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Solid State Physics II

Chapter 5 Response Theory

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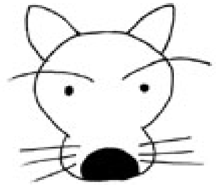


Green's Functions and Response Theory in Many Particle Systems

- How to understand the response of many electrons to external fields?
- What is Green's function?
- Physical implications of Green's function?
- Diagrammatic representation of physical processes?

A simple example of response function

Consider an electron trapped in a potential (e.g., Coulomb potential). If an external electric field $\mathbf{E}$ is applied to this system, then an electric dipole moment $\mathbf{p}$ will develop as a response to the external perturbation.

$$\mathbf{E}_{\rm external} \Rightarrow \mathbf{p} = \alpha \mathbf{E}$$

where the proportional coefficient α is called *polarizability* of the system.

How do understand this response of the system with respect to the external perturbation?

In general, for a system with an external field $\mathbf{H}$ coupled to an internal degree of freedom, μ, as

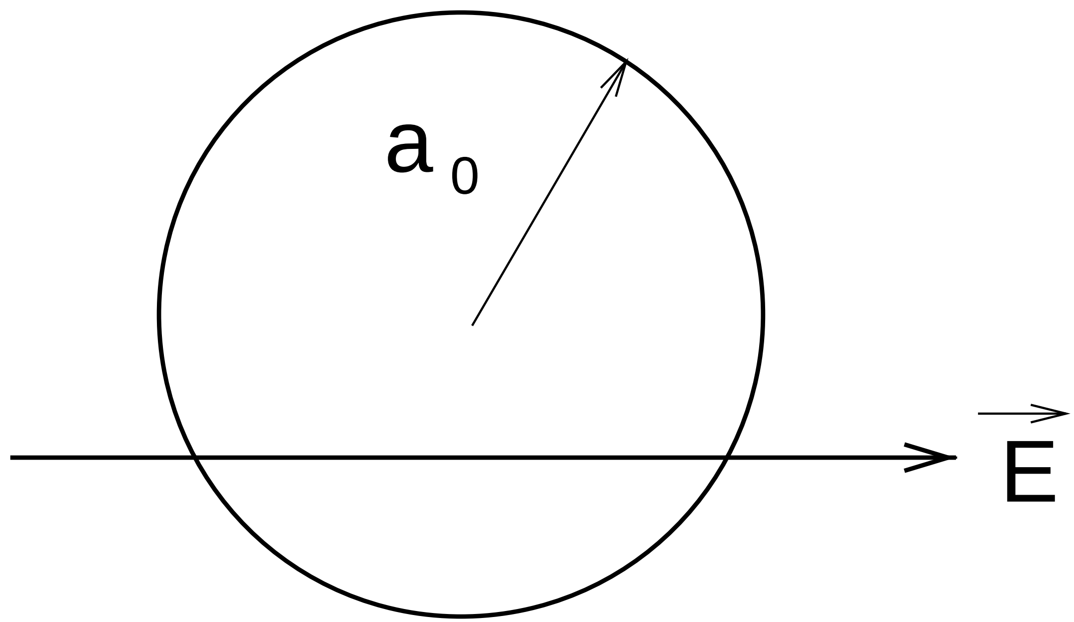
$$\mathcal{H}_1 = -\mu H$$

$$F = \langle \mathcal{H}_o + \mathcal{H}_1 \rangle - TS$$

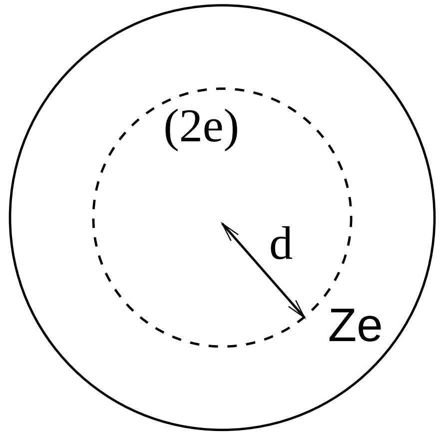
we can obtain the polarization μ of the system by

$$\langle \mu \rangle = -\frac{\partial F}{\partial H}.$$

An atom in an external electric field: a classical approach



First approximation:



$$\frac{1}{4\pi\epsilon_0}(Ze)^2(\frac{d}{a_0})^3 = (Ze)E$$

$$d = \frac{a_0^3}{(Ze)}E \cdot (4\pi\epsilon_0)$$

$$\therefore P = (Ze) \cdot d = a_0^3 E \cdot (4\pi\epsilon_0)$$

◎ **Polarizability:**

$$P = \alpha E$$

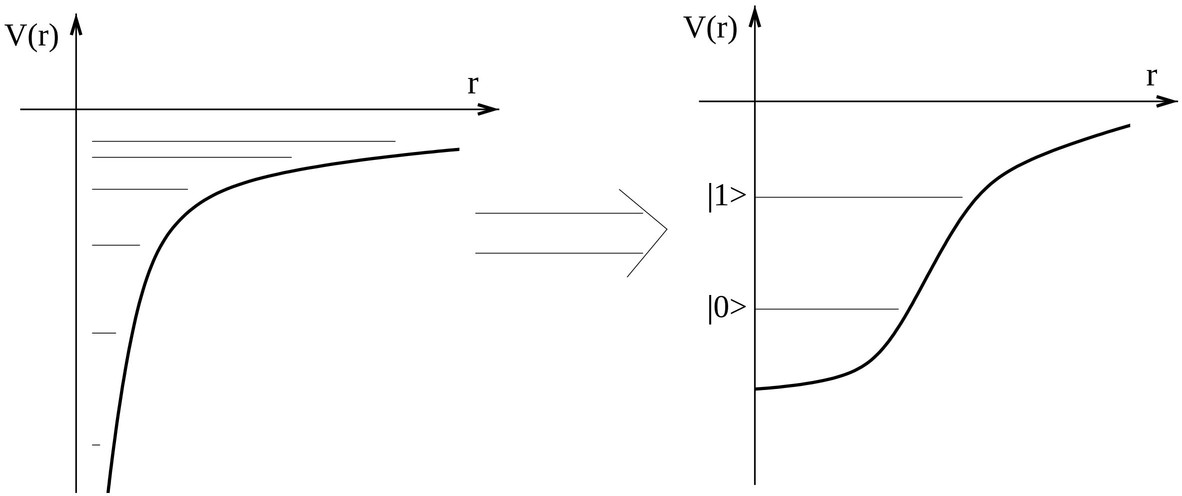
$$\therefore \alpha = 4\pi\epsilon_0 a_0^3$$

Remark: The larger the atom, the easier to be polarized! Why?

Why is this the *first* approximation?

Quantum Mechanical Approach

Instead of considering the real atom with $\frac{1}{r}$ potential, we assume a hypothetical "two level" atom:

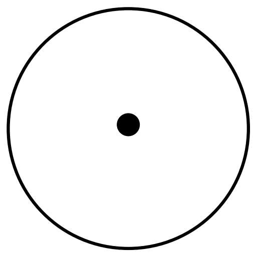


1-particle quantum mechanics

Hamiltonian:

$$\mathcal{H}_0|\varphi_n\rangle = \varepsilon_n|\varphi_n\rangle, \quad (n = 0, 1)$$

where $\varepsilon_0 = 0$, $\varepsilon_1 = \hbar\omega_0$.



$\Rightarrow |\varphi_0\rangle$ with ε_0 (Ground state)

External Field :

$$\mathbf{E} \longrightarrow \mathcal{H}_1 = +e\mathbf{x} \cdot \mathbf{E}$$

where $\langle\varphi_0|\mathcal{H}_1|\varphi_0\rangle = 0$.

- Perturbation of $\mathbf{E}_{\mathrm{ext}} \longrightarrow$

$$|\varphi_0\rangle \rightarrow |\varphi\rangle = |\varphi_0\rangle + |\varphi'\rangle$$

- first order correction to the wavefunction:

$$|\varphi^{(1)}\rangle = |\varphi_0\rangle + \sum_{n\neq 0} |\varphi_n\rangle \frac{\langle \varphi_n|\mathcal{H}_1|\varphi_0\rangle}{\varepsilon_0 - \varepsilon_n}$$

Assuming $\langle \varphi_1|\mathcal{H}_1|\varphi_0\rangle \neq 0$, we have

$$|\varphi^{(1)}\rangle = |\varphi_0\rangle - \frac{\langle \varphi_1|\mathcal{H}_1|\varphi_0\rangle}{\hbar\omega_0}|\varphi_1\rangle$$

- Polarization: $\mathbf{P} = -e\mathbf{x}$:

$$\begin{aligned} \langle \mathbf{P} \rangle &= \langle \varphi^{(1)} | (-e) \mathbf{x} | \varphi^{(1)} \rangle \\ &= 2 \frac{e^2}{\hbar \omega_0} |\langle \varphi_1 | \mathbf{x} | \varphi_0 \rangle|^2 \cdot \mathbf{E} \\ \therefore \alpha &= \frac{2e^2}{\hbar \omega_0} |\langle \varphi_1 | \mathbf{x} | \varphi_0 \rangle|^2 \end{aligned}$$

How is the α (of the QM result) compared with the one by the classical theory, $\alpha = 4\pi\epsilon_0 \cdot a_0^3$?

