via its own equation of motion, which depends on the two-particle correlation function L. To close the hierarchy, one uses functional derivatives. However, the resulting perturbation expansions are still complicated. Dyson equations reorganize these expansions into simpler integral forms that allow one to sum infinite series of diagrams. The goal is to understand why reformulating the problem in a Dyson form clarifies (i) how interactions renormalize quasi-particle energies, (ii) why one writes an additive *self-energy*, and (iii) how summing Dyson-like expansions resums infinite series of perturbation diagrams.

Summary of Key Results.

- A shortcoming of *directly* iterating the one-body equation of motion

$$G_u(1,1') \;=\; G_0(1,1') \;+\; G_0\left[u + v_H\right] G_u \;+\; i\, G_0\, v_c\, \frac{\delta G_u}{\delta u}$$

can be seen by simple examples (like the Hartree approximation). Iterating a finite series of diagrams may produce spurious multi-pole structures, rather than a pole shift. Recasting the equation into Dyson form avoids that proliferation of poles and allows one to handle many-body corrections with an additive self-energy.

- The *self-energy*, denoted Σ, captures exchange–correlation effects beyond the classical (Hartree) potential. One typically splits $\Sigma = \Sigma_H + \Sigma_{\mathrm{xc}}$; the latter is dynamic and non-local.
- Writing the Green's function as

$$G^{-1} \;=\; G_0^{-1} \;-\; \Sigma \qquad \text{(Dyson equation)},$$

  highlights that Σ modifies the non-interacting propagation to yield the full, dressed Green's function.
- The *Bethe–Salpeter approach* extends these ideas to the two-particle Green's function/correlation function L. One obtains a *kernel* Ξ (related to Σ) in an integral equation that captures collective excitations (e.g. electron–hole pairs).
- Solving (or approximating) Dyson-like equations leads to infinite resummations of many-body diagrams. This is a corner-stone of self-consistent perturbation theory and functional approaches.

4.1 Motivation: Why the Dyson Equation?

The one-body equation of motion,

$$G_u(1,1') \;=\; G_0(1,1') \;+\; G_0(1,2)\,\big[u(2)+v_H(2)\big]\,G_u(2,1') \;+\; i\,G_0(1,2)\,v_c(2,3)\,\frac{\delta G_u(2,1')}{\delta u(3^+)}, \tag{8}$$

is a functional-differential equation in which all many-body effects are built by iterating in the fictitious external field u. However, *simply* iterating such expansions may yield an ever-increasing number of poles, rather than the physically correct shift of the main quasi-particle pole.

A more robust route is to recast it in *inverse-operator* form, defining an *exchange–correlation self-energy* Σ_{xc}. This is reminiscent of how one solves simpler linear equations by factoring out known parts and collecting the "correction" in a single operator. In many-body theory, the resulting object Σ becomes the non-trivial element in the *Dyson equation*:

$$[G^{-1}](1,1') \;=\; [G_0^{-1}](1,1') \;-\; \Sigma(1,1').$$

4.2 From the Functional-Differential Equation to the Dyson Equation

4.2.1 Starting Point: Functional-Differential Equation

We begin with the equation of motion in the presence of a small fictitious potential u, sometimes called the "Schwinger–Dyson" or "functional-differential" equation:

$$G_u(1,1') = G_0(1,1') \;+\; G_0(1,2)\,\big[u(2)+v_H(2)\big]\,G_u(2,1') \;+\; i\,G_0(1,2)\,v_c(2,3)\,\frac{\delta G_u(2,1')}{\delta u(3^+)}. \tag{9}$$

Here:

- G_u is the one-body Green's function in the presence of the potential u.

- G_0 is the non-interacting Green's function.
- $v_H(2)$ is the Hartree potential.
- $\delta G_u/\delta u$ plays the role formerly occupied by G_2 in the Martin–Schwinger hierarchy.

Direct iteration of (9) can proliferate unphysical multi-pole structures. Instead, we recast the problem in *inverse-operator* form.

4.2.2 Introducing G_u^{-1}

Define the inverse Green's function G_u^{-1} by the usual integral relation

$$\int d1''\, G_u^{-1}(1,1'')\, G_u(1'',1') = \delta(1,1').$$

We wish to rewrite (9) so as to isolate a single operator capturing all many-body effects beyond G_0.

