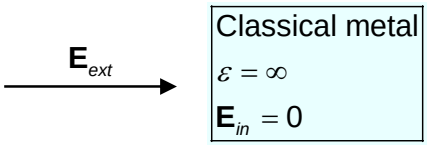
Screening (Electron-Electron Interaction)

Classical picture



The internal field is zero. Electrons are free to move; a layer of charge (**screening charge**) accumulates at the surface. The external field is screened.

Quantum picture: The field penetrates a short distance. Both the screening charge density and the internal field show damped oscillations (1D **Friedel oscillations**).

Problem: A solid is subjected to an external (applied) potential $\phi_{ext}(\mathbf{q},\omega)$; find the response $\phi_{total}(\mathbf{q},\omega)$ and $\rho_{total}(\mathbf{q},\omega)$.

Applications: (1) ϕ_{ext} from an ion core – crystal potential for band calculations.
(2) ϕ_{ext} from an electron – electron-electron interaction; independent electron approximation is good if the net interaction is weak.
(3) ϕ_{ext} from a charged (ionic) impurity – scattering, relaxation time, transport properties.

Definition: **dielectric function** $\phi_{total}(\mathbf{q},\omega) = \phi_{ext}(\mathbf{q},\omega)/\varepsilon(\mathbf{q},\omega)$

Consistent with $\mathbf{D}(\mathbf{q},\omega) = \varepsilon(\mathbf{q},\omega)\mathbf{E}(\mathbf{q},\omega)$

$$\mathbf{D}(\mathbf{r},t) = \frac{1}{(2\pi)^4}\int \mathbf{D}(\mathbf{q},\omega)\, e^{i(\mathbf{q}\cdot\mathbf{r}-\omega t)}\, d^3q\, d\omega = \frac{1}{(2\pi)^4}\int \varepsilon(\mathbf{q},\omega)\,\mathbf{E}(\mathbf{q},\omega) e^{i(\mathbf{q}\cdot\mathbf{r}-\omega t)}\, d^3q\, d\omega$$

$$= \frac{1}{(2\pi)^4}\int \varepsilon(\mathbf{q},\omega)\int d^3r'\, dt'\, \mathbf{E}(\mathbf{r}',t') e^{-i(\mathbf{q}\cdot\mathbf{r}'-\omega t')} e^{i(\mathbf{q}\cdot\mathbf{r}-\omega t)}\, d^3q\, d\omega$$

$$= \int\left\{\int \frac{1}{(2\pi)^4}\varepsilon(\mathbf{q},\omega) e^{i\mathbf{q}\cdot(\mathbf{r}-\mathbf{r}')-i\omega(t-t')} d^3q\, d\omega\right\}\mathbf{E}(\mathbf{r}',t')\, d^3r' dt'$$

$\mathbf{D}(\mathbf{r},t) = \int \varepsilon(\mathbf{r}-\mathbf{r}', t-t')\,\mathbf{E}(\mathbf{r}',t') d^3r'\, dt'$ $\varepsilon(\mathbf{r}-\mathbf{r}', t-t')$: nonlocal & noninstantaneous

Cf: in classical E&M, ε is often treated as a constant.

Computing ε:

Let $\phi_{total} \equiv \phi$. $\nabla^2\phi = -4\pi\rho$ $\rho = \rho_{ext} + \rho_{ind}$ Assume $\phi \propto \exp(i\mathbf{q}\cdot\mathbf{r})$.

$$q^2\phi = 4\pi\rho = 4\pi(\rho_{ext} + \rho_{ind}) = q^2\phi_{ext} + 4\pi\rho_{ind} = q^2\varepsilon\phi + 4\pi\rho_{ind}$$

$$\boxed{\varepsilon(\mathbf{q},\omega) = 1 - \frac{4\pi}{q^2}\,\frac{\rho_{ind}(\mathbf{q},\omega)}{\phi(\mathbf{q},\omega)}}$$

Computation scheme: $\phi \rightarrow$ Schrödinger equation $\rightarrow \psi \rightarrow \rho_{ind} \rightarrow \varepsilon$

Thomas-Fermi theory: semiclassical model, $\omega = 0$, long wavelength limit $\lambda \rightarrow \infty$.

$$\left(-\frac{\hbar^2}{2m}\nabla^2 - e\,\phi\right)\psi = E\psi,$$

where ϕ ~ constant in a small macroscopic volume about **r**.

