PROPAGATOR AND QUASI-PARTICLES
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I. THE 1-PARTICLE PROTAGONIST

Given a Hamiltonian with ground state with $N$ particles $|E^N_n\rangle$ and two single particle states $|u\rangle$ and $|u'\rangle$, the time-ordered 1-particle propagator is

$$iG(u,v,t',t) = \langle E^N_n|\Psi_u(t)\psi_{u'}(t')|E^N_n\rangle$$

$$= \left\{ \begin{array}{ll}
\langle E^N_n|\psi_{u'}(t')\psi_u(t)|E^N_n\rangle & t > t' \\
-\langle E^N_n|\psi_{u'}(t')\psi_u(t)|E^N_n\rangle & t' > t
\end{array} \right.$$  

If $t > t'$, it is proportional to the amplitude for the propagation from time $t'$ to time $t$ of a state formed by adding a particle $|u'\rangle$ to the ground state, to a state where a particle $|u\rangle$ is added to the ground state. If $t' > t$ the amplitude refers to a hole being created in $|u\rangle$ at time $t$ and destroyed in $|u'\rangle$ at later time $t'$.

Since it depends on $t - t'$, it has Fourier representation:

$$G(u,t;u',t') = \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} e^{-i\omega(t-t')} G(u,u';\omega)$$

The discontinuity at $t = t'$ implies a slow decay of the Fourier transform:

$$\lim_{|\omega|\to\infty} \omega G_{u,u'}(\omega) = \langle u|u'\rangle$$

Proof: $iG(u,t + \eta;u',t) - iG(u,t - \eta;u',t) = \langle u|u'\rangle$ for $\eta \to 0^+$. After Fourier transform:

$$\langle u|u'\rangle = \int_{-\infty}^{+\infty} \frac{d\omega}{\pi} \sin(\omega \eta) G(u,u';\omega)$$

$$= \int_{-\infty}^{+\infty} d\omega \sin \omega \left[ \omega G(u,u';\omega) \right]$$

where $\omega' = \omega/\eta$. Since $\omega'$ is as large as wanted, the relation is true for all $|u\rangle$ and $|u'\rangle$, if eq.(3) holds. □

If the system is confined in a box, the spectrum of the Hamiltonian is discrete, with eigenstates $|E^N_n\rangle$. Insertion of the identities $1 = \sum_a |E^N_{n0}\rangle \langle E^N_{n0}|$ in eq.(4) makes the time-dependence explicit. In frequency space the propagator for position-spin states has the following Lehmann’s representation:

$$G_{\mu\nu}(x',x;\omega) = \sum_a \langle E^N_n|\psi_{\mu}(x)|E^N_{n+1}\rangle \langle E^N_{n+1}|\psi_{\nu}(x')|E^N_n\rangle$$

$$= \frac{1}{\pi} \int_{-\infty}^{+\infty} \frac{d\omega}{\omega - \frac{1}{\hbar}(\mu + \epsilon^N_{n+1}) + i\eta}$$

$$+ \frac{\langle E^N_n|\psi_{\nu}(x')|E^N_{n-1}\rangle \langle E^N_{n-1}|\psi_{\mu}(x)|E^N_n\rangle}{\omega - \frac{1}{\pi}(\mu - \epsilon^N_{n-1}) - i\eta}$$

The values $E^N_{n+1} - E^N_{n} = \epsilon^N_{n+1} \geq 0$ are the excitation energies. In the differences $E^N_{n+1} - E^N_{n} = \pm \mu$, the chemical potential is insensitive to $N$, if $N$ is large.

A. Homogeneous systems

For a homogeneous system confined in the box the propagator has expansion

$$G_{\mu\nu}(x,x';\omega) = \frac{1}{V} \sum_{k} e^{ik(x-x')} G_{\mu\nu}(k,\omega)$$