♠ An example of perturbation methods:

A harmonic oscillator can be described by

$$\mathcal{H}_o = \hbar\omega_o(a^+ a + \frac{1}{2}),$$

with $\mathcal{H}_o|n\rangle = \epsilon_n^o|n\rangle$. And, the perturbation by the external electric field can be written as

$$\mathcal{H}_1 = +e\mathbf{x}\cdot\mathbf{E}_e = e\beta(a + a^+)E_e$$

where $x = \beta(a + a^+)$.

- 0th order:

  Without the external perturbation, the ground state $|\psi_o\rangle$ is

$$|\psi_o\rangle = |0\rangle$$

$$\mathcal{H}_o|\psi_o\rangle = \frac{\hbar\omega_o}{2}|\psi_o\rangle$$

  Thus, the polarization w.r.t. $|\psi_o\rangle$ becomes null.

$$\langle p\rangle = \langle 0|(-e)x|0\rangle = 0$$

- 1st order correction:

$$|\psi^{(1)}\rangle = |\psi_o\rangle + \sum_{n\neq 0} |n\rangle \frac{\langle n|\mathcal{H}_1|\psi_o\rangle}{\epsilon_o^o - \epsilon_n^o}$$

Thus, the polarization w.r.t. $|\psi_o\rangle$ becomes

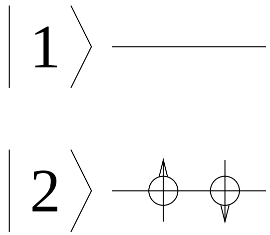
$$\langle p\rangle = \langle\psi^{(1)}|(-e)x|\psi^{(1)}\rangle$$

$$\cdots$$

$$\langle p\rangle = 2\frac{e^2}{\hbar\omega}|\langle 0|x|1\rangle|^2 E_e = \alpha E_e$$

$$\alpha = \frac{2e^2\beta^2}{\hbar\omega_o}$$

2-particle quantum mechanics in the first-quantization picture



Ground state $|\Psi_0\rangle$ with $E_0 = 2\varepsilon_0$

$$\Psi_0(x_1, x_2) = \varphi_0(x_1)\varphi_0(x_2)|\chi_s\rangle, \quad |\chi_s\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle|\downarrow\rangle - |\downarrow\rangle|\uparrow\rangle).$$

For the external field $\mathcal{H}_1 = +e\mathbf{x}\cdot\mathbf{E}$, we can apply the same perturbation scheme to calculate $|\Psi^{(1)}\rangle$:

$$|\Psi^{(1)}\rangle = |\Psi_0\rangle + \sum_{n\neq 0}{}' |\Psi_n\rangle \frac{\langle\Psi_n|\mathcal{H}_1|\Psi_0\rangle}{E_0 - E_n}$$

Here, a question arises:

how many excited states $\{|\Psi_n\rangle\}$ to be considered?

Answer: $2+3=5 \longrightarrow$ Why?

$\rightarrow$ List up all the state $|\Psi_n\rangle$:

$$\begin{aligned}
\Psi_1(x_1,x_2) &= [\varphi_0(x_1)\varphi_1(x_2)\varphi_0(x_2)\varphi_1(x_1)]\frac{1}{\sqrt{2}}\cdot\chi_s \\
\Psi_2(x_1,x_2) &= ...
\end{aligned}$$

$\rightarrow$ The basis functions become too complicated!

Here, a question arises:

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Answer: $2+3=5 \longrightarrow$ Why?

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$\rightarrow$ The basis functions become too complicated!

How many excited states need be considered if there are 3 (or "N") available states instead of 2?

Quantum Mechanics in the Second Quantization Picture for electrons

- ground state:

$$|\Psi_0\rangle = c^\dagger_{0\uparrow} c^\dagger_{0\downarrow}|0\rangle \text{with} \quad E_0 = 2\varepsilon_0$$

- excited state:

$$|\Psi_n\rangle = c^\dagger_{i\sigma} c^\dagger_{j\sigma'}|0\rangle \text{with} \quad E_n = \varepsilon_i + \varepsilon_j$$

$$|\Psi_n\rangle = |n_{0\uparrow}, n_{0\downarrow}, n_{1\uparrow}, n_{1\downarrow}\rangle = |\{n_{i\sigma}\}\rangle$$

where $n_{i\sigma} = 0, 1$ with $i = \{0, 1\}$ and $\sigma = \{\uparrow, \downarrow\}$.

$\Rightarrow$ Total number of 2-particle states with N available orbital-states (normal modes):

$${}_{2N}C_2 = 2N(2N-1)/2$$

Note: In this way, all the symmetrization issues are taken:

$$c^\dagger_{0\uparrow} c^\dagger_{0\uparrow} = 0$$

◎ Hamiltonian in a 2$^{\rm nd}$ quantization form

$$\mathcal{H}_0 = \sum_{i,\sigma} \varepsilon_i c^\dagger_{i\sigma} c_{i\sigma} = \sum_\sigma (\varepsilon_0 c^\dagger_{0\sigma} c_{0\sigma} + \varepsilon_1 c^\dagger_{1\sigma} c_{1\sigma})$$

$$\mathcal{H}_1 = ?$$

$\longrightarrow \langle \varphi_i | + e\mathbf{x} \cdot \mathbf{E} | \varphi_j \rangle = e\mathbf{V}_{ij} \cdot \mathbf{E}$ where $\mathbf{V}_{ij} = \langle \varphi_i | \mathbf{x} | \varphi_j \rangle$: dipole matrix element.

Let's assume $\mathbf{V}_{ij} = 0$ except for

$$\mathbf{V}_{10} = \mathbf{V}_{01} = V_0 \hat{e}_{01}, \quad (\hat{e}_{01} = \langle \varphi_i | \hat{x} | \varphi_j \rangle)$$

$$\rightarrow \quad \mathcal{H}_1 = \sum_\sigma V_0 (c^\dagger_{0\sigma} c_{1\sigma} + c^\dagger_{1\sigma} c_{0\sigma}) \hat{e}_{01} \cdot \mathbf{E}$$

$$\mathcal{H} | \Psi' \rangle = E' | \Psi' \rangle$$

$$\rightarrow \quad | \Psi' \rangle = | \Psi_0 \rangle + \sum_n{}' | \Psi_n \rangle \frac{\langle \Psi_n | \mathcal{H}_1 | \Psi_0 \rangle}{E_0 - E_n}$$

♠ Calculation of $\langle \Psi_n | \mathcal{H}_1 | \Psi_0 \rangle$;

$$
\begin{aligned}
\langle \Psi_n | \mathcal{H}_1 | \Psi_0 \rangle &= \langle 0 | c_{j\sigma'} c_{i\sigma} \left[\sum_{\sigma_1} E (c^\dagger_{0\sigma_1} c_{1\sigma_1} + c^\dagger_{1\sigma_1} c_{0\sigma_1}) \right] c^\dagger_{0\uparrow} c^\dagger_{0\downarrow} | 0 \rangle \\
&= \sum_{\sigma_1} E \langle 0 | c_{j\sigma'} c_{i\sigma} (c^\dagger_{1\sigma_1} c_{0\sigma_1}) c^\dagger_{0\uparrow} c^\dagger_{0\downarrow} | 0 \rangle \\
&= E \left(\langle 0 | c_{j\sigma'} c_{i\sigma} c^\dagger_{1\uparrow} c^\dagger_{0\downarrow} | 0 \rangle - \langle 0 | c_{j\sigma'} c_{i\sigma} c^\dagger_{1\downarrow} c^\dagger_{0\uparrow} | 0 \rangle \right) \\
&\Rightarrow \mathbf{P} = -e\mathbf{x} \\
&\Rightarrow \mathbf{P} = \sum_{\sigma} (-e a_0) \hat{e}_{01} (c^\dagger_{0\sigma} c_{1\sigma} + c^\dagger_{1\sigma} c_{0\sigma}) \\
\langle \mathbf{P} \rangle &= \langle \Psi' | \left[\sum_{\sigma} (-e a_0) \hat{e}_{01} (c^\dagger_{0\sigma} c_{1\sigma} + c^\dagger_{1\sigma} c_{0\sigma}) \right] | \Psi' \rangle
\end{aligned}
$$

