Propagator & Quasi-Particles

Notes by Luca G Molinari[26]

I. THE PROPAGATOR

Given a Hamiltonian with ground state $|E_0^N\rangle$ with N electrons and two one-particle states $|u\rangle$ and $|u'\rangle$, the time-ordered 1-particle propagator is

$$iG(u,t;u',t') = \langle E_0^N|\mathsf{T}\psi_u(t)\psi^\dagger_{u'}(t')|E_0^N\rangle \quad (1)$$
$$= \begin{cases} +\langle E_0^N|\psi_u e^{-\frac{i}{\hbar}(\hat H - E_0)(t-t')}\psi^\dagger_{u'}|E_0^N\rangle & t>t' \\ -\langle E_0^N|\psi^\dagger_{u'} e^{-\frac{i}{\hbar}(\hat H - E_0)(t'-t)}\psi_u|E_0^N\rangle & t'>t \end{cases}$$

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[27]. 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'.

The Fourier transform is

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

Since the propagator is discontinuous at $t=t'$

$$iG(u,t^+;u',t) - iG(u,t^-;u',t) = \langle u|u'\rangle,$$

the Fourier transform has slow decay in ω:

$$\boxed{\lim_{|\omega|\to\infty}\omega\, G(u,u';\omega) = \langle u|u'\rangle} \quad (3)$$

Proof: Evaluate the discontinuity in Fourier space:

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

While $\eta\to 0$, the limit of the integral exists. It must be $sG(u,u',s)\to\langle u|u'\rangle$ for $s\to\infty$. □

If the system is confined in a box, the spectrum of the Hamiltonian is discrete, with eigenstates $|E_a^N\rangle$. Insertion of the identities $1=\sum_a |E_a^{N\pm 1}\rangle\langle E_a^{N\pm 1}|$ in eq.(1) makes the time-dependence explicit. In frequency space the propagator for position-spin states has the following Lehmann's representation[5]

$$G_{\mu\mu'}(\mathbf{x},\mathbf{x}';\omega) = \sum_a \frac{\langle E_0^N|\psi_\mu(\mathbf{x})|E_a^{N+1}\rangle\langle E_a^{N+1}|\psi^\dagger_{\mu'}(\mathbf{x}')|E_0^N\rangle}{\omega - \frac{1}{\hbar}(\mu+\epsilon_a^{N+1})+i\eta}$$
$$+\frac{\langle E_0^N|\psi^\dagger_{\mu'}(\mathbf{x}')|E_a^{N-1}\rangle\langle E_a^{N-1}|\psi_\mu(\mathbf{x})|E_0^N\rangle}{\omega-\frac{1}{\hbar}(\mu-\epsilon_a^{N-1})-i\eta} \quad (4)$$

The values $E_a^{N\pm1}-E_0^{N\pm1}=\epsilon_a^{N\pm1}\ge 0$ are the excitation energies, and $E_0^{N\pm1}-E_0^N=\pm\mu$, the chemical potential μ being insensitive to small variations of N, if N is large.

II. HOMOGENEOUS SYSTEMS

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

$$G_{\mu\mu'}(\mathbf{x},\mathbf{x}',\omega) = \frac{1}{V}\sum_{\mathbf{k}} e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{x}')}G_{\mu\mu'}(\mathbf{k},\omega)$$

Let us assume that $G_{\mu\mu'}=\delta_{\mu\mu'}G$. Since H and $\mathbf{P}$ commute, they share a basis of eigenvectors $|E_a^N,\mathbf{k}\rangle$; in the rest frame the ground state has momentum equal to zero. By the operator identity

$$\psi_\mu(\mathbf{x}) = e^{-\frac{i}{\hbar}\mathbf{x}\cdot\mathbf{P}}\psi_\mu(\mathbf{0})e^{\frac{i}{\hbar}\mathbf{x}\cdot\mathbf{P}}$$

the Lehmann representation in $\mathbf{k}$ space is obtained:

$$G(\mathbf{k},\omega) = \tfrac{1}{2}V\sum_{a,\mu}\Big[\frac{|\langle E_0^N|\psi_\mu(\mathbf{0})|E_a^{N+1},\mathbf{k}\rangle|^2}{\omega-\frac{1}{\hbar}(\mu+\epsilon^{N+1}_{a,\mathbf{k}})+i\eta}$$
$$+\frac{|\langle E_0^N|\psi^\dagger_\mu(\mathbf{0})|E_a^{N-1},-\mathbf{k}\rangle|^2}{\omega-\frac{1}{\hbar}(\mu-\epsilon^{N-1}_{a,-\mathbf{k}})-i\eta}\Big]$$

