W6: Many-Body Perturbation Theory and Feynman Diagrams

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Section 9.1: The Coulomb Interaction and Perturbation Theory – Objective

The aim is to calculate material properties via Green's functions by treating the Coulomb interaction as a perturbation. Since the non-interacting problem can be solved exactly, the strategy is to expand around that solution.

Scattering Theory: Lippmann–Schwinger Equation

In scattering theory, an unperturbed state $|\phi_0\rangle$ is modified by a perturbation $\hat{V}$. The Lippmann–Schwinger equation is:

$$|\phi\rangle = |\phi_0\rangle + \frac{1}{\omega - \hat{H}_0 + i\eta}\,\hat{V}\,|\phi\rangle. \tag{9.1}$$

This can be rewritten using the non-interacting Green's function

$$G_0 \equiv \frac{1}{\omega + i\eta - \hat{H}_0},$$

yielding:

$$|\phi\rangle = \left(1 - G_0\,\hat{V}\right)^{-1}|\phi_0\rangle. \tag{9.2}$$

Connecting Scattering Theory to Perturbation Theory

The expansion

$$\left(1 - G_0\,\hat{V}\right)^{-1} = 1 + G_0\,\hat{V} + G_0\,\hat{V}\,G_0\,\hat{V} + \cdots,$$

is the perturbative (Born) series.

Each term in the series corresponds to successive scattering events.

This series forms the basis for constructing the full Green's function.

From Scattering to the Dyson Equation

The full Green's function is defined by:

$$G(\omega) \equiv \frac{1}{\omega + i\eta - \hat{H}},$$

where $\hat{H} = \hat{H}_0 + \hat{V}$.

Using the series expansion from scattering theory, we have:

$$G = G_0 + G_0\,\hat{V}\,G_0 + G_0\,\hat{V}\,G_0\,\hat{V}\,G_0 + \cdots .$$

This expansion is compactly written as the Dyson equation:

$$G = G_0 + G_0\,\Sigma\,G, \tag{9.3}$$

where the self-energy Σ summarizes all scattering (interaction) processes.

Scattering in the Continuum and Green's Functions

In the continuum, the eigenstates are extended (scattering states) rather than bound.

Physical observables (e.g. scattering amplitudes) depend on the **asymptotic behavior** of these states.

The Green's function, with its $i\eta$ prescription, encodes the causal propagation of scattering states.

Thus, in the continuum limit, we only need the asymptotic (scattered) part of the wavefunction to compute observables.

Continuum Eigenstates: Single-Particle vs. Many-Body

In scattering theory, energies in the continuum correspond to extended states.

For a non-interacting Hamiltonian, these eigenstates are typically single-particle states (e.g. plane waves) that are not normalizable.

In a full many-body system, the eigenstates are many-body states (often combinations of many Slater determinants) and are also extended.

When working with one-particle Green's functions, we usually consider transitions where an electron is added or removed. In this effective picture, the relevant excitations are often treated as single-particle (or quasi-particle) states.

Thus, while the full spectrum of the many-body Hamiltonian is built from many-body eigenstates, in practical scattering and Green's function calculations we often focus on the effective single-particle excitations that live in the continuum.

Section 9.1: Perturbation Theory Approaches

Brillouin–Wigner Perturbation Theory:

$$E = E_{ip} + \sum_{n=1}^{\infty} \langle \phi_{ip} | \hat{V} \left(\frac{1}{1-\hat{P}} \frac{1}{E-\hat{H}_0} \hat{V} \right)^{n-1} | \phi_{ip} \rangle, \tag{9.5}$$

and

$$|\Phi\rangle = \sum_{n=0}^{\infty} \left(\frac{1}{1-\hat{P}} \frac{1}{E-\hat{H}_0} \hat{V} \right)^{n} | \phi_{ip} \rangle. \tag{9.6}$$

Rayleigh–Schrödinger Perturbation Theory:

$$E = E_{ip} + \sum_{n=1}^{\infty} \langle \phi_{ip} | \hat{V} \left(\frac{1}{E_{ip}-\hat{H}_0} (E_{ip} - E + \hat{V}) \right)^{n-1} | \phi_{ip} \rangle, \tag{9.7}$$

and

$$|\Phi\rangle = \sum_{n=0}^{\infty} \left(\frac{1}{E_{ip}-\hat{H}_0} (E_{ip} - E + \hat{V}) \right)^{n} | \phi_{ip} \rangle. \tag{9.8}$$

Section 9.1: Møller–Plesset Perturbation Theory

Instead of treating the full Coulomb interaction as a perturbation, a part is incorporated into a mean-field Hamiltonian.