♠ Calculation of $\langle\Psi_n|\mathcal{H}_1|\Psi_0\rangle$;

$$\begin{aligned}
\langle\Psi_n|\mathcal{H}_1|\Psi_0\rangle &= \langle 0|c_{j\sigma'}c_{i\sigma}\left[\sum_{\sigma_1} E(c^\dagger_{0\sigma_1}c_{1\sigma_1}+c^\dagger_{1\sigma_1}c_{0\sigma_1})\right]c^\dagger_{0\uparrow}c^\dagger_{0\downarrow}|0\rangle \\
&= \sum_{\sigma_1} E\langle 0|c_{j\sigma'}c_{i\sigma}(c^\dagger_{1\sigma_1}c_{0\sigma_1})c^\dagger_{0\uparrow}c^\dagger_{0\downarrow}|0\rangle \\
&= E\left(\langle 0|c_{j\sigma'}c_{i\sigma}c^\dagger_{1\uparrow}c^\dagger_{0\downarrow}|0\rangle - \langle 0|c_{j\sigma'}c_{i\sigma}c^\dagger_{1\downarrow}c^\dagger_{0\uparrow}|0\rangle\right) \\
&\Rightarrow \mathbf{P} = -e\mathbf{x} \\
&\Rightarrow \mathbf{P} = \sum_\sigma (-ea_0)\hat{e}_{01}(c^\dagger_{0\sigma}c_{1\sigma}+c^\dagger_{1\sigma}c_{0\sigma}) \\
\langle\mathbf{P}\rangle &= \langle\Psi'|\left[\sum_\sigma (-ea_0)\hat{e}_{01}(c^\dagger_{0\sigma}c_{1\sigma}+c^\dagger_{1\sigma}c_{0\sigma})\right]|\Psi'\rangle
\end{aligned}$$

What's next? What happens when there are interactions among electrons?

One-Particle Green's function

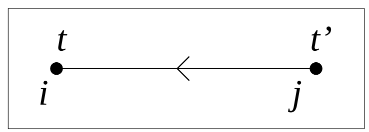
Definition:

(i) $c_i(t) = e^{-i\mathcal{H}_0 t} c_i e^{i\mathcal{H}_0 t}$

(ii) Time ordering operator: $T(A(t)B(t')) = \theta(t-t')A(t)B(t') \pm \theta(t'-t)B(t')A(t)$

(iii) Green's function:

$$\langle \varphi_i(t)|\varphi_j(t')\rangle \rightarrow iG^0_{ij}(t,t') = \langle \Phi_0| i\frac{\partial}{\partial t}[c_i(t)c_j^\dagger(t')]|\Phi_0\rangle$$

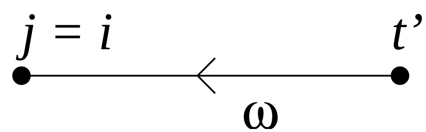


$$\begin{aligned} i\frac{\partial}{\partial t}[iG^0_{ij}(t,t')] &= \langle \Phi_0| i\frac{\partial}{\partial t}[T(c_i(t)c_j^\dagger(t'))]|\Phi_0\rangle \\ &= i\delta(t-t')\delta_{ij} + \epsilon_i^0[iG^0_{ij}(t,t')] \end{aligned}$$

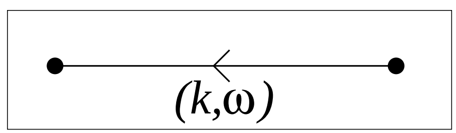
$$\left(i\frac{\partial}{\partial t} - \epsilon_i^0\right) G^0_{ij}(t,t') = \delta(t-t')\delta_{ij}$$: 1-ptl Green's function

Using Fourier transformation,

$$
\begin{aligned}
G^0_{ij}(t, t' = 0) &= \int \frac{d\omega}{2\pi i} e^{-i\omega t} G^0_{ij}(\omega) \\
&\rightarrow \quad (\omega - \epsilon^0_i) G^0_{ij}(\omega) = \delta_{ij} \\
&\rightarrow \quad G^0_{ij}(\omega) = \frac{\delta_{ij}}{\omega - \epsilon^0_i}
\end{aligned}
$$



$$(i = \mathbf{k}) \Longrightarrow G^0_{\mathbf{k}}(\omega) = \frac{1}{\omega - \varepsilon^0_{\mathbf{k}}}$$



$$G^0_{ij}(\omega) = \frac{\delta_{ij}}{\omega - \epsilon^0_i + i\eta \mathrm{sgn}(\epsilon^0_i - \mu)}$$

◎ Interacting System: interaction picture

$$
\begin{aligned}
iG(i,t;j,t') &= \frac{\langle\Psi|T[c_i(t)c_j^\dagger(t')]|\Psi\rangle}{\langle\Psi|\Psi\rangle} \\
&= \frac{\langle\Psi_0|T[U_I(\infty,t)c_{Ii}(t)U_I(t,t')c_{Ij}^\dagger(t')U_I(t',-\infty)]|\Psi_0\rangle}{\langle\Psi_0|U_I(\infty,-\infty)|\Psi_0\rangle}
\end{aligned}
$$

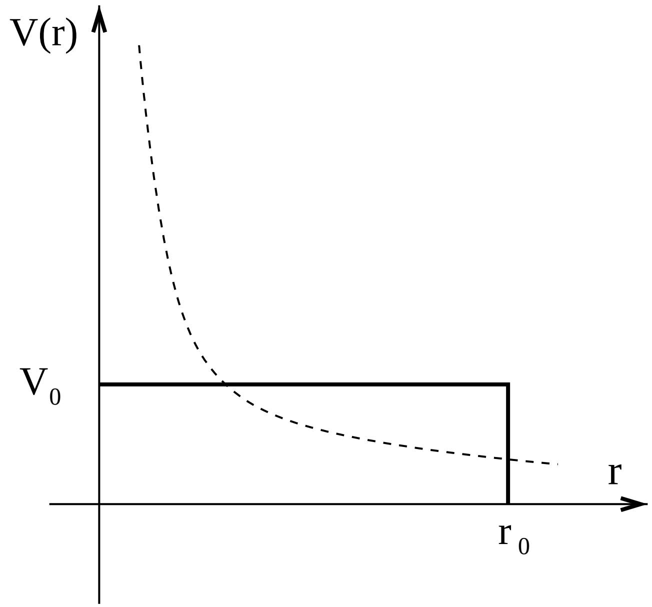
In general

$$
\langle O(t)\rangle = \frac{\langle\Psi_0|T[U_I(\infty,t)O_I(t)U_I(t',-\infty)]|\Psi_0\rangle}{\langle\Psi_0|U_I(\infty,-\infty)|\Psi_0\rangle}
$$

where

$$
\begin{aligned}
O_I(t) &= e^{i\mathcal{H}_0 t}O_H(t)e^{-i\mathcal{H}_0 t} \\
O_H(t) &= e^{-i\mathcal{H}t}O_S(t)e^{i\mathcal{H}t} \\
U_I(t,t') &= T\exp\left[-i\int_{t'}^{t} dt_1 H_I(t_1)\right] \\
&= 1 - i\int_{t'}^{t} dt_1 H_I(t_1) + \ldots.
\end{aligned}
$$

Coulomb Interactions



$$
\begin{aligned}
& \langle \varphi_{\alpha_1}(x_1)\varphi_{\alpha_2}(x_2)|V(x_1-x_2)|\varphi_{\alpha_1'}(x_1)\varphi_{\alpha_2'}(x_2)\rangle \\
\approx \quad & V_0\langle \varphi_{\alpha_1}(x_1)|\varphi_{\alpha_1'}(x_1)\rangle \cdot \langle \varphi_{\alpha_2}(x_2)\varphi_{\alpha_2'}(x_2)\rangle \\
= \quad & V_0\delta_{\alpha_1\alpha_1'}\delta_{\alpha_2\alpha_2'}
\end{aligned}
$$

