Longitudinal Response Functions in the Random Phase Approximation

The Random Phase Approximation is a scheme with which to treat electron-electron interaction in an electron gas. The procedure ultimately gives us the screening due to electron-electron interaction self-consistently, which is measured by the quantity $\epsilon(\vec{q},\omega)$, the dielectric function.

Let us consider the electron gas with a real time-dependent perturbation of the form:

$$\delta U(\vec{r}, t) = \lim_{\alpha\to 0}\left(U e^{i\vec{q}\cdot\vec{r}} e^{-i\omega t} e^{\alpha t} + U e^{-i\vec{q}\cdot\vec{r}} e^{i\omega t} e^{\alpha t}\right) \tag{1}$$

Time dependent perturbation theory up to first order gives (cf. Notes on Scattering, Linear Response and the Dielectric Function):

Link to Notes on Scattering, Linear Response and the Dielectric Function

$$\begin{aligned} c^{(0)}(t) &= \delta_{f,i} \\ c^{(1)}(t) &= -\frac{i}{\hbar}\int_{-\infty}^{t} \langle f \mid \delta U(\vec{r}, t') \mid i\rangle e^{i\omega_{\text{fi}} t'} dt' \end{aligned} \tag{2}$$

where the $c_n^{(i)}(t)$ are the perturbative expansion coefficients for $\mid \psi,\ t = -\infty;\ t\rangle = \sum_n c_n(t)\, e^{-i E_n t/\hbar} \mid n\rangle$. The first order term above has assumed that the perturbation starts at $t = -\infty$, which is the lower limit on integral.

Now, since we have a free electron gas, we may take the initial state to be $\mid \vec{k}\rangle$ (where $\langle\vec{r} \mid \vec{k}\rangle = \frac{1}{\sqrt{V}} e^{i\vec{k}\cdot\vec{r}}$) and the final state to be $\left|\vec{k}'\right\rangle$. We can then write:

$$c^{(0)}(t) = \delta_{\vec{k},\vec{k}'} \tag{3}$$

$$\begin{aligned} c^{(1)}(t) &= -\frac{i}{\hbar V}\int_{-\infty}^{t} dt' \int d^3 r \int d^3 r'\, e^{-i\vec{k}'\cdot\vec{r}'} \langle\vec{r}' \mid \delta U(\vec{r}, t') \mid \vec{r}\rangle e^{i\vec{k}\cdot\vec{r}} e^{i\omega_{\text{fi}} t'} \\ &= \lim_{\alpha\to 0} -\frac{i}{\hbar V}\int_{-\infty}^{t} dt' \int d^3 r\, e^{-i\vec{k}'\cdot\vec{r}} U e^{i\vec{q}\cdot\vec{r}} e^{-i\omega t'} e^{\alpha t'} e^{i\vec{k}\cdot\vec{r}} e^{i\omega_{\text{fi}} t'} - \\ &\frac{i}{\hbar V}\int_{-\infty}^{t} dt' \int d^3 r\, e^{-i\vec{k}'\cdot\vec{r}} U e^{-i\vec{q}\cdot\vec{r}} e^{i\omega t'} e^{\alpha t'} e^{i\vec{k}\cdot\vec{r}} e^{i\omega_{\text{fi}} t'} \\ &= \lim_{\alpha\to 0} -\frac{i}{\hbar V}\int_{-\infty}^{t} dt'\, V\delta_{k',k+q}\, U e^{i(\omega_{\text{fi}}-\omega-i\alpha) t'} - \frac{i}{\hbar V}\int_{-\infty}^{t} dt'\, V\delta_{k',k-q}\, U e^{i(\omega_{\text{fi}}+\omega-i\alpha) t'} \\ &= \lim_{\alpha\to 0}\left\{-\frac{i}{\hbar}\delta_{k',k+q}\frac{U}{-i(\omega-\omega_{\text{fi}}+i\alpha)} - \frac{i}{\hbar}\delta_{k',k-q}\frac{U}{-i(-\omega-\omega_{\text{fi}}+i\alpha)}\right\} \\ &= \lim_{\alpha\to 0}\left\{\delta_{k',k+q}\frac{U/\hbar}{(\omega-\omega_{\text{fi}}+i\alpha)} + \delta_{k',k-q}\frac{U/\hbar}{(-\omega-\omega_{\text{fi}}+i\alpha)}\right\} \end{aligned} \tag{4}$$

Having obtained the expansion coefficients up to first order, we can write for the final state ket:

$$\begin{aligned} \mid f\rangle &= \sum_{k'} c_{k'} \left|\vec{k}'\right\rangle \\ &\approx \lim_{\alpha\to 0}\sum_{k'}\left(\delta_{\vec{k},\vec{k}'} + \delta_{k',k+q}\frac{U/\hbar}{(\omega-\omega_{\text{fi}}+i\alpha)} + \delta_{k',k-q}\frac{U/\hbar}{(-\omega-\omega_{\text{fi}}+i\alpha)}\right)\left|\vec{k}'\right\rangle \end{aligned}$$

$$= \left|\vec{k}'\right\rangle + \lim_{\alpha\to 0} \frac{U}{(-E_{\text{fi}} + \hbar\omega + i\alpha)} \left|\vec{k}+\vec{q}\right\rangle + \lim_{\alpha\to 0} \frac{U/\hbar}{(-\hbar\omega - E_{\text{fi}} + i\alpha)} \left|\vec{k}-\vec{q}\right\rangle$$

$$= \left|\vec{k}'\right\rangle + \lim_{\alpha\to 0} \frac{U}{\left(E(\vec{k}) - E(\vec{k}+\vec{q}) + \hbar\omega + i\alpha\right)} \left|\vec{k}+\vec{q}\right\rangle + \lim_{\alpha\to 0} \frac{U}{\left(E(\vec{k}) - E(\vec{k}-\vec{q}) - \hbar\omega + i\alpha\right)} \left|\vec{k}-\vec{q}\right\rangle$$

We can therefore readily see that the final state is a superposition of the intial state with the states $\left|\vec{k}+\vec{q}\right\rangle$ and $\left|\vec{k}-\vec{q}\right\rangle$ as we might expect. Using this final state ket, we can now calculate the induced charge density:

$$\begin{aligned} \delta\rho(\vec{r}, t) &= e \sum_{k\,\epsilon\,\text{occupied}} \{\langle f \mid f\rangle - \langle i \mid i\rangle\} \\ &= e \sum_{k\,\epsilon\,\text{occupied}} \left\{|\psi_k(\vec{r}, t)|^2 - \frac{1}{V}\right\} \end{aligned} \tag{6}$$

where $|\psi_k(\vec{r}, t)|^2 = \langle f \mid f\rangle$ and the sum is over all **occupied** states k. Now to evaluate the expression above, we drop terms of order U^2(or equivalently $|b|^2$) so that we can write:

$$\delta\rho(\vec{r}, t) \approx e \sum_{k\,\epsilon\,\text{occupied}} \left\{\frac{1}{V} + \left(b_{k+q} + b^*{}_{k-q}\right)\frac{e^{i\vec{q}\cdot\vec{r}}}{V} + \left(b^*{}_{k+q} + b_{k-q}\right)\frac{e^{-i\vec{q}\cdot\vec{r}}}{V} - \frac{1}{V}\right\} \tag{7}$$

where $b_{k+q} = \lim_{\alpha\to 0} \frac{U}{\left(E(\vec{k})-E(\vec{k}+\vec{q})+\hbar\omega+i\alpha\right)}$. Therefore,

$$\delta\rho(\vec{r}, t) \approx \frac{e\,U}{V} \lim_{\alpha\to 0} \sum_{k\,\epsilon\,\text{occupied}} \left\{\left(\frac{1}{E(\vec{k}) - E(\vec{k}+\vec{q}) + \hbar\omega + i\alpha} + \frac{1}{E(\vec{k}) - E(\vec{k}-\vec{q}) - \hbar\omega - i\alpha}\right) e^{i\vec{q}\cdot\vec{r}} + c.c\right\} \tag{8}$$

For convenience, we now change the sum over all occupied states to a sum over **all** states using the Fermi-Dirac distribution, $f^0(\vec{k})$, as so:

$$\delta\rho(\vec{r}, t) \approx \frac{e\,U}{V} \lim_{\alpha\to 0} \sum_{k} \left\{\left(\frac{f^0(\vec{k})}{E(\vec{k}) - E(\vec{k}+\vec{q}) + \hbar\omega + i\alpha} + \frac{f^0(\vec{k})}{E(\vec{k}) - E(\vec{k}-\vec{q}) - \hbar\omega - i\alpha}\right) e^{i\vec{q}\cdot\vec{r}} + c.c\right\} \tag{9}$$

