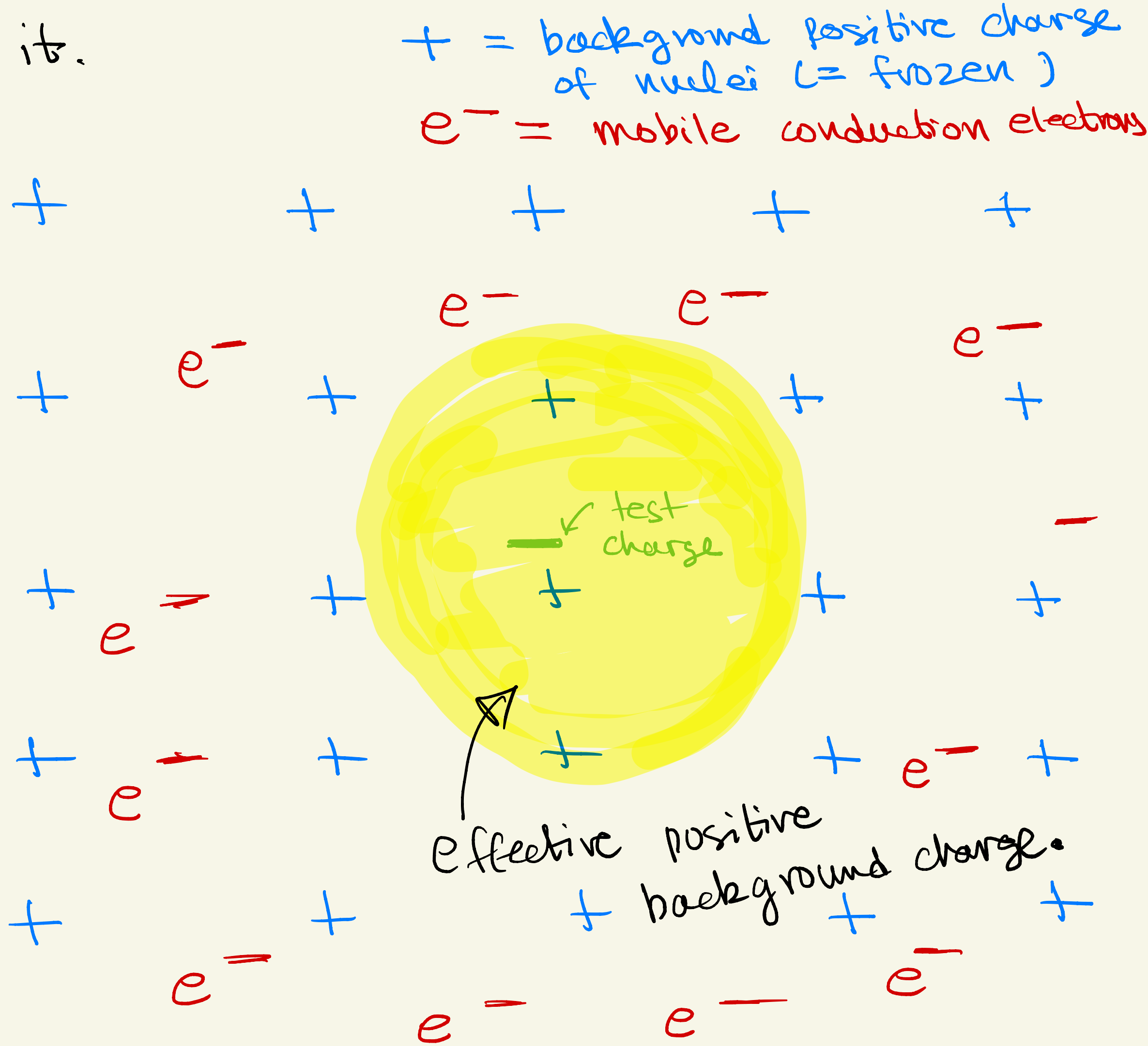
Applications of Linear Response : Screening, Plasmons and Instabilities

The density-density response fn, χ_{nn} encodes a lot of physics : (i) 'Non-collective modes' (= particle-hole excitations) and 'collective modes' (= plasmons).
(ii) Dielectric screening of charged fermions (iii) Instabilities of an interacting system with Fermi surface.