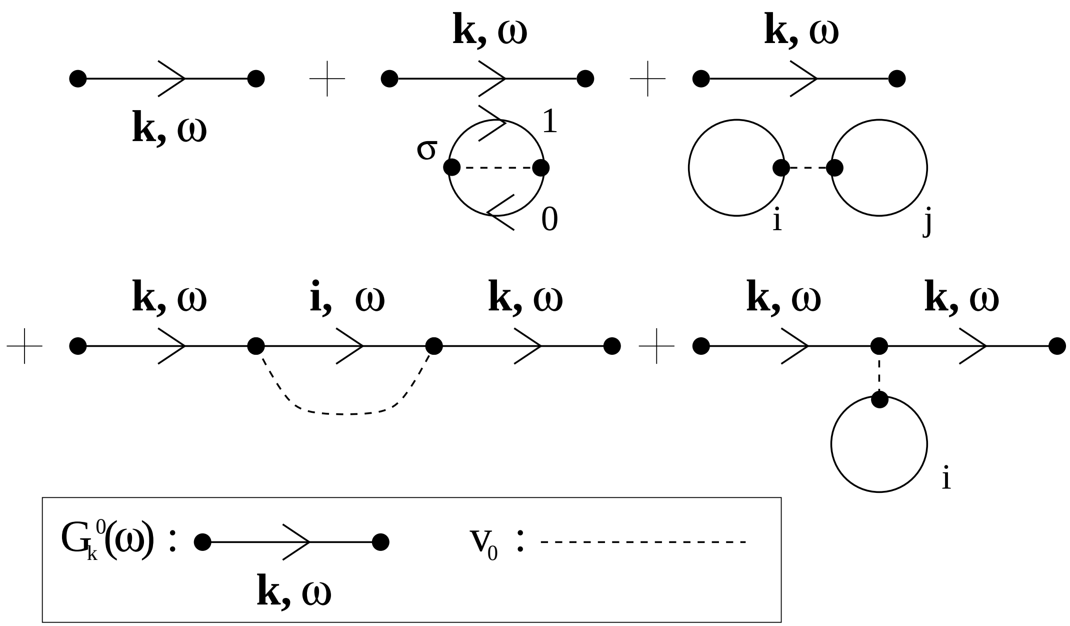
$$
\begin{aligned}
\mathcal{H}_1 &= \frac{1}{2} \sum_{\alpha_1 \alpha_1' \alpha_2 \alpha_2'} \langle \alpha_1 \alpha_2 | V | \alpha_1' \alpha_2' \rangle c^\dagger_{\alpha_1} c^\dagger_{\alpha_2} c_{\alpha_2'} c_{\alpha_1'} \\
&= \frac{1}{2} v_0 \sum_{\alpha_1 \alpha_2} c^\dagger_{\alpha_1} c^\dagger_{\alpha_2} c_{\alpha_2} c_{\alpha_1}
\end{aligned}
$$

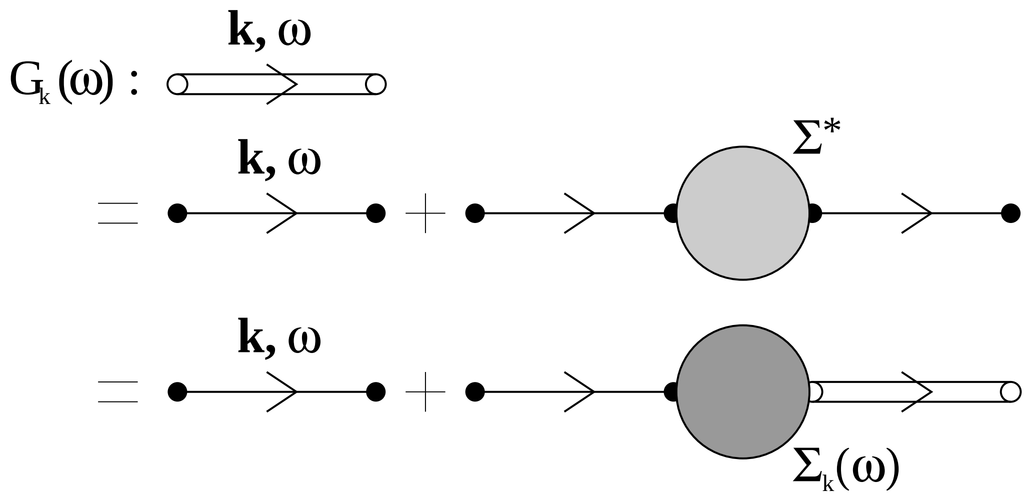
where $\alpha \equiv (i, \sigma)$.

$$
\begin{aligned}
\rightarrow \mathcal{H}_1 &= \frac{1}{2} v_0 \sum_{i\sigma j\sigma'} c^\dagger_{i\sigma} c^\dagger_{j\sigma'} c_{j\sigma'} c_{i\sigma} \\
&= \frac{1}{2} v_0 \sum_{ij\sigma} \left(c^\dagger_{i\sigma} c^\dagger_{j-\sigma} c_{j-\sigma} c_{i\sigma} + c^\dagger_{i\sigma} c^\dagger_{j\sigma} c_{j\sigma} c_{i\sigma} \right) \\
&= v_0 \left(\sum_i c^\dagger_{i\uparrow} c_{i\uparrow} \right) \left(\sum_j c^\dagger_{j\downarrow} c_{j\downarrow} \right) + v_0 \sum_\sigma c^\dagger_{0\sigma} c^\dagger_{1\sigma} c_{1\sigma} c_{0\sigma} \\
&= v_0 N_\uparrow N_\downarrow + v_0 \sum_\sigma c^\dagger_{0\sigma} c^\dagger_{1\sigma} c_{1\sigma} c_{0\sigma}
\end{aligned}
$$

How would the spin configuration of the ground state evolve for $\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_1$ as v_0 increases?

$$\mathcal{H}_1 = v_0 \left(\sum_i c_{i\uparrow}^\dagger c_{i\uparrow}\right)\left(\sum_j c_{j\downarrow}^\dagger c_{j\downarrow}\right) + v_0 \sum_\sigma c_{0\sigma}^\dagger c_{1\sigma}^\dagger c_{1\sigma} c_{0\sigma}$$





$$G_{\mathbf{k}}(\omega) = G^0_{\mathbf{k}}(\omega) + G^0_{\mathbf{k}}(\omega)\Sigma_{\mathbf{k}}(\omega)G_{\mathbf{k}}(\omega)$$

$$G_{\mathbf{k}}(\omega) = \frac{1}{\left(G^0_{\mathbf{k}}(\omega)\right)^{-1} - \Sigma_{\mathbf{k}}(\omega)}$$

Green's Function: Time-independent Formalism

Consider a Hamiltonian $\mathcal{H} = \mathcal{H}_o + \mathcal{H}_1$ such that

$$\frac{\partial \mathcal{H}}{\partial t} = 0$$

$$\mathcal{H}|\psi(t)\rangle = i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle$$

Then, assuming $|\psi(t)\rangle = e^{-i\epsilon t}|\psi(0)\rangle$, we have the time-independent Schrodinger equation:

$$\mathcal{H}|\psi(0)\rangle = \epsilon|\psi(0)\rangle$$

For a complete set of $\{|\varphi_n\rangle\}$ provided by

$$\mathcal{H}_o|\varphi_n\rangle = \epsilon_n^o|\varphi_n\rangle,$$

we can convert the equation into another form:

$$(\epsilon - \mathcal{H}_o)|\psi\rangle = \mathcal{H}_1|\psi\rangle$$

Looking for a solution

$$(\epsilon - \mathcal{H}_o)G_o(\epsilon) = 1$$

or, alternatively,

$$(\epsilon - \mathcal{H}_o(\mathbf{x}))G_o(\mathbf{x}, \mathbf{x}'; \epsilon) = \delta(\mathbf{x} - \mathbf{x}')$$

$$\begin{aligned} |\psi\rangle &= |\varphi_o\rangle + G_o(\epsilon)\mathcal{H}_1|\psi\rangle \\ &= |\varphi_o\rangle + (\epsilon - \mathcal{H}_o)^{-1}\mathcal{H}_1|\psi\rangle \end{aligned}$$

Equivalently,

$$\psi(\mathbf{x}) = \varphi_o(\mathbf{x}) + \int d\mathbf{x}' G_o(\mathbf{x}, \mathbf{x}'; \epsilon)\mathcal{H}_1(\mathbf{x}')\psi(\mathbf{x}')$$

Note that $\varphi_o\rangle$ is one of the null solution of $\mathcal{H}_o$:

$$(\epsilon - \mathcal{H}_o)|\varphi_o\rangle = 0$$

Calculation of G_o

$$G_o(\epsilon) = \sum_n a_n |\varphi_n\rangle$$

$$1 = \sum_n |\varphi_n\rangle\langle\varphi_n|$$

$$(\epsilon - \mathcal{H}_o)G_o = \sum_n |\varphi_n\rangle a_n(\epsilon - \epsilon_n^o) = 1$$

$$\therefore G_o(\epsilon) = \sum_n \frac{|\varphi_n\rangle\langle\varphi_n|}{\epsilon - \epsilon_n^o}$$