Now that we are summing over all k, we may change the sum in the second term from a sum over k to a sum over $k' = k - q$ so that:

$$\begin{aligned} \delta\rho(\vec{r}, t) &\approx \frac{e\,U}{V} \lim_{\alpha\to 0} \sum_{k} \left\{\left(\frac{f^0(\vec{k})}{E(\vec{k}) - E(\vec{k}+\vec{q}) + \hbar\omega + i\alpha} + \frac{f^0(\vec{k}+\vec{q})}{E(\vec{k}+\vec{q}) - E(\vec{k}) - \hbar\omega - i\alpha}\right) e^{i\vec{q}\cdot\vec{r}} + c.c\right\} \\ &= \frac{e\,U}{V} \lim_{\alpha\to 0} \sum_{k} \left\{\left(\frac{f^0(\vec{k}) - f^0(\vec{k}+\vec{q})}{E(\vec{k}) - E(\vec{k}+\vec{q}) - \hbar\omega + i\alpha}\right) e^{i\vec{q}\cdot\vec{r}} + c.c\right\} \end{aligned} \tag{10}$$

If we assume that the induced potential energy has the same wavelength and frequency response as the induced charge (which Fourier analysis ensures), then we may write:

$$\vec{\nabla}^2 \phi(\vec{r}, t) = \frac{-e\,\delta\rho(\vec{r}, t)}{\epsilon_0} \qquad \left(\text{with}\quad \phi(\vec{r}, t) \sim \phi\, e^{i\vec{q}\cdot\vec{r}}\, e^{-i\omega t}\, e^{\alpha t} + c.c.\right) \tag{11}$$

Equating Fourier components on each side, we can write:

$$\phi = \left(\frac{e^2}{\epsilon_0\,\vec{q}^2} \frac{1}{V} \lim_{\alpha\to 0} \sum_{k} \frac{f^0(\vec{k}) - f^0(\vec{k}+\vec{q})}{E(\vec{k}) - E(\vec{k}+\vec{q}) - \hbar\omega + i\alpha}\right) U \tag{12}$$

This expression gives the induced potential energy due a potential energy perturbation. However, the question arises: is the potential energy perturbation due solely to external potential or does is already include effects due to polarization of the electron gas? The answer is the latter. This is because the electron within the electron gas does not feel the potential of an external source, but feels the effective potential due to the external source plus the screening effects. Therefore, $\delta U(\vec{r}, t)$ is actually the total potential, which will now be referred to as $U_{\text{tot}}(\vec{r}, t)$. Thus, we need to include this effect self-consistently by writing:

$$U_{\text{tot}}(\vec{r}, t) = U_{\text{ext}}(\vec{r}, t) + \phi(\vec{r}, t) \qquad \left(\text{with} \quad U_{\text{ext}}(\vec{r}, t) \sim U_{\text{ext}}\, e^{i\,\vec{q}\cdot\vec{r}}\, e^{-i\omega t}\, e^{\alpha t} + c.c.\right)$$

$$= U_{\text{ext}} + \left(\frac{e^2}{\epsilon_0 \vec{q}^{\,2}} \frac{1}{V} \lim_{\alpha\to 0} \sum_k \frac{f^0(\vec{k}) - f^0(\vec{k}+\vec{q})}{E(\vec{k}) - E(\vec{k}+\vec{q}) - \hbar\omega + i\alpha}\right) U_{\text{tot}} \tag{13}$$

Hence we have the dielectric function from the relation:

$$U_{\text{tot}} = \frac{U_{\text{ext}}}{\epsilon(\vec{q}, \omega)} \qquad \text{with} \quad \boxed{\epsilon(\vec{q}, \omega) = 1 + \frac{e^2}{\epsilon_0 \vec{q}^{\,2}} \frac{1}{V} \lim_{\alpha\to 0} \sum_k \frac{f^0(\vec{k}) - f^0(\vec{k}+\vec{q})}{E(\vec{k}+\vec{q}) - E(\vec{k}) - \hbar\omega + i\alpha}} \tag{14}$$

The fact that we have obtained the dielectric function self-consistently raises the following question. Since we have used an external potential and calculated the response of the electron gas to that perturbation, does it apply to the electron gas itself since we have separated one electron from the others? A heuristic answer can be seen from the following argument. Suppose we have an electron-electron interaction term in the Hamiltonian of the form:

$$H_I = \frac{1}{2V} \sum_q U_{\boldsymbol{q}}\, \rho_{\boldsymbol{q}}\, \rho_{-\boldsymbol{q}} \tag{15}$$

where $U_{\boldsymbol{q}} = e^2 / (\epsilon_0 q^2)$. Using a mean-field approximation, we can generally make the substitution $\rho_{\mathbf{q}}\, \rho_{-\mathbf{q}} \to \langle \rho_{\mathbf{q}} \rangle\, \rho_{-\mathbf{q}} + \rho_{\mathbf{q}}\, \langle \rho_{-\mathbf{q}} \rangle$, which turns the interacting term in the Hamiltonian into:

$$H_I = \frac{1}{V} \sum_q V_{\boldsymbol{q}}\, \rho_{\boldsymbol{q}} \tag{16}$$

where $V_{\boldsymbol{q}} = U_q \langle \rho_q \rangle$. This shows that the mean-field approximation gives a term that looks identical to an external potential and each electron responds to the average charge density i.e. the interacting electrons give rise to an "external-looking" potential. In a similar sense, the Random Phase Approximation gives an effective interaction implying that the electron gas can actually screen itself.

The Susceptibility and Polarization Function

For many perturbations that do not disturb the system significantly, we can safely assume that the system of interest (usually a solid for the purposes presented here), gives rise to a response that is linear with respect to the perturbing probe. This can be formulated as so **for a translational invariant system** (which is what concerns us here):

$$\begin{aligned} \delta n(\vec{r}, t) &= \int\!\!\int \chi(\vec{r} - \vec{r}\,', t - t')\, U_{\text{ext}}(\vec{r}\,', t')\, d^3 r'\, dt' \\ \delta n(\vec{r}, t) &= \int\!\!\int \Pi(\vec{r} - \vec{r}\,', t - t')\, U_{\text{tot}}(\vec{r}\,', t')\, d^3 r'\, dt' \\ U_{\text{ext}}(\vec{r}, t) &= \int\!\!\int \epsilon(\vec{r} - \vec{r}\,', t - t')\, U_{\text{tot}}(\vec{r}\,', t')\, d^3 r'\, dt' \end{aligned} \tag{17}$$

Here the susceptibility, $\chi(\vec{r} - \vec{r}\,', t - t')$, is the density response function that includes screening effects while the polarization function, $\Pi(\vec{r} - \vec{r}\,', t - t')$, does **not** include screening effects. Also, $\delta n(\vec{r}, t) = \delta\rho(\vec{r}, t) / e$ is the induced **number density**. We can Fourier transform the equations with the following convention:

$$\begin{aligned} f(\vec{r}, t) &= \frac{1}{V} \int \tilde{F}(\vec{q}, t)\, e^{i \vec{q} \cdot \vec{r}}\, d^3 q \\ \tilde{F}(\vec{q}, t) &= \int f(\vec{r}, t)\, e^{-i \vec{q} \cdot \vec{r}}\, d^3 r\, dt \\ f(\vec{r}, t) &= \frac{1}{2\pi} \int \tilde{F}(\vec{r}, \omega)\, e^{-i \omega t}\, d\omega \\ \tilde{F}(\vec{r}, \omega) &= \int f(\vec{r}, t)\, e^{i \omega t}\, dt \end{aligned} \tag{18}$$

to write:

$$\begin{aligned} \delta n(\vec{q}, \omega) &= \chi(\vec{q}, \omega)\, U_{\text{ext}}(\vec{q}, \omega) \\ \delta n(\vec{q}, \omega) &= \Pi(\vec{q}, \omega)\, U_{\text{tot}}(\vec{q}, \omega) \\ U_{\text{ext}}(\vec{q}, \omega) &= \epsilon(\vec{q}, \omega)\, U_{\text{tot}}(\vec{q}, \omega) \end{aligned} \tag{19}$$

Using the Poisson equation, we may write:

$$\begin{aligned} &\vec{\nabla}^2 \phi(\vec{r}, t) = \frac{-e\, \delta\rho(\vec{r}, t)}{\epsilon_0} \qquad \text{and in Fourier Space :} \\ &-\vec{q}^{\,2} \phi(\vec{q}, \omega) = \frac{-e\, \delta\rho(\vec{q}, \omega)}{\epsilon_0} = \frac{-e^2\, \delta n(\vec{q}, \omega)}{\epsilon_0} \\ &\text{OR :} \quad \phi(\vec{q}, \omega) = \frac{e^2\, \delta n(\vec{q}, \omega)}{\epsilon_0\, \vec{q}^{\,2}} \equiv V(q)\, \delta n(\vec{q}, \omega) \end{aligned} \tag{20}$$

Using this relation, we may write:

$$\delta n(\vec{q}, \omega) = \Pi(\vec{q}, \omega)\, (U_{\text{ext}}(\vec{q}, \omega) + V(q)\, \delta n(\vec{q}, \omega)) \tag{21}$$

or more familiarly:

$$\delta n(\vec{q}, \omega) = \frac{U_{\text{ext}}(\vec{q}, \omega)\, \Pi(\vec{q}, \omega)}{1 - V(q)\, \Pi(\vec{q}, \omega)} \tag{22}$$

and using equation (17) above, we can equate:

$$\chi(\vec{q}, \omega) = \frac{\Pi(\vec{q}, \omega)}{1 - V(q)\, \Pi(\vec{q}, \omega)} \tag{23}$$

Dividing the first two of the equations in (17) we can also get that:

$$\boxed{\frac{U_{\text{tot}}(\vec{q}, \omega)}{U_{\text{ext}}(\vec{q}, \omega)} = \frac{\chi(\vec{q}, \omega)}{\Pi(\vec{q}, \omega)} = \frac{1}{1 - V(q)\, \Pi(\vec{q}, \omega)} = \frac{1}{\epsilon(\vec{q}, \omega)} = 1 + V(q)\, \chi(\vec{q}, \omega)} \tag{24}$$

Our expression above for the dielectric function subsequently determines the other linear response functions as well. So far, equation (24) is exact within the linear response regime. The calculation in the previous section gives us a way to calculate these response functions. We can therefore conclude that within the Random Phase Approximation:

$$\Pi(\vec{q}, \omega) = \frac{1}{V} \lim_{\alpha \to 0} \sum_k \frac{f^0(\vec{k}+\vec{q}) - f^0(\vec{k})}{E(\vec{k}+\vec{q}) - E(\vec{k}) - \hbar\omega + i\alpha} \tag{25}$$

which is the Lindhard expression for the polarization function.

