1 Dielectric Response Function

We reformulate the screening problem in terms of χ_{nn} by rewriting the perturbing field as

$$H' = \int d\mathbf{r} \, n(\mathbf{r}, t) \, U(\mathbf{r}, t), \tag{1}$$

where $U(\mathbf{r}, t)$ is the local electrostatic potential energy of the charge Q, which we take to be the Coulomb interaction. We must determine the net field felt by other electrons as a result of the test charge Q placed at the origin. We start by writing equation

$$U_{eff}(\mathbf{r},t) = U(\mathbf{r}) + \int e^2 \frac{\langle \delta n(\mathbf{r}',t) \rangle}{|\mathbf{r} - \mathbf{r}'|} d\mathbf{r}'.$$
 (2)

Fourier transforming this expression with respect to \mathbf{r} and t,

$$U_{eff}(\mathbf{k},\omega) = U(\mathbf{k}) + \frac{4\pi e^2}{k^2} \langle \delta n(\mathbf{k},\omega) \rangle, \qquad (3)$$

and using the linear response expression for the fluctuation (equation ??) $\left(\chi_{nn}(\mathbf{r}t,\mathbf{r}'t') = -\frac{i}{\hbar} \langle [n(\mathbf{r},t),n(\mathbf{r}',t')] \rangle \right)$

$$\langle \delta n(\mathbf{k},\omega) \rangle = \chi_{nn}(\mathbf{k},\omega)U(\mathbf{k})$$
 (4)

we obtain

$$U_{eff}(\mathbf{k},\omega) = \left[1 + U(\mathbf{k})\chi_{nn}(\mathbf{k},\omega)\right]U(\mathbf{k},\omega)$$

= $\varepsilon^{-1}(\mathbf{k},\omega)U(\mathbf{k}),$ (5)

with $\epsilon(\mathbf{k}, \omega)$ the dielectric function and $U(\mathbf{k}) = 4\pi^2/k^2$. It is the dielectric function that contains the dynamics of the screening process (described in the introduction to this chapter).

To make contact with our previous treatment of screening, we introduce a generalized screening function, χ_{SC} , through

$$\langle \delta n(\mathbf{r},t) \rangle = \langle n(\mathbf{r},t) \rangle - n_e = \int d\mathbf{r}' \chi_{SC}(\mathbf{r},\mathbf{r}',t) U_{eff}(\mathbf{r}').$$
(6)

The generalized screening function χ_{SC} , describes the response of the system to the screened potential in contrast to χ_{nn} , which is simply the response to the bare potential. From Eq.(??), we see that the Thomas-Fermi screening function is simply

$$\chi_{SC}(\mathbf{r}, \mathbf{r}', t) = -\frac{\partial n_e}{\partial \mu} \delta(\mathbf{r} - \mathbf{r}') \delta(t).$$
(7)

The Fourier transform of Eq.(6) yields

$$\langle \delta n(\mathbf{k},\omega) \rangle = \chi_{SC}(\mathbf{k},\omega) U_{eff}(\mathbf{k},\omega),$$
(8)

Prithvi Narayan Campus

which, together with Eq.(3), implies that

$$U_{eff}(\mathbf{k},\omega) = \left[1 - \frac{4\pi e^2}{k^2} \chi_{SC}(\mathbf{k},\omega)\right]^{-1} U(\mathbf{k})$$
(9)

is an equivalent expression for the total effective electrostatic potential in the presence of the test charge Q. Equating Eqs.(9) and (5), we see immediately that

$$\chi_{nn} = \varepsilon^{-1} \chi_{SC} = \frac{\chi_{SC}}{1 - \frac{4\pi e^2 \chi_{SC}}{\nu^2}}$$
(10)

It is generally easier to construct a theory for χ_{SC} because it describes the response to the total field of the system. The lowest-order theory for χ_{SC} is the random-phase approximation(RPA) in which it is assumed that

$$\chi_{SC}(\mathbf{k},\omega) = \chi_{nn}^{\circ}(\mathbf{k},\omega) \tag{11}$$

Alternately, the effective interaction is given by the geometric series

$$U_{eff}(\mathbf{k},\omega) = U(\mathbf{k})(1 + U(\mathbf{k})\chi_{nn}^{\circ}(\mathbf{k},\omega) + (U(\mathbf{k})\chi_{nn}^{\circ}(\mathbf{k},\omega))^{2} + \cdots)$$

$$= \frac{U(\mathbf{k})}{1 - U(\mathbf{k})\chi_{nn}^{\circ}(\mathbf{k},\omega)}.$$
(12)

This approximation leaves out exchange effects and is essentially time-dependent Hartee-Fock. As shown in the previous section, the zero-frequency limit of χ_{nn}° is the Thomas-Fermi approximation.