Zeroth-order energy: Sum of occupied HF eigenvalues.

First-order correction is

$$E^{(1)} = \langle \phi_{ip} | \hat{V} | \phi_{ip} \rangle = -\sum_{i<j} \left(v_{ijji} - v_{ijij} \right), \tag{9.9}$$

so that $E_{ip} + E^{(1)}$ equals the HF total energy.

Second-order correction (MP2):

$$E^{(2)} = \sum_{i<j}^{\text{occ}} \sum_{a<b}^{\text{empty}} \frac{|v_{ijab} - v_{ijba}|^2}{\varepsilon_i + \varepsilon_j - \varepsilon_a - \varepsilon_b}. \tag{9.11}$$

Section 9.2: Objective

This section addresses the difficulty that the interacting ground state appears explicitly in the Green's function expressions. The strategy is to connect the non-interacting and interacting systems via **adiabatic switching**.

Adiabatic Switching-On of the Interaction

The Coulomb interaction is slowly switched on using a time-dependent form:

$$v_\eta(t) = v_c\, e^{-\eta|t|}, \quad \eta \to 0^+.$$

At $t \to \pm\infty$, the interaction is off; at $t = 0$, the full interaction is present.

Time Evolution Operator in the Interaction Picture

In the interaction picture, the full Hamiltonian is split as:

$$H = H_0 + V,$$

where H_0 is the non-interacting (free) part and V is the interaction.
The time evolution operator $U_I(t, t_0)$ evolves states according to the interaction:

$$|\psi_I(t)\rangle = U_I(t, t_0)\,|\psi_I(t_0)\rangle.$$

$U_I(t, t_0)$ satisfies the differential equation:

$$\frac{d}{dt}U_I(t, t_0) = -i\,V_I(t)\,U_I(t, t_0), \quad U_I(t_0, t_0) = I,$$

where the interaction-picture operator is given by:

$$V_I(t) = e^{iH_0(t-t_0)}\,V\,e^{-iH_0(t-t_0)}.$$

The formal solution is expressed as a time-ordered exponential:

$$U_I(t, t_0) = T\left\{\exp\left[-i\int_{t_0}^{t} V_I(t')\,dt'\right]\right\}.$$

Understanding the Time-Ordered Series

The time evolution operator in the interaction picture is defined as

$$U_I(t, t_0) = T\left\{\exp\left[-i\int_{t_0}^{t} V_I(t')\,dt'\right]\right\},$$

where T denotes time ordering.
The role of T is to rearrange operators so that those with later times appear to the left:

$$T\{V_I(t_1)V_I(t_2)\} = \begin{cases} V_I(t_1)V_I(t_2), & t_1 > t_2, \\ V_I(t_2)V_I(t_1), & t_2 > t_1. \end{cases}$$

Expanding the exponential yields:

$$U_I(t, t_0) = 1 + (-i)\int_{t_0}^{t} dt_1\, V_I(t_1) + \frac{(-i)^2}{2!}\int_{t_0}^{t} dt_1 \int_{t_0}^{t} dt_2\, T\{V_I(t_1)V_I(t_2)\} + \cdots.$$

Equivalently, by using ordered integration limits we can write:

$$U_I(t, t_0) = 1 + (-i)\int_{t_0}^{t} dt_1\, V_I(t_1) + (-i)^2\int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2\, V_I(t_1)V_I(t_2) + \cdots.$$

Each term is "sorted in orders of V" – the nth term is proportional to V^n.

Propagating the Ground State In the interaction picture

In the interaction picture, we propagate the non-interacting ground state $|\phi_{ip}\rangle$ from $t = -\infty$ to time t and further to $t = \infty$.

The time evolution operator $U_I(t, t_0)$ connects the non-interacting state to the interacting state.

This gives the relation:

$$\langle \phi_\eta^+ | \hat{O}_H(t) | \phi_\eta^- \rangle = \langle \phi_{ip} | U_I(\infty, t)\, \hat{O}_I(t)\, U_I(t, -\infty) | \phi_{ip} \rangle.$$

Here, $\hat{O}_H(t)$ is the operator in the Heisenberg picture and $\hat{O}_I(t)$ in the interaction picture.

Normalization and Removal of Divergent Phases

Direct propagation introduces divergent phases due to adiabatic switching.

To cancel these divergences, we normalize the expectation value by the overlap of the evolved states.

The normalized expression is:

$$\frac{\langle \phi_\eta^+ | \hat{O}_I(t) | \phi_\eta^- \rangle}{\langle \phi_\eta^+ | \phi_\eta^- \rangle} = \frac{\langle \phi_{ip} | U_I(\infty, t)\, \hat{O}_I(t)\, U_I(t, -\infty) | \phi_{ip} \rangle}{\langle \phi_{ip} | U_I(\infty, -\infty) | \phi_{ip} \rangle}.$$

This ratio ensures that the divergent phase factors cancel, leaving a well-defined expression.