Note: *It is worth noting that within the Random Phase Approximation, the polarization function is often denoted by $\Pi^0(\vec{q}, \omega)$ or $\Pi^{RPA}(\vec{q}, \omega)$ to explicitly dissociate it from the exact polarization funcion $\Pi(\vec{q}, \omega)$.*

Density-Density Correlations: Relation to Susceptibility and Polarization Functions

There is a slightly different and more general method by which to obtain the polarization function above which does not only apply to the electron gas. The reason that this method was not presented from the beginning is that the above method provides one with a more intuitive grasp of the essential physics. However, it does not generalize as easily. The following method uses a standard result of linear response theory that says that correlation functions are a directly related to susceptibilties (cf. Notes on Quantum Mechanical Linear Response).

Link to Notes on Quantum Mechanical Linear Response

Suppose we have a perturbation of the form $\int n(\vec{x}', t')\, U_{\text{ext}}(\vec{x}', t')\, d^3x'$, where the perturbation couples to the number density in the sample. This would be the case for an incoming electron scattering from a solid, for example, where $U_{\text{ext}}(\vec{x}', t')$ would be equal to $\int d^3x \frac{e^2\, n(\vec{x})}{4\pi\epsilon_0 |\vec{x}-\vec{x}'|}$. From this perturbation, we can read off the susceptibility from the relation:

$$\delta n(\vec{x}, t) = \frac{i}{\hbar} \int_{-\infty}^{t} dt' \int d^3x'\, U_{\text{ext}}(\vec{x}', t') \langle [n(\vec{x}', t'),\ n(\vec{x}, t)] \rangle \tag{26}$$

Comparing this equation to equation (17) above, we can write:

$$\chi(\vec{x}, \vec{x}'; t-t') = -\frac{i}{\hbar} \Theta(t-t') \langle [n(\vec{x}, t-t'),\ n(\vec{x}', 0)] \rangle \tag{27}$$

where we have used the fact that the susceptibility must be time-translationally invariant. To compare with the relations above, we require the Fourier Transform of the susceptibility. We can therefore write:

$$\chi(\vec{x}, \vec{x}'; \omega) = -\frac{i}{\hbar} \int_0^{\infty} d\tau\, e^{i\omega\tau} \langle [n(\vec{x}, \tau),\ n(\vec{x}', 0)] \rangle \tag{28}$$

Now we insert a complete set of states, and we use the fact that $n(\vec{x}, \tau) = e^{i H_0 t/\hbar}\, n(\vec{x})\, e^{-i H_0 t/\hbar}$ in going from the interaction representation to the Schroedinger representation. Equation (28) then becomes:

$$\chi(\vec{x}, \vec{x}', \omega) = -\frac{i}{\hbar} \int_0^{\infty} d\tau\, e^{i\omega\tau} \sum_i e^{-i(E_i-E_0)\tau/\hbar} \langle G \mid n(\vec{x}) \mid i \rangle \langle i \mid n(\vec{x}') \mid G \rangle - e^{i(E_i-E_0)\tau/\hbar} \langle G \mid n(\vec{x}') \mid i \rangle \langle i \mid n(\vec{x}) \mid G \rangle \tag{29}$$

where we have assumed zero temperature and $|G\rangle$ and $|i\rangle$ are the ground state and intermediate state respectively. To explicitly evaluate the integral above, we need to regularize the integral by adding $\lim_{\alpha\to 0} = e^{-\alpha t}$ and we get that:

$$\lim_{\alpha\to 0} \int_0^{\infty} d\tau\, e^{i\omega\tau}\, e^{-i(E_i-E_0)\tau/\hbar}\, e^{-\alpha\tau} = \frac{i}{\omega + E_0/\hbar - E_i/\hbar + i\alpha} \tag{30}$$

which gives us for the susceptibility:

$$\chi(\vec{x}, \vec{x}', \omega) = \lim_{\alpha\to 0} \sum_i \left(\frac{\langle G \mid n(\vec{x}) \mid i\rangle \langle i \mid n(\vec{x}') \mid G\rangle}{\hbar\omega + E_0 - E_i + i\alpha} - \frac{\langle G \mid n(\vec{x}') \mid i\rangle \langle i \mid n(\vec{x}) \mid G\rangle}{\hbar\omega + E_i - E_0 + i\alpha} \right) \tag{31}$$

Lastly, we need to Fourier Transform the spatial variables:

$$\chi(\vec{x} - \vec{x}', \omega) = \frac{1}{V} \int \lim_{\alpha\to 0} \sum_i \left(\frac{\langle G \mid n(\vec{q}) \mid i\rangle \langle i \mid n(-\vec{q}) \mid G\rangle}{\hbar\omega + E_0 - E_i + i\alpha} - \frac{\langle G \mid n(-\vec{q}) \mid i\rangle \langle i \mid n(\vec{q}) \mid G\rangle}{\hbar\omega + E_i - E_0 + i\alpha} \right) e^{i\vec{q}\cdot(\vec{x}-\vec{x}')}\, d^3 q \tag{32}$$

where we have assumed translational invariance in space for simplicity. We can read off the Fourier Transformed susceptibility to get:

$$\chi(\vec{q}, \omega) = \lim_{\alpha\to 0} \frac{1}{V} \sum_i \left(\frac{\left|\langle i \mid n^\dagger(\vec{q}) \mid G\rangle\right|^2}{\hbar\omega + E_0 - E_i + i\alpha} - \frac{\left|\langle i \mid n(\vec{q}) \mid G\rangle\right|^2}{\hbar\omega + E_i - E_0 + i\alpha} \right) \tag{33}$$

We should now note that had we used $U_{\text{tot}}(\vec{x}', t')$ for $U_{\text{ext}}(\vec{x}', t')$, we would have obtained an identical looking expression for the polarization function $\Pi(\vec{q}, \omega)$. Therefore, we can also write:

$$\begin{aligned} \Pi(\vec{q}, \omega) &= \lim_{\alpha\to 0} \frac{1}{V} \sum_i \left(\frac{\left|\langle i \mid n^\dagger(\vec{q}) \mid G\rangle\right|^2}{\hbar\omega + E_0 - E_i + i\alpha} - \frac{\left|\langle i \mid n(\vec{q}) \mid G\rangle\right|^2}{\hbar\omega + E_i - E_0 + i\alpha} \right) \\ &\overset{\text{TRI}}{=} \lim_{\alpha\to 0} \frac{1}{V} \sum_i \left|\langle i \mid n^\dagger(\vec{q}) \mid G\rangle\right|^2 \left(\frac{1}{\hbar\omega + E_0 - E_i + i\alpha} - \frac{1}{\hbar\omega + E_i - E_0 + i\alpha} \right) \end{aligned} \tag{34}$$

where the last equality holds true if the system is time-reversal invariant. There is a **critical** difference between the expressions of the polarization function and the susceptibility! The matrix elements in the expression for the susceptibility, $\chi(\vec{q}, \omega)$, would need to be evaluated between the **full interacting states (bare electrons)** whereas for the polarization function, $\Pi(\vec{q}, \omega)$, we can evaluate it between the **weakly-interacting states (quasi-particles)**. The expression here for the polarization function enables us to evaluate the matrix elements for different band structures and does not limit the calculation to the electron gas. However, we should evaluate it for the case of free electrons to see that we obtain the same expression as in equation (25). First, the density operator for free electrons in second quantization can be written as:

$$n^\dagger(\vec{q}) = \sum_k c_{k+q}^\dagger c_k \qquad \text{and} \qquad n(\vec{q}) = \sum_k c_{k-q}^\dagger c_k \tag{35}$$

so that the matrix element can be written as:

$$\langle i \mid n^\dagger(\vec{q}) \mid G\rangle = \sqrt{f^0(\vec{k})\left(1 - f^0(\vec{k} + \vec{q})\right)} \qquad \text{and} \qquad \left|\langle i \mid n^\dagger(\vec{q}) \mid G\rangle\right|^2 = f^0(\vec{k})\left(1 - f^0(\vec{k} + \vec{q})\right) \tag{36}$$