To understand the role played by the frequency dependence, we expand the denominator in Eq.(28 *in lecture -03*) for large ω . In this limit, we find that

$$\lim_{\omega \to \infty} \chi_{nn}^{\circ}(\mathbf{k}, \omega) \to 2 \int \frac{dp}{(2\pi\hbar)^3} (f_p - f_{p+\hbar k}) \left[\frac{1}{\hbar\omega} - \frac{\epsilon_p - \epsilon_{p+\hbar k}}{(\hbar\omega)^2} + \cdots \right]$$
$$= -\frac{2}{(\hbar\omega)^2} \int \frac{dp}{(2\pi\hbar)^3} (f_p - f_{p+\hbar k}) (\epsilon_p - \epsilon_{p+\hbar k})$$
$$= \frac{2k^2}{m\omega^2} \int \frac{dp}{(2\pi\hbar)^3} f_p = \frac{k^2}{m\omega^2} n_e$$
(13)

The high-frequency limit of the dielectric function,

$$\epsilon = 1 - \frac{4\pi e^2 n_e}{mk^2} \frac{k^2}{\omega^2}$$

= $1 - \left(\frac{\omega_p}{\omega}\right)^2$, (14)

is fundamentally related to the plasma frequency. In fact, as we will see later, the plasma frequency is an exact zero of the dielectric function.



Figure 1: Diagramatic expansion in the RPA for the screened electron-electron interaction. Each bubble represents a particle-hole excitation. Mathematically, these excitations are described by the polarization function $\chi_{nn}^{\circ}(\mathbf{k},\omega)$. The momentum exchanged between the particle and the hole is carried away by the Coulomb interaction at each dotted line, as indicated. As a result, the argument of the Coulomb interaction is decoupled from the momentum summation in each bubble. Consequently, all such terms can be summed exactly. The result is Eq. (12)

1.1 Structure Function

The time-dependent density response function defined in the previous section is a fundamental quantity in many-body theorem. In addition to the screening function, the structure function, as well as the total energy of an interacting system, can all be written in terms of χ_{nn} . The principal reason for this is that the potential in most many-body systems is typically a sum of pair-wise interactions. In this section, we focus on calculating the structure function, as it will play a prominent role in later topics.

The structure function is defined as the auto-correlation function of the Fourier components

$$S(\mathbf{k}) = \frac{1}{N} \langle n_{\mathbf{k}} n_{-\mathbf{k}} \rangle \tag{15}$$

of the particle density. In equilibrium neutron-scattering experiments, the central quantity that is measured is the structure factor. As advertised, we can also write the total average energy of an interacting electron system in terms of $S(\mathbf{k}, \omega)$. This can be done trivially by computing the average value of the Hamiltonian for an interacting electron gas

$$\langle H \rangle = E_0 = \epsilon_{kin} + \sum_{\mathbf{k}} \frac{2\pi e^2}{k^2} \left[S(\mathbf{k}) - N \right]$$
(16)

in momentum space(see Eq.8.18).

In the time domain, the structure function becomes

$$S(\mathbf{k},t) = \frac{1}{N} \left(\sum_{i} e^{ik \cdot r_i(0)} \sum_{j} e^{-ik \cdot r_j(t)} \right).$$
(17)

By noting that

$$e^{i\mathbf{k}\cdot\mathbf{r}_{i}} = \int d\mathbf{r}e^{i\mathbf{k}\cdot\mathbf{r}}\delta(\mathbf{r}-\mathbf{r}_{i})$$
(18)

and the density at **r** is

$$n(\mathbf{r}) = \sum_{i=1}^{N} \delta(\mathbf{r} - \mathbf{r}_i), \qquad (19)$$

we rewrite Eq. (17) as

$$S(\mathbf{k},t) = \frac{1}{N} \int d\mathbf{r} d\mathbf{r}' \langle n(\mathbf{r},t=0)n(\mathbf{r}',t) \rangle e^{i\mathbf{k}.(\mathbf{r}-\mathbf{r}')}.$$
(20)