With the introduction of the *spectral function*

$$A(\mathbf{k},\omega) =$$
$$\tfrac{V}{2}\sum_{a\mu}|\langle E_0^N|\psi_\mu(\mathbf{0})|E_a^{N+1},\mathbf{k}\rangle|^2\delta(\omega-\tfrac{1}{\hbar}(\epsilon^{N+1}_{a,\mathbf{k}}+\mu))$$
$$+|\langle E_0^N|\psi^\dagger_\mu(\mathbf{0})|E_a^{N-1},-\mathbf{k}\rangle|^2\delta(\omega+\tfrac{1}{\hbar}(\epsilon^{N-1}_{a,-\mathbf{k}}-\mu))$$

we get the remarkable expression:

$$\boxed{G(\mathbf{k},\omega) = \int_{-\infty}^{\infty}d\omega'\frac{A(\mathbf{k},\omega')}{\omega-\omega'+i\eta\,\mathrm{sign}\,(\hbar\omega'-\mu)}} \quad (5)$$

The spectral function is non-negative. As $|\omega|G(\mathbf{k},\omega)\to 1$ for $|\omega|\to\infty$, the spectral function is normalized in frequency for all $\mathbf{k}$, and is a probability measure

$$\boxed{\int_{-\infty}^{+\infty}d\omega\, A(\mathbf{k},\omega) = 1} \quad (6)$$

The Lehmann representation (5) pictures G as a *superposition of independent-particle propagators* G^0, weighted by the spectral function.

The propagator for independent particles

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

has a pole at Re $\omega=\omega^0_{\mathbf{k}}$, which is the dispersion relation of the particle (e.g. $\omega^0_{\mathbf{k}}=\hbar k^2/2m$). The imaginary part of the pole is infinitesimal. The spectral function is a delta-function peaked at the pole:

$$A^0(\mathbf{k},\omega) = \delta(\omega - \omega^0_{\mathbf{k}})$$

As the two-particle interaction is turned on, the spectral function is expected to broaden and gain structure, and a "quasi-particle" pole to remain, with modified dispersion and finite imaginary part.

The spectral function can be measured through the photocurrent intensity of outgoing electrons in angle-resolved photoemission spectroscopy (ARPES) in the sudden-approximation[2].
In the homogeneous electron gas (HEG) it is sharply peaked, with small equally spaced satellites denoting plasmon excitations[24]. A high frequency expansion gives the spectral moments

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

$m_\ell(\mathbf{k}) = \int_{-\infty}^{\infty} \omega^\ell A(\mathbf{k},\omega) d\omega$. The first ones were evaluated for HEG by Vogt et al.[25]. The variance $m_2 - m_1^2$ measures the width, that depends on $\mathbf{k}$.

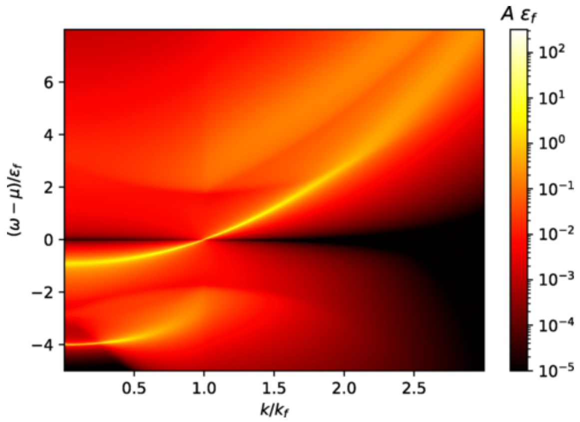

FIG. 1: The spectral function $A(k,\omega)$ for HEG $r_s = 4$ in G_0W_0 approximation[3]. At $\hbar\omega = \mu$ it is zero (black) for all k. The bright approximate parabola is the peak of the quasi-particle dispersion. A plasmon satellite appears a bright segment.

Exercise II.1 *Show that:*

$$iG_{\mu\mu'}(\mathbf{k};t) = \langle E^N_0 | \mathsf{T} a_{\mathbf{k},\mu}(t) a^\dagger_{\mathbf{k},\mu'} | E^N_0\rangle \tag{7}$$

$$n_\mu(\mathbf{k}) = -iG_{\mu\mu}(\mathbf{k},0^-) = \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi i} G_{\mu\mu}(\mathbf{k},\omega) e^{i\omega\eta} \tag{8}$$

Exercise II.2 *Show that if $t > 0$:*

$$iG(\mathbf{k},t) = \int_{\mu/\hbar}^{\infty} d\omega\, e^{-i\omega t} A(\mathbf{k},\omega) \tag{9}$$

$$n(\mathbf{k}) = \langle E^N_0 | a^\dagger_{\mathbf{k}\mu} a_{\mathbf{k}\mu} | E^N_0 \rangle = \int_{-\infty}^{\mu/\hbar} d\omega A(\mathbf{k},\omega) \tag{10}$$

For independent fermions: $iG^0(\mathbf{k},t) = e^{-i\omega^0_{\mathbf{k}} t}\theta(\hbar\omega^0_{\mathbf{k}} - \mu^0)$ and $n^0(\mathbf{k}) = \theta(\mu^0 - \hbar\omega^0_{\mathbf{k}}) = \theta(k_F - k)$.