This expresses the fact that the ground state has probability $f^0(\vec{k})$ for the state $\vec{k}$ to be occupied and $1 - f^0(\vec{k} + \vec{q})$ for the state $\vec{k} + \vec{q}$ to be unoccupied. We now substitute this into the polarization function to obtain:

$$\begin{aligned} \Pi(\vec{q}, \omega) &= \lim_{\alpha\to 0} \frac{1}{V} \sum_k \left(\frac{f^0(\vec{k})\left(1 - f^0(\vec{k} + \vec{q})\right)}{\hbar\omega + E(\vec{k}) - E(\vec{k} + \vec{q}) + i\alpha} - \frac{f^0(\vec{k})\left(1 - f^0(\vec{k} - \vec{q})\right)}{\hbar\omega + E(\vec{k} - \vec{q}) - E(\vec{k}) + i\alpha} \right) \\ &= \lim_{\alpha\to 0} \frac{1}{V} \sum_k \left(\frac{f^0(\vec{k} + \vec{q}) - f^0(\vec{k})}{E(\vec{k} + \vec{q}) - E(\vec{k}) - \hbar\omega + i\alpha} \right) \end{aligned} \tag{37}$$

$$= \lim_{\alpha\to 0} \frac{1}{V} \sum_k f^0(\vec{k})\left(1 - f^0(\vec{k}+\vec{q})\right)\left(\frac{1}{E(\vec{k}) - E(\vec{k}+\vec{q}) + \hbar\omega + i\alpha} - \frac{1}{E(\vec{k}+\vec{q}) - E(\vec{k}) + \hbar\omega + i\alpha}\right)$$

where the second equality is the same as equation (25) above and the third equality uses equation (34).

Static Screening (the $\omega \ll v_F\, q$)

Static Screening in 3D

To gain further physical insight into the Lindhard expression and what it means for the solid, it is useful to examine certain limits. The first limit we will examine is the $\omega \ll v_F\, q$ limit i.e. the static limit. This is particularly useful in that it gives the screening in the absence of movement. For example, it would give us how an impurity in the metal would be screened. To obtain this expression we use the standard trick in going from a sum to an integral, $\sum_k \to 2 \frac{V}{(2\pi)^3} \int d^3k$, to write:

$$\Pi(\vec{q}, \omega) = \frac{2}{(2\pi)^3} \int d^3k \left(\frac{f^0(\vec{k}+\vec{q}) - f^0(\vec{k})}{E(\vec{k}+\vec{q}) - E(\vec{k})}\right) \tag{38}$$

where the factor of two comes from summing over the spin states. If $\vec{q}$ is small, we can write for the numerator and denominator respectively:

$$f^0(\vec{k}+\vec{q}) - f^0(\vec{k}) \approx \frac{\partial f^0(k)}{\partial E} \vec{\nabla}_{\vec{k}} E(\vec{k})\cdot\vec{q} \qquad \text{and} \qquad E(\vec{k}+\vec{q}) - E(\vec{k}) \approx \vec{\nabla}_{\vec{k}} E(\vec{k})\cdot\vec{q} \tag{39}$$

It is worth noting that for small $\vec{q}$, $\vec{\nabla}_{\vec{k}} E(\vec{k})\cdot\vec{q} \approx v_F\, \hat{k}\cdot\vec{q}$, which is why we take the limit $\omega \ll v_F\, q$. Now we can write for the polarization function, knowing that $f^0(\vec{k})$ is actually $f^0(E(\vec{k}))$:

$$\Pi(\vec{q}, \omega) = \frac{2}{(2\pi)^3} \int d^3k \left(\frac{\frac{\partial f^0(k)}{\partial E} \vec{\nabla}_{\vec{k}} E(\vec{k})\cdot\vec{q}}{\vec{\nabla}_{\vec{k}} E(\vec{k})\cdot\vec{q}}\right) = \int dE\, \rho(E) \frac{\partial f^0(\vec{k})}{\partial E} \tag{40}$$

where $\rho(E)$ is the density of single-particle states for both spins. Then noticing that the $\partial f^0(\vec{k})/\partial E$ factor is sharply peaked at the Fermi energy, we can write:

$$\Pi(\vec{q}, \omega) = -\rho_{3d}(E_F) = -\frac{\sqrt{2 m^3 E_F}}{\pi^2 \hbar^3} = -\frac{m k_F}{\pi^2 \hbar^2} \qquad \text{and} \qquad \epsilon(\vec{q}, \omega) = 1 + \frac{q_{TF}^2}{\vec{q}^2} \tag{41}$$

where $q_{TF} = \sqrt{e^2 \rho_{3d}(E_F)/\epsilon_0}$ is the Thomas-Fermi wavevector. Now we can write that the external potential is screened by this factor giving:

$$U_{tot}(\vec{q}, \omega) = \frac{e^2}{\epsilon_0(\vec{q}^2 + q_{TF}^2)} \qquad \text{or after Fourier Transforming} \qquad U_{tot}(\vec{r}, t) = \frac{e^2}{4\pi\epsilon_0} \frac{1}{r} e^{-q_{TF} r} \tag{42}$$

and we can readily see that as $\vec{q} \to 0$, we no longer have the divergence at long wavelength (or long distances). The interaction is effectively damped after a couple Thomas-Fermi lengths, $1/q_{TF}$, which is usually on the order of half a lattice spacing (e.g. for copper, $q_{TF} \approx 0.55$ Å^{-1}).

Static Screening in 2D

The extension to two dimensions is quite straightforward in the case of Thomas-Fermi screening. The essential formulae stay the same besides a dimensional reduction. We get for the polarization and dielectric functions respectively:

$$\Pi(\vec{q},\,\omega) \;=\; -\rho_{2\,d}(E_F) \;=\; \frac{-m}{\pi\,\hbar^2} \qquad \text{and} \qquad \epsilon(\vec{q},\,\omega) \;=\; 1 \;+\; \frac{\kappa_{\text{TF}}}{\vec{q}} \tag{43}$$

where we now must use the 2D Coulomb interaction [a] $V(q) \;=\; \frac{e^2}{2\,\epsilon_0\,q}$ to obtain the dielectric function. The screening length is usually smaller in 2D, but in real space, the potential falls off as $\sim r^{-3}$, so we cannot immediately deduce whether the screening effects are more important in 3D or 2D.

Static Screening in 3D: the expression for arbitrary wavevector and the Kohn Anomaly

The expression above in the 3D case is taken in the limit of small $\vec{q}$. While this served as an excellent example for demonstrating the effect known as Thomas-Fermi screening, there is a more general expression for the polarization function for all $\vec{q}$ that contains physics beyond aforementioned approximation. For ease of calculation, $T \;=\; 0$ is assumed throughout. We can then write for the polarization function, akin to equation (38):

$$\Pi(\vec{q},\,\omega) \;=\; \frac{2}{(2\,\pi)^3}\int d^3\,k\left(\frac{f^0(\vec{k}+\vec{q})-f^0(\vec{k})}{E(\vec{k}+\vec{q})-E(\vec{k})}\right) \tag{44}$$

We can simplify this by writing substituting for the second integral $k' \;=\; -(k+q)$ and then $k \;=\; -k'$ to write:

$$\Pi(\vec{q},\,\omega) \;=\; \frac{2}{(2\,\pi)^3}\int d^3\,k\,f^0(\vec{k})\left(\frac{1}{E(\vec{k})-E(\vec{k}+\vec{q})} - \frac{1}{E(\vec{k}+\vec{q})-E(\vec{k})}\right) \tag{45}$$

The integral is most easily evaluated in spherical coordinates, so we can write:

$$= \frac{-16\,\pi\,m}{(2\,\pi)^3\,\hbar^2}\int d(\cos\theta)\,k^2\,dk\left(\frac{\Theta(\vec{k}-k_F)}{2\,\vec{k}\cdot\vec{q}+\vec{q}^{\,2}}\right) \tag{46}$$

$$= \frac{-16\,\pi\,m}{(2\,\pi)^3\,\hbar^2}\int_{-1}^{1} d(\cos\theta)\int_0^{k_F} k^2\,dk\left(\frac{1}{2\,k\,q\cos\theta+\vec{q}^{\,2}}\right) \tag{47}$$

$$= \frac{-m}{\pi^2\,\hbar^2\,q}\int_0^{k_F} k\,\text{Ln}\left|\frac{q+2\,k}{q-2\,k}\right| dk \tag{48}$$