As we have seen, $\langle n(\mathbf{r}, t)n(\mathbf{r}', t') \rangle$ depends only on $\mathbf{r} - \mathbf{r}'$ and t - t'. Hence, our choice of the time origin at t = 0 does not affect our results. The dynamic structure factor is the time Fourier transform

$$S(\mathbf{k},\omega) = \int_{-\infty}^{\infty} dt e^{-i\omega t} S(\mathbf{k},t)$$
(21)

Kapil Adhikari

of $S(\mathbf{k}, t)$. It is $S(\mathbf{k}, \omega)$ that is measured in angle-resolved x-ray or neutron-scattering experiments. The static and dynamic structure factors are related through the simple sum rule

$$S(\mathbf{k}) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} S(\mathbf{k}, \omega).$$
(22)

For systems with inversion symmetry, such as most solids and all fluids, $S(\mathbf{k}, \omega)$ is invariant under a change of sign of $\mathbf{k} : S(\mathbf{k}, \omega) = S(-\mathbf{k}, \omega)$. From Eq.(??), it follows that $S(\mathbf{k}, \omega) = e^{\beta \hbar \omega} S(\mathbf{k}, -\omega)$. This relationship reflects the principle of detailed balance. From Eq.(??), we have

$$i\hbar\chi_{nn}(\mathbf{k},\omega) = n_e \int_{-\infty}^{0} dt e^{-i\omega t} \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} e^{i\omega' t} \Big[S(\mathbf{k},\omega') - S(\mathbf{k},-\omega') \Big]$$

$$= n_e \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi i} \frac{S(\mathbf{k},\omega') - S(\mathbf{k},-\omega')}{\omega' - \omega}$$

$$= n_e \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi i} (1 - e^{-\beta\hbar\omega'}) \frac{S(\mathbf{k},\omega')}{\omega' - \omega}.$$
 (23)

We see, then, that the density response function, $\chi_{nn}(\mathbf{k}, \omega)$, can in principle be determined from experiment, once $S(\mathbf{k}, \omega)$ is known.

An expression identical to Eq.(16) can be derived, using parameter differentiation. We consider a variation of the ground state energy with respect to e^2 :

$$\frac{\partial}{\partial e^2} E_0(e^2) = \frac{\partial}{\partial e^2} \langle \psi(e^2) | H | \psi(e^2) \rangle$$

$$= \left(\frac{\partial}{\partial e^2} \langle (e^2) \rangle | H | \psi(e^2) \rangle + \langle \psi(e^2) | H \left(\frac{\partial}{\partial e^2} | \psi(e^2) \rangle \right) + \langle \psi(e^2) | \frac{\partial H}{\partial e^2} | \psi(e^2) \rangle$$

$$= E_0(e^2) \frac{\partial}{\partial e^2} \langle \psi(e^2) | \psi(e^2) \rangle + \langle \frac{\partial H}{\partial e^2} \rangle = \langle \psi | \frac{\partial H}{\partial e^2} | \psi \rangle.$$
(24)

We have used the fact that $H|\psi(e^2)\rangle = E_0|\psi(e^2)\rangle$. Because the kinetic energy is independent of e^2 and $V \sim e^2$, we have that

$$\frac{\partial E_0}{\partial e^2} = \frac{1}{e^2} \langle \psi | V_e | \psi \rangle, \tag{25}$$

where V_e is the total potential for our interacting system:

$$V_e = V_{ee} + V_{ion-ion} + V_{e-ion}$$

= $e^2 \bigg[\frac{1}{2} \sum_{j,j'} \frac{1}{|\mathbf{r}_j - \mathbf{r}'_j|} + \frac{1}{2} \int d\mathbf{r} d\mathbf{r}' \frac{n_e^2}{\mathbf{r} - \mathbf{r}'} - \sum_j \int d\mathbf{r} \frac{n_e}{|\mathbf{r} - \mathbf{r}_j|} \bigg].$ (26)

The second and third terms in the total potential represent the ion-ion and electron-ion interactions, respectively. The ions provide a homogeneous back-ground of compensating positive charge for the electron gas. If we substitute the form for the density in Eq. (19), we can rewrite the total

potential as

$$\frac{V_e}{e^2} = \frac{1}{2} \int d\mathbf{r} d\mathbf{r}' \frac{n(\mathbf{r})n(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} + \frac{n_e^2}{2} \int \frac{d\mathbf{r} d\mathbf{r}'}{|\mathbf{r} - \mathbf{r}'|} - n_e \int d\mathbf{r} d\mathbf{r}' \frac{n(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} \\
= \frac{1}{2} \int d\mathbf{r} d\mathbf{r}' \frac{(n(\mathbf{r}) - n_e)(n(\mathbf{r}') - n_e)}{|\mathbf{r} - \mathbf{r}'|}.$$
(27)