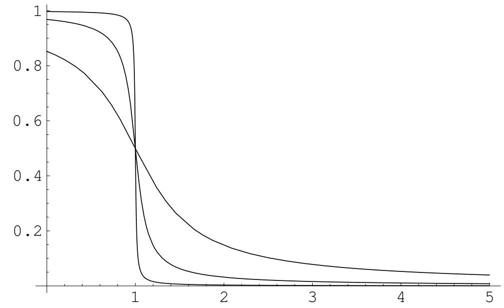

FIG. 2: The distribution $n_\sigma(k)$ for the Lorentzian spectral function. Units are such that $\mu = 1$, $\hbar\Gamma/\mu = 0.1$, 0.5, 0.01.

A. Lorentzian approximation

A weak interaction produces a broadening of the δ-shaped spectral line of the ideal gas. A useful approximation is a Lorentzian of half-width $\Gamma_{\mathbf{k}} > 0$,

$$A(\mathbf{k},\omega) = \frac{1}{\pi}\frac{\Gamma_k}{(\omega-\omega_k)^2 + \Gamma_k^2} \tag{11}$$

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

$$G(\mathbf{k},\omega) = \frac{1}{\omega - \omega_k + i\Gamma_k \,\mathrm{sign}(\hbar\omega - \mu)} \tag{12}$$

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 ($t > 0$):

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

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

The average occupation number in momentum space is (see fig.2):

$$n(k) = \frac{1}{2} + \frac{1}{\pi}\mathrm{arctg}\frac{\mu - \hbar\omega_k}{\hbar\Gamma_k} \tag{13}$$

For infinitesimal broadness Γ_k we recover the step distribution of noninteracting fermions.

B. The Fermi surface

The imaginary part of eq.(5) changes sign only once, at $\hbar\omega = \mu$, and for all $\mathbf{k}$:

$$\mathrm{Im}\, G(\mathbf{k},\omega) = \begin{cases} \pi A(\mathbf{k},\omega) > 0 & \text{if } \mu > \hbar\omega \\ -\pi A(\mathbf{k},\omega) < 0 & \text{if } \mu < \hbar\omega \end{cases} \tag{14}$$

This important property identifies the chemical potential μ of the system of interacting particles as the value $\hbar\omega$ at which Im G changes sign.
For the homogeneous electron gas (HEG) Luttinger[?] showed that, near $\hbar\omega = \mu$, it is

$$|\mathrm{Im}\, G(k,\omega)| \approx C(k)(\mu - \hbar\omega)^2$$

The change of sign of Im G reflects in another representation of the propagator:

$$\boxed{G(\mathbf{k},\omega) = \frac{1}{\omega - \omega^0_{\mathbf{k}} - \Sigma^\star(\mathbf{k},\omega)}} \tag{15}$$

where $\hbar\omega^0_{\mathbf{k}}$ is the single particle energy. It implies that

$$\mathrm{Im}\,\Sigma^\star(\mathbf{k},\omega) = \begin{cases} > 0 & \text{if } \mu > \hbar\omega \\ < 0 & \text{if } \mu < \hbar\omega \end{cases} \tag{16}$$

and

$$A(\mathbf{k},\omega) = \frac{1}{\pi} \frac{|\mathrm{Im}\Sigma^*|}{(\omega - \omega^0_{\mathbf{k}} - \mathrm{Re}\Sigma^*)^2 + (\mathrm{Im}\Sigma^*)^2}$$

The frequency value where the imaginary part of the self-energy changes sign (vanishes), identifies the chemical potential μ of the interacting system of fermions. To this special value there corresponds a surface in $\mathbf{k}$ space:

Definition II.3 (Fermi surface) *The Fermi surface of the system is the set of* $\mathbf{k}$ *vectors such that*

$$\boxed{\frac{\mu}{\hbar} - \omega^0_{\mathbf{k}} - \Sigma^\star(\mathbf{k}, \frac{\mu}{\hbar}) = 0} \tag{17}$$

Theorem II.4 (Luttinger and Ward, 1960)
The volume enclosed by the Fermi surface equals the density (per spin direction)

$$\int \frac{d\mathbf{k}}{(2\pi)^3}\, \theta\left(G(\mathbf{k},\mu/\hbar)\right) = n \tag{18}$$

A proof is given in appendix.
A consequence is: If the strength of the interaction is varied at fixed density, while the Fermi surface may change, the inner volume does not change.
For isotropic systems the Fermi surface, both for non-interacting and the interacting system, is the surface of a sphere of radius k_F fixed by the density.

C. Quasi-particles

In *Fermi liquids*, in a certain energy range, the propagation of the many-particle state may be describes as the propagation of a single *quasi-particle*, the effect of the particles being a renormalisation of the bare particle parameters, such as mass and dispersion law. Normal metals are Fermi liquids, and to some extent the conduction electrons can be described in terms of non-interacting quasi-electrons.

The concept of quasi-particle was introduced phenomenologically in 1957 by Landau[12,17] and applied with success to the study of ^{3}He. As the interaction is turned on, the 1-particle states of the ideal Fermi gas evolve into quasi-particle excitations of a Fermi liquid. The identification is not sharp and involves the notion of *lifetime* and *weight* of the quasi-particle. The origin of this simple picture is the property that in Fermi liquids the interaction preserves a Fermi surface, wherein most degrees of freedom are frozen. A microscopic justification was then provided by Galitskii, who evaluated self-energy corrections of the one-particle propagator by resumming ladder diagrams for two-particle scattering[5,6].