Let us assume that $G_{\mu\nu} = \delta_{\mu\nu} G$. Since $H$ and $P$ commute, they share a basis of eigenvectors $|E^N_n,k\rangle$; the ground system has momentum equal to zero. By using the operator identity and its adjoint

$$\psi_{\mu}(x) = \exp(-i/\hbar x \cdot P) \psi_{\mu}(0) \exp(i/\hbar x \cdot P)$$

the Lehmann representation in $k$ space is obtained:

$$G(k,\omega) = \frac{1}{V} \sum_{a,\mu} |\langle E^N_n|\psi_{\mu}(0)|E^N_{n+1},k\rangle|^2$$

$$\omega - \frac{1}{\hbar}(\mu + \epsilon^N_{n+1}(k)) + i\eta$$

$$+ |\langle E^N_n|\psi_{\mu}(0)|E^N_{n-1},-k\rangle|^2$$

$$- \omega - \frac{1}{\hbar}(\mu - \epsilon^N_{n-1}(-k)) - i\eta$$

With the introduction of the spectral function

$$A(k,\omega) = \frac{1}{V} \sum_{a,\mu} |\langle E^N_n|\psi_{\mu}(0)|E^N_{n+1},k\rangle|^2 \delta(\omega - \frac{1}{\hbar}(\epsilon^N_{n+1}(k) + \mu))$$

$$+ |\langle E^N_n|\psi_{\mu}(0)|E^N_{n-1},-k\rangle|^2 \delta(\omega + \frac{1}{\hbar}(\epsilon^N_{n-1}(-k) - \mu))$$

we get the remarkable expression:

$$G(k,\omega) = \int_{-\infty}^{+\infty} d\omega' \frac{A(k,\omega')}{\omega - \omega' + i\eta \text{sign}(\hbar\omega' - \mu)}$$

(5)

It pictures $G$ as a superposition of independent-particle propagators

$$G^0(k,\omega) = \frac{1}{\omega - \omega^0_k + i\eta \text{sign}(\hbar\omega^0 - \mu^0)}$$

(6)

The independent-particle propagator

has a pole with Re $\omega = \omega^0_k$ (the dispersion relation of the particle; for free fermions $\omega^0_k = \hbar^2/2m$) and infinitesimal imaginary part. The spectral function is a delta-function peaked on the pole: $A^0(k,\omega) = \delta(\omega - \omega^0_k)$. As the two-particle interaction is turned on, the spectral function is expected to broaden and take structure, and a "quasi-particle" pole to survive.

The imaginary part of eq.(7) changes sign for all $k$ at the chemical potential:

$$\text{Im} G(k,\omega) = \left\{ \begin{array}{ll}
\pi A(k,\omega) > 0 & \text{if } \mu > \hbar \omega \\
-\pi A(k,\omega) < 0 & \text{if } \mu < \hbar \omega
\end{array} \right.$$
This important property identifies the chemical potential $\mu$ of the system with interacting particles: it is the frequency value at which $\text{Im } G$ changes sign for all $k$. Actually, $\text{Im } G(k, \mu/h) = 0$.

For the homogeneous electron gas (HEG) Luttinger\cite{Luttinger} showed that, near $\omega = \mu/h$, it is $\text{Im } G(k, \omega) \approx C(k) (\mu - \hbar \omega)^2 \text{sign}(\mu - \hbar \omega)$, with $C(k) > 0$.

The spectral function can be measured through the photocurrent intensity of outgoing electrons in angle-resolved photoemission spectroscopy (ARPES)\cite{ARPES}. In HEG it is sharply peaked, with small equally spaced satellites denoting plasmon excitations\cite{Luttinger}.

A high frequency expansion gives the spectral moments

$$G(k, \omega) \approx \frac{1}{\omega} + \frac{m_1(k)}{\omega^2} + \frac{m_2(k)}{\omega^3} + \ldots$$

$m_{\ell}(k) = \int_{-\infty}^{\infty} \omega^\ell A(k, \omega) d\omega$. The first ones were evaluated for HEG by Vogt et al.\cite{Vogt}. The variance $m_2 - m_1^2$ measures the width, that depends on $k$.

**Exercise I.1** Show that, for a homogeneous system, and $t > 0$:

$$iG(k, t) = \int_{-\infty}^{\infty} \frac{d\omega}{\mu/h} e^{-i\omega t} A(k, \omega)$$

(8)

$$n(k) = (E_0^N | a_{k_0}^\dagger a_{kn}^\dagger | E_0^N) = \int_{-\infty}^{\mu/h} d\omega A(k, \omega)$$

(9)

For independent fermions: $iG_0^0(k, t) = e^{-i\omega k t} \theta(\omega^0_k - \mu/\pi)$ and $n^0(k) = \theta(h\mu^0_k - \omega^0_k)$.