Cosequently,

$$\frac{\delta E_0}{\delta e^2} = \frac{1}{2} \int d\mathbf{r} d\mathbf{r}' \frac{\langle \delta n(\mathbf{r}) \delta n(\mathbf{r}') \rangle}{|\mathbf{r} - \mathbf{r}'|}
= \frac{n_e}{2} \int d\mathbf{r} d\mathbf{r}' \int \frac{d\mathbf{k}}{(2\pi)^3} \frac{e^{i\mathbf{k}(\mathbf{r} - \mathbf{r}')}}{|\mathbf{r} - \mathbf{r}'|} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \tilde{S}(k, \omega)
= \frac{n_e V}{2} \int \frac{d\mathbf{k}}{(2\pi)^3} \frac{4\pi}{k^2} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \tilde{S}(k, \omega),$$
(28)

where we introduced a rescaled structure factor

$$n_e \tilde{S}(\mathbf{k},\omega) = \int_{-\infty}^{\infty} dt e^{-i\hbar t} e^{-i\mathbf{k}(\mathbf{r}-\mathbf{r}')} \langle \delta n(\mathbf{r}) \delta n(\mathbf{r}',t) \rangle d(\mathbf{r}-\mathbf{r}').$$
(29)

The advantage of this definition of the structure factor is that it eliminates the n_e^2 -term that would normally appear in the energy. This term simply shifts the zero of the potential energy and, hence, is of no real consequence.

Using the sum rule in Eq.(22) for $S(\mathbf{k}, \omega)$ yields

$$E_0(e^2) = E_0(e^2 = 0) + \frac{N}{2} \int_0^{e^2} de'^2 \int \frac{d\mathbf{k}}{(2\pi)^3} \frac{4\pi}{k^2} \tilde{S}(\mathbf{k}; e'^2),$$
(30)

where we have allowed for explicit e^2 -dependence in the static structure factor. This is an exact expression. If the free-particle form for $\tilde{S}(\mathbf{k})$ is used, Hartee-Fock theory results. Inclusion of the effects of screening allows us then to reduce $E_0(e^2)$ to the Gell-Mann-Brueckner perturbative expansion.

1.2 Evaluation of $\chi_{SC}(k, \omega)$

Our goal now is to evaluate completely the effects of screening in the RPA. We start by rewriting the screening function as

$$\chi_{SC}(\mathbf{k},\omega) = \chi_{nn}^{\circ}(\mathbf{k},\omega) = 2 \int \frac{d\mathbf{p}}{(2\pi\hbar)^3} \frac{(f_{\mathbf{p}} - f_{\mathbf{p}+\hbar k})}{(\hbar\omega + \epsilon_{\mathbf{p}} - \epsilon_{\mathbf{p}} + \hbar \mathbf{k})}$$

$$= 2 \lim_{\eta \to 0} \int_{-\infty}^{\infty} \frac{d\omega'}{\omega - \omega' + i\eta} \int \frac{d\mathbf{p}}{(2\pi\hbar)^3} (f_{\mathbf{p}} - f_{\mathbf{p}+\hbar \mathbf{k}}) \times \delta(\hbar\omega' - \epsilon_{\mathbf{p}+\hbar \mathbf{k}} + \epsilon_{\mathbf{p}}).$$
(31)

Using Eq.(23), we rewrite the right side in terms of the structure factor. We find that

$$4\pi\hbar\int \frac{d\mathbf{p}}{(2\pi\hbar)^3} (f_{\mathbf{p}} - f_{\mathbf{p}} + \hbar\mathbf{k}) \delta(\hbar\omega' - \epsilon_{\mathbf{p}} + \hbar\mathbf{k} + \epsilon_{\mathbf{p}}) = n_e (1 - e^{-\beta\hbar\omega'}) S_0(k, \omega'), \tag{32}$$