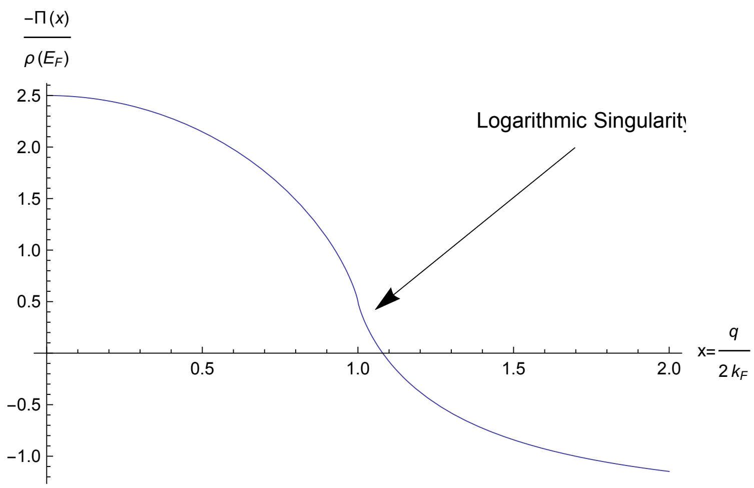
This integral can be readily evaluated to yield:

$$= \frac{-m\,k_F}{8\,\pi^2\,\hbar^2\,q}\left(4\,q+4\,k_F\left[1-\left(\frac{q}{2\,k_F}\right)^2\right]\text{Ln}\left|\frac{\frac{q}{2\,k_F}+1}{\frac{q}{2\,k_F}-1}\right|\right) \tag{49}$$

This expression can be written in terms of the density of states, $\rho_{3\,d}(E_F)$, as:

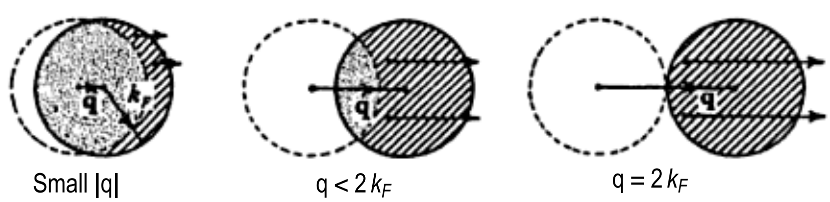
$$\Pi(\vec{q},\;\omega) \;=\; -\,\rho_{3\,d}(E_F)\left(\frac{1}{2}+\frac{1}{4\,x}\left[1-x^2\right]\text{Ln}\left|\frac{x+1}{x-1}\right|\right) \;\equiv\; -\,\rho_{3\,d}(E_F)\,F(x) \tag{50}$$

where $x \;=\; q\,/\,2\,k_F$. Therefore one can see that the Thomas-Fermi screening length now is a function of $\vec{q}$ unlike before. This expression is peculiar for what happens at $q \;=\; 2\,k_F$. There is a singularity at this wavevector and it can readily be seen that there is an abrupt change in the ability of the electrons to screen perturbations. The plot below to gives an idea of the singular nature of the above function.



Since this singularity also carries over to the dielectric function, and that is what measures screening, we can deduce that there will be a singularity in the screening at $q = 2\, k_F$ as well. This is further evidenced by the fact that the derivative of both $\Pi(\vec{q}, \omega)$ and $\epsilon(\vec{q}, \omega)$ diverge at this point, again indicating an abrupt change in screening.

An intuitive way of understanding the singularity that gives rise to the Kohn anomaly is by examining the polarization function and drawing the corresponding Fermi surfaces (see below). The polarization function contains a sum over $f(\vec{k} + \vec{q}) - f(\vec{k})$. Therefore, the state $|\vec{k}\rangle$ needs to be occupied and the state $|\vec{k} + \vec{q}\rangle$ need to be unoccupied or vice versa for the sum to have non-zero contribution. As $|\vec{q}|$ is increased, these regions expand so that the sum increases. Eventually, a critical value of $|\vec{q}| = q_c$ is reached where there is no longer any overlap of the two spheres. At this point, the functional form of the of the polarization function still changes because of the factor in the denominator, but the numerator has no new contributions. However, the contribution from the last few points before $|\vec{q}|$ reaches q_c is not large so that the singularity is not serious. This can be easily generalized to non-spherical Fermi surfaces. All that is needed is a critical $|\vec{q}|$ where the Fermi surfaces no longer overlap[1].



The next question that naturally arises is: **does this abrupt change in screening have any experimental consequences?** The answer is yes. We will examine a slightly oversimplified example, but one that extracts the essential points. Let us consider an ionic plasma, which is appropriate for modeling long wavelength longitudinal lattice vibrations. The equation of motion is therefore simple and we may write:

$$M \frac{d^2 \vec{x}}{d t^2} = \frac{-N Z^2 e^2 \vec{x}}{\epsilon_0} \tag{51}$$

Now, we must take into account the effect of the electrons. To take this into consideration, we notice that the electrons modify all external perturbations. Therefore, the electrons should modify the forces due to the polarization of the ionic plasma, in which case we must divide the right hand side of equation (51) by the dielectric function. We can therefore write:

$$M \frac{d^2 \vec{x}}{d t^2} = \frac{-N Z^2 e^2 \vec{x}}{\epsilon(\vec{q}, \omega) \epsilon_0} \tag{52}$$

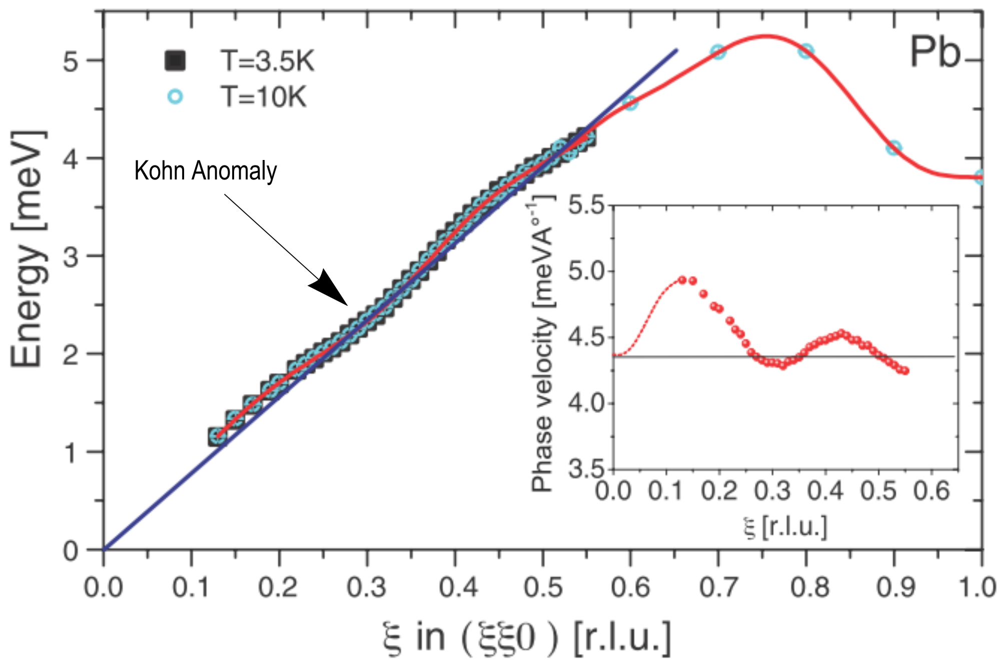
It is therefore easy to read off the frequency of vibration of the phonon and its renormalized value:

$$\nu_q{}^2 = \frac{\Omega_p{}^2}{\epsilon(\vec{q}, \omega)} \tag{53}$$

where $\Omega_p{}^2$ is the bare ionic plasma freqency. We can take the derivative on both sides yield:

$$\frac{d \nu_q}{d \vec{q}} = -\frac{\Omega_p}{2 \epsilon(\vec{q}, \omega)^{3/2}} \frac{d \epsilon(\vec{q}, \omega)}{d \vec{q}} \tag{54}$$

and we can readily see that the dispersion in the renormalized phonon frequency as a function of wavevector will have a singularity just as for the dielectric function. This is an observable effect, as can be seen below in the phonon dispersion for lead (Pb) in the [110] direction[2]:



Plasmons (the $\omega \gg v_F q$ limit)

For this particular limit, let us examine the case where $T = 0$. The polarization function can then be written as for the case of time-reversal symmetric systems (i.e. $E(\vec{k}) = E(-\vec{k})$):

$$\Pi(\vec{q}, \omega) = \frac{2}{V} \sum_k \frac{E(\vec{k}+\vec{q}) - E(\vec{k})}{(\hbar\omega + i\alpha)^2 - \left(E\left(\vec{k}+\vec{q}\right) - E(\vec{k})\right)^2} \tag{55}$$

The numerator can be written as $E(\vec{k}+\vec{q}) - E(\vec{k}) = \frac{\hbar^2}{2m}\left(\vec{q}^2 + 2\vec{k}\cdot\vec{q}\right)$ in which case, in the $\omega \gg v_F q$, we can write:

$$\Pi(\vec{q}, \omega) = \frac{1}{2m} \frac{2}{V} \sum_k \frac{\vec{q}^2 + 2\vec{k}\cdot\vec{q}}{\omega^2} \tag{56}$$

We now note that $\sum_k \vec{k}\cdot\vec{q} = 0$ because for every $\vec{k}$ there will be a corresponding contribution from $-\vec{k}$. Hence, we can write:

$$\Pi(\vec{q},\omega) = \frac{\vec{q}^2}{2\,m\,\omega^2}\,\frac{2}{V}\sum_k = \frac{n_{3d}\,\vec{q}^2}{m\,\omega^2} \tag{57}$$

And we get for the dielectric function:

$$\epsilon(\vec{q},\omega) = 1 - \frac{n\,e^2}{\epsilon_0\,m\,\omega^2} \equiv 1 - \frac{{\omega_p}^2}{\omega^2} \tag{58}$$

where $n_{3d} = N/V$ is the density of free electrons. This demonstrates that for $\omega = \omega_p$, the dielectric function goes to zero and $U_{\text{tot}}(\vec{q},\omega)$ diverges. The physical meaning of this divergence is that an external perturbation at this energy will give rise to a self-sustaining oscillation, also known as a plasmon.