Quasi-particles may result from canonical transformations, that bring a Hamiltonian to a quadratic form in creation and destruction operators of new entities, with no direct link to the particles in the Hamiltonian, such as magnons, plasmons, phonons, bogolons, ...

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

$$\boxed{0 = \omega - \omega^0_{\mathbf{k}} - \Sigma^\star(\mathbf{k},\omega)} \tag{19}$$

With the pole at $\omega_1(\mathbf{k}) + i\omega_2(\mathbf{k})$, the propagator has the form of a quasi-particle propagator plus a regular part:

$$G(\mathbf{k},\omega) = \frac{Z(\mathbf{k})}{\omega - \omega_1(\mathbf{k}) - i\omega_2(\mathbf{k})} + G^{\mathrm{reg}}(\mathbf{k},\omega) \tag{20}$$

The residue $Z(\mathbf{k})$ is the "quasi-particle weight". The normalization of the spectral function implies that $0 \le Z(\mathbf{k}) \le 1$. In the region $Z(\mathbf{k}) \approx 1$, the quasi-particle term effectively describes the whole system.
The Lehmann representation tells us that ω_2 has the sign of $\mu - \hbar\omega_1$. Accordingly, back to time:

$$\begin{aligned} iG(\mathbf{k},t) =& iG^{reg}(\mathbf{k},t) \\ &+ \begin{cases} +Z(\mathbf{k})e^{-i\omega_1(\mathbf{k})t + \omega_2(\mathbf{k})t}\theta(\hbar\omega_1 - \mu) & t > 0 \\ -Z(\mathbf{k})e^{-i\omega_1(\mathbf{k})t + \omega_2(\mathbf{k})t}\theta(\mu - \hbar\omega_1) & t < 0 \end{cases} \end{aligned}$$

In both cases the product $\omega_2(\mathbf{k})t < 0$ describes the *damping of the quasi-particle mode.*
If the pole is near the real axis, the lifetime is long and a frequency integral of the propagator is strongly enhanced in its vicinity, with a particle-like contribution weighted by the residue. The concept of quasi-particle is useful when ω_2 is small.
From eq.(19), we obtain

$$\omega_1(\mathbf{k}) - \omega^0_{\mathbf{k}} - \mathrm{Re}\,\Sigma^\star(\mathbf{k},\omega_1(\mathbf{k})) = 0 \tag{21}$$

$$\omega_2(\mathbf{k}) = Z(\mathbf{k})\,\mathrm{Im}\,\Sigma^\star(\mathbf{k},\omega_1(\mathbf{k})) \tag{22}$$

$$Z(\mathbf{k}) = \left[1 - \frac{\partial}{\partial\omega}\mathrm{Re}\,\Sigma^\star(\mathbf{k},\omega)\right]^{-1}_{\omega=\omega_1(\mathbf{k})} \tag{23}$$

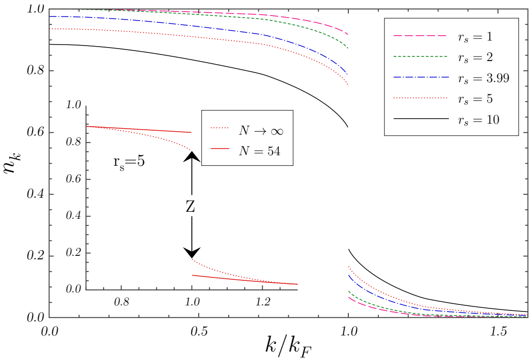

FIG. 3: The distribution $n(k)$ for HEG, at various r_s. For small r_s (large density) the gas is closer to ideal, with step distribution (Ceperley et al.[10]).

The smallness of ω_2 is ensured by $\hbar\omega_1(\mathbf{k})$ close to to the Fermi surface, where $\text{Im}\Sigma^\star(\mathbf{k},\omega)$ vanishes. The requirement is then: $|\omega_2| \ll |\omega_1 - \mu/\hbar|$.

In conclusion, these are the properties that characterize a quasi-particle:
i) it is a pole of the propagator, in complex ω plane,
ii) the residue $Z(\mathbf{k})$ is not negligible (order 1),
iii) $|\omega_2| \ll |\omega_1 - \mu/\hbar|$.

The presence of a quasi-particle reflects in a discontinuity of the momentum density $n_\sigma(\mathbf{k}) = \langle gs|a^\dagger_{\mathbf{k},\sigma} a_{\mathbf{k},\sigma}|gs\rangle$ across the Fermi surface (17), a fact first proven by Migdal[15]. The proof is straightforward. By evaluating (8) with the pole expansion (20), the residue theorem gives:

$$n_\sigma(\mathbf{k}) = n^{\text{reg}}_\sigma(\mathbf{k}) + \begin{cases} Z(\mathbf{k}) & \text{if } \hbar\omega_1(\mathbf{k}) < \mu \\ 0 & \text{if } \hbar\omega_1(\mathbf{k}) > \mu \end{cases}$$

The equation for the Fermi surface (17) is $\hbar\omega_1(\mathbf{k}) = \mu$. At a point $\mathbf{k}$ of the surface, the jump is:

$$n(\mathbf{k}^{in}) - n(\mathbf{k}^{out}) = Z(\mathbf{k})$$

For metals, the step can be measured in Compton scattering experiments[14]. For HEG, an accurate Montecarlo evaluation of the momentum distribution near k_F was done by Holzmann et al.[10] (Fig.3).