where $S_0(\mathbf{k}, \omega')$ is the structure factor for the free system. We simplify the left side of this expression by noting that $f_{\mathbf{p}} - f_{\mathbf{p}+\hbar\mathbf{k}} = f_{\mathbf{p}}(1 - f_{\mathbf{p}+\hbar\mathbf{k}}) - f_{\mathbf{p}+\hbar\mathbf{k}}(1 - f_{\mathbf{p}})$ and $1 - f_{\mathbf{p}} = e^{\beta(\epsilon_{\mathbf{p}}-\mu)}f_{\mathbf{p}}$. Consequently,

$$f_{\mathbf{p}} - f_{\mathbf{p}+\hbar\mathbf{k}} = f_{\mathbf{p}}(1 - e^{\beta}(\epsilon_{\mathbf{p}} - \epsilon_{\mathbf{p}+\hbar\mathbf{k}})), \tag{33}$$

and the explicit temperature-dependent factor multiplying the free-particle structure function can be eliminated to yield

$$n_e S_0(\mathbf{k},\omega) = 4\pi\hbar \int \frac{d\mathbf{p}}{(2\pi\hbar)^3} f_{\mathbf{p}}(1 - f_{\mathbf{p}+\hbar\mathbf{k}}) \delta(\hbar\omega - \epsilon_{\mathbf{p}+\hbar\mathbf{k}} = \epsilon_{\mathbf{p}}).$$
(34)

The factor $1 - f_{\mathbf{p}+\hbar\mathbf{k}}$ is the probability that the state with momentum $\mathbf{p} + \hbar\mathbf{k}$ is empty. Hence, $S_0(\mathbf{k}, \omega)$ is determined by the number of ways a particle can exchange energy with a hole with a total energy change $\hbar\omega = \epsilon_{\mathbf{p}} - \epsilon_{\mathbf{p}+\hbar\mathbf{k}}$. In this sense, $S_0(\mathbf{k}, \omega)$ can be thought of as the effective density of states for particle-hole excitations.

To evaluate the integral in Eq.(34) at T = 0, we shift the momentum in $f_{\mathbf{p}+\hbar\mathbf{k}}$ by $-\hbar\mathbf{k}$, so that the resultant integrand

$$\int \frac{d\mathbf{p}}{(2\pi\hbar)^2} (f_{\mathbf{p}} - f_{\mathbf{p}+\hbar\mathbf{k}}) \delta(\hbar\omega - \epsilon_{\mathbf{p}+\hbar\mathbf{k}} + \epsilon_{\mathbf{p}})$$

$$= \int \frac{d\mathbf{p}}{(2\pi\hbar)^2} f_{\mathbf{p}} \Big[\delta(\hbar\omega - \epsilon_{\mathbf{p}+\hbar\mathbf{k}} + \epsilon_{\mathbf{p}}) - \delta(\hbar\omega - \epsilon_{\mathbf{p}} + \epsilon_{\mathbf{p}-\hbar\mathbf{k}}) \Big]$$

$$= \int \frac{d\mathbf{p}}{(2\pi\hbar)^2} f_{\mathbf{p}} \Big[\delta \Big(\hbar\omega - \frac{(\hbar k)^2}{2m} - \frac{\mathbf{p}.\hbar\mathbf{k}}{m} \Big) - \delta \Big(\hbar\omega + \frac{(\hbar k)^2}{2m} + \frac{\mathbf{p}.\hbar\mathbf{k}}{m} \Big) \Big]$$

$$= I_{\omega} - I_{-\omega}$$
(35)

will contain a single Fermi distribution function. We now transform to spherical coordinates and obtain

$$T_{\omega} = \frac{1}{\pi\hbar^{2}} \int_{0}^{p_{F}} p^{2} dp \int_{-1}^{1} d\mu \delta \left(\hbar\omega - \frac{(\hbar k)^{2}}{2m} - \frac{\hbar k p \mu}{m} \right)$$

$$= \frac{m}{\pi k\hbar^{3}} \int_{0}^{p_{F}} p dp \Theta \left(1 - \left| \frac{m}{\hbar k p} \left(\hbar\omega - \frac{(\hbar k)^{2}}{2m} \right) \right| \right)$$

$$= \frac{m}{\pi k\hbar^{3}} \int_{\frac{m}{\hbar bark} \left| \hbar\omega - \frac{(\hbar k)^{2}}{2m} \right|} p dp$$

$$= \frac{m}{2\pi k\hbar^{3}} \left[p_{F}^{2} - \left(\frac{m}{\hbar k} \left(\omega - \frac{(\hbar k)^{2}}{2m} \right) \right)^{2} \right] \times \Theta \left(p_{F} - \frac{m}{\hbar k} \left| \hbar\omega - \frac{(\hbar k)^{2}}{2m} \right| \right)$$
(36)