**Exercise I.2** Show that for homogeneous (and, in general, interacting) systems, if the total energy per particle is a function of the density, $E/N = c(n)$, then the chemical potential and the pressure are (Hugenholtz)

$$\mu(n) = \frac{\partial E}{\partial N} \bigg|_V = \frac{d}{dn} [n c(n)]$$

(10)

$$p(n) = \frac{\partial E}{\partial V} \bigg|_N = n [\mu(n) - c(n)]$$

(11)

Show that, for non-interacting fermions, it is $\mu^0 = \hbar \omega_F$.

**Exercise I.3** Show that the retarded propagator for the ideal electron gas $G^{\text{ret}}(k, \omega) = (\omega - \omega_k^0 + i\eta)^{-1}$, in real space, coincides with the matrix element of the forward time-evolution operator of a single particle\cite{Luttinger}:

$$iG^{\text{ret}}(\mathbf{x}, \mathbf{x}', t′) = 0 \theta(t′ - t) \langle \mathbf{x}' | \mathbf{e}^{i \mathbf{k} \cdot \mathbf{x}' - i \mathbf{r}^2 \mathbf{t}' / 2 m (t - t') | \mathbf{x} \rangle$$

$$= \theta(t - t′) \left[ \frac{m}{2\pi i \hbar (t - t′)} \right]^{\frac{3}{2}} \exp \left[ \frac{i m}{2 \hbar} \frac{|\mathbf{x} - \mathbf{x}'|^2}{t - t′} \right].$$

**Example I.4** (Lorentzian approximation) A weak interaction produces a broadening of the $\delta$-shaped spectral line of the ideal gas. A useful approximation is a Lorentzian of half-width $\Gamma_k > 0$,

$$A(k, \omega) = \frac{1}{\pi} \frac{\Gamma_k}{(\omega - \omega_k)^2 + \Gamma_k^2}$$

(12)

![FIG. 1: The distribution $n_\sigma(k)$ for the Lorentzian spectral function. Units are such that $\mu = 1$, $\hbar/\mu = 0.1, 0.5, 0.01$.](image)

This distribution decays too slowly to have finite momenta. The propagator has the simple expression:

$$G(k, \omega) = \frac{1}{\omega - \omega_k + i\Gamma_k \text{sign}(\hbar \omega - \mu)}$$

(13)

The imaginary part has a finite (“pathological”) discontinuity. For $\Gamma_k \to 0$ the propagator of the ideal Fermi gas is reproduced, with the correct imaginary part of the pole. In the time domain $(t > 0)$:

$$iG(k, t) = e^{-i\omega_k t - \Gamma_k t} - \Gamma_k \int_{-\infty}^{\mu/h} d\omega \frac{e^{-i\omega t}}{\pi (\omega - \omega_k)^2 + \Gamma_k^2}$$

For $k$ values $\omega_k \gg \mu/h + \Gamma_k$ the integral is negligible, and the first term describes the propagation of a quasi-particle with dispersion $\omega = \omega_k$, that decays with lifetime $\Gamma_k^{-1}$.

The average occupation number in momentum space is (see fig. 1):

$$n(k) = \frac{1}{2} + \frac{1}{\pi} \arctg \frac{\mu - \hbar \omega_k}{\hbar \Omega_k}$$

(14)

For infinitesimal broadness $\Gamma_k$ we recover the step distribution of noninteracting fermions.

**B. The Fermi surface**

The change of sign of $\text{Im } G$ reflects in another representation of the propagator:

$$G(k, \omega) = \frac{1}{\omega - \omega_k - \Sigma^*(k, \omega)}$$

(15)

where $\omega_k^0$ is the single particle energy. It implies that

$$\text{Im } \Sigma^*(k, \omega) = \begin{cases} > 0 & \text{if } \mu > \hbar \omega \\ < 0 & \text{if } \mu < \hbar \omega \end{cases}$$

(16)

The frequency value where the imaginary part of the self-energy changes sign (vanishes), identifies the chemical potential $\mu$ of the interacting system of fermions. To this special value there corresponds a surface in $k$ space:
Definition I.5 (Fermi surface) The Fermi surface of the system is the set of \( k \) vectors such that

\[
\mu/h − ω^0_k − \Sigma^*(k, \mu/h) = 0
\]  

(17)

(the imaginary part of the self energy is zero for all \( k \)).