D. Effective mass

Long-lived quasi-particles are found near the Fermi surface. If the residue $Z(\mathbf{k})$ is close to unity at the surface, then the Fermi surface is sharp, i.e. the momentum density $n(\mathbf{k})$ has a finite (in general $\mathbf{k}$-dependent) discontinuouity across it. It is meaningful to expand the dispersion relation near the Fermi surface.

For simplicity we consider the isotropic case. In the interacting case, the Fermi surface has equation

$$\mu - \omega^0_k - \hbar\,\Sigma^\star(k, \frac{\mu}{\hbar}) = 0 \tag{24}$$

while for the free electrons it is $\mu^0 - \omega^0_k = 0$. The two surfaces coincide as they bound the same Fermi sphere in $\mathbf{k}$ space, of radius k_F (Luttinger-Ward theorem).
We expand the dispersion laws near the surface:

$$\hbar\,\omega^0_k = \mu^0 + \frac{\hbar^2 k_F}{m}(k - k_F) + \dots$$
$$\hbar\,\omega_1(k) = \mu + \frac{\hbar^2 k_F}{m^*}(k - k_F) + \dots$$

where m^* is the effective mass of the quasi-particle.
Linearization of eq.(21) near k_F gives:

$$\frac{m}{m^*} = Z(k_F)\left[1 + \frac{m}{\hbar k_F}\frac{\partial}{\partial k}\text{Re}\,\Sigma^\star(k, \frac{\mu}{\hbar})\right]_{k=k_F} \tag{25}$$

The imaginary part $\omega_2(k)$ of the pole defines the life-time of the quasi-particle, which is finite because of scattering processes, and diverges near the Fermi surface:

$$\frac{\hbar}{\tau(k)} = -2\,Z(k)\,\text{Im}\,\Sigma^\star(k, \omega_1(k)) \tag{26}$$

The *mean free path* is the length $\ell = \frac{\hbar k_F}{m^*}\tau(k_F)$.

The quasi-particle parameters m^*, $Z(k_F)$ and $\tau(k)$ have been evaluated for HEG in several approximations: R.P.A. (Quinn and Ferrell[20], 1958), GW (Krakovsky and Percus[11], 1996), GW with vertex corrections (Takada[24], 2001), Quantum Monte Carlo (Azadi et al.[1], 2021) .

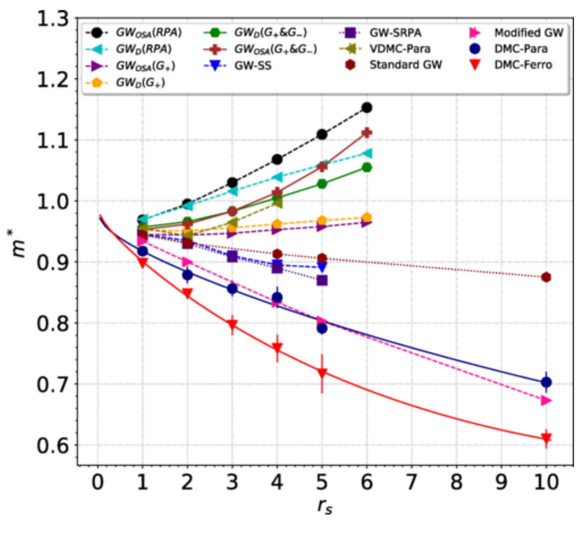

FIG. 4: The effective mass $m^\star$ for HEG at various r_S with different methods. Monte Carlo calculations (DMC) show that $m^\star$ decreases with r_S, in contradiction with many-body perturbation theory (from Azadi et al.[1])

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 is given in Mahan's book[14,22].

Exercise II.5 *The self-energy diagram for HEG with screened Coulomb potential in the Thomas-Fermi approximation is*

$$\Sigma^\star(k) = -\frac{1}{\hbar}\int \frac{d\mathbf{q}}{(2\pi)^3}\frac{4\pi e^2}{|\mathbf{k}-\mathbf{q}|^2+k_{TF}^2}\theta(k_F-q)$$
$$= -\frac{\hbar k_F^2}{m}\frac{4}{3\pi^2}r_s^{3/2}\Big\{1+\frac{1+a^2}{4x}\log\frac{(1+x)^2+a^2}{(1-x)^2+a^2}$$
$$-(a+\frac{x}{2a})\left[\arctan\frac{x+1}{a}-\arctan\frac{x-1}{a}\right]\Big\}$$