Expansion of the Expectation Value

The time evolution operator U_I can be expanded in a Dyson series, order by order in the interaction V_I.

The expansion for the expectation value of an operator $\hat{O}_H(t)$ becomes:

$$\lim_{\eta\to 0}\langle\phi_\eta^+|\hat{O}_H(t)|\phi_\eta^-\rangle = \lim_{\eta\to 0}\sum_{p=0}^{\infty}\frac{(-i)^p}{p!}\int_{-\infty}^{\infty}dt_1\cdots\int_{-\infty}^{\infty}dt_p\; e^{-\eta(|t_1|+\cdots+|t_p|)}$$

$$\times\langle\phi_{ip}|T\{V_I(t_1)\cdots V_I(t_p)\hat{O}_I(t)\}|\phi_{ip}\rangle\,\langle\phi_{ip}|S_\eta|\phi_{ip}\rangle. \tag{9.20}$$

Here:

- T denotes time ordering.
- $S_\eta = U_I(\infty,-\infty)$ is the full time-evolution (scattering) operator.
- The exponential factors $e^{-\eta|t_i|}$ implement adiabatic switching.

This expansion forms the basis for the diagrammatic representation of the interacting Green's function.

Connecting Ground States and the Gell-Mann–Low Theorem

Propagate the non-interacting ground state $|\phi_{ip}\rangle$ from $t = -\infty$ to $t = 0$ using U_I.

Define the states $|\phi_\eta^-(t)\rangle$ and $|\phi_\eta^+(t)\rangle$ by forward and backward propagation, respectively.

In the limit $\eta \to 0$, these states converge to the true interacting ground state $|\phi_0\rangle$ (This is the main hypotehsis of adiabatic switching).

Expectation values are computed as:

$$\langle O \rangle = \frac{\langle \phi_\eta^+ | O | \phi_\eta^- \rangle}{\langle \phi_\eta^+ | \phi_\eta^- \rangle}.$$

This is the Gell-Mann–Low theorem guarantees that adiabatic switching connects the non-interacting ground state to an interacting state (No necessarily the ground state!!, although we assume so.).

Interacting Green's Function

The zero-temperature interacting Green's function is:

$$G(x,t;x',t') = -i\,\frac{\langle\phi_{ip}|\; T\{\psi_I(x,t)\psi_I^\dagger(x',t')\,S_\eta\}\;|\phi_{ip}\rangle}{\langle\phi_{ip}|\;S_\eta\;|\phi_{ip}\rangle},$$

where

$$S_\eta \equiv U_I(\infty,-\infty).$$

Diagrammatic Expansion of the Green's Function

The interacting Green's function at zero temperature is given by:

$$G(x,t;x',t') = -i\,\frac{\langle\phi_{ip}|\;T\left[\psi(x,t)\psi^{\dagger}(x',t')\,\hat{S}\right]|\phi_{ip}\rangle}{\langle\phi_{ip}|\hat{S}|\phi_{ip}\rangle}, \tag{9.22}$$

where $\hat{S}_{\eta} = U_I(\infty,-\infty)$.

The Coulomb interaction in the interaction picture is:

$$\hat{V}_I(t) = \frac{1}{2}\int dx\,dx'\,\psi_I^{\dagger}(x,t)\,\psi_I^{\dagger}(x',t)\,v_c(r,r')\,\psi_I(x',t)\,\psi_I(x,t). \tag{9.23}$$

Expanding the numerator yields a series in powers of v_c.

Compact Notation for the Diagrammatic Expansion

In compact notation, the expansion becomes (schematically):

$$
\begin{aligned}
-i\langle\phi_{ip}|\, T\Big[\psi(x,t)\psi^{\dagger}(x',t')\,\hat{S}\Big]|\phi_{ip}\rangle &= G_0(x,t;x',t') \\
&+ \sum_{p=1}^{\infty}\left(\frac{i}{2}\right)^{p}\frac{1}{p!}\int\cdots\int d1\,d1'\cdots dp\,dp'\,v_c(1,1')\cdots v_c(p,p') \\
&\times\; G^0_{2p+1}\Big(x,t,1,1',\ldots,p,p';\,x',t',1,1',\ldots,p,p'\Big).
\end{aligned}
$$

Here, G^0_s denotes the non-interacting Green's function involving s pairs of field operators).