Theorem I.6 (Luttinger and Ward)

1) The volume enclosed by the Fermi surface is independent of the interaction:

\[
\frac{N}{V} = \int \frac{dk}{(2\pi)^3} \theta \left( \frac{\mu}{h} − ω^0_k − \Sigma^*(k, \mu/h) \right)
\]  

(18)

2) The occupation number \( n_k \) is discontinuous across the Fermi surface.

See the papers by Luttinger and Ward\(^a\), Luttinger\(^b\), the dissertation by Praž\(^c\) a lesson by Gurarii\(^d\) and, on a similar line, the book by Giuliani and Vignale\(^e\).

For isotropic systems the Fermi surface is the surface of a sphere of radius \( k_F \) fixed by the density.

C. Quasi-particles

In analogy with the propagator of independent particles, a property that defines a quasi-particle is to be a pole of the propagator:

\[
0 = ω − ω^0_k − \Sigma^*(k, ω)
\]  

(19)

If the pole is \( ω_1(k) + iω_2(k) \), the propagator has the form of a quasi-particle propagator plus a regular part:

\[
G(k, ω) = \frac{Z(k)}{ω − ω_1(k) − iω_2(k)} + G^{reg}(k, ω)
\]  

(20)

The residue \( Z(k) \) is the “quasi-particle weight”, and the sum rule for the spectral function implies that \( 0 ≤ Z(k) ≤ 1 \). The Lehmann representation tells us that \( ω_2 \) has the sign of \( μ − hω_1 \). Accordingly, for \( t > 0 \) and \( hω_1(k) > μ \) it is

\[
iG(k, t) = Z(k)e^{−iω_1(k)t + ω_2(k)t} + iG^{reg}(k, t)
\]  

(21)

where \( ω_2(k) < 0 \) describes the damping of the quasi-particle mode. For a quasi-particle weight close to unity, the quasi-particle term effectively describes the whole system in a region of \( k \) vectors. If the pole is near the real axis, the lifetime is long and a frequency integral containing the propagator is strongly enhanced in its vicinity, with a particle-like contribution weighted by the residue.

In conclusion, these are the properties that characterize a quasi-particle:

i) it is a complex pole of the propagator,

ii) the residue \( Z(k) \) is not negligible (order 1),

iii) \( |ω_2(k)| \) is small (more precisely, \( |ω_2| ≪ |ω_1 − μ/h| \)).

The presence of a quasi-particle reflects in a discontinuity of the occupation number

\[
n(k) = \int_{−∞}^{∞} dω \frac{G(k, ω)e^{iωt}}{2πi}
\]  

(22)

across the Fermi surface (17), a fact first proven by Migdal\(^f\). The proof is straightforward. By evaluating (22) with the pole expansion (21), the residue theorem gives:

\[
n(k) = n^{reg}(k) + \begin{cases} Z(k) & \text{if } hω_1(k) < μ \\ 0 & \text{if } hω_1(k) > μ \end{cases}
\]

The equation for the Fermi surface (17) is equivalent to \( hω_1(k) = μ \). At a point \( k_μ \) of the surface, the jump is:

\[
n(k_μ^−) − n(k_μ^+) = Z(k_μ).
\]

For metals, this step can be measured in Compton scattering experiments\(^g\). For HEG, an accurate Monte Carlo evaluation of the momentum distribution near \( k_F \) was done by Holzmann et al.\(^h\) (Fig.2).

The concept of quasi-particle is useful if we require that \( ω_2 \) is small. From eq. (19), we obtain

\[
ω_1(k) − ω^0_k − \text{Re} \Sigma^*(k, ω_1(k)) = 0
\]

(23)

\[
ω_2(k) = Z(k) \text{Im} \Sigma^*(k, ω_1(k))
\]

(24)

\[
Z(k) = \left[ 1 − \frac{∂}{∂ω} \text{Re} \Sigma^*(k, ω) \right]_{ω=ω_1(k)}^{-1}
\]

(25)

The smallness of \( ω_2 \) is ensured by \( hω_1 \) close to to the Fermi surface, where \( \text{Im} \Sigma^*(k, ω) \) vanishes. The requirement is then: \( |ω_2| < |ω_1 − μ/h| \).

D. Effective mass

Long-living quasi-particles are found near the Fermi surface. If the residue is close to unity, this means that
the Fermi surface is sharp, i.e. the occupation numbers have finite (variable from point to point) discontinuity across it. It is then meaningful to expand the dispersion relations near the Fermi surface.