Dielectric Screening

Despite long range Coulomb repulsion, electrons in a system with Fermi surface have effectively short-range interactions. The physical picture is that due to free movement of charge (which is a consequence of system being a metal), a 'test electron' repels electrons close to it.



Quantitatively,

$$U_{tot}(r) = U_0(r) + e^2 \int \frac{\langle \delta n(r') \rangle}{|r - r'|} dr'$$

where $\langle \delta n(r') \rangle$ is the change in the density due to introduction of the test charge and $U_0(r) = \frac{e^2}{r}$ is the bare Coulomb potential. Fourier transforming,

$$U_{tot}(k, \omega) = U_0(k) + \frac{4\pi e^2}{k^2} \langle \delta n(k, \omega) \rangle.$$

The key point is that, from linear response,

$$\langle \delta n(k, \omega) \rangle = \chi_{nn}(k, \omega)\, U_0(k)$$

$$\Rightarrow \quad U_{tot}(k, \omega) = \frac{U_0(k)}{\varepsilon(k, \omega)} \quad \text{where}$$

$$\frac{1}{\epsilon(k, \omega)} = 1 + \frac{4\pi e^2}{k^2} \chi_{nn}(k, \omega)$$

Here $\chi_{nn}(k,\omega)$ is the density-density response of the interacting electrons which we haven't determined yet. It is not

$$\chi^0_{nn}(k,\omega) = \sum_q \frac{n(\varepsilon_q) - n(\varepsilon_{k+q})}{\omega + i\varepsilon + \varepsilon_q - \varepsilon_{k+q}}$$

that we derived for non-interacting $\bar{e}$s.

One can approximately relate $\chi_{nn}(k,\omega)$ to $\chi^0_{nn}(k,\omega)$ in two equivalent ways.

first method: let us imagine that we turn on the charge for all the $\bar{e}$s, including the test charge, slowly at $t = -\infty$, and do a linear response in the coupling strength e^2. Now we are perturbing around a non-interacting limit, and therefore, we can write

$$U_{tot}(k,\omega) = U_0(k) + \frac{4\pi e^2}{k^2} \langle \delta n(k,\omega) \rangle$$

where $\langle \delta n(k,\omega) \rangle = \chi^0_{nn}(k,\omega)\, U_{tot}(k,\omega)$

Note the difference with above equation, where we wrote $\langle \delta n(k,\omega) \rangle = \chi_{nn}(k,\omega)\, U_0(k)$

$$\Rightarrow \quad U_{tot}(k,\omega) = \frac{U_0(k)}{1 - \frac{4\pi e^2}{k^2} \chi^0_{nn}(k,\omega)}$$

$$\Rightarrow \quad \boxed{\varepsilon(k,\omega) = 1 - \frac{4\pi e^2}{k^2} \chi^0_{nn}(k,\omega)}$$

Further, $\boxed{1 + \frac{4\pi e^2}{k^2} \chi_{nn}(k,\omega) = \frac{1}{1 - \frac{4\pi e^2}{k^2} \chi^0_{nn}(k,\omega)}}$

$$\Rightarrow \quad \chi_{nn}(k,\omega) = \frac{-\chi^0_{nn}(k,\omega)}{1 - U_0(k)\, \chi^0_{nn}(k,\omega)}$$

where $U_0(k) = \frac{4\pi e^2}{k^2}$.

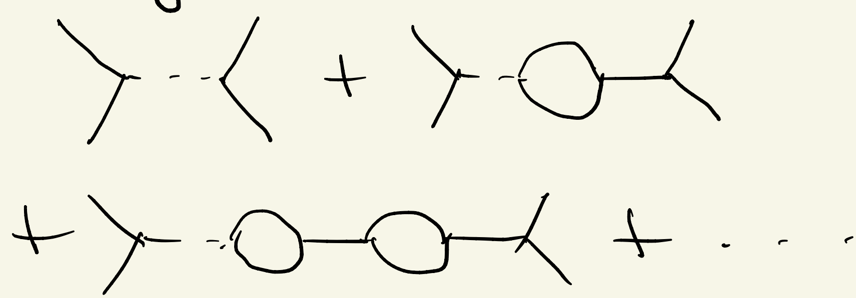
Note that this is just an approximate relation obtained within the above self-consistent approach.