Plasmons in 2D (the $\omega \gg v_F\, q$ limit)

Let us examine plasmons in 2D as this is relavant to High-Resolution Electron Energy Loss Spectroscopy (HREELS) experiments. Again, we start with the similar expression for the polarization function in 2D for time-reversal symmetric systems:

$$\Pi_{2d}(\vec{q},\omega) = \frac{2}{A}\sum_k \frac{E(\vec{k}+\vec{q}) - E(\vec{k})}{(\hbar\omega + i\alpha)^2 - \left(E\left(\vec{k}+\vec{q}\right) - E(\vec{k})\right)^2} \tag{59}$$

Again, we see that $\sum_k \vec{k}\cdot\vec{q} = 0$ and we can write for the polarization function (again using the usual approximation in going from the sum to the integral in two dimensions):

$$\Pi_{2d}(\vec{q},\omega) = \frac{2}{A}\,\frac{A}{(2\,\pi)^2}\,2\int d^2k\,\frac{\vec{q}^2}{2\,m\,\omega^2} \tag{60}$$

where the extra factor of two accounts for the electron spin. Therefore, we may write:

$$\Pi_{2d}(\vec{q},\omega) = \frac{1}{\pi^2}\,\frac{\vec{q}^2}{2\,m\,\omega^2}\,2\,\pi\,\frac{{k_F}^2}{2} = \frac{{k_F}^2\,\vec{q}^2}{2\,\pi\,m\,\omega^2} \tag{61}$$

and using the fact that $k_F = \sqrt{2\,\pi\,N/A}$ in 2D enables us to write for the polariation function and the dielectric function:

$$\Pi_{2d}(\vec{q},\omega) = \frac{n_{2d}\,\vec{q}^2}{m\,\omega^2} = d\cdot\Pi_{3d}(\vec{q},\omega) \qquad \text{and} \qquad \epsilon(\vec{q},\omega) = 1 - \frac{e^2}{2\,\epsilon_0}\,\frac{n_{2d}\,\vec{q}}{m\,\omega^2} \equiv 1 - \frac{\omega_{p_{2d}}(\vec{q})^2}{\omega^2} \tag{62}$$

where d is the lattice spacing between two-dimensional sheets and we have used the fact that $V(q) = \frac{e^2}{2\,\epsilon_0\,q}$ in 2D [a]. We notice now that the two-dimensional plasma frequency is **disperses as** $\sim\sqrt{q}$, and is also decreased in magnitude from the 3D plasma frequency by a factor of $\sqrt{2}$.

Current-Current Correlations: A Different Formulation

Throughout, we have examined the polarization function and the dielectric function as they relate to density perturbations in the solid. In our derivation of density-density correlations, however, we assumed that the external probe was in the form of a perturbing scalar potential. Of course, a gauge can be chosen where the electric field is completely specified by a scalar potential. However, one can also choose a gauge where the electric field is completely specified by the time derivative of a vector potential. This leads to a different formulation of the Random Phase Approximation based on the current density response function. From Ohm's Law, we can write (**again assuming translational invariance**):

$$\delta \vec{J}(\vec{q}, \omega) = -e\, \delta \vec{j}(\vec{q}, \omega) = \sigma_{\alpha\beta}(\vec{q}, \omega)\, \vec{E}(\vec{q}, \omega) = i\, \omega\, \sigma_{\alpha\beta}(\vec{q}, \omega)\, \vec{A}_{\text{tot}}(\vec{q}, \omega) \tag{63}$$

where $\delta \vec{J}(\vec{q}, \omega)$ is the induced electrical current density, $\delta \vec{j}(\vec{q}, \omega)$ is the induced number current density, $\sigma_{\alpha\beta}$ is the conductivity tensor and we have used the fact that $\vec{E}(\vec{r}, t) = -\partial \vec{A}(\vec{r}, t) / \partial t$. For an isotropic medium, the conductivity tensor can be separated into its longitudinal and transverse components, in which case we can write:

$$\delta \vec{J}^L(\vec{q}, \omega) = -e\, \delta \vec{j}^L(\vec{q}, \omega) = \sigma^L(\vec{q}, \omega)\, \vec{E}^L(\vec{q}, \omega) = i\, \omega\, \sigma^L(\vec{q}, \omega)\, \vec{A}^L_{\text{tot}}(\vec{q}, \omega)$$

and

$$\delta \vec{J}^T(\vec{q}, \omega) = -e\, \delta \vec{j}^T(\vec{q}, \omega) = \sigma^T(\vec{q}, \omega)\, \vec{E}^T(\vec{q}, \omega) = i\, \omega\, \sigma^T(\vec{q}, \omega)\, \vec{A}^T_{\text{tot}}(\vec{q}, \omega) \tag{64}$$

Now, just as we defined the responses to U_{tot} and U_{ext}, we can also define the corresponding quantities for responses to $e\, \vec{A}_{\text{tot}}$ and $e\, \vec{A}_{\text{ext}}$. Therefore we can write:

$$\begin{aligned} \delta \vec{j}^L(\vec{q}, \omega) &= \chi^L_j(\vec{q}, \omega)\, e\, \vec{A}^L_{\text{ext}}(\vec{q}, \omega) \\ \delta \vec{j}^L(\vec{q}, \omega) &= P^L(\vec{q}, \omega)\, e\, \vec{A}^L_{\text{tot}}(\vec{q}, \omega) \end{aligned} \tag{65}$$

where $\chi^L_j(\vec{q}, \omega)$ is the **screened** current density response function (analogous to the susceptibility) and $P^L(\vec{q}, \omega)$ is the **unscreened** current density response function (analogous to the polarization function). One should note that because $\delta \vec{j}(\vec{q}, \omega)$ and $\vec{A}^L_{\text{ext}}(\vec{q}, \omega)$ are vector quantities, $\chi^L_j(\vec{q}, \omega)$ and $P^L(\vec{q}, \omega)$ are actually tensors which we have separated into their longitudinal and transverse components after assuming an **isotropic medium**.

However, there is difference between how the perturbation enters the Hamiltonian in contrast to the scalar potential case. When including the vector potential, the Hamiltonian is written as:

$$\begin{aligned} H_A &= \frac{1}{2\,m} \sum_i \left(\vec{p}_i + e\, \vec{A}_{\text{ext}}(\vec{r}_i, t)\right)^2 + \sum_{i<j} \frac{e^2}{4\, \pi \epsilon_0\, |\vec{r}_i - \vec{r}_j|} \\ H_A &= H + e \int \vec{j}_p(\vec{r}, t) \cdot \vec{A}_{\text{ext}}(\vec{r}, t)\, d^3 r + \sum_i \frac{e^2}{2\, m} A^2_{\text{ext}}(\vec{r}_i, t) \end{aligned} \tag{66}$$

where H is the original Hamiltonian without the perturbing potential and $\vec{j}_p(\vec{r}, t)$ is the paramagnetic current density and is given by:

$$\vec{j}_p(\vec{r}, t) = \frac{1}{2\, m} \sum_i \left(\vec{p}_i\, \delta(\vec{r} - \vec{r}_i) + \delta(\vec{r} - \vec{r}_i)\, \vec{p}_i\right) \tag{67}$$

because $\vec{A}_{\text{ext}}(\vec{r}_i, t)$ and $\vec{p}_i$ do not necessarily commute unless one is using the transverse gauge (i.e. $\vec{\nabla} \cdot \vec{A}_{\text{ext}}(\vec{r}_i, t) = 0$). This is not the entire current however, as there is a contribution from the last term in the H_A. One can obtain the current density in the presence of a vector potential using:

$$\delta \vec{j}(\vec{r}, t) = \frac{1}{2\, m} \left(\psi^*(\vec{r}, t)\, \hat{p}\, \psi(\vec{r}, t) - \psi(\vec{r}, t)\, \hat{p}\, \psi^*(\vec{r}, t)\right) = \vec{j}_p(\vec{r}, t) + \frac{\hat{n}(\vec{r}, t)}{m}\, e\, A_{\text{ext}}(\vec{r}, t) \tag{68}$$

where $\hat{p}$ is the **canonical momentum** and $n(\vec{r}, t) = \sum_i \delta(\vec{r} - \vec{r}_i)$ is the number density operator. The last term in the current density is called the diamagnetic current. It should be noted that the quantity defined above is gauge invariant, whereas the paramagnetic current alone is not. We now note that the form of the perturbation for the paramagnetic current is identical to that of the density perturbation when deriving the susceptibility. To obtain an expression for $\chi^L_{j_p}(\vec{q}, \omega)$, we can therefore appeal to the same logic that helped us obtain the susceptibility when considering the density perturbation. Here, $\chi^L_{j_p}(\vec{q},\omega)$ is the paramagnetic current response to the external vector potential define to be:

$$\vec{j}^{\,L}_p(\vec{q},\omega) = \chi^L_{j_p}(\vec{q},\omega)\, e\, \vec{A}^{\,L}_{\text{ext}}(\vec{q},\omega) \tag{69}$$