Calculation of the Polarization $\mathbf{p}$

$$
\begin{aligned}
\mathbf{p} &= \langle \psi | (q\mathbf{d}) | \psi \rangle \\
&= \langle \varphi_o | (q\mathbf{d}) | \varphi_o \rangle \\
&\quad + \langle \varphi_o | (q\mathbf{d}) G_o \mathcal{H}_1 | \psi \rangle \\
&\quad + \langle \psi | \mathcal{H}_1 G_o (q\mathbf{d}) | \varphi_o \rangle \\
&\quad + \langle \psi | \mathcal{H}_1 G_o (q\mathbf{d}) G_o \mathcal{H}_1 | \psi \rangle \\
&\approx \langle \varphi_o | (q\mathbf{d}) G_o \mathcal{H}_1 | \varphi_o \rangle \\
&\quad + \langle \varphi_o | \mathcal{H}_1 G_o (q\mathbf{d}) | \varphi_o \rangle
\end{aligned}
$$

For the case of a response to the electric field,

$$\mathcal{H}_1 = -q\mathbf{x} \cdot \mathbf{E}_e$$

$$\mathbf{p} = \left[2q^2 \langle \varphi_o | \mathbf{x} G_o \mathbf{x} | \varphi_o \rangle \right] \cdot \mathbf{E}_e$$

Green's Function: Time-dependent Formalism

Suppose $\mathcal{H}_1 = \mathcal{H}_1(t)$, i.e., $\partial\mathcal{H}_1/\partial t \neq 0$,

$$\left(i\frac{\partial}{\partial t} - \mathcal{H}_o\right)|\psi(t)\rangle = \mathcal{H}_1|\psi(t)\rangle$$

Now look for a Green's function:

$$\left(i\frac{\partial}{\partial t} - \mathcal{H}_o\right)G_o(t,t') = 1\delta(t-t')$$

From the results of the previous pages, we can guess

$$\begin{aligned} G_o(t,t') &= \int \frac{d\epsilon}{2\pi} G_o(\epsilon+i\eta) e^{-i\epsilon(t-t')} \\ &= \int \frac{d\epsilon}{2\pi} \frac{e^{-i\epsilon(t-t')}}{\epsilon-(\epsilon_n^o - i\eta)} |\varphi_n\rangle\langle\varphi_n| \\ &= -i\theta(t-t') \sum_n e^{-i\epsilon_n^o(t-t')} |\varphi_n\rangle\langle\varphi_n| \\ &= -i\theta(t-t') e^{-i\mathcal{H}_o(t-t')} \end{aligned}$$

$$\begin{aligned} \Rightarrow |\psi(t)\rangle &= |\varphi_o(t)\rangle + \int_{-\infty}^{t} dt' G_o(t,t')\mathcal{H}_1(t')|\psi(t')\rangle \\ &= |\varphi_o(t)\rangle + \int_{-\infty}^{t} dt' G_o(t,t')\mathcal{H}_1(t')|\varphi_o(t')\rangle \\ &\quad + \int_{-\infty}^{t} dt' \int_{-\infty}^{t'} dt'' G_o(t,t')\mathcal{H}_1(t')G_o(t',t'')\mathcal{H}_1(t'')|\varphi_o(t'')\rangle + \ldots \end{aligned}$$

Introducing the “interaction picture”,

$$\mathcal{H}_I(t) = e^{i\mathcal{H}_o t}\mathcal{H}_1(t)e^{-i\mathcal{H}_o t}$$

$$|\psi_I(t)\rangle = e^{i\mathcal{H}_o t}|\psi(t)\rangle$$

$$|\varphi_{oI}\rangle = |\varphi_o(0)\rangle = e^{i\mathcal{H}_o t}|\varphi_o\rangle$$

$$\begin{aligned}
\Rightarrow |\psi_I(t)\rangle &= |\varphi_o(0)\rangle \\
&\quad +(-i)\int^t dt'\mathcal{H}_I(t')|\varphi_o\rangle \\
&\quad +\frac{(-i)^2}{2!}\int^t\int^t dt'dt''\mathcal{T}[\mathcal{H}_I(t')\mathcal{H}_I(t'')]|\varphi_o\rangle \\
&\quad +\dots \\
&= \mathcal{T}\exp\left[-i\int_{-\infty}^t dt'\mathcal{H}_I(t')\right]|\varphi_o\rangle \\
&= U_I(t,-\infty)|\varphi_o\rangle
\end{aligned}$$

Expectation value of an operator $\mathcal{O}$

$$
\begin{aligned}
\langle \mathcal{O} \rangle (t) &= \langle \psi(t) | \mathcal{O} | \psi(t) \rangle / \langle \psi(t) | \psi(t) \rangle \\
&= \langle \psi_I(t) | e^{i\mathcal{H}_o t} \mathcal{O} e^{-i\mathcal{H}_o t} | \psi_I(t) \rangle / \langle \psi(t) | \psi(t) \rangle \\
&= \langle \psi_I(t) | \mathcal{O}_I(t) | \psi_I(t) \rangle / \langle \psi(t) | \psi(t) \rangle \\
&= \frac{\langle \varphi_o | \mathcal{T} \exp\left[-i \int_t^\infty dt' \mathcal{H}_I(t')\right] \mathcal{O}_I(t) \exp\left[-i \int_{-\infty}^t dt' \mathcal{H}_I(t')\right] | \varphi_o \rangle}{\langle \varphi_o | \mathcal{T} \exp\left[-i \int_{-\infty}^\infty dt' \mathcal{H}_I(t')\right] | \varphi_o \rangle} \\
&= \langle \varphi_o | U_I(\infty, t) \mathcal{O}_I(t) U_I(t, -\infty) | \varphi_o \rangle / \langle \varphi_o | U_I(\infty, -\infty) | \varphi_o \rangle \\
&= \langle \varphi_o | U_I(\infty, t) \mathcal{O}_I(t) U_I(t, -\infty) | \varphi_o \rangle_{\mathrm{conn}}
\end{aligned}
$$

Green's Function in 2nd Quantization Formalism

Definition: One-particle Green's function

$$G(x't';xt) = -i\langle \mathcal{T}[\hat{\psi}(x't')\hat{\psi}^{+}(xt)]\rangle$$

Time-ordering operator $\mathcal{T}$:

$$\mathcal{T}[\psi(t')\psi^{+}(t)] \equiv \theta(t'-t)\psi(t')\psi^{+}(t) + \zeta\theta(t-t')\psi^{+}(t)\psi(t')$$

where $\zeta = +1$ for bosons and -1 for fermions.

Here the one-particle Green's function $G^{o}(x't', xt)$ satisfies

$$\left(i\frac{\partial}{\partial t} - h_o\right) G^{o}(t,t') = \delta(\mathbf{x}-\mathbf{x}')\delta(t-t')$$

To calculate the expectation value of $G(x't';xt)$,

$$\begin{aligned} G(x't';xt) &= -i\langle \mathcal{T}[\hat{\psi}(x't')\hat{\psi}^+(xt)]\rangle_{\rm conn} \\ &= -i\langle \Phi_o|\mathcal{T}\left[U_I(\infty,t')\hat{\psi}_I(x't')U_I(t',t)\hat{\psi}_I^+(xt)U_I(t,-\infty)\right]|\Phi_o\rangle_{\rm conn} \end{aligned}$$

Free Fermion Gas

Consider a fermion system with the ground state

$$|\Phi_o\rangle = \prod_{k\sigma} \theta(k_F - k) c^+_{k\sigma} |0\rangle$$

Fermion Field Operator:

$$\psi(\mathbf{x}) = \sum_{k\sigma} c_{k\sigma} \varphi_k(\mathbf{x})$$

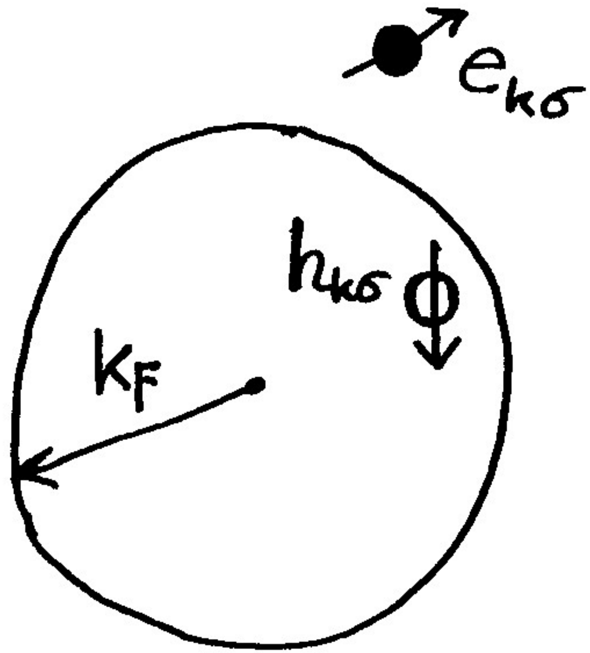
where $\varphi_k(\mathbf{x}) = e^{i\mathbf{k}\cdot\mathbf{x}}$.

$$\begin{aligned}
\psi_I(\mathbf{x}, t) &= e^{i\mathcal{H}_o t} \psi(\mathbf{x}) e^{-i\mathcal{H}_o t} \\
&= \sum_{k\sigma} e^{i\mathcal{H}_o t} c_{k\sigma} e^{-i\mathcal{H}_o t} \varphi_k(\mathbf{x}) \\
&= \sum_{k\sigma} e^{-i\omega_k t} c_{k\sigma} \varphi_k(\mathbf{x})
\end{aligned}$$

Note that

$$\theta(k - k_F) c_{k\sigma} |\Phi_o\rangle = 0$$

$$\theta(k_F - k) c^+_{k\sigma} |\Phi_o\rangle = 0$$



Consider a transformation of $c_{k\sigma}$:

$$c_{k\sigma} = e_{k\sigma}\theta(k - k_F) + h_{k\sigma}^{+}\theta(k_F - k)$$

so that

$$e_{k\sigma}|\Phi_o\rangle = h_{k\sigma}|\Phi_o\rangle = 0$$

where $e_{k\sigma}$ ($h_{k\sigma}$) is defined only in the range of $k > k_F$ ($k < k_F$).