4.2.3 Moving to Inverse Form: Combine with G_0^{-1}

A standard route (see many-body texts) is to multiply or operate with G_0^{-1} on (9), and use the fact that

$$G_0^{-1}(1,1') - G_u^{-1}(1,1') \quad = \quad (\text{'interactions' dressing}).$$

After appropriate rearrangements and applying the chain rule, one finds an expression of the form:

$$G_u^{-1}(1,1') = G_0^{-1}(1,1') \;-\; \big[u(1) + v_H(1)\big]\delta(1,1') \;-\; i\, v_c(1,2)\, \frac{\delta G_u(1,3)}{\delta u(2^+)}\, G_u^{-1}(3,1'). \tag{10}$$

This is the *inverse-operator* statement corresponding to (9). The last term arises via the chain rule for $\delta G_u/\delta u$.

4.2.4 Defining the Self-Energy Σ

Group everything *beyond* G_0^{-1} into one operator, called the *self-energy*:

$$\Sigma(1,1') \;\equiv\; \underbrace{\big[u(1) + v_H(1)\big]\delta(1,1')}_{\text{local potential}} \;+\; \underbrace{i\, v_c(1,2)\, \frac{\delta G_u(1,3)}{\delta u(2^+)}\, G_u^{-1}(3,1')}_{\text{correlation \& exchange}}.$$

Hence (10) becomes

$$G_u^{-1}(1,1') = G_0^{-1}(1,1') \;-\; \Sigma(1,1').$$

When $u \to 0$, we identify $\Sigma = \Sigma_H + \Sigma_{\text{xc}}$ (Hartree + exchange–correlation) for the physical system.

4.2.5 The Dyson Equation

Inverting the relation

$$G_u^{-1} = G_0^{-1} - \Sigma$$

yields the well-known *Dyson equation* for G_u:

$$G_u = G_0 + G_0\, \Sigma\, G_u,$$

or in integral notation,

$$G_u(1,1') = G_0(1,1') \; + \; \int d2\, d3 \;\; G_0(1,2)\, \Sigma(2,3)\, G_u(3,1'). \tag{11}$$

In the limit $u \to 0$, we revert to the physical interacting Green's function G, with the corresponding Dyson equation capturing all orders of many-body diagrams.

4.2.6 Pole Structure

By writing the theory in an inverse-operator form, we avoid spurious multi-poles in partial expansions. Instead, a *single* pole (or broadened resonance) is shifted or damped by Σ. Mathematically,

$$G(\mathbf{k},\omega) = \frac{1}{\omega - \epsilon_{\mathbf{k}} - \Sigma(\mathbf{k},\omega)},$$

which physically describes the quasi-particle energy renormalizations and lifetimes, rather than generating multiple unphysical poles by naive iteration.

4.2.7 Conclusion of the Inverse-Form Logic

1. We began with (9), the functional-differential equation in u.
2. We introduced G_u^{-1} and combined G_0^{-1} with the chain rule to identify Σ as an additive correction.
3. Solving the integral Dyson equation (11) now resums infinitely many diagrammatic contributions once an approximation for Σ is chosen (e.g. Hartree–Fock, GW, T-matrix, etc.).

Thus, the *inverse-operator* method reorganizes expansions into a *single self-energy* operator Σ, which we then solve via the Dyson equation to incorporate infinitely many many-body diagrams in a controlled manner.

4.3 Interpretation and Practical Value

Infinite Summation of Diagrams. The self-energy Σ can itself be expanded in diagrams (for instance, Fock, second-order, ring diagrams, etc.). Solving the Dyson equation with that Σ amounts to an infinite resummation. This is crucial for capturing long-range screening, plasmons, and repeated scattering processes, making the Dyson approach indispensable in computational many-body theory.

Connection to the Bethe–Salpeter Equation. One can similarly write a Dyson-like integral equation for the two-particle correlation function, leading to the Bethe–Salpeter equation. The *interaction kernel* there is closely related to Σ. This is vital for excitonic and optical-absorption analysis.

Conserving Approximations. If Σ is built from skeleton diagrams in terms of the full G, one obtains a "Φ-derivable" or "conserving" approximation, satisfying macroscopic conservation laws. This highlights how the Dyson concept enforces gauge invariance and continuity equations, provided Σ is derived consistently.