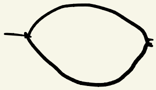
Another way to arrive at the same answer is to obtain $U_{tot}(k,\omega)$ by summing an infinite number of terms within a perturbation theory in e^2.

$$V_{eff}(k,\omega) = V_0(k) + V_0(k)\,\chi^0_{nn}(k,\omega)\,V^0(k) + V_0(k)\left(\chi^0_{nn}(k,\omega)\right)^2 V^0(k) + \dots$$

Diagramatically:

$U_{tot} =$



The bubble  precisely corresponds to $\chi^0_{nn}(k,\omega)$ as one may readily verify.

Summing the geometric series,

$$V_{tot}(k,\omega) = \frac{V_0(k)}{1 - V^0(k)\,\chi^0_{nn}(k,\omega)}$$

which is precisely the equation we derived above using a self-consistent approach.

Short-range interactions between e^-s :

$$\chi^0_{nn}(k \approx 0, \omega = 0) = \sum_q \frac{n(\varepsilon_q) - n(\varepsilon_{k+q})}{\varepsilon_q - \varepsilon_{k+q}}$$

$$\approx \int \frac{\partial n}{\partial \varepsilon} N(\varepsilon)\, d\varepsilon$$

$-\delta(\varepsilon - \varepsilon_F)$

density of states

$$\approx -N(\varepsilon_F)$$

fermi energy

$\Rightarrow$ at small k

$$U_{tot}(k, \omega=0) \approx \frac{V_0(k)}{1 + V_0(k) N(\varepsilon_F)}$$

Clearly as $k \to 0$ $U_{tot}(k, \omega=0)$ <u>does not</u> diverge $\Rightarrow$ short range interactions.

Fourier transforming,

$$U_{tot}(r) \sim e^2 \frac{e^{-r/\xi}}{r}$$

2.718....

charge

where $\xi^2 \sim \dfrac{1}{N(\varepsilon_F) e^2}$

Thus, as $N(\varepsilon_F) \to 0$, the interaction becomes long-ranged (e.g. in a system with Fermi points such as graphene at neutrality)

Friedel oscillations:

The only singularity of $\chi^0_{nn}(k, \omega=0)$ is at $k \approx 2k_F$ due to absence of any particle-hole excitations at $k > 2k_F$ for $\omega = 0$.

In particular, $\varepsilon(x) \sim 1 + x \log x$

where $x \doteq \dfrac{q - 2k_F}{2k_F}$. This singularity leaves its imprint in $V_{tot}(k \approx 2k_F, \omega=0)$ and relatedly, in the screening charge.

Fourier transforming, one can show that

$$V_{tot}(r) \sim \frac{\cos(2k_F r)}{r^3}$$

To obtain the screening charge, Q^{ind}.

$$\nabla^2 U_0(r) = 4\pi Q^{test}$$

$$\nabla^2 U_{tot}(r) = 4\pi \left[Q^{test} + Q^{ind}\right]$$

$$\Rightarrow \quad \nabla^2 \left[U_{tot} - U_0\right] = 4\pi Q^{ind}(r)$$

$$\Rightarrow \quad \nabla^2 \left[\frac{U_0}{\varepsilon} - U_0\right] = 4\pi Q^{ind}(r)$$

$$\Rightarrow \quad Q^{ind}(r) = Q \int d^3k \left[\frac{1}{\varepsilon(k)} - 1\right] e^{ik\cdot r}.$$

Again, by using the fact that $\varepsilon(k)$ has $x \log x$ singularity where $x = k - 2k_F$, one can show that

$$Q^{ind}(r) \sim \frac{\cos(2k_F r)}{r^3}.$$

Excitations and $\chi^0_{nn}(k,\omega)$:

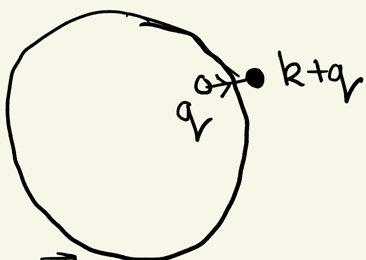
particle-hole excitation spectrum and plasmons.