Understanding the Notation $G^0_{(2p+1)}$

The one-body Green's function is defined as

$$G^0(x,t;x',t') = \langle \phi_{ip}|\, T\left[\psi_I(x,t)\psi_I^\dagger(x',t')\right]|\phi_{ip}\rangle,$$

which we can denote as $G_0^{(1)}$ (i.e. one pair of field operators or one propagator line).

In our perturbative expansion (Eq. (9.24)), each Coulomb vertex (a two-body operator) effectively adds one extra pair of field operators.

Therefore, when p vertices are inserted:

$$\text{Total number of operator pairs} = 1 + 2p = 2p + 1,$$

meaning that the corresponding Green's function involves $2p+1$ propagator lines (or equivalently, $2(2p+1)$ individual field operators).

Thus, the notation $G^0_{(2p+1)}$ denotes the non-interacting Green's function constructed from a time-ordered product corresponding to $2p+1$ propagator lines. Here, p is the order of the perturbation (i.e. the number of Coulomb interaction insertions).

Recap and Physical Interpretation

The expansion in Eq. (9.24) reads schematically as:

$$-i\langle\phi_{ip}|\,T\left[\psi(x,t)\psi^{\dagger}(x',t')\,\hat{S}\right]|\phi_{ip}\rangle = G^{0}(x,t;x',t') + \sum_{p=1}^{\infty}\left(\frac{i}{2}\right)^{p}\frac{1}{p!}\int\cdots\int d1\,d1'\cdots dp\,dp'\,v_c(1,1')\cdots v_c(p,p') \times G^{0}_{(2p+1)}\big(x,t,1,1',\ldots,p,p';\,x',t',1,1',\ldots,p,p'\big).$$

The subscript $2p+1$ in $G^{0}_{(2p+1)}$ indicates that, after inserting p Coulomb vertices,

- The original two external operators are supplemented by $2p$ operators from the vertices.
- This results in a Green's function containing a total of $2p+1$ propagator lines.

In this context, p is indeed the order of the perturbation, and the notation reflects how the diagrammatic structure grows with each interaction insertion.

Wick's theorem: Determinant Structure of $G_0^{(2n+1)}$

Wick's theorem lets us express a time-ordered product of many field operators as a sum over all possible complete contractions.

For the higher-order non-interacting Green's function, which involves $2n+1$ pairs of field operators, this sum can be written compactly as a determinant:

$$G_0^{(2n+1)}(c,1,1',2,2',\ldots,n,n';\ c',1,1',2,2',\ldots,n,n') = \sum_P (-1)^P\, G_0(c,\tilde{c}')\cdots G_0(n,\tilde{n})\, G$$

Here:

- The sum is over all permutations P connecting the field operator pairs from the bra and ket.
- $(-1)^P$ is the sign of the permutation, ensuring the overall antisymmetry required for fermions.
- $G_0(c,\tilde{c}')$, etc., represent the one-body non-interacting Green's functions obtained from each contraction.

This determinant structure compactly encodes all the direct and exchange contributions arising from all possible pairings.

It is a powerful simplification that naturally accounts for the antisymmetry of the

Linked Cluster Theorem

The linked cluster theorem guarantees that disconnected (vacuum) diagrams cancel out when the Green's function is properly normalized.

Although the expansion contains many disconnected diagrams, they appear in both the numerator and denominator and cancel.

Thus, only the connected diagrams contribute to the physical Green's function.

Application to the Calculation of the Green's Function (Overview)

Our goal is to construct the perturbation series for the interacting Green's function G and to express it in a compact form using Feynman diagrams.

The zeroth-order term is simply the non-interacting one-body Green's function, G_0.

At order p in the perturbation, we introduce p Coulomb interaction vertices.

Each Coulomb vertex (depicted as a dashed line) is a two-body operator and has two endpoints (vertices) where a G_0 line is attached.

Thus, each interaction vertex adds two *pairs* (or propagator lines) to the diagram. Combined with the original external G_0 (one pair), the diagram at order p will have $1 + 2p = 2p + 1$ G_0 lines.

Constructing the Diagrams

Step 1: Building Blocks

For each Coulomb interaction vertex, add one G_0 line to each of its two endpoints.

Each endpoint is a vertex (labeled by a space–spin–time coordinate $m = (r_m, \sigma_m, t_m)$) and is marked with a dot.

Step 2: Assembling the Diagram

Combine these building blocks so that every vertex is saturated by two G_0 lines, and the whole diagram is closed, except for one extra G_0 line that forms a single leg.

Finally, add one external G_0 to saturate the last vertex, yielding two external points c and c'.

Counting: At order p, the diagram has $2p + 1$ propagator lines corresponding to the $2p + 1$ pairs of field operators.