Approximate local solution: $E(\mathbf{k};\mathbf{r}) \cong \frac{\hbar^2 k^2}{2m} - e\phi(\mathbf{r})$ **r** treated as a parameter.

For $\phi = 0$, $n_o(\mathbf{r}) = \frac{1}{4\pi^3}\int d^3k \;\; \frac{1}{\exp\left[\left(\frac{\hbar^2k^2}{2m} - \mu\right)\Big/ kT\right] + 1}$

For $\phi \neq 0$, $n(\mathbf{r}) = \frac{1}{4\pi^3}\int d^3k \;\; \frac{1}{\exp\left[\left(\frac{\hbar^2k^2}{2m} - e\phi - \mu\right)\Big/ kT\right] + 1} \cong n_o(\mathbf{r}) + \frac{\partial n_o}{\partial \mu}(e\phi)$

$$\rho_{ind}(\mathbf{r}) = -e\left(n(\mathbf{r}) - n_o(\mathbf{r})\right) = -e^2\,\frac{\partial n_o}{\partial \mu}\,\phi(\mathbf{r})$$

Fourier transform: $\rho_{ind}(\mathbf{q},0) = -e^2\,\frac{\partial n_o}{\partial \mu}\,\phi(\mathbf{q},0)$, treating $\frac{\partial n_o}{\partial \mu}$ (slowly varying) as a constant.

$$\boxed{\varepsilon_{TF}(\mathbf{q},0) = 1 + \frac{4\pi e^2}{q^2}\frac{\partial n_o}{\partial \mu} \equiv 1 + \frac{k_0^2}{q^2}}$$

k_0 = **Thomas-Fermi wave vector** $= \left(4\pi e^2\,\frac{\partial n_o}{\partial \mu}\right)^{\frac{1}{2}}$

For a free electron gas at $T \ll T_F$, $\mu \sim E_F$, $n_o = \frac{k_F^3}{3\pi^2} = \frac{1}{3\pi^2}\left(\frac{2mE_F}{\hbar^2}\right)^{\frac{3}{2}}$

$$\frac{\partial n_o}{\partial \mu} \simeq \frac{\partial n_o}{\partial E_F} = g(E_F) = \frac{mk_F}{\pi^2\hbar^2}$$

$\boxed{k_0 = \sqrt{\frac{4e^2 m k_F}{\pi\hbar^2}}}$ ~ 1-2 Å^{-1}, typically.

Example: $\phi_{ext}(\mathbf{r}) = \frac{Q}{r}$ associated with an ion core, an electron, or a charged impurity.

$$\phi_{ext}(\mathbf{q}) = \int \frac{Q}{r}\ e^{-i\mathbf{q}\cdot\mathbf{r}}\ d^3r = Q\int \frac{1}{r}\frac{\nabla^2 e^{-i\mathbf{q}\cdot\mathbf{r}}}{-q^2}\,d^3r = -\frac{Q}{q^2}\int \nabla^2\left(\frac{1}{r}\right)e^{-i\mathbf{q}\cdot\mathbf{r}}d^3r = \frac{4\pi Q}{q^2}$$

where we employed integration-by-parts twice and used $\nabla^2\left(\frac{1}{r}\right) = -4\pi\delta(\mathbf{r})$.

$\phi(\mathbf{q}) = \dfrac{\phi_{ext}(\mathbf{q})}{\varepsilon} = \dfrac{4\pi Q}{q^2 + k_0^2}$ $\qquad$ $\phi(\mathbf{r}) = \dfrac{1}{(2\pi)^3}\int \phi(\mathbf{q})\, e^{i\mathbf{q}\cdot\mathbf{r}} d^3q$ = … (straightforward calculation)

$\boxed{\phi(\mathbf{r}) = \dfrac{Q}{r}e^{-k_0 r}}$ = **screened Coulomb potential** (Yukawa potential). Range $\sim \dfrac{1}{k_0}$ ~ 1 Å.

Coulomb potential is long range. After screening, it becomes a short-range potential (about atomic dimension).