The imaginary part of $\chi^0_{nn}(k,\omega)$ encodes real particle-hole excitations:

$$\text{Im}\, \chi^0_{nn}(k,\omega) = \frac{1}{V} \sum_q \left[n(\varepsilon_q) - n(\varepsilon_{k+q}) \right] \delta(\omega + \varepsilon_q - \varepsilon_{k+q})$$

Let's consider various limits:

(i) $\omega \gtrsim 0$, $k \gtrsim 0$.



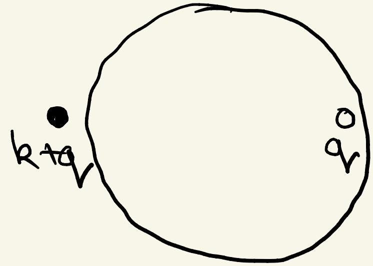
ω is maximized when $\vec{k}$ is perpendicular to the Fermi surface. $\omega = \varepsilon_{k+q} - \varepsilon_q \approx \frac{\vec{k}\cdot\vec{q}}{m} \approx v_F k$

where v_F is the Fermi velocity.

$\Rightarrow$ If $\omega > v_F k$, particle-hole excitation is impossible.

(ii) $\omega \approx 0$, $k \approx 2k_F$

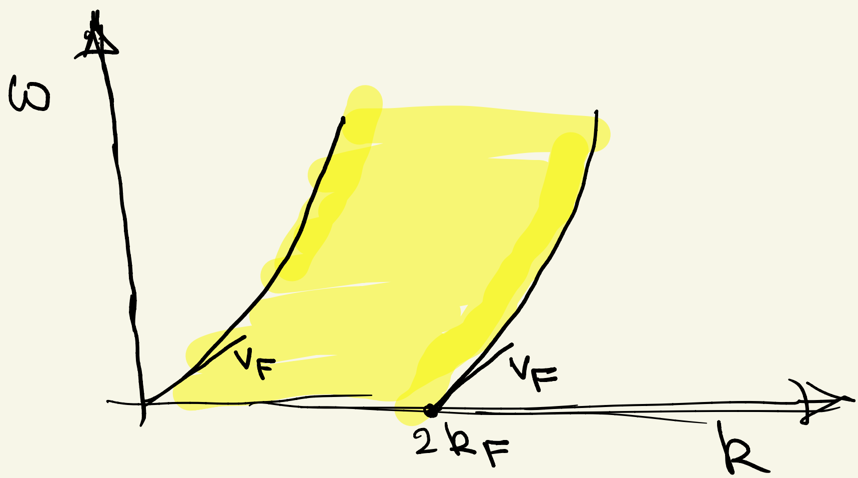
For $k \approx 2k_F$, ω is minimized if q and $k+q$ are close to fermi surface and antipodal.



$\omega = \varepsilon_{k+q} - \varepsilon_q \approx (k-2k_F)v_F$

$\Rightarrow$ If $\omega < v_F(k-2k_F)$, particle-hole excitation is impossible

Allowed range of particle-hole excitations:



Plasmons:

Recall that plasmons are collective oscillations of a charged system. Classically, a density fluctuation $\delta n(q)$ generates electrostatic potential $\varphi_q = -\frac{4\pi e}{q^2}\delta n(q)$ which

generates an electric field $-i\vec{q}\,\varphi_q = \frac{4\pi i e\,\delta n(q)}{q}$

The force due to this electric field generates current $\vec{j} = -\rho_0 e \vec{v}$ whose time derivative is (using Newton's law),

$$\frac{d\vec{j}}{dt} = -\rho_0 e \frac{d\vec{v}}{dt} = \rho_0 e \frac{e\vec{E}}{m}$$

Continuity equation $\vec{\nabla}\cdot\vec{j} = e\frac{\partial n}{\partial t}$ combined with Gauss's law $\nabla\cdot E = -4\pi e n$ implies

$$\frac{d}{dt}(\vec{\nabla}\cdot\vec{j}) = \rho_0 \frac{e^2}{m} - 4\pi e n$$

$$\Rightarrow \quad \frac{\partial^2 n}{\partial t^2} + \frac{4\pi e^2 \rho_0 n}{m} = 0$$

Thus, the system oscillates at a frequency $\Omega_p = \sqrt{\frac{4\pi e^2 \rho_0}{m}}$, which is called Plasma frequency.