We can therefore immediately write for the paramagnetic current density response function:

$$\begin{aligned}\chi^L_{j_p}(\vec{q},\omega) &= \lim_{\alpha\to 0}\frac{1}{V}\sum_i\left(\frac{\left|\langle i\mid j^{L\dagger}_p(\vec{q})\mid G\rangle\right|^2}{\hbar\omega+E_0-E_i+i\alpha}-\frac{\left|\langle i\mid j^L_p(\vec{q})\mid G\rangle\right|^2}{\hbar\omega+E_i-E_0+i\alpha}\right)\\ &\overset{\text{TRI}}{=} \lim_{\alpha\to 0}\frac{1}{V}\sum_i\left|\langle i\mid j^L_p(\vec{q})\mid G\rangle\right|^2\left(\frac{1}{\hbar\omega+E_0-E_i+i\alpha}-\frac{1}{\hbar\omega+E_i-E_0+i\alpha}\right)\end{aligned} \tag{70}$$

where $j^L_p(\vec{q})$ is the component of the paramagnetic current density along $\vec{q}$ or $\vec{A}^{\,L}_{\text{ext}}(\vec{q},\omega)$ and the last equality holds if the system probed is time-reversal invariant. Now that we have dealt with the paramagnetic term, we move onto the diamagnetic response, which does **not** enter the Hamiltonian in a form that one is used to. However, the response can be obtained easily enough by noting that the diamagnetic current is linearly proportional to the external vector potential. Therefore, to linear order in $\vec{A}_{\text{ext}}(\vec{q},\omega)$, we may approximate the density operator by its average value and write for the screened current density response function:

$$\chi^L_j(\vec{q},\omega) = \chi^L_{j_p}(\vec{q},\omega) + \frac{n}{m} \tag{71}$$

Before proceeding, one should note that we may write the unscreened current density response function in much the same way, proceeding as above with $\vec{A}_{\text{tot}}(\vec{q},\omega)$ instead of $\vec{A}_{\text{ext}}(\vec{q},\omega)$. We can therefore write for $P^L(\vec{q},\omega)$:

$$P^L(\vec{q},\omega) = P^L_{j_p}(\vec{q},\omega) + \frac{n}{m} \tag{72}$$

where

$$\begin{aligned}P^L_{j_p}(\vec{q},\omega) &= \lim_{\alpha\to 0}\frac{1}{V}\sum_i\left(\frac{\left|\langle i\mid j^{L\dagger}_p(\vec{q})\mid G\rangle\right|^2}{\hbar\omega+E_0-E_i+i\alpha}-\frac{\left|\langle i\mid j^L_p(\vec{q})\mid G\rangle\right|^2}{\hbar\omega+E_i-E_0+i\alpha}\right)\\ &\overset{\text{TRI}}{=} \lim_{\alpha\to 0}\frac{1}{V}\sum_i\left|\langle i\mid j^{L\dagger}_p(\vec{q})\mid G\rangle\right|^2\left(\frac{1}{\hbar\omega+E_0-E_i+i\alpha}-\frac{1}{\hbar\omega+E_i-E_0+i\alpha}\right)\end{aligned} \tag{73}$$

where again it is stressed that the matrix elements for the **unscreened** response function are evaluated between the **dressed quasi-particle states** whereas the matrix elements of the **screened** response function are evaluated between the **bare electronic states**. Also, the last equality only holds when the system posseses time-reversal invariance.

Two Important Calculational Tools

Before we calculate $P^L_{j_p}(\vec{q},\omega)$ in the Random Phase Approximation, there are two important relations that one needs to derive. One is the relation between the diagmagetic response and the paramagnetic response, i.e. we can calculate the diamagnetic current density response function just by knowing thse paramagnetic current density reponse function. The other is the relationship between the longitudinal current density response function and the density response functions. This enables one to compare the result of our Random Phase Approximation calculation in both cases.

Let us first write the diamagnetic current density response function in terms of the paramagnetic one. We first start with the static current density response function:

$$\chi^L_{j_p}(\vec{q},0) = \frac{1}{V}\sum_i \left|\langle i \mid j_p^{L\dagger}(\vec{q}) \mid G\rangle\right|^2 \left(\frac{1}{E_0-E_i} - \frac{1}{E_i-E_0}\right) = \frac{2}{V}\sum_i \frac{\left|\langle i \mid j_p^{L\dagger}(\vec{q}) \mid G\rangle\right|^2}{E_0-E_i} \tag{74}$$

A Small Digression into Sum Rules

At this juncture, we need digress and derive an important sum rule. We note from the Fourier Transformed continuity equation that:

$$i\frac{\partial\,\hat{n}(\vec{q})}{\partial t} = \frac{1}{\hbar}[\hat{n}(\vec{q}),H] = q\,\delta\,j^L(\vec{q}) \tag{75}$$

where H is the Hamiltonian. Let us now take the commutator of the second and third terms with $\hat{n}^\dagger(\vec{q})$ and take the expectation value in the ground state. We then get:

$$\langle G \left|\left[[\hat{n}(\vec{q}),H],\hat{n}^\dagger(\vec{q})\right]\right| G\rangle = \hbar\,q\,\langle G\left|\left[\delta\,j^L(\vec{q}),\hat{n}^\dagger(\vec{q})\right]\right| G\rangle \tag{76}$$

Evaluating the left hand side of the above equation gives:

$$\langle G \left|\left[[\hat{n}(\vec{q}),H],\hat{n}^\dagger(\vec{q})\right]\right| G\rangle = \sum_i (E_i-E_0)\left(|\langle G \mid n(\vec{q}) \mid i\rangle|^2 + \left|\langle G\mid n^\dagger(\vec{q}) \mid i\rangle\right|^2\right) \overset{\text{TRI}}{=} 2\sum_i (E_i-E_0)\,|\langle G \mid n(\vec{q}) \mid i\rangle|^2 \tag{77}$$

where the last equality holds for time-reversal invariant systems. Now, evaluating the right hand side of the above equation gives:

$$\hbar\,q\,\langle G\left|\left[\delta\,j^L(\vec{q}),\hat{n}^\dagger(\vec{q})\right]\right| G\rangle = \frac{\hbar\,q}{2\,m}\sum_l \langle G\left|\left[p_l\,e^{-i\vec{q}\cdot\vec{r}_l} + e^{-i\vec{q}\cdot\vec{r}_l}\,p_l,\,e^{i\vec{q}\cdot\vec{r}_l}\right]\right| G\rangle \tag{78}$$

after Fourier Transforming equation (67). We then evaluate the commutator to get:

$$\hbar\,q\,\langle G\left|\left[\delta\,j^L(\vec{q}),\hat{n}^\dagger(\vec{q})\right]\right| G\rangle = \frac{N\,\hbar^2\,q^2}{m} \tag{79}$$

where $N = \sum_l(1)$ is thte total number of electons in the sample. Therefore, we can write:

$$\sum_i (E_i-E_0)\,|\langle G\mid n(\vec{q}) \mid i\rangle|^2 = \frac{N\,\hbar^2\,q^2}{2\,m} \tag{80}$$

which is our desired sum rule, often referred to as the ***f*-sum rule**. Physically, it reflects that the excitations in a solid are constrained by the total number of electrons, (i.e. conservation of particle number). Let us now write this in terms of the current density using the continuity equation (75):

$$(E_i-E_0)\,\langle G\mid \hat{n}(\vec{q}) \mid i\rangle = \hbar\,q\,\langle G \mid \delta\,j^L(\vec{q}) \mid i\rangle \tag{81}$$

Hence, we can also write the f-sum rule as:

$$\sum_i \frac{\left|\langle G\mid \delta\,j^L(\vec{q}) \mid i\rangle\right|^2}{(E_i-E_0)} = \frac{N}{2\,m} \tag{82}$$

Now, armed with the f-sum rule, we may write equation (74) as:

$$\chi^L_{j_p}(\vec{q},0) = -\frac{n}{m} \tag{83}$$

And we get the result that:

$$\chi_j^L(\vec{q},0) = \chi_{j_p}^L(\vec{q},0) + \frac{n}{m} = 0 \tag{84}$$

for all $\vec{q}$! While at first this may seem surprising, it reflects the physical principle that a static (i.e. ω=0) vector potential does not give rise to an electric field. In general therefore, the current density response function can be written as:

$$\chi_j^L(\vec{q},\omega) = \chi_{j_p}^L(\vec{q},\omega) - \chi_{j_p}^L(\vec{q},0) \tag{85}$$