Translating Diagrams into Equations

Once the diagram is constructed, we translate it into an equation by following these rules:

Vertex Labeling: Each vertex is labeled as $m = (r_m, \sigma_m, t_m)$.
Propagators: An arrow from vertex m' to vertex m denotes the non-interacting Green's function $G_0(m, m')$.
Interaction Lines: A dashed line is used to represent the Coulomb interaction:

$$i\, v_c(m, m') = i\, \frac{e^2}{|r_m - r_{m'}|}\, \delta(t_{m'} - t_m).$$

Integration: Integrate over all internal vertex coordinates (space, time, and spin).
Closed Loops: Each closed loop (where a G_0 line forms a self-loop, representing the density) contributes an extra factor of -1.

Only *connected* and topologically distinct diagrams are retained (vacuum fluctuations cancel between numerator and denominator).

Bare Propagator

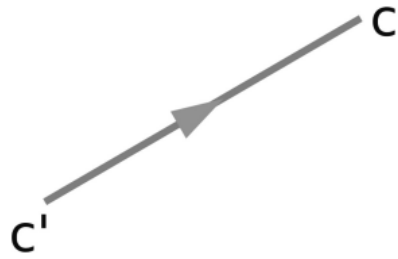

Figure 9.1. Graphical representation of $G^0(x, t, x', t')$: a Feynman diagram. Space, spin, and time are combined in one coordinate, $x, t \to c$.

First Order Diagrams

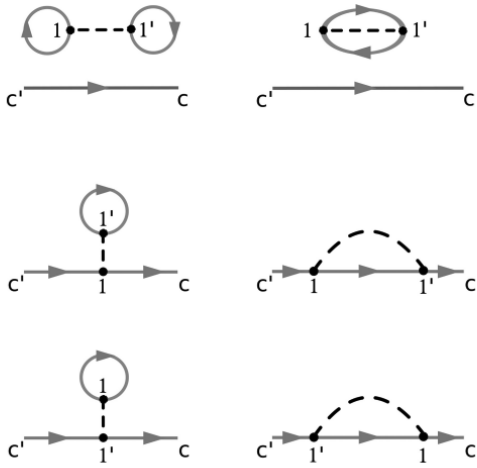

Figure 9.2. Propagation of an interacting electron from $c' = (x', t')$ to $c = (x, t)$: first-order processes contributing to the numerator of Eq. (9.22). The diagrams in the first row are *disconnected*, the others are *connected* diagrams. Continuous line: non-interacting Green's function. Closed circle: non-interacting density. Dashed line: bare Coulomb interaction v_c. Dots: internal points called *vertices*; these are integrated over. To obtain the final results, one has to use the Feynman rules specified in the text and summarized in the last subsection of Sec. 9.4.

Second order Diagrams (Incomplete)

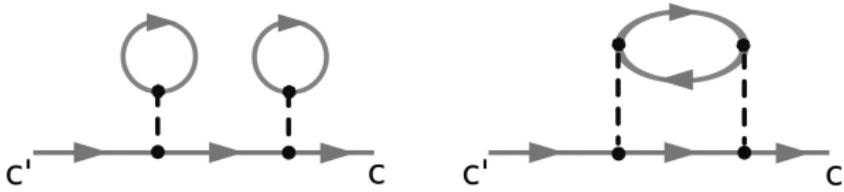

Figure 9.4. Two of the second-order contributions to G: two subsequent interactions with the density, and a polarization diagram.

From diagrams to Equations

Table 9.1. Conversion of diagrams into equations. Each closed loop carries a factor (-1). In the last column the expressions are given in the space of momentum and frequency, which are carried by the Green's functions and internally integrated as $\frac{1}{\beta}\sum_{\omega_n\sigma}\int d\mathbf{k}$. It is understood that $G^0_{\mathbf{k}}$ is scalar in a homogeneous system, and a matrix in an inhomogeneous system.

	$T=0$	$T\neq 0$ (space, imaginary time)	$T\neq 0$ (reciprocal space, Matsubara frequency)
n	$\mathbf{r}_n, \sigma_n, t_n$	$\mathbf{r}_n, \sigma_n, \tau_n$	
$n\bullet$	$\int d\,x_n \int_{-\infty}^{\infty} d\,t_n$	$\int d\,x_n \int_0^{\beta} d\,\tau_n$	
n ← m	$G^0(n,m)$	$G^0(n,m)$	$G^0_{\mathbf{k}\sigma}(\omega_n)$
n ← m	$G(n,m)$	$G(n,m)$	$G_{\mathbf{k}\sigma}(\omega_n)$
	$n^0(\mathbf{r}_m)$ and $n(\mathbf{r}_m)$	$n^0(\mathbf{r}_m)$ and $n(\mathbf{r}_m)$	n^0 and n
n - - - - m	$iv_c(\mathbf{r}_1,\mathbf{r}_2)\delta(t_1^+ - t_2)$	$-v_c(\mathbf{r}_1,\mathbf{r}_2)\delta(\tau_1^+ - \tau_2)$	$-v_c(\mathbf{k})$