From a linear-response perspective, when $\omega \sim \Omega_p$, instead of screening, the response to an external potential is <u>infinitely</u> enhanced, similar to a resonance. That is why, at $\omega = \Omega_p$, system oscillates by itself, without any external input. That is, the plasma oscillations are a collective excitation of the system. This suggests that when $\omega \approx \Omega_p$, dielectric constant $\varepsilon(k, \omega) \to 0$, so that $U_{tot} = U_0 / \varepsilon(k, \omega)$ diverses.

To find Ω_p, we therefore need to find zero of $\varepsilon(k, \omega)$.

$\varepsilon(q \simeq 0,\ \omega$ large$)$

$$= 1 - \frac{4\pi e^2}{k^2}\frac{1}{V}\sum_q \frac{[n(\varepsilon_q) - n(\varepsilon_{q+k})]}{\omega + \varepsilon_q - \varepsilon_{q+k}}$$

(Taylor expanding in $1/\omega$)

$$\simeq 1 - \frac{4\pi e^2}{k^2}\frac{1}{(2\pi)^3}\int d^3q \, \underbrace{\frac{[n(\varepsilon_q) - n(\varepsilon_{q+k})]}{\omega}}_{\to 0}$$

$$+ \frac{1}{(2\pi)^3}\frac{4\pi e^2}{k^2\,\omega^2}\underbrace{\int_q [n(\varepsilon_q) - n(\varepsilon_{q+k})][\varepsilon_q - \varepsilon_{q+k}]}_{\approx k^2 \text{ at small } \vec{k}}$$

$$\simeq 1 - \frac{4\pi e^2 \rho_0}{m\,\omega^2}$$

$$\Rightarrow \varepsilon = 0 \quad \text{at} \quad \omega = \Omega_p = \left(\frac{4\pi e^2 \rho_0}{m}\right)^{1/2}$$

Linear Response and Instabilities

Above we derived,

$$\chi_{nn}(k,\omega) = \frac{-\chi^0_{nn}(k,\omega)}{1 - U_0(k)\,\chi^0_{nn}(k,\omega)}$$

Where χ^0 is the linear-response (i.e. linear susceptibility) for a non-interacting system and χ_{nn} is that for an interacting system. Within a mean-field / self-consistent approximation, such an expression works for more general settings.

As a toy example, consider the Ising model: $H = -J\sum_{i} s_i s_j - h\sum_i s_i$

Within mean-field approximation,

$$H_{MF} = \sum_i -\overbrace{(Jzm+h)}^{h_{eff}} s_i$$

where $m = \langle s_i \rangle$ and z is the coordination number.

$$\Rightarrow \quad m = \chi_0 h_{eff}$$

where $h_{eff} = h + Jzm$ and χ_0 is the susceptibility in the absence of interactions (i.e at $J=0$). Explicity, when $J=0$.

$$m = \tanh(\beta h) \Rightarrow \chi_0 \sim \frac{1}{T}.$$

Solving $m = \chi_0 \, (Jzm + h)$

$$\Rightarrow \quad m = \frac{\chi_0 h}{1 - \chi_0 Jz}$$

Compare this with $\chi_{mm} = \dfrac{-\chi_0}{1 - \chi_0 U_0(k)}$

The above argument for the Ising model works for any model, within mean-field approximation.

For example, consider

$$H = \underbrace{-\sum_{\langle ij \rangle}(c^+_i c_j + h.c.) + \mu \sum_i c^+_i c_i}_{H_0}$$

$$+ \quad V \sum_{\langle ij \rangle} n_i n_j$$

where $n_i = c^+_i c_i$

The density response for H_0 is χ_0 i.e.