5 A Starting Point for Approximations

Motivation. We want a practical scheme for Σ. The formal structure is given by Schwinger–Dyson equations, but we must choose which diagrams or which functional derivatives to keep. Section 10.5 shows how to group diagrams to produce standard approximations.

5.1 Analysis of the Self Energy equation

In this section, we examine how Eqs. (10.34), (10.35), (10.36), and (10.37) are derived in sequence. These equations come from expressing the self-energy $\Sigma(1,2)$ as a functional of the Green's function G and its variation with respect to the external potential u. We assume the usual decomposition

$$G^{-1} = G_0^{-1} - (u + v_H + \Sigma)$$

and that all arguments (1), (2), etc., each contain both space–spin and time labels, such as (r_1, σ_1, t_1).

We start with:

$$\Sigma(1,2) \;=\; v_H(1,2) \;-\; i\, v_c(1,4)\, G(1,3)\, \frac{\delta G^{-1}(3,2)}{\delta u(4^+)}. \tag{10.34}$$

Recall that $v_H(1,2) \equiv v_H(1)\,\delta(1,2)$ is the Hartree contribution, and v_c is the Coulomb interaction. The factor $\frac{\delta G^{-1}(3,2)}{\delta u(4^+)}$ arises because the Green's function G (and hence G^{-1}) depends on the external potential u.

Splitting δG^{-1}. We use the fact that

$$G^{-1}(3,2) \;=\; G_0^{-1}(3,2) \;-\; u(3)\,\delta(3,2) \;-\; v_H(3,2) \;-\; \Sigma(3,2).$$

Hence the variation $\frac{\delta G^{-1}(3,2)}{\delta u(4^+)}$ naturally separates into two parts:

$$\frac{\delta G^{-1}(3,2)}{\delta u(4^+)} \;=\; \frac{\delta}{\delta u(4^+)}\Big[-\,u(3)\,\delta(3,2)\Big] \;-\; \frac{\delta\Sigma(3,2)}{\delta u(4^+)},$$

where the derivative of the local piece $-\,u(3)\delta(3,2)$ is $-\,\delta(3,4)\,\delta(3,2)$. Hence,

$$\frac{\delta G^{-1}(3,2)}{\delta u(4^+)} \;=\; -\,\delta(3,4)\,\delta(3,2) \;-\; \frac{\delta\Sigma(3,2)}{\delta u(4^+)}.$$

Substituting this back into Eq. (10.34) yields two contributions: one from the local delta-function piece, and one from $\frac{\delta\Sigma}{\delta u}$.

Collecting the terms leads to Eq. (10.35). The local variation $-\,\delta(3,4)\,\delta(3,2)$ coupled with the factor $-\,i\,v_c(1,4)\,G(1,3)$ becomes a plus sign overall and gives the first bracket $\delta(3,2)\delta(3,4)$. The second piece is recognized as the chain rule expression that involves $\frac{\delta\Sigma}{\delta u}$. Thus one obtains

$$\Sigma(1,2) \;=\; v_H(1,2) \;+\; i\, v_c\big(1^+,4\big)\, G(1,3)\Big[\delta(3,2)\,\delta(3,4) \;+\; \frac{\delta\Sigma(3,2)}{\delta u(4)}\Big]. \tag{10.35}$$

This is exactly the statement of Eq. (10.35). To proceed to Eq. (10.36), one notices that $\Sigma_x(1,2) = i\,G(1,2)\,v_c(1^+,2)$ is essentially the Fock exchange term, plus a correction from Σ_c. The presence of $\delta(3,4)\,\delta(3,2)$ implies a short-range local contact $(3 = 2, 3 = 4)$.

Identifying the derivative $\delta(v_H+\Sigma_{\mathrm{xc}})$. The term $\frac{\delta\Sigma}{\delta u(4)}$ is interpreted as part of $\frac{\delta(v_H+\Sigma_{\mathrm{xc}})}{\delta G}$ times $\frac{\delta G}{\delta u}$.

The final result re-expresses these local manipulations and derivative chain-rules into

$$\Sigma(1,2) \;=\; v_H(1,2) \;+\; i\,v_c(1^+,4)\,G(1,3)\Big[\delta(3,2)\,\delta(3,4) \;+\; \delta\big(v_H+\Sigma_{\mathrm{xc}}\big)/\delta G \;\times\; \frac{\delta G}{\delta u(4)}\Big], \qquad (10.36)$$

matching the structure in the text. One sees the local piece $\delta(3,2)\delta(3,4)$ plus the functional derivative involving Σ.