Problem: we assumed ϕ was slowly varying. The answer is not slowly varying. So, TF theory does not really apply to the Coulomb potential. It is fine for many other cases (for which ϕ is slowly varying).

Lindhard theory (a quantum theory within the Hartree approximation; better than TF)

Unperturbed system (free electron gas) $\left|\psi_{\mathbf{k}}^0\right\rangle = e^{i\mathbf{k}\cdot\mathbf{r} - iE(\mathbf{k})t/\hbar}$ $\qquad$ (assume volume V = 1)

Perturbation $\phi(\mathbf{r},t) = \phi(\mathbf{q},\omega)\, e^{i(\mathbf{q}\cdot\mathbf{r}-\omega t)+\alpha t} + c.c.$ with $\alpha \to 0$ (needed for convenience)

Apply 1st order time dependent perturbation theory; $\left|\psi_{\mathbf{k}}\right\rangle = \left|\psi_{\mathbf{k}}^0\right\rangle + b_{\mathbf{k}+\mathbf{q}}\left|\psi_{\mathbf{k}+\mathbf{q}}^0\right\rangle + b_{\mathbf{k}-\mathbf{q}}\left|\psi_{\mathbf{k}-\mathbf{q}}^0\right\rangle$

$$b_{\mathbf{k}+\mathbf{q}} = e\phi(\mathbf{q},\omega)\,\frac{\exp\left(i\dfrac{\left(E(\mathbf{k}+\mathbf{q}) - E(\mathbf{k}) - \hbar\omega\right)t}{\hbar}\right)\exp(\alpha t)}{E(\mathbf{k}+\mathbf{q}) - E(\mathbf{k}) - \hbar\omega - i\,\hbar\alpha}$$

$$b_{\mathbf{k}-\mathbf{q}} = e\phi^*(\mathbf{q},\omega)\,\frac{\exp\left(i\dfrac{\left(E(\mathbf{k}-\mathbf{q}) - E(\mathbf{k}) + \hbar\omega\right)t}{\hbar}\right)\exp(\alpha t)}{E(\mathbf{k}-\mathbf{q}) - E(\mathbf{k}) + \hbar\omega - i\,\hbar\alpha}$$

$\rho_{ind} = -e\sum_{\mathbf{k},s} f\left(E(\mathbf{k})\right)\left[\left|\psi_{\mathbf{k}}\right|^2 - 1\right]$ = … keeping 1st order term only (linear response)

Substituting into $\varepsilon(\mathbf{q},\omega) = 1 - \dfrac{4\pi}{q^2}\ \dfrac{\rho_{ind}(\mathbf{q},\omega)}{\phi(\mathbf{q},\omega)}$,

$$\boxed{\varepsilon = 1 + \frac{4\pi e^2}{q^2}\sum_{\mathbf{k},s}\frac{f(\mathbf{k}) - f(\mathbf{k}+\mathbf{q})}{E(\mathbf{k}+\mathbf{q}) - E(\mathbf{k}) - \hbar\omega - i\hbar\alpha}} \qquad \alpha \to 0$$

In general complex, because $\dfrac{1}{x + i\alpha} = P\left(\dfrac{1}{x}\right) - i\pi\delta(x)$

It involves transitions between occupied and unoccupied states: $f(\mathbf{k}) - f(\mathbf{k}+\mathbf{q})$.

Various limits (derivations not shown):

(1) $\omega = 0,\ q \ll k_F\ (\lambda \to \infty)$: $\varepsilon(\mathbf{q},0) = 1 + \dfrac{k_0^2}{q^2}$, same as Thomas-Fermi results.

(2) $\varepsilon(q=0,\omega) = 1 - \dfrac{\omega_p^2}{\omega^2}$, same as Drude results.

(3) q finite, $\hbar\omega \gg E(\mathbf{k}+\mathbf{q}) - E(\mathbf{k})$ and $E(\mathbf{k}) - E(\mathbf{k}-\mathbf{q})$ for all $\mathbf{k}$ with $f(\mathbf{k}) \neq 0$ (high frequency limit), $\varepsilon = 1 - \dfrac{\omega_p^2}{\omega^2}$.