Example: First- and Second-Order Contributions

First Order ($p = 1$):

Two contributions arise (see Fig. 9.2):

The *Hartree term*: a modification of the propagation due to the mean-field potential, written as

$$-i\, G_0\, v_c\, G_0\, G_0 = G_0\, v_H\, G_0.$$

The *Exchange term*: similar to the Hartree term but with an opposite sign due to exchange.

Second Order ($p = 2$):

Diagrams involve two interaction vertices. For instance, one diagram might have two successive interactions where the external propagator is modified by two density insertions, and other diagrams include bubble structures (electron–hole pair creation).

The final, compact expression for the interacting Green's function is given by

$$G(c, c') = \sum_{p=0}^{\infty} i^p \int \prod_{j=1}^{p} \Big[v_c(j, j')\, d(j, j') \Big] \, \det\Big[G_0 \Big]_{cd}, \tag{9.36}$$

First and Second order Diagrams

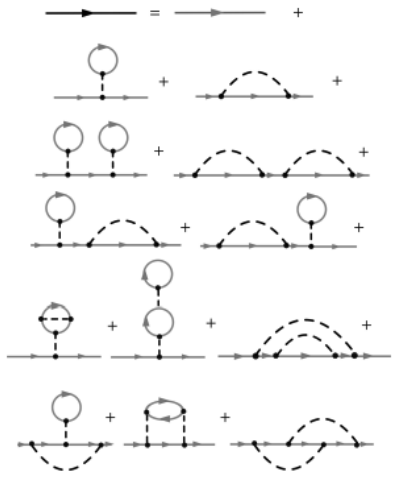

Figure 9.5. All diagrams contributing to the interacting Green's function up to second order in the Coulomb interaction.

Example: Diagrammatic Setup for $p = 2$

External Points:

$c = (x, t)$ (entry point)
$c' = (x', t')$ (exit point)

Interaction Vertices:

Two vertices (labeled 1 and 2), depicted as dots.
Each vertex corresponds to a Coulomb interaction (dashed line) and adds two pairs of field operators.

Density Lines (Self-Loops):

At each vertex, one of the attached propagators forms a closed loop.
These self-loops represent the density at that vertex (e.g., $G_0(1, 1^+)$ at vertex 1).

Overall Counting:

At zeroth order, G_0 involves 1 pair.
With $p = 2$ vertices, the total number of propagator pairs is $1 + 2 \times 2 = 5$.

Translating the $p = 2$ Diagram into an Equation

Step 1: External Propagator The external propagation from c to c' is given by $G_0(c, c')$.

Step 2: First Interaction Vertex (at Point 1)

The external line propagates from c to vertex 1: $G_0(c, 1)$.

At vertex 1, a Coulomb interaction occurs, represented by $i\, v_c(1, 1')$, where in the equal-time limit $1' \to 1^+$.

A self-loop (density line) attaches at vertex 1: $G_0(1, 1^+)$.

Step 3: Connection Between Vertices A propagator $G_0(1, 2)$ connects vertex 1 to vertex 2.

Step 4: Second Interaction Vertex (at Point 2)

At vertex 2, a Coulomb interaction $i\, v_c(2, 2')$ occurs (with $2' \to 2^+$).

A self-loop attaches at vertex 2: $G_0(2, 2^+)$.

Step 5: Final External Propagation A propagator $G_0(2, c')$ connects vertex 2 to the external point c'.

Final Equation and Interpretation

Combining all pieces, the contribution from this $p = 2$ diagram is:

$$\Delta G(c, c') = i^2 \int d^4 1\, d^4 2\; G_0(c, 1)\Big[i\, v_c(1, 1')\, G_0(1, 1^+)\Big]\; G_0(1, 2)\Big[i\, v_c(2, 2')\, G_0(2, 2^+)\Big]\; G_0($$

where:

$d^4 1$ and $d^4 2$ denote integration over the space-time (and spin) coordinates at points 1 and 2.

The interaction is given by

$$v_c(1, 1') = \frac{e^2}{|r_1 - r_{1'}|}\, \delta(t_{1'} - t_1),$$

and similarly for $v_c(2, 2')$.

The limits $1' \to 1^+$ and $2' \to 2^+$ indicate the self-loop (density) structure.