We can label the effective vertex $\Xi \equiv \delta(v_H+\Sigma_{\mathrm{xc}})/\delta G$, or recognize that $\delta(v_H)/\delta G = \delta(1,2)$ is local, whereas $\delta\Sigma_{\mathrm{xc}}/\delta G$ is the nontrivial part. Then

$$\Sigma(1,2) \;=\; v_H(1,2) \;+\; i\,G(1,3)\,v_c(1^+,4)\,\Big[\delta(3,2)\,\delta(3,4) \;+\; \dots\Big].$$

One more rearrangement or naming of terms gives the final expression in the text,

$$\Sigma(1,2) \;=\; v_H(1,2) \;+\; i\,G(1,3)\;W(1^+,4)\;\Lambda(3,2;4), \qquad (10.37)$$

where $W \equiv \epsilon^{-1}v_c$ is the screened interaction, and Λ (sometimes $\tilde{\Gamma}$, or $\widetilde{\Xi}$) is the "reducible vertex." In various references, one sees this step described as the chain rule leading to

$$\Sigma_{\mathrm{xc}}(1,2) \;=\; i\int d3\,d4\;\,G(1,3)\,\Gamma(3,2;4)\,W(1^+,4),$$

matching the canonical Hedin or Bethe–Salpeter forms. Essentially, Eq. (10.37) says $\Sigma = G \times W$ plus a vertex correction, but the last portion is simplified if we define $\Gamma \equiv \delta G^{-1}/\delta v_{\mathrm{cl}}$.

5.2 Interpretation: Σ as a Generalized Potential

Equation (10.37) shows that we can interpret Σ as the sum of a classical piece (Hartree) plus an induced non-local part (exchange–correlation), which can be thought of as a 'screened' potential felt by an added electron.

Equation (10.37) reveals a *physical picture* of the self-energy Σ as a "generalized potential." One can view it as combining three main effects:

1. **Hartree potential**:
$$\Sigma_H(1) \;=\; v_H(1) \;=\; -\,i\,v_c(1,3)\,G\big(3,3^+\big),$$
where the diagonal of G acts like a density $n(3)$. This produces the *classical Coulomb* contribution, effectively a local potential.

2. **Fock (exchange) term**:
$$\Sigma_x(1,2) \;=\; i\,G(1,2)\,v_c(1^+,2).$$
Here, the nonlocal propagation in $G(1,2)$ gives rise to an *exchange potential* that couples points 1 and 2. In a many-electron system, this removes self-interaction and introduces long-range exchange.

3. **Correlation part Σ_c**: Interpreted as a *generalized induced potential.* Just as, in classical electrostatics, an external test charge ρ_{ext} is screened by χ (the density–density response) leading to $v_{\mathrm{ind}} = v_c\,\chi\,v_c\,\rho_{\mathrm{ext}}$, likewise, the correlation part of Σ can be written as
$$\Sigma_c \;=\; v_c\,L\big(i\Xi\big)\,G,$$

where G acts like the external charge, and L is analogous to χ. The operator $i\Xi$ (sometimes $\tilde{\Gamma}$) is a generalized vertex function, including both the classical Coulomb interaction and additional exchange–correlation effects. Hence, $v_c\,L$ generalizes the usual screening $v_c\,\chi$.

Altogether, Σ_c is a "dynamically induced" nonlocal potential beyond simple Hartree or Fock exchange, capturing the response of the medium to a propagating electron or hole. This viewpoint suggests how one might approximate Σ:

- In strongly screened materials, one needs a good approximation for L, so that $v_c\,L$ is described well.
- If the effective interaction is not the bare Coulomb, then refining the vertex Ξ may be more crucial.

In practice, we use Eq. (10.37) as a starting point for familiar self-energy approximations such as *Hartree–Fock*, *GW*, and *T-matrix* forms. A concise overview can be found, for instance, in Table 10.1 of the text.

5.3 Common Approximations

(a) **Hartree–Fock**: Keep only the bare Fock term. No dynamical screening, no satellites, but is fully conserving.

(b) **GW Approximation**: Replace v_c by the dynamically screened interaction W, neglect vertex corrections beyond unity ($\Gamma = 1$). This recovers plasmon excitations, more accurate bandgaps, etc.