For simplicity we consider the isotropic case. The equation for the Fermi surface

$$\mu - \omega_k^0 - \hbar \Sigma^*(k, \frac{\mu}{\hbar}) = 0$$

is solved by \( k \) equal to a constant, i.e. a spherical surface with the same radius \( k_F \) for the free and interacting cases (Luttinger theorem). We then expand the dispersion laws near the surface:

$$\hbar \omega_k^0 = \mu^0 + \frac{\hbar^2 k_F}{m} (k - k_F) + \ldots$$

$$\hbar \omega_1(k) = \mu + \frac{\hbar^2 k_F}{m^*} (k - k_F) + \ldots$$

where \( m^* \) is the effective mass of the quasi-particle. Linearization of eq. (23) near \( k_F \) gives:

$$m^* = Z(k_F) \left[ 1 + \frac{m}{\hbar k_F} \frac{\partial}{\partial k} \Re \Sigma^*(k, \frac{\mu}{\hbar}) \right]_{k=k_F}$$

The imaginary part of the pole defines the life-time of the quasi-particle, which is finite because of scattering processes, and diverges near the Fermi surface:

$$\frac{\hbar}{\tau(k)} = -2 Z(k) \Im \Sigma^*(k, \omega_1(k))$$

The mean free path is the length \( \ell = \hbar k_F \tau(k) \). The quasi-particle parameters \( m^*, Z(k_F) \) and \( \tau(k) \) have been evaluated for the homogeneous electron gas in several approximations: R.P.A. (Quinn and Ferrell, 1958), G.W.A. (Krauskov and Percus, 1996) G.W.A. with vertex corrections (Takada, 2001). We report the quasi-particle data in R.P.A.:[4]

$$\tau(k)^{-1} = 0.252 \sqrt{\pi} \frac{r_s \hbar (k - k_F)^2}{2m} + \ldots$$

$$m^* = 1 - 0.083 r_s (\log r_s + 0.203) + \ldots$$

The interaction with phonons gives a much stronger renormalization, about 40% in metals like Na or Al, and 15% in Cs. An evaluation of self-energy with 1-phonon exchange in made in Mahan’s book.[5]

**Exercise I.7** The self-energy diagram for HEG with screened Coulomb potential in the Thomas-Fermi approximation is

$$\Sigma^*(k) = -\frac{1}{\hbar} \int \frac{dq}{(2\pi)^3} \frac{4\pi e^2}{|k - q|^2 + k_T^2} \theta(k_F - q)$$

$$= -\frac{e^2}{2\pi \hbar x} \int_1^{\infty} dy \log[(y + x)^2 + a^2]$$

$$= -\frac{\hbar k_F^2}{m} \frac{4}{3\pi^2} \frac{x^3/2}{x} \left\{ 1 + \frac{1 + a^2}{4x} \log \left[ \frac{(1 + x)^2 + a^2}{(1 - x)^2 + a^2} \right] - \frac{(a + x)}{2a} \left[ \arctan \frac{x + 1}{a} - \arctan \frac{x - 1}{a} \right] \right\}$$

where \( x = k/k_F \) and \( a = k_T/k_F = \sqrt[3]{16/(3\pi^2)} \sqrt{r_s} \approx 0.8145 \sqrt{r_s} \). Evaluate the effective mass \( m^* \).

**Exercise I.8** Consider the self-energy diagram for HEG with 1-phonon exchange:

$$\Sigma^*(k) = \frac{i}{\hbar} \int \frac{dq'k'}{(2\pi)^3} G^0(k - k') D(k')$$

$$D(k) = g^2 \frac{\omega_k^2}{(\omega + i\eta)^2 + \omega_k^2} \theta(\omega_D - \omega_k)$$

where \( \omega_D \) is Debye’s cutoff and \( \omega_k = ck \) (c is the velocity of sound waves in the solid). Show that \( \Im \Sigma^*(k, \omega) \) changes sign once, as a function of \( \omega \).