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

Exercise II.6 *Consider the self-energy diagram for HEG with 1-phonon exchange:*

$$\Sigma^\star(k) = \frac{i}{\hbar}\int\frac{d^4k'}{(2\pi)^4}G^0(k-k')D(k')$$
$$D(k) = g^2\frac{\omega_k^2}{\omega^2-(\omega_k-i\eta)^2}\theta(\omega_D-\omega_k)$$

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

III. INHOMOGENEOUS SYSTEMS

In the general expression of Lehmann's representation (4) it is useful to introduce the functions $f'_{a\mu}(\mathbf{x})$ and $f''_{a\mu}(\mathbf{x})$, which carry the quantum numbers $\mathbf{x},\mu$ of a single particle, and the frequencies ω'_a and ω''_a:

$$f'_{a\mu}(\mathbf{x}) = \langle E_0^N|\psi_\mu(\mathbf{x})|E_a^{N+1}\rangle,\quad \hbar\omega'_a=\mu+\epsilon_a^{N+1} \tag{27}$$
$$f''_{a\mu}(\mathbf{x}) = \langle E_0^N|\psi^\dagger_\mu(\mathbf{x})|E_a^{N-1}\rangle,\quad \hbar\omega''_a=\mu-\epsilon_a^{N-1} \tag{28}$$

It is $\hbar\omega'_a>\mu$ and $\hbar\omega''_a<\mu$. Eq.(4) becomes

$$G_{\mu\mu'}(\mathbf{x},\mathbf{x}',\omega)$$
$$=\sum_a \frac{f'_{a\mu}(\mathbf{x})f'_{a\mu'}(\mathbf{x}')^*}{\omega-\omega'_a+i\eta}+\frac{f''_{a\mu'}(\mathbf{x}')f''_{a\mu}(\mathbf{x})^*}{\omega-\omega''_a-i\eta}$$
$$=\sum_a\frac{f_{a\mu}(\mathbf{x})f_{a\mu'}(\mathbf{x}')^*}{\omega-\omega_a+i\eta\,\mathrm{sign}(\mu-\hbar\omega_a)} \tag{29}$$

where $f_a=f'_a$ or f''_a respectively for $\hbar\omega_a>\mu$ or $\hbar\omega_a<\mu$. Completeness of the eigenstates $|E_{a\mu}^{N\pm1}\rangle$ in the subspaces with $N\pm1$ particles implies

$$\sum_a f'_{a\mu}(\mathbf{x})f'_{a\mu'}(\mathbf{x}')^* = \langle E_0^N|\psi_\mu(\mathbf{x})\psi^\dagger_{\mu'}(\mathbf{x}')|E_0^N\rangle \tag{30}$$
$$\sum_a f''_{a\mu}(\mathbf{x})f''_{a\mu'}(\mathbf{x}')^* = \langle E_0^N|\psi^\dagger_{\mu'}(\mathbf{x}')\psi_\mu(\mathbf{x})|E_0^N\rangle \tag{31}$$

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

$$\sum_a f_{a\mu}(\mathbf{x})f_{a\mu'}(\mathbf{x}')^*=\langle\mathbf{x}\mu|\mathbf{x}'\mu'\rangle \tag{32}$$

In general, the functions are not orthogonal.

In eq.(29) 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[8], which was derived in 1952 by Julian Schwinger. Consider the equation for the Green function:

$$(\hbar\omega-\hat h_{\mathbf{x}})G_{\mu\mu'}(\mathbf{x},\mathbf{x}',\omega)$$
$$=\hbar\langle\mathbf{x}\mu|\mathbf{x}'\mu'\rangle+\int d\mathbf{x}''\Sigma^\star_{\mu\mu''}(\mathbf{x},\mathbf{x}'',\omega)G_{\mu''\mu'}(\mathbf{x}'',\mathbf{x}',\omega)$$

where h 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 (29) and take the limit $\omega\to\omega_a$:

$$(\hat h f_{a\mu})(\mathbf{x})+\sum_{\mu''}\int d\mathbf{x}''\hbar\Sigma^\star_{\mu\mu''}(\mathbf{x},\mathbf{x}'',\omega_a)f_{a\mu''}(\mathbf{x}'')$$
$$=\hbar\omega_a f_{a\mu}(\mathbf{x}) \tag{33}$$

The ground-state average of a one-particle observable is

$$\langle E_0^N|O|E_0^N\rangle=\sum_{\mu\mu'}\int d\mathbf{x}d\mathbf{x}'\langle\mathbf{x}\mu|\hat o|\mathbf{x}'\mu'\rangle f''_{a\mu}(\mathbf{x})^*f''_{a\mu}(\mathbf{x}')$$
$$=\sum_a\langle f_a|\hat o|f_a\rangle\theta(\mu-\hbar\omega_a) \tag{34}$$

where the functions f_a are treated as elements of the Hilbert space of one particle with spin. In particular the ground-state density of particles with spin μ is

$$\langle E_0^N|n_\mu(\mathbf{x})|E_0^N\rangle=\sum_a|f_{a\mu}(\mathbf{x})|^2\theta(\mu-\hbar\omega_a) \tag{35}$$

