Many-Body Perturbation Theory via Functional Derivatives

Leading into RPA and the GW Approximation

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Introduction and Motivation (1)

- In many-body theory, the one-body Green's function G is a cornerstone.
- Naively, the equation of motion for G references higher-order $G_2, G_3, \ldots$ (the Martin–Schwinger hierarchy).
- Goal: find a closed equation for G by employing functional derivatives.
- This sets up the RPA (random phase approximation) and GW expansions in extended systems.

Introduction and Motivation (2)

- The functional-derivative trick: add a fictitious external potential $u(3)$, then remove it $(u \to 0)$.
- It's analogous to source fields in quantum field theory or linear-response expansions in condensed matter.

Definitions and Background (1)

Time-ordered one-body Green's function:

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

where $(1) \equiv (x_1, t_1)$ and $\hat{\psi}(1)$ annihilates an electron at $(\mathbf{r}_1, \sigma_1, t_1)$.
Note: For finite T, one can switch to Matsubara or contour ordering.

Definitions and Background (2)

Hamiltonian:

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

- $h(x) = -\frac{1}{2}\nabla^2 + v_{\text{ext}}(x)$: single-particle part.
- $v_c(x, x')$: instantaneous Coulomb interaction.

Equation of Motion for G

From the Heisenberg EoM, we get

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

Key: G_2 is the two-particle Green's function.

Two-Particle Green's Function G_2

$$G_2(1, 2; 1', 2') = (-i)^2 \langle 0 | T[\hat{\psi}(1)\hat{\psi}(2)\hat{\psi}^\dagger(2')\hat{\psi}^\dagger(1')] | 0 \rangle.$$

- Equation of motion for G_2 references G_3, etc.
- Leads to the Martin–Schwinger hierarchy.

Martin–Schwinger Hierarchy

- Each G_s references G_{s+1} in its EoM.
- An infinite chain, correct but not practical.
- We seek a closure scheme to avoid direct $G_2, G_3, \ldots$

Introducing L: The Two-Particle Correlation Function

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

- For non-interacting electrons, $L = 0$.
- For interactions, L accounts for excess correlation beyond $G \times G$.

Substitute into G's EoM

Original:

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

Replace G_2 by $-L + G\,G$:

$$\ldots$$

Rearranged Equation for G

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

- G_0: non-interacting Green's function.
- v_H: Hartree potential.
- L: still unknown, capturing correlation.

Summary and Motivation for Next Step

- The one-body EoM now depends on L.
- We still don't have a closed form for G alone.
- **Next:** Use functional derivatives ($\delta G/\delta u$) to express L.
- This will close the problem at the one-body level.

Functional Derivative Approach

- Direct EoM for G references G_2, leading to an infinite hierarchy $(G_3, G_4, \ldots)$.
- **Functional-derivative trick:** turn G_2 into $\delta G/\delta u$, avoiding separate G_2 equations.

Adding an External Potential u

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

- $u(3)$ couples to electron density $\hat{n}(3)$.
- Denote the new 1-body Green's function by G_u.
- Eventually, $u \rightarrow 0$, i.e. purely formal.

Relating G_2 to $\delta G/\delta u$

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

- L_u is the two-particle correlation function *with* the potential u.
- In the limit $u \to 0$, we recover the physical L.

Replacing $G_2 \mapsto \frac{\delta G}{\delta u}$

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

- Single integral-differential eq. in G_u.

One Equation for G

- All references to G_2 are gone, replaced by $\delta G/\delta u$.
- At the end, set $u = 0$ to recover the physical system.
- This is still nonlinear, but *only one* function G is unknown.

Physical Meaning of $u \to 0$

- u is a formal probe, not an actual external field.
- Similar to source fields in QFT or small potentials in Kubo response.
- The derivative $\delta G/\delta u$ at $u = 0$ encodes correlation that would appear in G_2.

Advantages & Implications

- Avoid explicit G_2 (or $G_3, G_4, \ldots$).
- Systematic approach to correlation.
- Next: we rewrite in a Dyson-like form, incorporate self-energy approximations (RPA, GW).

Summary (Functional Derivative Approach)

- We introduced a small $u(3)$, letting L appear as $\delta G/\delta u$.
- The final eq. is an integral–differential eq. for G alone.
- **Next Steps:** Move to self-energy Σ and Dyson eq.

Dyson Equations: Motivation

Context: We introduced how the one-body Green's function G depends on the two-particle correlation function L, but the resulting expansions can be complicated.