(c) ***T*-Matrix Approaches**: Summation of repeated scattering (ladder) diagrams more relevant in low-density or strongly correlated systems.

Higher-level approaches add partial vertex corrections or combine GW with T-matrix physics.

5.4 First Glance at GW: The Screened Interaction Approximation

We now explicitly discuss how the correlation part of the self-energy naturally leads to the *GW approximation* by approximating the effective two-particle interaction.

Including Correlation Effects. Starting from Eq. (10.37), we first retain only the classical Hartree potential in the effective two-particle interaction Γ. Thus, the correlation portion of the self-energy Σ_{xc} simplifies to:

$$\Sigma_{\text{xc}}(1,2) = \Sigma_x(1,2) + v_c(1^+,\bar{3})G(1,2)L(\bar{4},\bar{3};\bar{4}^+,\bar{3}^+)v_c(2,\bar{4}^+), \tag{12}$$

which corresponds to Eq. (10.38). The Fock term $\Sigma_x = iGv_c$ is included explicitly.

Connection to Polarizability and Screened Interaction. From our functional derivative definitions, we know:

$$-iL(3,2;3^+,2^+) = \frac{\delta n(3)}{\delta u(2)} = \chi(3,2), \tag{13}$$

where χ is the density-density response function (polarizability), symmetric and causal in time or contour ordering. Therefore, the object $-iv_cLv_c$ is precisely the classical induced potential created by a test charge, leading directly to the screened Coulomb interaction W:

$$W(1,2) = v_c(1,2) + v_c(1,\bar{3})\chi(\bar{3},\bar{4})v_c(\bar{4},2). \tag{14}$$

Deriving the GW Approximation. Putting these together, we obtain the standard GW form:

$$\Sigma_{\mathrm{xc}}(1,2) = iG(1,2)W(1^+,2), \tag{15}$$

which replaces the bare Coulomb interaction v_c by a screened interaction W. Thus, the crucial physical improvement over Hartree–Fock ($\Sigma_x = iGv_c$) is screening. Hence, instead of an unscreened Fock exchange, the electron experiences a dynamic, frequency-dependent potential encoding the rearrangement of all other electrons.

Approximating the Polarizability: L_0 vs. RPA. In practice, χ (or equivalently L) must be approximated. The simplest choice is $L \approx L_0$, where:

$$L_0(1,2;1',2') = G(1,2')G(2,1'). \tag{16}$$

This defines GW^{L_0}, meaning no further bubbles or repeated interactions are summed. Such a choice may suffice in finite systems (e.g., small molecules) but is problematic for extended systems, where repeated scattering or bubble diagrams are critical for describing proper screening.

Instead, one typically approximates the irreducible two-particle function $\tilde{L}$ by L_0, and then solves the Bethe–Salpeter (Dyson) equation:

$$L = \tilde{L} - i\tilde{L}v_cL, \tag{17}$$

to obtain the full L. This procedure automatically includes infinite repeated bubble diagrams, and thus provides the *Random Phase Approximation (RPA)* for χ. The resulting GW approximation with RPA screening is called GW$^{\mathrm{RPA}}$.

GW^{L_0} vs. GW$^{\mathrm{RPA}}$.

- **GW^{L_0}**: No repeated bubbles (just one bubble diagram). Useful only for finite systems.
- **GW$^{\mathrm{RPA}}$**: Solves the Dyson/BSE equation, summing infinite repeated bubbles, yielding a screened Coulomb interaction W consistent with RPA. This is standard and robust for extended systems.

In extended solids, GW$^{\mathrm{RPA}}$ significantly improves the physical accuracy over unscreened approximations like Hartree–Fock or GW^{L_0}. This infinite resummation, intrinsic to solving a Dyson equation, incorporates interactions to all orders.

Conserving Nature of the GW Approximation. The GW approximation remains conserving at every level, as evidenced by its diagrammatic structure. Even when additional bubbles (higher-order diagrams) are included, the conserving property remains intact.

Compact Representation with the $\Phi[G, W]$-functional. The functional $\Phi[G, W]$ representation of the GW approximation simplifies significantly by expressing it directly in terms of the screened interaction W:

$$\Phi_{GW}[G, W] = -\frac{1}{2}\mathrm{Tr}(GWG). \tag{18}$$

This succinct diagrammatic form highlights the powerful simplification achieved by summing bubble diagrams into the single screened interaction W.