One should note that all of the above logic also applies for the unscreened current density response function, in which case:

$$P_{j_p}^L(\vec{q},0) = -\frac{n}{m} \tag{86}$$

and

$$P^L(\vec{q},\omega) = P_{j_p}^L(\vec{q},\omega) - P_{j_p}^L(\vec{q},0)\,. \tag{87}$$

With this equation, we may now relate density response functions to the longitudinal current density response functions. This can be done using equations (70) and (85) to write:

$$\begin{aligned}
\chi_j^L(\vec{q},\omega) = \lim_{\alpha\to 0}\frac{1}{V}\\
\sum_i\left(\left|\langle i\mid j_p^{L\dagger}(\vec{q})\mid G\rangle\right|^2\left(\frac{1}{\hbar\omega+E_0-E_i+i\alpha}-\frac{1}{\hbar\omega+E_i-E_0+i\alpha}\right)-2\left|\langle i\mid j_p^L(\vec{q})\mid G\rangle\right|^2\left(\frac{1}{E_i-E_0}\right)\right)\\
= \lim_{\alpha\to 0}\frac{1}{V}\sum_i\left|\langle i\mid j_p^{L\dagger}(\vec{q})\mid G\rangle\right|^2\left(\frac{\hbar^2\omega^2}{(E_0-E_i)^2}\frac{2(E_i-E_0)}{(\hbar\omega+i\alpha)^2-(E_0-E_i)^2}\right)\\
= \lim_{\alpha\to 0}\frac{\omega^2}{q^2}\frac{1}{V}\sum_i\left|\langle i\mid \hat{n}^\dagger(\vec{q})\mid G\rangle\right|^2\left(\frac{2(E_i-E_0)}{(\hbar\omega+i\alpha)^2-(E_0-E_i)^2}\right)\\
= \lim_{\alpha\to 0}\frac{\omega^2}{q^2}\frac{1}{V}\sum_i\left|\langle i\mid \hat{n}^\dagger(\vec{q})\mid G\rangle\right|^2\left(\frac{1}{\hbar\omega+E_0-E_i+i\alpha}-\frac{1}{\hbar\omega+E_i-E_0+i\alpha}\right)\\
\boxed{\chi_j^L(\vec{q},\omega) = \frac{\omega^2}{q^2}\chi(\vec{q},\omega)}
\end{aligned} \tag{88}$$

and similarly:

$$\boxed{P^L(\vec{q},\omega) = \frac{\omega^2}{q^2}\Pi(\vec{q},\omega)} \tag{89}$$

Longitudinal Current Density Response in the Random Phase Approximation

We can now, armed with the formalism above, obtain a similar Lindhard-esque expression for the longitudinal current density response function. As before, we must calculate the unscreened response function, as this is the one that is tractable. Then we can compare to equation (89) above. Let us begin with the second line of equation (88) to calculate the unscreened current density response function. We can write:

$$P^L(\vec{q},\omega) = \lim_{\alpha\to 0} \frac{1}{V}\sum_i \left|\langle i \mid j_p^{L\dagger}(\vec{q}) \mid G\rangle\right|^2 \left(\frac{\hbar^2\omega^2}{(E_0-E_i)^2}\,\frac{2\,(E_i-E_0)}{(\hbar\omega+i\alpha)^2-(E_0-E_i)^2}\right) \tag{90}$$

To evaluate the above sum, we must first Fourier Transform the paramagnetic current density operator:

$$\begin{aligned}\vec{j}_p(\vec{q}) &= \frac{1}{2m}\int d^3r\, e^{-i\vec{q}\cdot\vec{r}}\sum_i\left(\vec{p}_i\,\delta(\vec{r}-\vec{r}_i)+\delta(\vec{r}-\vec{r}_i)\,\vec{p}_i\right) = \frac{1}{2m}\sum_i \vec{p}_i\,e^{-i\vec{q}\cdot\vec{r}_i} + e^{-i\vec{q}\cdot\vec{r}_i}\,\vec{p}_i \\ &= \frac{1}{2m}\sum_i \vec{p}_i\,e^{-i\vec{q}\cdot\vec{r}_i} + e^{-i\vec{q}\cdot\vec{r}_i}\,\vec{p}_i = \frac{1}{m}\sum_i\left(\vec{p}_i+\frac{\hbar\vec{q}}{2}\right)e^{-i\vec{q}\cdot\vec{r}_i}\end{aligned} \tag{91}$$

using $[f(\vec{r}),\vec{p}] = i\hbar\vec{\nabla}f(\vec{r})$ in the last equality. The longitudinal component is parallel to $\vec{q}$. Therefore, in second quantization, we can write:

$$\vec{j}_p^{L\dagger}(\vec{q}) = \frac{\hbar}{m}\sum_k\left(k\cos\theta+\frac{\vec{q}}{2}\right)c_{k+q}^{\dagger}\,c_k \tag{92}$$

where we have used that $\hat{p}\mid k\rangle = k\mid k\rangle$ when evaluating the matrix element $\langle k' \mid j_p^L(q)\mid k\rangle$. We can therefore write for the matrix element:

$$\left|\langle i \mid j_p^{L\dagger}(\vec{q}) \mid G\rangle\right|^2 = \frac{\hbar^2}{m^2}\left(k\cos\theta+\frac{\vec{q}}{2}\right)^2 f^0(\vec{k})\left(1-f^0(\vec{k}+\vec{q})\right) \tag{93}$$

And the unscreened current density response function becomes:

$$\begin{aligned}P^L(\vec{q},\omega) &= \lim_{\alpha\to 0}\frac{1}{V}\sum_k\frac{\hbar^2}{m^2}\left(k\cos\theta+\frac{\vec{q}}{2}\right)^2 f^0(\vec{k})\left(1-f^0(\vec{k}+\vec{q})\right)\left(\frac{\hbar^2\omega^2}{\left(\frac{\hbar^2 q}{m}\left(k\cos\theta+\frac{q}{2}\right)\right)^2}\,\frac{2\,\frac{\hbar^2 q}{m}\left(k\cos\theta+\frac{q}{2}\right)}{(\hbar\omega+i\alpha)^2-\left(\frac{\hbar^2 q}{m}\left(k\cos\theta+\frac{q}{2}\right)\right)^2}\right) \\ &= \lim_{\alpha\to 0}\frac{1}{V}\sum_k f^0(\vec{k})\left(1-f^0(\vec{k}+\vec{q})\right)\left(\frac{\omega^2}{q^2}\,\frac{2\,\frac{\hbar^2 q}{m}\left(k\cos\theta+\frac{q}{2}\right)}{(\hbar\omega+i\alpha)^2-\left(\frac{\hbar^2 q}{m}\left(k\cos\theta+\frac{q}{2}\right)\right)^2}\right) \\ &= \lim_{\alpha\to 0}\frac{1}{V}\frac{\omega^2}{q^2}\sum_k f^0(\vec{k})\left(1-f^0(\vec{k}+\vec{q})\right)\left(\frac{1}{\hbar\omega+i\alpha+\frac{\hbar^2 q}{m}\left(k\cos\theta+\frac{q}{2}\right)^2}-\frac{1}{\hbar\omega+i\alpha-\frac{\hbar^2 q}{m}\left(k\cos\theta+\frac{q}{2}\right)^2}\right) \\ &= \lim_{\alpha\to 0}\frac{1}{V}\frac{\omega^2}{q^2}\sum_k f^0(\vec{k})\left(1-f^0(\vec{k}+\vec{q})\right)\left(\frac{1}{\hbar\omega+i\alpha-E(\vec{k}+\vec{q})+E(\vec{k})}-\frac{1}{\hbar\omega+i\alpha+E(\vec{k}+\vec{q})-E(\vec{k})}\right) \\ &= \lim_{\alpha\to 0}\frac{1}{V}\frac{\omega^2}{q^2}\sum_k\left|\langle i \mid \hat{n}^{\dagger}(\vec{q}) \mid G\rangle\right|^2\left(\frac{1}{\hbar\omega+i\alpha-E(\vec{k}+\vec{q})+E(\vec{k})}-\frac{1}{\hbar\omega+i\alpha+E(\vec{k}+\vec{q})-E(\vec{k})}\right) \\ &= \frac{\omega^2}{q^2}\,\Pi(\vec{q},\omega)\end{aligned} \tag{94}$$

which is just the polarization function in equation (34). Therefore, as long as one knows the relationship between the response functions and physically measurable quantities like the dielectric function or the conductivity, either method can be used.

Notes

a) Note: *The Fourier Transform of the Coulomb potential can be evaluated in the following way:*

$$V_{2d}(q) = \int d^2 x \, \frac{e^{-i \vec{q}\cdot\vec{x}}}{|\vec{x}|} = \int_0^\infty dr \int_0^{2\pi} d\theta \, e^{-i q r \cos\theta} = 2\pi \int_0^\infty dr \, J_0(q r) = \frac{2\pi}{q}$$

where $J_0(x)$ *is the zeroth order Bessel Function of the* 1^{st} *kind*.

References

1 J.M. Ziman, *Principles of the Theory of Solids*. (Cambridge University Press, 1972).

2 P. Aynajian, T. Keller, L. Boeri, S. M. Shapiro, K. Habicht, and B. Keimer, Science **319** (5869), 1509 (2008).