- **Goal:** Reorganize expansions via Dyson equations to handle infinite series of diagrams more cleanly.
- (i) Understand how interactions shift quasi-particle energies.
- (ii) Define an additive self-energy Σ that captures exchange–correlation effects.
- (iii) Summation of Dyson-like expansions to include infinite orders systematically.

Outcome:

- The self-energy Σ modifies non-interacting G_0 to produce the *dressed* G.
- Higher-order correlations become manageable in a single integral equation.

Key Results (Summary)

- Iterating the equation of motion directly (*e.g.*, Hartree expansions) can cause undesired extra poles instead of a shifted main peak.
- Recasting into *inverse* form reveals an additive self-energy, Σ.
- The Dyson equation
$$G^{-1} = G_0^{-1} - \Sigma$$
  shows how interactions (beyond Hartree) enter as dynamic and non-local corrections.
- Bethe–Salpeter approach: an analogous construction for the two-particle Green's function L, yielding a kernel related to Σ.
- Solving Dyson-like equations $\Longrightarrow$ infinite diagrammatic resummation. Essential for self-consistent many-body methods.

Equation of Motion and Functional Derivatives

Original functional-differential equation (Schwinger–Dyson form):

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

- u = small fictitious potential; G_u = Green's function in that potential.
- Directly iterating can produce unphysical multi-pole expansions.
- We want a more stable reorganized approach.

Inverse-Operator Strategy

Define G_u^{-1}: so that

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

Key step: combine G_0^{-1} with the chain rule in the equation of motion to isolate "interaction dressing" as a single operator, Σ:

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

This is the inverse form of the Schwinger–Dyson equation.

- Σ lumps all exchange–correlation effects beyond G_0.
- When $u \to 0$, $\Sigma \equiv \Sigma_H + \Sigma_{\mathrm{xc}}$ for the physical system.

Dyson Equation: Final Integral Form

Invert $G_u^{-1} = G_0^{-1} - \Sigma$ to get the Dyson equation:

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

- Summation over all many-body corrections encoded in Σ.
- At $u = 0$, recovers the *physical* G.
- Poles in $G(\mathbf{k}, \omega)$ now shift via $\mathrm{Re}\, \Sigma(\mathbf{k}, \omega)$.

Advantage: avoids spurious poles from naive expansions, capturing instead a single shifted quasi-particle peak and possible satellites.

Pole Structure and Physical Meaning

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

- Shifts $\epsilon_{\mathbf{k}}$ by $\mathrm{Re}\,\Sigma$.
- Quasi-particle lifetimes from $\mathrm{Im}\,\Sigma$.
- Summation of infinite classes of diagrams once Σ is suitably approximated.

Physical content:

- Σ_H: local Hartree potential from electron density.
- Σ_{xc}: dynamic exchange–correlation capturing interactions, screening, etc.

Wrap-Up of the Inverse-Operator Logic

1. Start: functional-differential equation in a fictitious field u.
2. Multiply by G_0^{-1}, gather all extra terms into Σ.
3. Dyson equation yields infinite diagrammatic resummation for G once Σ is chosen (HF, GW, T-matrix, …).

Conclusion: The Dyson approach systematically reorganizes expansions, giving a single self-energy operator that encapsulates correlation corrections. This powerful viewpoint underlies modern many-body perturbation theory.

Next steps:

- Approximate or derive expressions for Σ (e.g., GW).
- Possibly solve self-consistently for G (or not, in a one-shot approach).
- Similar logic extends to two-particle correlation with Bethe–Salpeter eq.

A starting Point For Approximations

- We seek a *practical scheme* for the self-energy Σ.
- Formally, Schwinger–Dyson equations or infinite diagram expansions exist, but we must decide which diagrams / derivatives to keep.
- Key question: *How do we systematically derive or approximate* Σ*?*

Eqs. (10.34)–(10.37): The Self-Energy as a Functional

Goal: express $\Sigma(1,2)$ in terms of G and $\delta G/\delta u$.

Decomposition:

$$G^{-1} \;=\; G_0^{-1} \;-\; \big[u + v_H + \Sigma\big].$$

→ all arguments are space/spin/time (r_1, σ_1, t_1), etc.

Starting expression (Eq. (10.34)):

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

- $v_H(1,2) \equiv v_H(1)\, \delta(1,2)$ is Hartree.
- Variation w.r.t. u encodes the *correlation* via $\delta G^{-1}/\delta u$.