Here $\Theta(x)$ is the Heaviside step function. Subtracting the $\omega \rightarrow -\omega$ contribution, we find that

$$I_{\omega} - I_{-\omega} = \frac{m}{2\pi k\hbar^3} \left[p_F^2 - \left(\frac{m}{\hbar k} \left(\omega - \frac{(\hbar k)^2}{2m} \right) \right)^2 \right] \\ \times \Theta \left(p_F - \frac{m}{\hbar k} \left| \hbar \omega - \frac{(\hbar k)^2}{2m} \right| \right) \\ - \frac{m}{2\pi k\hbar^3} \left[p_F^2 - \left(\frac{m}{\hbar k} \left(\hbar \omega + \frac{(\hbar k)^2}{2m} \right) \right)^2 \right] \\ \times \Theta \left(p_F - \frac{m}{\hbar k} \left| \hbar \omega + \frac{(\hbar k)^2}{2m} \right| \right)$$
(37)

results. The Heaviside step function imposes the constraint

$$\frac{(\hbar k)^2}{2m} - \hbar k v_F \le \omega \le \frac{(\hbar k)^2}{2m} + \hbar k v_F \tag{38}$$

for the first term and

$$0 \le \omega \le hbarkv_F - \frac{(\hbar k)^2}{2m}$$
(39)

for the second. For $\omega \ge 0$, the restrictions are represented graphically in Fig.(1.2) with ω_{\pm} = $\frac{(\hbar k)^2}{2m} \pm \hbar k v_F.$

Because the range of ω for the first term in Eq.(37) exceeds that for the second, we consider three separate cases corresponding to

a) both terms contributing, b)only the first, and c)neither: Case a) $0 \le \omega \le \hbar k v_F - \frac{(\hbar k)^2}{2m}$

$$\mathbf{I}_{\omega} - \mathbf{I}_{-\omega} = n_e S_0(\mathbf{k}, \omega) = \frac{m}{2\pi k \hbar^3} \left[p_F^2 - \left(\frac{m}{\hbar k} \left(\hbar \omega - \frac{(\hbar k)^2}{2m}\right)\right)^2 - \left[p_F^2 - \left(\frac{m}{\hbar k} \left(\hbar \omega + \frac{(\hbar k)^2}{2m}\right)\right)^2 \right] \right]$$
(40)

$$\Rightarrow n_e S_0(\mathbf{k},\omega) = \frac{m^2 \omega}{\pi \hbar^2 k}; \tag{41}$$

Kapil Adhikari

Case b) $\hbar k v_F - \frac{(\hbar k)^2}{2m} \le \omega \le \frac{(\hbar k)^2}{2m} + \hbar k v_F$

$$\Rightarrow n_e S_0(\mathbf{k},\omega) = \frac{m}{2\pi k\hbar^3} \left[p_F^2 - \left(\frac{m}{\hbar k} \left(\hbar\omega - \frac{(\hbar k)^2}{2m}\right)\right)^2 \right]; \tag{42}$$

Case c) $\hbar \omega \ge \frac{(\hbar k)^2}{2m} + \hbar k v_F$

$$\Rightarrow n_e S_0(\mathbf{k},\omega) = 0. \tag{43}$$

Figure (1.2) contains the composite graph for all three cases.

At finite temperature, an explicit expression can also be obtained for $n_e S_0(\mathbf{k}, \omega)$. We simply need to compute \mathbf{I}_{ω} and then let $\omega \to -\omega$.



Figure 2: Frequency range for the zero-temperature structure function.