Rewriting the Hamiltonian in terms of $e_{k\sigma}$ and $h_{k\sigma}$,

$$\begin{aligned}
\mathcal{H}_o &= \sum_{k\sigma}(\omega_k - \mu)c_{k\sigma}^{+}c_{k\sigma} \\
&= \sum_{k>k_F,\sigma}(\omega_k - \mu)e_{k\sigma}^{+}e_{k\sigma} + \sum_{k<k_F,\sigma}(\mu - \omega_k)h_{k\sigma}^{+}h_{k\sigma} + \sum_{k\sigma}\omega_k\theta(k_F - k) \\
&= \sum_{k>k_F,\sigma}\xi_{ek}e_{k\sigma}^{+}e_{k\sigma} + \sum_{k<k_F,\sigma}\xi_{hk}h_{k\sigma}^{+}h_{k\sigma} + E_o
\end{aligned}$$

Free Fermion Green's Function

$$\begin{aligned} G^o_{\alpha\beta}(xt, x't') &= -i\langle\Phi_o|\mathcal{T}[\psi_\alpha(xt)\psi^+_\beta(x't')]|\Phi_o\rangle \\ &= -i\delta_{\alpha\beta}\sum_k e^{ik(x-x')}e^{-i\xi_k(t-t')}[\theta(t-t')\theta(k-k_F)-\theta(t'-t)\theta(k_F-k)] \\ &= \delta_{\alpha\beta}\int\frac{d^3k d\omega}{(2\pi)^4}e^{ik(x-x')}e^{-i\omega(t-t')}\left[\frac{\theta(k-k_F)}{\omega-\xi_k+i\eta}+\frac{\theta(k-k_F)}{\omega-\xi_k-i\eta}\right] \end{aligned}$$

$$G^o_{\alpha\beta}(\mathbf{k},\omega) = \delta_{\alpha\beta}\left[\frac{\theta(k-k_F)}{\omega-\xi_k+i\eta}+\frac{\theta(k_F-k)}{\omega-\xi_k-i\eta}\right] = \frac{\delta_{\alpha\beta}}{\omega-\xi_k-i\eta\,\mathrm{sgn}(k-k_F)}$$

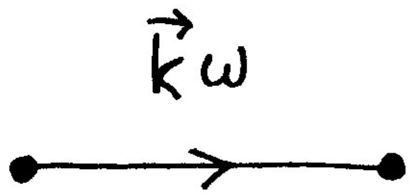
Here we used the relation:

$$\theta(t-t') = -\int_{-\infty}^{\infty}\frac{d\omega}{2\pi i}\frac{e^{-i\omega(t-t')}}{\omega+i\eta}$$

Physical Interpretation of Green's Function

Green's Function in Momentum Space

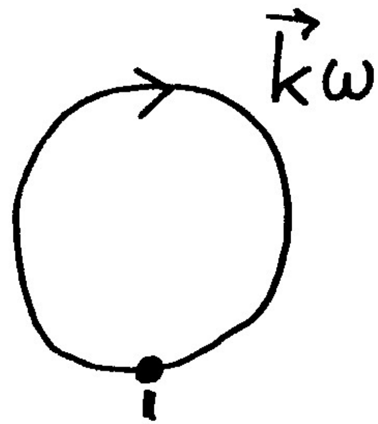
$$
\begin{aligned}
G^o_{\alpha\beta}(xt;00) = \delta_{\alpha\beta} G^o(xt) &= -i \langle \Phi_o | \mathcal{T}[\psi_\alpha(xt)\psi^+_\beta(00)] | \Phi_o \rangle \\
&= \delta_{\alpha\beta} \sum_k \int \frac{d\omega}{2\pi} e^{i(kx-\omega t)} G^o(k\omega)
\end{aligned}
$$



$$
G^o(k\omega) = \frac{1}{\omega - \xi_k + i\eta \,\mathrm{sgn}(k - k_F)}
$$

Electron Density

$$
\begin{aligned}
n_o(x=0) &= \sum_\alpha \langle \Phi_o | \psi_\alpha^+(00)\psi_\alpha(0,-0)|\Phi_o\rangle \\
&= -2iG^o(x=0,t=-0) \\
&= 2\sum_k \theta(k_F - k)
\end{aligned}
$$



Interacting Electron System

$$G(xt) = -i\langle\Phi_o|\mathcal{T}\left[U_I(\infty,-\infty)\psi(xt)\psi^+(00)\right]|\Phi_o\rangle_{\rm conn}$$

where

$$\begin{aligned} U_I(+\infty,-\infty) &= \mathcal{T}\exp[-i\int_{-\infty}^{\infty}dt' H_I(t')] \\ &= 1 - i\int_{-\infty}^{\infty}dt' H_I(t') \\ &\quad + \frac{(-i)^2}{2!}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}dt'dt''\mathcal{T}[H_I(t')H_I(t'')] + \ldots \end{aligned}$$

$$
\begin{aligned}
\Rightarrow G(xt) &= -i\langle\Phi_o|\mathcal{T}[\psi(xt)\psi^+(00)|\Phi_o\rangle_{\rm conn} \\
&\quad +(-i)^2\langle\Phi_o|\mathcal{T}\left[\int_{-\infty}^{\infty} dt' H_I(t')\psi(xt)\psi^+(00)\right]|\Phi_o\rangle_{\rm conn} \\
&\quad +\ldots \\
&= G^o(xt) + G^{(1)}(xt) + \ldots
\end{aligned}
$$

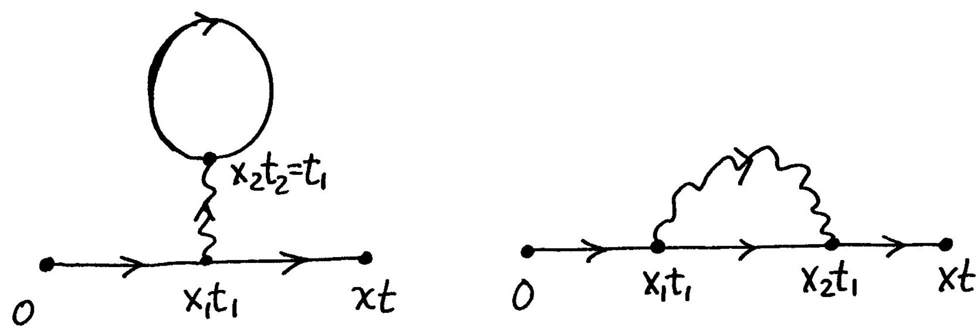
Here it is noted that

$$
\int_{-\infty}^{\infty} dt' H_I(t') = \int d^4x_1 d^4x_2 V(\mathbf{x}_1-\mathbf{x}_2)\delta(t_1-t_2)\psi^+(\mathbf{x}_1t_1)\psi^+(\mathbf{x}_2t_2)\psi(\mathbf{x}_2t_2)\psi(\mathbf{x}_1t_1)
$$