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

$$N=\sum_{a\mu}\|f_a\|^2\theta(\mu-\hbar\omega_{a\mu}) \tag{36}$$

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

$$NE_0^N-\sum_\mu\int d\mathbf{x}\,\langle E_0^N|\psi^\dagger_\mu(\mathbf{x})H\psi_\mu(\mathbf{x})|E_0^N\rangle=\langle H_1+2H_2\rangle$$

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

$$\langle H_1 + 2H_2\rangle = NE_0^N - \sum_a E_a^{N-1}\|f_a\|^2\theta(\mu - \hbar\omega_a)$$
$$= \sum_{a\mu} \hbar\omega_a\|f_a\|^2\theta(\mu - \hbar\omega_a)$$

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

$$\boxed{E_0^N = \tfrac{1}{2}\sum_a \langle f_a|\hat{h} + \hbar\omega_a|f_a\rangle\theta(\mu - \hbar\omega_a)} \qquad (37)$$

A. Approximate quasi-particle evaluation

In applications, one may solve the quasi-particle equation (33) 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 μ and the ground state energy E_0^N 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:

$$(\hat{h}f_{a\mu}^0)(\mathbf{x}) + v_{KS}(\mathbf{x})f_{a\mu}^0(\mathbf{x}) = \hbar\,\omega_a^0 f_{a\mu}^0(\mathbf{x}) \qquad (38)$$

The functions f_a^0 form an orthonormal system, and the eigenvalues are real. If the potential v_{KS} were exactly known, the solutions f_a^0, though different from the quasi-particle functions f_a, 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.(33) and take the scalar product with f_b^0, and use the KS equation to eliminate $\hat{h}$:

$$\sum_{\mu,\mu'}\int d\mathbf{x}d\mathbf{y}\, f_{b\mu}^0(\mathbf{x})^*\Sigma^\star_{\mu\mu'}(\mathbf{x},\mathbf{y},\omega_a)f_{a\mu'}(\mathbf{y})$$
$$-\tfrac{1}{\hbar}\langle f_b^0|v_{KS}|f_a\rangle = (\omega_a - \omega_b^0)\langle f_b^0|f_a\rangle$$

The formula is rewritten as

$$(f_b^0|\Sigma^\star(\omega_a)|f_a) - \frac{1}{\hbar}\langle f_b^0|v_{KS}|f_a\rangle = (\omega_a - \omega_b^0)\langle f_b^0|f_a\rangle.$$

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

$$\mathrm{Re}\,\omega_a = \omega_a^0 + Z_a(f_a^0|\,\mathrm{Re}\,\Sigma^\star(\omega_a^0) - \tfrac{1}{\hbar}v_{KS}\delta|f_a^0) \qquad (39)$$
$$\mathrm{Im}\,\omega_a = Z_a\,(f_a^0|\,\mathrm{Im}\,\Sigma^\star(\omega_a^0)|f_a^0) \qquad (40)$$
$$Z_a^{-1} = 1 - \frac{\partial}{\partial\omega}(f_a^0|\,\mathrm{Re}\,\Sigma^\star(\omega)|f_a^0)\Big|_{\omega=\omega_a^0} \qquad (41)$$

Z_a is the quasi-particle weight, δ means $\delta(\mathbf{x}-\mathbf{y})$.

IV. PROOF OF THE LUTTINGER-WARD TH.

There are several similar proofs: the original one by Luttinger and Ward[13], the dissertation by Praz[19], the book by Giuliani and Vignale[7], Dzyaloshinski[4], Pieri and Strinati[18], Heath et al.[9], Najak[16]. In all cases, a proof is *a waltzer in the complex plane.*
The particle density per spin value is:

$$n = \int\frac{d\mathbf{k}}{(2\pi)^3}n_{\mathbf{k}}, \quad n_{\mathbf{k}} = \int_{-\infty}^{\infty}\frac{d\omega}{2\pi i}e^{i\omega\eta}G(\mathbf{k},\omega)$$

Now, in the integral for $n_{\mathbf{k}}$, insert the identity

$$G(\mathbf{k},\omega) = G(\mathbf{k},\omega)\frac{\partial}{\partial\omega}\Sigma(\mathbf{k},\omega) - \frac{\partial}{\partial\omega}\log G(\mathbf{k},\omega)$$

and integrate by parts; the boundary term vanishes because $G(\omega) \approx 1/\omega$ and $\Sigma(\omega)/\omega \to 0$,

$$n_{\mathbf{k}} = -\int_{\mathbb{R}}\frac{d\omega}{2\pi i}e^{i\omega\eta}\left[\Sigma(\mathbf{k},\omega)\frac{\partial}{\partial\omega}G(\mathbf{k},\omega) + \frac{\partial}{\partial\omega}\log G(\mathbf{k},\omega)\right]$$