**II. INHOMOGENEOUS SYSTEMS**

In the general expression of Lehmann’s representation[4] it is useful to introduce the functions \( f'_{a\mu}(x) \) and \( f''_{a\mu}(x) \), which carry the quantum numbers \( x, \mu \) of a single particle, and the frequencies \( \omega_a^\prime \) and \( \omega_a^\prime\prime \):

$$f'_{a\mu}(x) = \langle E_{a0}^N | \psi_\mu(x) | E_{aN+1}^N \rangle, \quad \omega_a^\prime = \mu + \epsilon_{aN+1}^\prime$$

$$f''_{a\mu}(x) = \langle E_{a0}^N | \psi_\mu(x) | E_{aN-1}^N \rangle, \quad \omega_a^\prime\prime = \mu - \epsilon_{aN-1}^\prime$$

It is \( \omega_a^\prime > \mu \) and \( \omega_a^\prime\prime < \mu \). Eq. (4) becomes

$$G_{\mu\mu'}(x, x', \omega) = \sum_a \frac{f'_{a\mu}(x) f'_{a\mu'}(x')^* + f''_{a\mu}(x) f''_{a\mu'}(x')^*}{\omega - \omega_a^\prime - i\eta}$$

$$= \sum_a \frac{f'_{a\mu}(x) f_{a\mu'}(x')^*}{\omega - \omega_a^\prime - i\eta \text{ sign}(\mu - \omega_a^\prime)}$$

where the sum is on the set \( \{ f'_{a\mu}(x), f''_{a\mu}(x) \} \) corresponding to \( \omega_a^\prime > \mu \) and \( \omega_a^\prime\prime < \mu \). Completeness of the eigenstates \( |E_{aN+1}^N\rangle \) in the subspaces with \( N \pm 1 \) particles implies

$$\sum_a f'_{a\mu}(x) f'_{a\mu'}(x')^* = \langle E_{00}^N | \psi_\mu(x) \psi_\mu^\dagger(x') | E_{00}^N \rangle$$

$$\sum_a f''_{a\mu}(x) f''_{a\mu'}(x')^* = \langle E_{00}^N | \psi_\mu(x) \psi_\mu^\dagger(x') | E_{00}^N \rangle$$

Their sum gives a completeness property in 1-particle space:

$$\sum_a f_{a\mu}(x) f_{a\mu'}(x')^* = \langle x\mu | x\mu' \rangle$$

In general, the functions are not orthogonal.

In eq. (33) the propagator has the form of the propagator of non-interacting particles or of the Hartree-Fock approximation. Then, the functions \( f_a \) would be eigenstates of a one-particle Hamiltonian, or solutions of the H.F. equations. For this analogy, the \( f_a \) are called “quasi-particle” states.

The functions solve a Schrödinger-like equation, which
was derived in 1952 by Julian Schwinger. Consider the equation for the Green function:

\[(\hbar \omega - \hat{h}) G_{\mu \nu}(x, x', \omega) = \hbar(x \mu | x' \mu') + \int d\mathbf{x}'' \Sigma_{\mu \nu}(\mathbf{x}, \mathbf{x}', \omega) G_{\mu' \nu'}(\mathbf{x}'', \mathbf{x}', \omega)\]

where \(\hbar\) is the single particle operator, and the self-energy acts as bi-local potential (the local term is included in \(\hat{h}\)). Insert the representation of the ground state density of particles with spin \(\mu\) with \(\hbar\omega_0\) and take the limit \(\omega \rightarrow \omega_0\):

\[
(\hbar f_{\mu \nu})(x) + \sum_{\mu'} \int d\mathbf{x}'' h \Sigma_{\mu \mu'}(x, x', \omega_0) f_{\mu \nu''}(x'') = \hbar \omega_0 f_{\mu \nu}(x)
\]

where the functions \(f_{a \mu}\) are treated as elements of the Hilbert space of one particle with spin. In particular the ground-state density of particles with spin \(\mu\) is

\[
\langle E_0^N | n_\mu(x) | E_0^N \rangle = \sum_a | f_{a \mu}(x) |^2 \theta(\mu - \hbar \omega_0)
\]

Integration and spin summation give a sum rule for the squared norms in the one-particle Hilbert space:

\[
N = \sum_{a \mu} | f_{a \mu} |^2 \theta(\mu - \hbar \omega_0)
\]

The total energy can be evaluated with the operator identity \(\sum_{\mu} \int d\mathbf{x} \psi_{\mu}^\dagger(\mathbf{x}) [\psi_{\mu}(\mathbf{x}), H] = H_1 + 2H_2\), where \(H = H_1 + \hat{H}_2\) is the Hamiltonian, and \(H_1, H_2\) are 1 and 2-particle operators. The average of the ground state \(| E_0^N \rangle\) gives

\[
NE_0^N = \sum_{\mu} \int d\mathbf{x} \langle E_0^N | \phi_{\mu}(\mathbf{x}) H \phi_{\mu}(\mathbf{x}) | E_0^N \rangle = \langle H_1 + 2H_2 \rangle
\]