Interpretation: This equation represents a scenario in which the external particle propagates from c to c' while being scattered twice. Each scattering event at vertices 1 and 2 introduces an interaction with the electron density (density loop) at that vertex.

The Dyson Equation for the one-particle Green's function, and the self-energy

The goal is to express the interacting one-body Green's function G in terms of the non-interacting propagator G_0 and the self-energy.

Starting from the diagrammatic expansion, each diagram has an ingoing and an outgoing G_0 line.

Schematically, we write:

$$G = G_0 + G_0 \, \Sigma_{\mathrm{red}} \, G_0$$

where Σ_{red} is the *reducible* (or improper) self-energy.

Σ_{red} represents the sum of all diagrams with no external lines.

Reducible vs. Proper Self-Energy

The reducible self-energy, Σ_{red}, contains diagrams that can be separated into lower-order pieces by cutting a single G_0 line.

We introduce the *proper* (irreducible) self-energy Σ, which is the sum of only those diagrams that remain connected when any single G_0 line is cut.

The reducible self-energy is built by concatenating proper self-energy parts with G_0 lines:

$$\Sigma_{\mathrm{red}} = \Sigma + \Sigma\, G_0\, \Sigma + \Sigma\, G_0\, \Sigma\, G_0\, \Sigma + \cdots = \Sigma + \Sigma\, G_0\, \Sigma_{\mathrm{red}}.$$

Combining to Obtain the Dyson Equation

By substituting Eq. (9.38) into Eq. (9.37), we obtain the Dyson equation:

$$G = G_0 + G_0 \, \Sigma[G_0] \, G$$

where $\Sigma[G_0]$ indicates that the self-energy is, at this stage, expressed as a functional of G_0.

Diagrammatically, this corresponds to an infinite series of terms in which lower-order self-energy insertions are summed to yield the full interacting Green's function.

In later chapters, the self-energy is re-expressed as a functional of the fully interacting G; however, at this point the functional dependence on G_0 (and v_c) is universal.

Summary and Physical Interpretation

The Dyson equation,

$$G = G_0 + G_0\,\Sigma[G_0]\,G,$$

provides a compact way to sum an infinite series of Feynman diagrams.

Σ_{red} (the reducible self-energy) is built from proper self-energy diagrams Σ linked by G_0 propagators.

This formulation effectively resums many interaction processes, capturing both direct and exchange contributions.

Ultimately, only connected, topologically distinct diagrams contribute to the physical Green's function, ensuring that the final result describes the true interacting system.

Appendix I: Time Evolution in the Interaction Picture

Split the full Hamiltonian:

$$H = H_0 + V.$$

Operator evolution:

$$O_I(t) = e^{iH_0(t-t_0)}\, O_S\, e^{-iH_0(t-t_0)}.$$

State evolution:

$$|\psi_I(t)\rangle = U_I(t, t_0)\, |\psi_I(t_0)\rangle,$$

with

$$U_I(t, t_0) = T\left\{\exp\left[-i \int_{t_0}^{t} V_I(t')\, dt'\right]\right\}.$$

Appendix II: Feynman Diagrams in Many-Body Theory – Basics

Propagators: The bare propagator $G_0(\omega)$ represents the amplitude for a particle to propagate:

$$G_0(\omega) = \frac{1}{\omega + i\eta - \varepsilon_k}.$$

Interaction Vertices: The Coulomb interaction:

$$v_c(r - r') = \frac{e^2}{|r - r'|},$$

is depicted by dashed lines.

Appendix II: Feynman Diagrams – Rules and Expansion

Feynman Rules:

(a) Assign a propagator G_0 to each line.

(b) Each interaction vertex contributes a factor of v_c and an integration over space-time.

(c) Include symmetry factors and minus signs (for fermions).

Diagrammatic Expansion: The full Green's function is expanded as:

$$G = G_0 + G_0 \hat{V} G_0 + G_0 \hat{V} G_0 \hat{V} G_0 + \cdots .$$

Appendix II: Single & Double Excitations and Brillouin's Theorem

Single Excitations: Promoting one electron from an occupied to an unoccupied orbital. Brillouin's theorem tells us:

$$\langle \Phi_{\mathrm{HF}} | \hat{H} | \Phi_i^a \rangle = 0.$$

Double Excitations: Simultaneous excitation of two electrons. These contribute at second order.

Appendix II: Vacuum Fluctuations and the Linked Cluster Theorem

Disconnected (vacuum) diagrams appear in the expansion.

The linked cluster theorem guarantees that these cancel in the normalized Green's function.

Appendix III: Overview of the Slater–Condon Rules

The Slater–Condon rules provide a systematic way to evaluate matrix elements of one-body and two-body operators between Slater determinants.