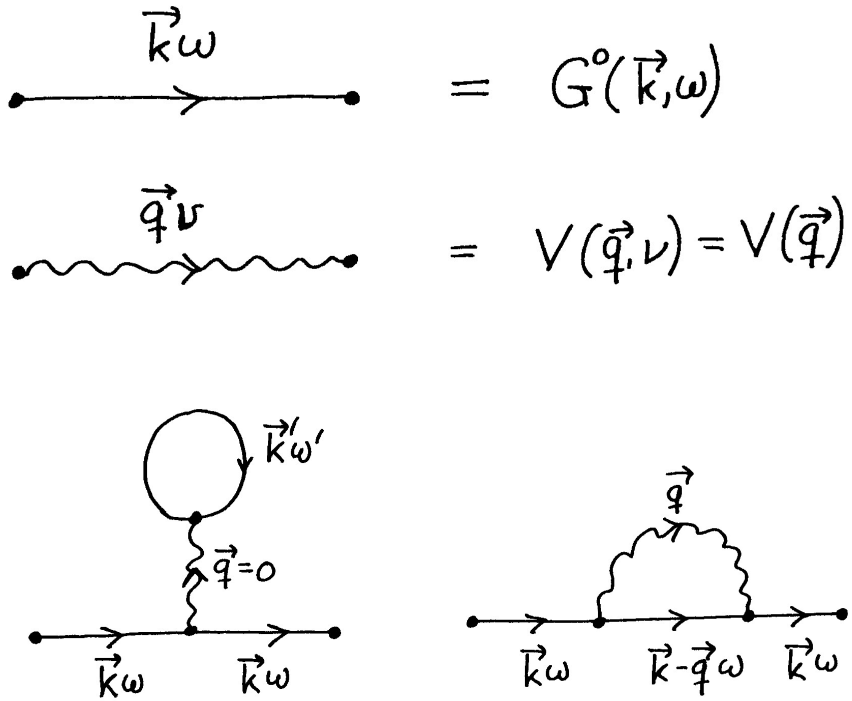
$$
\begin{aligned}
G^{(1)}(xt) &= (-i)^2\int d^4x_1 d^4x_2 V(\mathbf{x}_1-\mathbf{x}_2)\delta(t_1-t_2) \\
&\quad \times\langle\Phi_o|\mathcal{T}[\psi^+(\mathbf{x}_1t_1)\psi^+(\mathbf{x}_2t_2)\psi(\mathbf{x}_2t_2)\psi(\mathbf{x}_1t_1)\psi(\mathbf{x}t)\psi^+(00)]|\Phi_o\rangle_{\rm conn}
\end{aligned}
$$

Wick's Theorem

$$
\begin{aligned}
G^{(1)}(xt) &= (-i)^2 \int d^4x_1 d^4x_2 V(\mathbf{x}_1 - \mathbf{x}_2)\delta(t_1 - t_2) \\
&\quad \times \langle \Phi_o | \mathcal{T}[\psi^+(\mathbf{x}_1 t_1)\psi^+(\mathbf{x}_2 t_2)\psi(\mathbf{x}_2 t_2)\psi(\mathbf{x}_1 t_1)\psi(\mathbf{x}t)\psi^+(00)] | \Phi_o \rangle_{\text{conn}} \\
&= (-i)^2 (i)^{2+1} \int d^4x_1 d^4x_2 V(\mathbf{x}_1 - \mathbf{x}_2)\delta(t_1 - t_2) \\
&\quad \times [-G^o(xt; x_1t_1)G^o(x_1t_1; 00)G^o(x_2t_2^{-0}; x_2t_2) \\
&\quad + G^o(xt; x_2t_2)G(x_2t_2; x_1t_1)G^o(x_1t_1; 00)]
\end{aligned}
$$



Diagrammatic Rule



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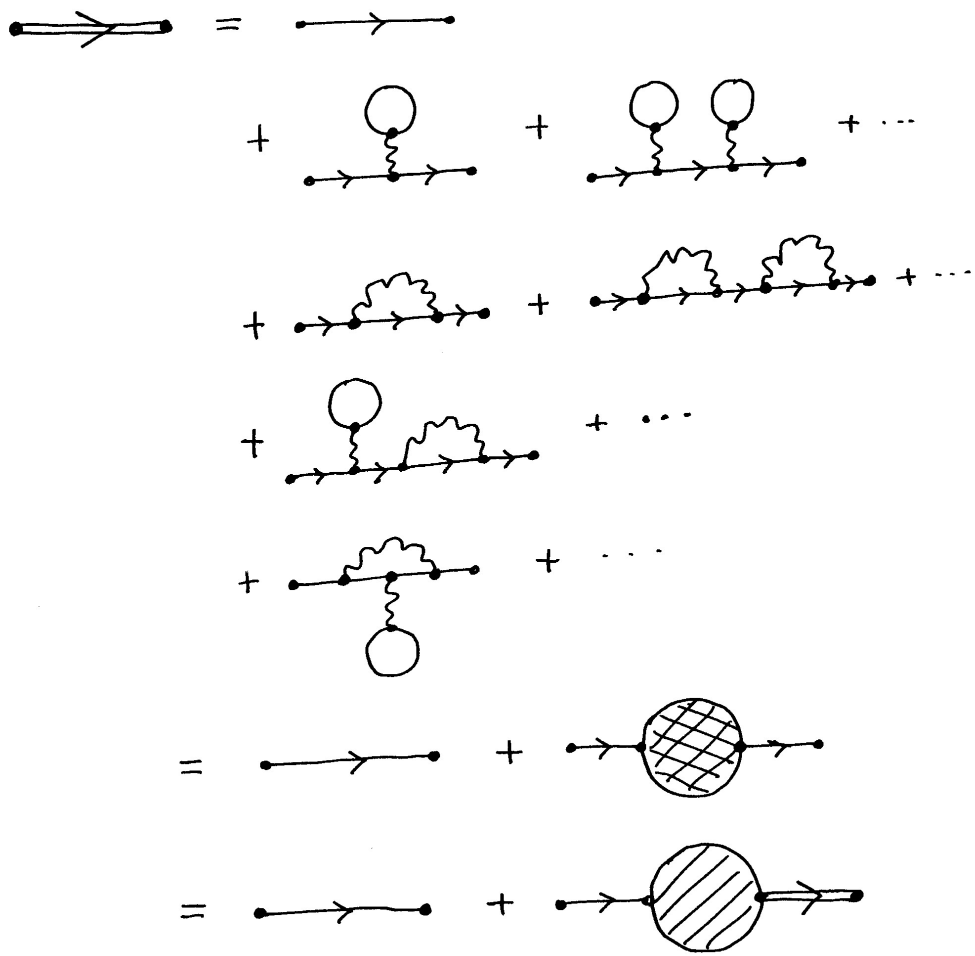
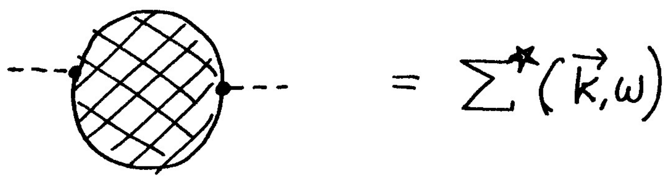
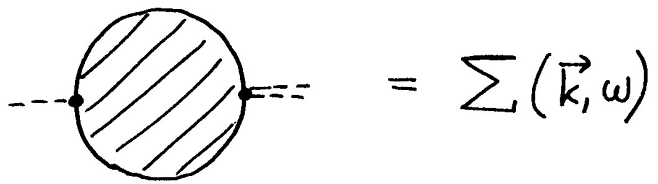


Self-Energy

$$G = G^o + G^o \Sigma^\star G^o = G^o + G^o \Sigma G$$

$$G = (1 - G^o\Sigma)^{-1} G^o = (G^{o-1} - \Sigma)^{-1} = \frac{1}{\omega - \xi_k - \Sigma_k(\omega)}$$



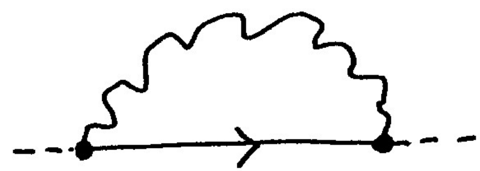


Physical Content of the Self-Energy

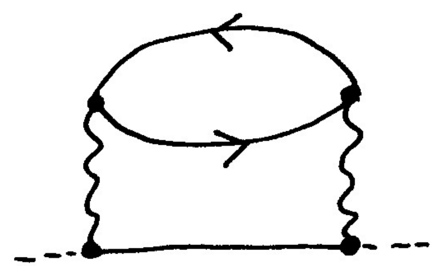
$$G^o(k\omega) = \frac{1}{\omega - \xi_k + i\eta \mathrm{sgn}(\omega)}$$