A resolution of identity with states \(| E_0^{N-1} \rangle\) is inserted to obtain an expression with quasi-particle states

\[
\langle H_1 + 2H_2 \rangle = N E_0^N - \sum_{\mu} E_0^{N-1} | f_{a \mu} |^2 \theta(\mu - \hbar \omega_0)
\]

By adding the ground-state expectation value of \(H_1\) one obtains the energy of the ground state:

\[
E_0^N = \frac{1}{2} \sum_a \langle f_{a} | \hbar + \hbar \omega_0 | f_{a} \rangle \theta(\mu - \hbar \omega_0)
\]

A. Approximate quasi-particle evaluation

In applications, one may solve the quasi-particle equation perturbatively, by starting from approximate functions. In density functional theory (DFT) the interacting many body problem is replaced by a problem with independent particles in a self-consistent Kohn-Sham potential. The particle density \(n(\mathbf{x})\), the chemical potential \(\mu\) and the ground state energy \(E_0^0\) so obtained, are in principle the same as in the many-body problem. However, the accuracy of experimental data show the limits of approximations to the unknown Kohn-Sham potential. For this reason, DFT is often used as the zero order for a many body calculation.

Let us then start from the Kohn-Sham equation:

\[
(\hbar f_{a \mu}^0 + v_{KS}(\mathbf{x}) f_{a \mu}^0)(\mathbf{x}) = \hbar \omega_0 f_{a \mu}^0(\mathbf{x})
\]

The functions \(f_{a \mu}^0\) form an orthonormal system, and the eigenvalues are real. If the potential \(v_{KS}\) were exactly known, the solutions \(f_{a \mu}^0\), though different from the quasi-particle functions \(f_{a \mu}\), would provide the same density, chemical potential and total energy of the many-body problem. Since this is not the case, let’s go back to Schwinger’s eq. and take the scalar product with \(f_{a \mu}^0\), and use the KS equation to eliminate \(\hat{h}\):

\[
\sum_{\mu, \mu'} \int d\mathbf{x} d\mathbf{y} f_{a \mu}^0(\mathbf{x}) \Sigma_{\mu \mu'}(\mathbf{x}, \mathbf{y}, \omega_0) f_{a \mu'}(\mathbf{y})
\]

The formula is rewritten as

\[
(f_{a \mu}^0 | \Sigma^*(\omega_0) | f_{a \mu}^0) - \frac{1}{\hbar} (f_{a \mu}^0 | v_{KS} | f_{a \mu}^0) = (\omega_0 - \omega_0) (f_{a \mu}^0 | f_{a \mu}^0).
\]

At first order, the unknown amplitudes \(f_{a \mu}(x)\) are replaced with \(f_{a \mu}^0(x)\), and the self-energy is expanded at the Kohn-Sham frequency: \(\Sigma^*(\omega_0) \approx \Sigma^*(\omega_0^0) + \frac{\partial \Sigma^*(\omega_0^0)}{\partial \omega}(\omega_0 - \omega_0)\). In the hypothesis that the functions \(f_{a \mu}^0\) are real, one obtains:

\[
\text{Re} \omega_0 = \omega_0^0 + Z_a (f_{a \mu}^0 | \text{Re} \Sigma^*(\omega_0^0) - \frac{1}{\hbar} v_{KS} \delta(f_{a \mu}^0))
\]

\[
\text{Im} \omega_0 = Z_a (f_{a \mu}^0 | \text{Im} \Sigma^*(\omega_0^0) | f_{a \mu}^0)
\]

\[
Z_a^{-1} = 1 - \frac{\partial}{\partial \omega} (f_{a \mu}^0 | \text{Re} \Sigma^*(\omega) | f_{a \mu}^0) \bigg|_{\omega=\omega_0^0}
\]

\(Z_a\) is the quasi-particle weight, \(\delta\) means \(\delta(x - y)\).


24. The states $\psi_{\chi}^\dagger |E_0\rangle$ are not normalised, therefore the Green function is only proportional to a probability amplitude.