Splitting $\frac{\delta G^{-1}}{\delta u}$: Local vs. Correlation Parts

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

Hence,

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

$\Longrightarrow$ Substituting back splits Eq. (10.34) into two terms:

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

$\Longrightarrow$ *Local piece* + *Chain-rule piece* → Eq. (10.35).

From (10.35) to (10.36): Identifying the Exchange and Derivatives

$$\Sigma_x(1,2) \;=\; i\,G(1,2)\,v_c(1^+,2) \quad \text{(bare Fock term).}$$

The remainder is

$$\Sigma_c(1,2) \;=\; i\,v_c(1^+,4)\,G(1,3)\,\big[\dots\big].$$

We rewrite $\frac{\delta\Sigma}{\delta u}$ as $\frac{\delta(v_H+\Sigma_{\mathrm{xc}})}{\delta G}\cdot\frac{\delta G}{\delta u}$.

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

This is Eq. (10.36).

Final Form: Eq. (10.37)

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

One often defines $W \equiv \epsilon^{-1} v_c$ as *the screened interaction*, and Λ or Γ as a vertex function:

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

$\Longrightarrow$ The self-energy Σ is a *generalized potential*:

$$\Sigma \;=\; \underbrace{v_H}_{\text{classical}} \;+\; \underbrace{\Sigma_x = i\,G\,v_c}_{\text{Fock exchange}} \;+\; \underbrace{\Sigma_c = \dots}_{\text{induced correlation}} \quad .$$

Σ as a Generalized Potential

- **Hartree term:** classical density → local v_H.
- **Fock (exchange):** nonlocal $i\,G\,v_c$. Cancels self-interaction, introduces long-range exchange.
- **Correlation:** a "generalized induced potential" akin to $v_c\,\chi\,v_c$ but with G in place of ρ_{ext}.

$\Longrightarrow$ Distinction:

- *Strongly screened* system: emphasize χ in $v_c\,\chi\,v_c$.
- *Less classical* regime or strong correlation: refine vertex Γ.

Common Approximations

1. **Hartree–Fock (HF)**
   - Keep only the bare Fock term.
   - No dynamical screening or satellites.
   - Fully conserving.
2. **GW Approximation**
   - Replace bare Coulomb interaction v_c by dynamically screened interaction W.
   - Neglect vertex corrections (set $\Gamma = 1$).
   - Recovers plasmon excitations and accurate bandgaps.
3. **T-Matrix Approaches**
   - Summation of ladder diagrams (repeated scattering).
   - Important in low-density or strongly correlated systems.

Screened Interaction and Polarizability

- Correlation self-energy Σ_{xc} simplifies to:

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

- Connection to Polarizability χ:

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

- Screened Interaction W:

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

The GW Approximation

- GW Approximation for self-energy:

$$\Sigma_{\mathrm{xc}}(1,2) = iG(1,2)W(1^{+},2) \tag{4}$$

- Improvement over Hartree–Fock:
  - Dynamical screening replaces unscreened Coulomb interaction.
  - Captures electron rearrangements (plasmonic excitations).
- Conserving approximation at every level.

Polarizability Approximation: L_0 vs. RPA

- Simplest Approximation $L \approx L_0$:

$$L_0(1,2;1',2') = G(1,2')G(2,1') \tag{5}$$

- Suitable for finite systems (small molecules).
- Insufficient for extended systems (solids).

- **Random Phase Approximation (RPA)**:

$$L = \tilde{L} - i\tilde{L}v_c L \tag{6}$$

- Summation of infinite bubble diagrams.
- Robust for extended solids ($\mathrm{GW}^{\mathrm{RPA}}$).

Comparing GW^{L_0} and GW$^{\mathrm{RPA}}$

GW^{L_0}

- Single bubble diagram.
- Suitable for finite, localized systems.
- Simpler but limited accuracy.

GW$^{\mathrm{RPA}}$

- Infinite bubble resummation.
- Essential for extended systems.
- Improved physical accuracy.
- Standard in solid-state applications.

Functional Representation $\Phi[G, W]$

- Compact representation with functional $\Phi[G, W]$:

$$\Phi_{GW}[G, W] = -\frac{1}{2}\mathrm{Tr}(GWG) \tag{7}$$

- Highlights simplification through screening.
- Powerful diagrammatic formulation.