Figure 3: Zero-temperature function as predicted from Eqs. (41)-(43)

Froom Eq.(34), we have that

$$\mathbf{I}_{\omega} = \frac{m}{\pi k \hbar^3} \int_{\frac{1}{2\hbar k} \left| 2m\hbar\omega - k^2\hbar^2 \right|}^{p_F} \frac{pdp}{e^{\beta(\epsilon_{\mathbf{p}}-\mu)} + 1}$$
$$= \frac{m^2}{\beta \pi k \hbar^3} \int_{a}^{p_F} \frac{\beta p}{m} dp \frac{1}{e^{\beta(\epsilon_{\mathbf{p}}+)} + 1}$$
$$= \frac{m^2}{\beta \pi k \hbar^3} \int_{\frac{\beta a^2}{2m}}^{\frac{\beta p_F^2}{2m}} \frac{dx}{e^{x-\beta\mu} + 1}.$$
(44)

With the help of the integral

$$\int \frac{dx}{1+be^{cx}} = \frac{1}{\alpha c} \Big[cx - \ln(\alpha + be^{cx}) \Big],\tag{45}$$

which implies that

$$\mathbf{I}_{\omega} = \frac{m^2}{\beta \pi \hbar^3 k} \bigg[x - \ln \big(1 + e^{x - \beta \mu} \big) \bigg]_{\frac{\beta a^2}{2m}}^{\frac{\beta p_F^2}{2m}},\tag{46}$$

we obtain the final expression for the temperature-dependent structure

$$(1 - e^{\beta\hbar\omega})n_e S_0(\mathbf{k},\omega) = \mathbf{I}_{\omega} - \mathbf{I}_{\omega} = \frac{m^2}{\beta\pi\hbar^3 k} \left[\beta\hbar\omega + \ln\left[\frac{1 + exp\left(\beta\left(\frac{1}{2m}\left(\frac{m\hbar\omega}{k}\frac{\hbar k}{2}\right)^2 - \mu\right)\right)}{1 + exp\left(\beta\left(\frac{1}{2m}\left(\frac{m\hbar\omega}{k} + \frac{\hbar k}{2}\right)^2 - \mu\right)\right)}\right] \right]$$

. In the limit of zero temperature, we obtain the expression previously derived at T = 0.

1.3 Dielectric Function

We turn now to the calculation of the dielectric-response function, $\epsilon(\mathbf{k}, \omega) = 1 - 4\pi e^2 \chi_{SC}(\mathbf{k}, \omega)/k^2$, where the screening function at the RPA level,

$$\chi_{SC}(\mathbf{k},\omega) = \lim_{\eta \to 0} \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi\hbar} \frac{n_e S_0(\mathbf{k},\omega')(1-e^{-\beta\hbar\omega'})}{\omega-\omega'+i\eta},$$
(47)

is a convolution of the structure function. In the limit that $\eta \to 0$, the screening function will acquire real and imaginary parts through

$$\lim_{\eta \to 0} \frac{1}{\omega - \omega' + i\eta} = P \frac{1}{\omega - \omega'} - i\pi \delta(\omega' - \omega).$$
(48)

Kapil Adhikari

The corresponding real $(1 + \epsilon_R(\mathbf{k}, \omega))$ and imaginary (ϵ_I) parts of the dielectric function are

$$1 + \epsilon_R(\mathbf{k}, \omega) = 1 - \frac{4\pi e^2}{k^2} P \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi\hbar} \frac{n_e S_0(\mathbf{k}, \omega')(1 - e^{-\beta\hbar\omega'})}{(\omega - \omega')}$$
(49)

and

$$e_I = \frac{2\pi e^2}{k^2 \hbar} n_e S_0(\mathbf{k}, \omega) (1 - e^{-\beta \hbar \omega}), \qquad (50)$$

respectively. In the limit of zero temperature, $S_0(\mathbf{k}, \omega)$ is linear in frequency and, hence, ϵ_l is an odd function of frequency.

The real and imaginary parts of the dielectric function are related as a result of the causal nature of the response to the test charge. From the definition of ϵ_R and ϵ_I , it follows immediately that

$$\epsilon_R = \frac{1}{\pi} P \int_{-\infty}^{\infty} \frac{d\omega' \epsilon_I(\mathbf{k}, \omega')}{\omega' - \omega}$$
(51)

and

$$\epsilon_I = \frac{-P}{\pi} \int_{-\infty}^{\infty} \frac{d\omega' \epsilon_R(\mathbf{k}, \omega')}{\omega' - \omega}.$$
(52)

These relationships are known as the *Kramers-Kronig relationships*.Relationships of this sort are true in general for any complex function that is analytic in either the upper- or lower-half planes. In the context of linear-response theory, they stem fundamentally from the causal nature of the response to the time-dependent perturbation.