$$G(k\omega) = \frac{1}{\omega - \xi_k - \Sigma(k\omega)}$$

$$\Sigma_1(\vec{k}) =$$



$$\Sigma_2(\vec{k}_1, \omega) =$$

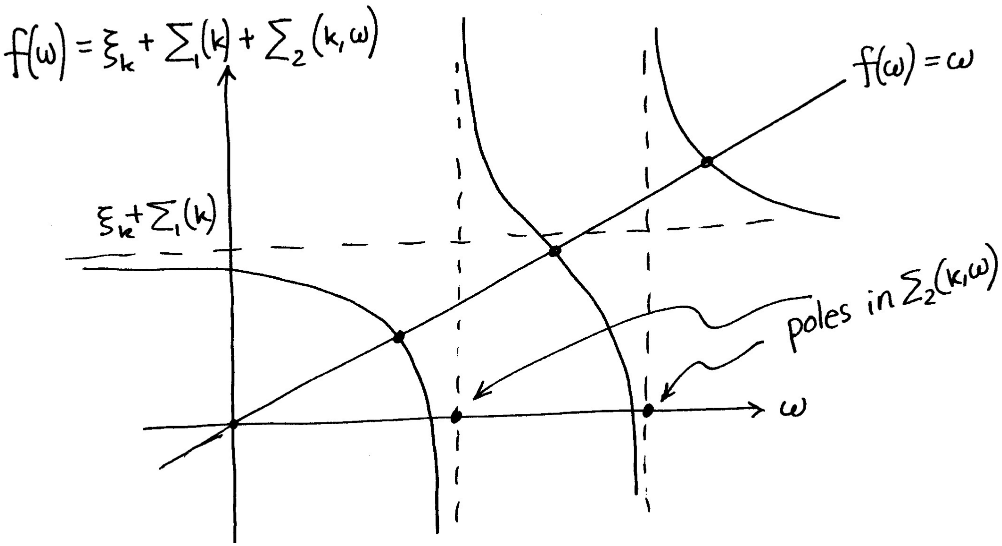


Quasi-Particle Pole in $G(k\omega)$

$$G(k\omega) = \frac{1}{\omega - \xi - \Sigma_1(k) - \Sigma_2(k\omega)}$$

Quasi-particle pole:

$$G^{-1}(k, \omega = E_k) = 0 \rightarrow \; E_k = \xi_k + \Sigma_1(k) + \Sigma_2(k, E_k)$$



Analysis of the pole structure in $G(k\omega)$

Assume that $\Sigma_2(\omega)$ has one two poles,

$$\Sigma_2(\omega) = \frac{A_1}{\omega - E_1} + \frac{A_2}{\omega - E_2}$$

$$\Rightarrow G(\omega) = \frac{1}{\omega - E_o - \Sigma_2(\omega)}$$

where $E_o = \xi + \Sigma_1$. Further, assuming that

$$\frac{A_i}{|E_i - E_o||E_j - E_o|} < \eta << 1 \qquad (i, j = 1, 2)$$

Around each pole ω_s, i.e., $\omega_s = E_o + \Sigma_2(\omega_s)$,

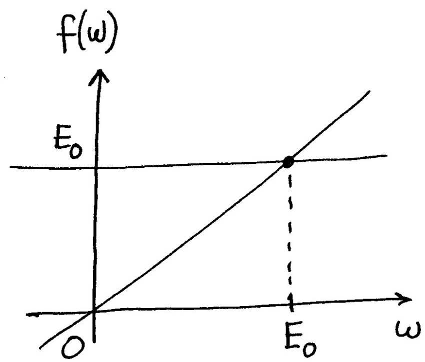
$$\begin{aligned} \omega - E_o - \Sigma_2(\omega) &\approx \omega - E_o - \Sigma_2(\omega_s) - (\omega - \omega_s)\Sigma_2'(\omega_s) \\ &= (\omega - \omega_s)\left(1 - \Sigma_2'(\omega_s)\right) \end{aligned}$$

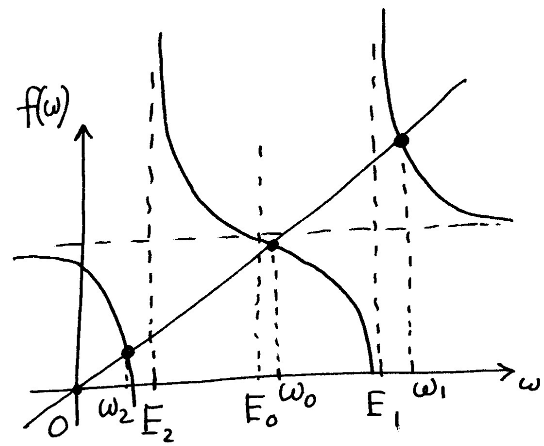
$$\therefore \quad G(\omega) \approx \sum_s \frac{[1 - \Sigma_2'(\omega_s)]^{-1}}{\omega - \omega_s}$$

$$G(\omega) \approx \sum_{s=0}^{2} \frac{[1-\Sigma_2'(\omega_s)]^{-1}}{\omega - \omega_s}$$

$$[1-\Sigma_2'(\omega_o)]^{-1} = \frac{1}{1+\sum_{i=1}^{2} \frac{A_i}{(\omega_o - E_i)^2}} \approx 1 - \sum_{i=1}^{2} \frac{A_i}{(\omega_o - E_i)^2}$$

$$[1-\Sigma_2'(\omega_i)]^{-1} = \frac{1}{1+\sum_{j=1}^{2} \frac{A_j}{(\omega_o - E_j)^2}} \approx \frac{1}{1+\frac{A_i}{(\omega_i - E_i)^2}} \approx \frac{A_i}{(\omega_i - E_o)^2} \quad \text{for } i = 1,2$$





Fermi Liquid State

Green's Function:

$$G(k\omega) = \frac{1}{\omega - \xi_k - \Sigma(k\omega)}$$

Quasi-particle energy:

$$E_k = \epsilon_k - \mu + \mathrm{Re}\Sigma(k, E_k)$$

Near the pole E_k

$$\begin{aligned} & \omega - \xi_k - \Sigma(k,\omega) \\ \approx\ & \omega - \xi_k - \mathrm{Re}\Sigma(k, E_k) - (\omega - E_k) \left.\frac{\partial \mathrm{Re}\Sigma_k}{\partial \omega}\right|_{E_k} - i\mathrm{Im}\Sigma_k \\ =\ & \left(1 - \left.\frac{\partial \mathrm{Re}\Sigma_k}{\partial \omega}\right|_{E_k}\right)(\omega - E_k - i\Gamma_k) \end{aligned}$$

$$\therefore \quad G(k\omega) \approx \frac{Z_k}{\omega - E_k - i\Gamma_k} + \varphi(k\omega)$$

where the renormalization constant Z_k ($0 < Z_k \leq 1$) is given by

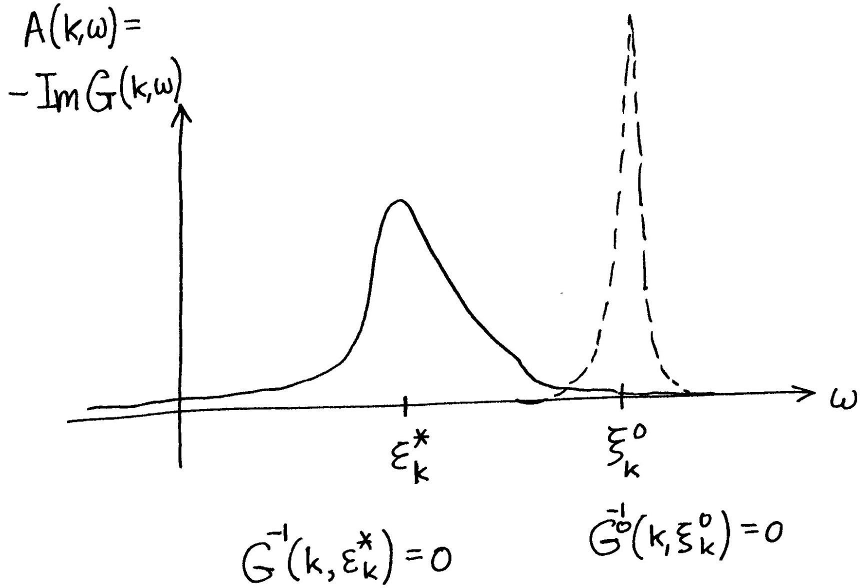
$$Z_k = \left(1 - \left. \frac{\partial \mathrm{Re}\Sigma_k}{\partial \omega} \right|_{E_k} \right)^{-1}$$

and the regular function $\varphi(k\omega)$ represents multi-particle excitation contribution to $G(k\omega)$ near E_k.

Spectral Function

$$G(k\omega) = \frac{1}{\omega - \xi_k - \Sigma_k(\omega)}$$

$$A(\mathbf{k},\omega) = -2\mathrm{Im}G(\mathbf{k},\omega)$$



Green's Function for the Fermi Liquid State

$$G_{\mathrm{FL}}(k\omega) = \frac{Z_k}{\omega - \xi_k + i\eta \mathrm{sgn}(\omega)}$$

Note: Unless there is a breakdown of perturbation theory (e.g., a phase transition), excitations of the true interacting system have the same quantum numbers (conserved quantities) as the non-interacting one.

Momentum Distribution Function $n(\mathbf{k})$