For a free electron gas at $T = 0$, ε can be evaluated exactly. $\varepsilon = \varepsilon_1 + i\varepsilon_2$

$$\varepsilon_1 = 1 + \frac{k_0^2}{q^2}\ \frac{1}{8\beta}\left\{4\beta + \left(1-\beta^2-\gamma^2\right)\ln\left|\frac{(1+\beta)^2-\gamma^2}{(1-\beta)^2-\gamma^2}\right| + 2\beta\gamma\ln\left|\frac{(1-\gamma)^2-\beta^2}{(1+\gamma)^2-\beta^2}\right|\right\}$$

$$\varepsilon_2 = \frac{\pi k_0^2}{q^2}\frac{1}{8\beta}\cdot\ (\mathrm{a})\ 0,\quad 4\beta + 4\beta^2 \le \delta$$

$$(\mathrm{b})\left[1 - \left(\beta - \frac{\delta}{4\beta}\right)^2\right],\quad \left|4\beta - 4\beta^2\right| \le \delta \le 4\beta + 4\beta^2$$

$$(\mathrm{c})\ \delta,\quad \delta \le \left|4\beta - 4\beta^2\right| \text{ and } \beta \le 1$$

$$(\mathrm{d})\ 0,\quad \delta \le \left|4\beta - 4\beta^2\right| \text{ and } 1 \le \beta$$

where $\beta = \dfrac{q}{2k_F} \ge 0;\ \delta = \dfrac{\hbar\omega}{E_F} \ge 0;\quad \gamma = \dfrac{\delta}{4\beta} \ge 0$

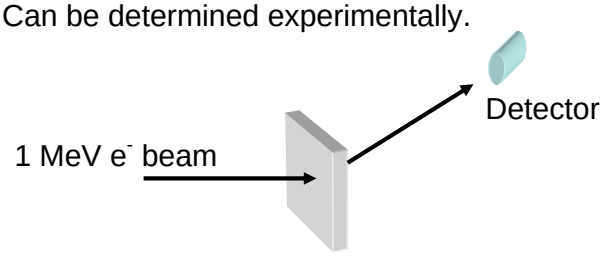
Application: find $\omega_P(q)$ = plasmon frequency as a function of q.

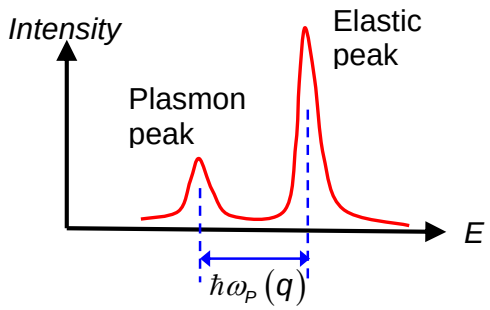
Condition for plasmon resonance: $\varepsilon = 0$. ω_p is usually large, $\varepsilon_2 = 0$ if q is small.

The condition reduces to $\varepsilon_1 = 0$. After a lot of algebra, we find

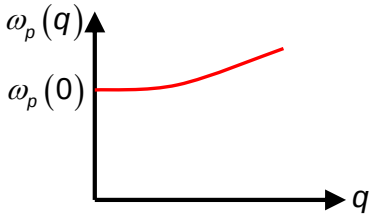
$$\boxed{\omega_p(q) \cong \omega_p(0)\left[1 + \frac{3}{10}\ \frac{q^2 v_F^2}{\omega_p^2(0)}\right]},\ \text{where } \omega_p^2(0) = \frac{4\pi n e^2}{m} = \text{Drude results.}$$

Can be determined experimentally.

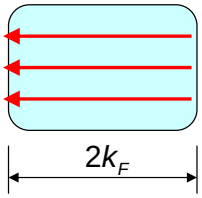




q (momentum transfer) is determined by scattering geometry.



Static limit $\omega = 0$, $\varepsilon = 1 + \dfrac{4\pi e^2}{q^2} \sum_{ks} \dfrac{f(\mathbf{k}) - f(\mathbf{k}+\mathbf{q})}{E(\mathbf{k}+\mathbf{q}) - E(\mathbf{k}) - i\hbar\alpha}$



Large contribution to ε if two regions of Fermi surface are parallel.