Lindhard has shown that at T = 0, ϵ_R is given by

$$\epsilon_{R} = \frac{k_{TF}^{2}}{k^{2}} \left\{ \frac{1}{2} + \frac{k_{F}}{4k} \left[\left\{ 1 - \frac{(\omega - \frac{\hbar k^{2}}{2m})^{2}}{k^{2} v_{F}^{2}} \right\} \ln \left| \frac{\omega - kv_{F} - \frac{\hbar k^{2}}{2m}}{\omega + kv_{F} - \frac{\hbar k^{2}}{2m}} \right| + \left\{ 1 - \frac{(\omega + \frac{\hbar ka^{2}}{2m})^{2}}{k^{2} v_{F}^{2}} \right\} \ln \left| \frac{\omega + kv_{F} + \frac{\hbar k^{2}}{2m}}{\omega - kv_{F} + \frac{\hbar k^{2}}{2m}} \right| \right\}$$
(53)



Figure 4: Real (ε_R) and imaginary (ε_I) parts of the dielectric function at T = 0.

Note first that this function is independent of the sign of ω . Hence, its parity is opposite that of ϵ_I . The general frequency dependence of the dielectric function is shown in Fig.(1.3). The large value of ϵ_R for $\omega \to 0$ indicates that the static screening is large. Another feature of the dielectric-response function is that $\epsilon(\mathbf{k}, \omega) = 0$ at the plasma frequency. The poles of $\epsilon^{-1}(\mathbf{k}, \omega)$ occur at the excitation frequencies of the electron gas. Recall that this is precisely the result we derived previously in the context of a small k and large ω expansion for the dielectric function. When $\epsilon(\mathbf{k}, \omega) = 0$, fluctuations in the electron density diverge as a result of the collective nature of plasma oscillations. At this point, the whole theory we have formulated breaks down, because we assumed that the electron density was a slowly varying function of the perturbing field. Let us investigate the behaviour of $\epsilon(\mathbf{k}, \omega)$ for small ω . Setting $\omega = 0$ in our expression for ϵ_R results in

$$\epsilon(x,\omega=0) = 1 + \epsilon_R(x,\omega=0) = 1 + \frac{k_{TF}^2}{k^2} \left[\frac{1}{2} + \frac{1-x^2}{4x} \ln \left| \frac{1+x}{1-x} \right| \right],$$
(54)

the dielectric function in the static limit with $x = k/2k_F$. The x = 0 limit of $\epsilon(x, \omega = 0) = 1 + k_{TF}^2/k^2$ is exactly the Thomas-Fermi approximation to the screening of a positive charge at the origin. As in the Thomas-Fermi case, we can construct the spatial potential that results from this kind of screening effect. To do so, we use the equation for the effective field $U_{eff}(k, \omega) = \epsilon^{-1}(\mathbf{k}, \omega)U(\mathbf{k}, \omega)$. For an electron gas, $U(\mathbf{k}, \omega = 0) = 4\pi e^2/k^2$. If we use our expression for $\epsilon(\mathbf{k}, \omega = 0)$, we find that

$$\phi_{eff}(\mathbf{r}) = 4\pi e \int \frac{d\mathbf{k}}{(2\pi)^3} \frac{e^{-i\mathbf{k}\cdot\mathbf{r}}}{k^2 + k_{TF}^2 Q(\mathbf{k})}$$
(55)

is the spatial dependence of the effective potential, where $Q(\mathbf{k})$ denotes the bracketed term in Eq.(55). When $k = 2k_F$, $Q(\mathbf{k})$ is logarithmically divergent. This divergence yields a contribution to the electrostatic potential of the form

$$\phi_{eff} \sim \frac{\cos 2k_F r}{r^3},\tag{56}$$

as $r \to \infty$. This oscillatory behavior of the electrostatic potential is a consequence solely of screening and is known as a **Friedel oscillation**. At long distances, then, we find that the charge is not sufficiently screened to give rise to the $e^{-k_{TF}r}/\mathbf{r}$ of Thomas-Fermi theory. Algebraic decay of the electrostatic potential signifies that a localized external charge affects the charge density everywhere in the electron gas. Kohn was first to argue that this slow decay of the screened electrostatic potential arises from the sharpness of the Fermi surface. This effect shows up in the phonon spectrum of a metal for excitations with net momentum transfer $k \ge 2k_F$. He also pointed out with Luttinger that the negative contribution from ϕ_{eff} gives rise to a superconducting instability in an electron gas at T = 0. This observation is significant because it illustrates that if left alone, an electron gas with bare repulsive interactions can become superconducting without the assistance of phonons.