A **Slater determinant** is an antisymmetrized product of single-particle orbitals representing a many-electron wave function.

These rules are essential in quantum chemistry and many-body physics for simplifying calculations in methods like Hartree–Fock and configuration interaction.

One-Body Operators

A one-body operator, $\hat{O}^{(1)}$, (e.g. kinetic energy or an external potential) acts on a single electron.

Diagonal matrix elements:

$$\langle \Phi | \hat{O}^{(1)} | \Phi \rangle = \sum_{i \in \text{occ}} \langle \phi_i | \hat{o}^{(1)} | \phi_i \rangle.$$

Off-diagonal matrix elements: Nonzero only if the two Slater determinants differ by one orbital. The matrix element is given by the single-particle integral:

$$\langle \Phi_i^a | \hat{O}^{(1)} | \Phi \rangle = \langle \phi_a | \hat{o}^{(1)} | \phi_i \rangle,$$

where $|\Phi_i^a\rangle$ is obtained by replacing the occupied orbital ϕ_i with a virtual orbital ϕ_a.

Two-Body Operators

A two-body operator, $\hat{O}^{(2)}$, (e.g. the Coulomb interaction) acts on pairs of electrons.

Diagonal matrix elements:

$$\langle \Phi | \hat{O}^{(2)} | \Phi \rangle = \frac{1}{2} \sum_{i,j \in \text{occ}} \left(\langle \phi_i \phi_j | \hat{o}^{(2)} | \phi_i \phi_j \rangle - \langle \phi_i \phi_j | \hat{o}^{(2)} | \phi_j \phi_i \rangle \right).$$

Off-diagonal matrix elements: Nonzero only if the determinants differ by at most two orbitals.

For determinants that differ by two orbitals (say, ϕ_i, ϕ_j replaced by ϕ_a, ϕ_b):

$$\langle \Phi_{ij}^{ab} | \hat{O}^{(2)} | \Phi \rangle = \langle \phi_a \phi_b | \hat{o}^{(2)} | \phi_i \phi_j \rangle - \langle \phi_a \phi_b | \hat{o}^{(2)} | \phi_j \phi_i \rangle.$$

If the determinants differ by more than two orbitals, the matrix element is zero.

Appendix IV: Interaction Picture for time evolution of Operators and States

Heisenberg Representation

In the Heisenberg picture, all time dependence is transferred to the operators. The time evolution of an operator $\hat{O}$ is given by:

$$\hat{O}_H(t) = e^{\frac{iHt}{\hbar}}\, \hat{O}_S\, e^{-\frac{iHt}{\hbar}},$$

where H is the **full** Hamiltonian.

State vectors: They remain time-independent.

Splitting the Hamiltonian

In the interaction picture, the Hamiltonian is split as:

$$H = H_0 + H_I,$$

where:

- H_0 is the "free" (solvable) part.
- H_I is the interaction (perturbation).

Operator Evolution in the Interaction Picture

Operators evolve according to the free Hamiltonian H_0:

$$\hat{O}_I(t) = e^{\frac{iH_0 t}{\hbar}} \, \hat{O}_S \, e^{-\frac{iH_0 t}{\hbar}}.$$

This is similar to the Heisenberg picture but with H_0 replacing H.

State Evolution in the Interaction Picture

The state vectors in the interaction picture are defined as:

$$|\psi_I(t)\rangle = e^{\frac{iH_0 t}{\hbar}} |\psi_S(t)\rangle.$$

They evolve with the **interaction Hamiltonian** in the interaction picture:

$$i\hbar \frac{d}{dt}|\psi_I(t)\rangle = H_I'(t)\,|\psi_I(t)\rangle,$$

where the interaction Hamiltonian is

$$H_I'(t) = e^{\frac{iH_0 t}{\hbar}}\, H_I\, e^{-\frac{iH_0 t}{\hbar}}.$$

Heisenberg vs. Interaction Picture

Heisenberg Representation:

Operators: $\hat{O}_H(t) = e^{\frac{iHt}{\hbar}}\,\hat{O}_S\,e^{-\frac{iHt}{\hbar}}$ (full H).
States: Time-independent.

Interaction Representation:

Operators: $\hat{O}_I(t) = e^{\frac{iH_0t}{\hbar}}\,\hat{O}_S\,e^{-\frac{iH_0t}{\hbar}}$ (only H_0).
States: Evolve with the interaction:

$$i\hbar\frac{d}{dt}|\psi_I(t)\rangle = H_I'(t)\,|\psi_I(t)\rangle.$$

Key Point: The interaction picture isolates the perturbative part H_I into the state evolution, making it ideal for perturbation theory.