$$\langle n(k,\omega) \rangle = \mu(k,\omega)\, \chi_0(k,\omega).$$

Again, within mean-field,

$$H_{MF} = -\sum_{\langle ij \rangle}(c^+_i c_j + h.c.) + \sum_i (Vz\langle n_i \rangle + \mu) n_i$$

$$\Rightarrow \quad \langle n \rangle = \chi_0 (Vz \langle n \rangle + \mu)$$

$$\Rightarrow \quad \langle n \rangle = \frac{\chi_0 \mu}{1 - \chi_0 V z}$$

$$\Rightarrow \quad \chi_{\text{interacting}} = \frac{\chi_0}{1 - \chi_0 V z}$$

The expressions such as these encode potential instabilities (similar to plasmon resonance), when $\chi_{\text{interacting}} = \infty$, i.e. when the denominator vanishes. For example, in the Ising model, χ diverges when $1 - \chi_0 J z = 0$, Using $\chi_0 \sim \frac{1}{T}$

$\Rightarrow$ it diverges at $T = T_c = Jz$, which precisely corresponds to the mean-field critical temperature.

Now consider interacting models at $T = 0$ e.g. in the above example where

$$\chi_{\text{interacting}} = \frac{\chi_0}{1 - \chi_0 V z}$$

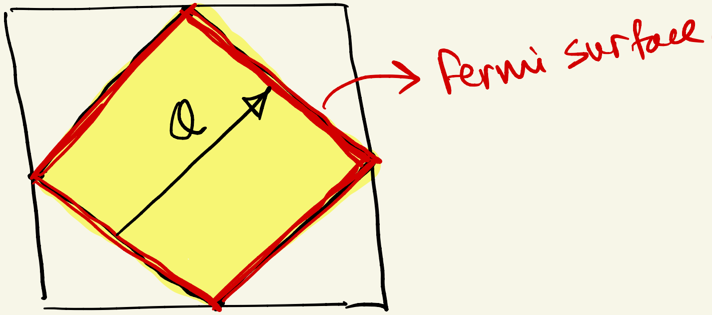
χ interacting diverges when $V > \dfrac{1}{\chi_0 Z} = V_c$.

This expression illustrates two qualitatively different scenarios : (a) If χ_0 is finite, then $V_c > 0$ i.e. there is a non-zero threshold for instability i.e. spontaneous symmetry breaking. (b) If χ_0 is infinite, then $V_c = 0$ i.e. the system is unstable.

To give an example of (a), consider $\chi_0^{nn}(k, \omega \to 0)$ for a non-nested fermi surface is non-divergent for any k.

As an example of (b), lets consider the nested Fermi surface in $d = 2$.

$$H_0 = -2t \sum_k \left[\cos(k_x) + \cos(k_y)\right].$$

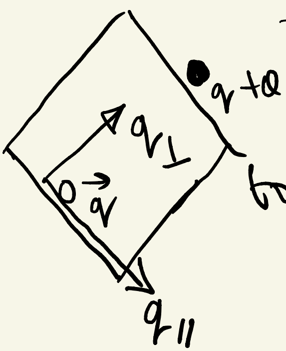


Consider $\chi_0(k,\omega) = \frac{1}{V}\sum_q \left[\frac{n(\varepsilon_q) - n(\varepsilon_{k+q})}{\omega + i\varepsilon + \varepsilon_q - \varepsilon_{k+q}}\right]$

Let's consider $\chi_0(k = Q, \omega)$

$$= \frac{1}{V}\sum_q \left[\frac{n(\varepsilon_q) - n(\varepsilon_{q+Q})}{\omega + i\varepsilon + \varepsilon_q - \varepsilon_{q+Q}}\right]$$

The dominant contribution comes from the following terms, where both $\vec{q}$ and $\vec{q} + \vec{Q}$ are very close to the Fermi surface.



$$\chi_0^{nn}(k = Q, \omega) \sim \int \frac{dq_\perp\, dq_\parallel}{\omega + v_F q_\perp}$$

$$\sim \log\left(\frac{\omega}{E_F}\right).$$

Thus, $\chi(k=Q, \omega=0) = \infty$.

Therefore turning on density-density interactions for a nested Fermi surface is expected to lead to an instability (charge-ordered spontaneous symmetry breaking state). i.e. if

$$H = H_0 + V \sum_{\langle ij \rangle} n_i n_j \,, \quad \text{then}$$

free-fermion nested Fermi surface

one expects $V_c \sim \dfrac{1}{\chi(k=Q, \omega=0)} = 0$.