The first integral will be shown to be zero (Lemma 1). What remains is rewritten as follows (see[16])

$$n = -\int\frac{d\mathbf{k}}{(2\pi)^3}\int_{-\infty}^{\infty}\frac{d\omega}{2\pi i}e^{i\omega\eta}\frac{\partial}{\partial\omega}\log G(\mathbf{k},\omega)$$
$$= -\int\frac{d\mathbf{k}}{(2\pi)^3}\frac{d\omega}{2\pi i}e^{i\omega\eta}\frac{\partial}{\partial\omega}\left[\log G^R(\mathbf{k},\omega) + \log\frac{G(\mathbf{k},\omega)}{G^R(\mathbf{k},\omega)}\right]$$

The first integral is zero because G^R is analytic in the upper half-plane (Lemma 2); G/G^R is 1 for $\hbar\omega > \mu$. Then:

$$n = -\int\frac{d\mathbf{k}}{(2\pi)^3}\int_{-\infty}^{\frac{\mu}{\hbar}}\frac{d\omega}{2\pi i}\frac{\partial}{\partial\omega}\log\frac{G(\mathbf{k},\omega)}{G^R(\mathbf{k},\omega)}$$
$$= \int\frac{d\mathbf{k}}{(2\pi)^3}\int_{-\infty}^{\frac{\mu}{\hbar}}\frac{d\omega}{2\pi i}\frac{\partial}{\partial\omega}\log\frac{G^R(\mathbf{k},\omega)}{G^R(\mathbf{k},\omega)^\star}$$
$$= \int\frac{d\mathbf{k}}{(2\pi)^3}\frac{1}{\pi}[\phi_{\mathbf{k}}(-\infty) - \phi_{\mathbf{k}}(\frac{\mu}{\hbar})]$$

where we put $G^R(\mathbf{k},\omega) = |G^R(\mathbf{k},\omega)|\exp i\phi_{\mathbf{k}}(\omega)$.
Given the spectral representation

$$G^R(\mathbf{k},\omega) = \int_{-\infty}^{+\infty}d\omega'\frac{A(\mathbf{k},\omega)}{\omega-\omega'+i\eta}$$

it is $\mathrm{Im}\,G^R(\omega) = -\pi A(\omega) < 0$ and $\mathrm{Re}\,G^R(\omega) \approx 1/\omega$ for large $|\omega|$. Then, $\phi_{\mathbf{k}}(-\infty) = \pi$.
Since $\mathrm{Im}\,G(\mathbf{k},\frac{\mu}{\hbar}) = 0$, we obtain

$$G(\mathbf{k},\frac{\mu}{\hbar}) = \mathrm{Re}\,G^R(\mathbf{k},\frac{\mu}{\hbar}) = |G(\mathbf{k},\frac{\mu}{\hbar})|\cos\phi_{\mathbf{k}}(\frac{\mu}{\hbar})$$

Then $\phi_{\mathbf{k}}(\frac{\mu}{\hbar})$ can be either 0 or π. Since $\phi_{\mathbf{k}}(-\infty) = \pi$, only $\mathbf{k}$ values where the phase is zero do contribute. The result is (18). □

Lemma 1: $\int \frac{d^4k}{(2\pi)^4}\Sigma(k)\frac{\partial}{\partial\omega}G(k) = 0$.
To prove it, we require the existence of the Phi functional:

$$\Phi[G,v] = \sum_{n=1}^{\infty} \frac{1}{2n}\int \frac{d^4k}{(2\pi)^4}\Sigma^{(n)}(k)G(k)$$

where $\Sigma^{(n)}$ is the sum of self-energy skeleton diagrams with n interaction lines v and $2n-1$ dressed propagators G. It has the property:

$$\frac{\delta\Phi}{\delta G(k)} = \sum_n \frac{1}{2n}\left[\int \frac{d^4k'}{(2\pi)^4}\frac{\delta\Sigma^{(n)}(k')}{\delta G(k)}G(k') + \Sigma^{(n)}(k)\right]$$
$$= \sum_n \frac{1}{2n}\left[(2n-1)\Sigma^{(n)}(k) + \Sigma^{(n)}(k)\right] = \Sigma(k)$$

Then: $\delta\Phi = \int \frac{d^4k}{(2\pi)^4}\Sigma(k)\delta G(k)$. Among possible first order variations we consider $\delta G(k) = G(\mathbf{k},\omega+\delta\omega) - G(\mathbf{k},\omega) = (\partial G/\partial\omega)\delta\omega$

$$0 = \frac{\delta\Phi}{\delta\omega} = \int \frac{d^4k}{(2\pi)^4}\Sigma(\mathbf{k},\omega)\frac{\partial G(\mathbf{k},\omega)}{\partial\omega} = -\int \frac{d^4k}{(2\pi)^4}\frac{\partial\Sigma}{\partial\omega}G(\mathbf{k},\omega)$$

Lemma 2: $\int_{-\infty}^{\infty}\frac{d\omega}{2\pi i}e^{i\omega\eta}\frac{\partial}{\partial\omega}\log G^R(\mathbf{k},\omega) = 0$.
By the Argument principle of complex analysis, the contour integral counts the number of zeros minus the number of poles in the upper half plane. We are assuming that G^R has no zeros, while its poles are in the lower half-plane.

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[27] the states $\psi_u^\dagger|E_0\rangle$ are not normalised, therefore the Green function is only proportional to a probability amplitude.