Say, $E(\mathbf{k})$ is occupied and $E(\mathbf{k}+\mathbf{q})$ is unoccupied.

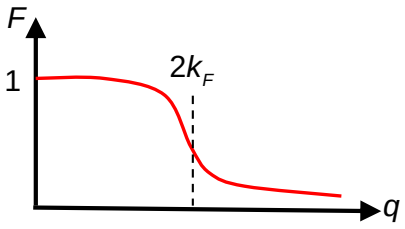
Both are ~ at the Fermi level. $E(\mathbf{k}+\mathbf{q}) - E(\mathbf{k})$ ~ 0. $f(\mathbf{k})$ = 1; $f(\mathbf{k}+\mathbf{q})$ = 0.

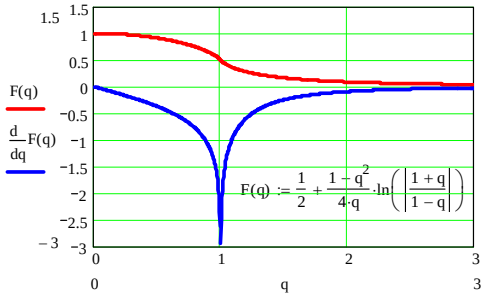
This condition (**Fermi surface nesting**) can lead to a large response of the system at $q = 2k_F$. Specifically, the phonon dispersion relations can show kinks (**Kohn anomalies**). Or, the lattice could spontaneously distort (**Peierls distortion**), leading to a **charge density wave** (CDW) state. This is more common for low dimensional systems; perfect nesting condition is automatically satisfied in 1D.

Free electron gas in the static limit at T = 0: $\omega = 0$, $\varepsilon_2 = 0$

$$\varepsilon_L(\mathbf{q},0) = 1 + \frac{k_0^2}{q^2}\left\{\frac{1}{2} + \frac{4k_F^2 - q^2}{8k_F q} \ln\left|\frac{2k_F + q}{2k_F - q}\right|\right\} \equiv 1 + \frac{k_0^2}{q^2} F$$

- $\varepsilon_1(q,0)$ not analytic at $q = 2k_F$; its slope is divergent (weak logarithmic divergence) (Kohn anomalies).





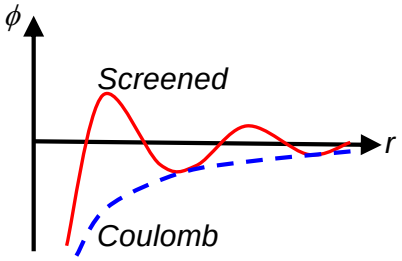
- $q \to 0$, $F \to 1$, $\varepsilon_L \to 1 + \dfrac{k_0^2}{q^2} \to$ Thomas Fermi results
- Effective screening length $\lambda(q)$: $\varepsilon = 1 + \dfrac{(1/\lambda)^2}{q^2}$ $\lambda(q) = \lambda(0)/\sqrt{F}$

As $q \to \infty$, $\lambda(q) \to \infty$. It is difficult to screen out short wave length perturbation.

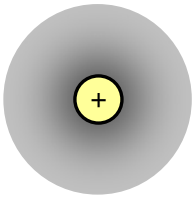
For the Coulomb potential, $\phi_{ext} = \dfrac{Q}{r}$, $\phi_{TF} = \dfrac{Q}{r}\exp(-k_0 r)$ (Thomas-Fermi).

Lindhard: $\phi_L \propto \dfrac{\cos(2k_F r)}{r^3} + \cdots$ in the asymptotic region

Decays like r^{-3} and oscillates as $\cos(2k_F r)$ -- **Friedel oscillations**. This "$2k_F$" wave vector is relevant to many physical phenomena.



The screening charge density ρ also shows Friedel oscillations.



Thomas Fermi: the screening charge is negative.

Lindhard: the screening charge shows damped oscillations.

In each case, the system is neutral when integrated over a large volume (classical limit).

Z + 1 approximation:

Example: Na crystal Na atomic configuration: $1s^2 2s^2 2p^6 3s^1$

Assume incoming x-rays excite and eject a 1s core electron. $Na \rightarrow Na^+$ ($1s^1 2s^2 2p^6 3s^1$)

Screening: $Na^+ \rightarrow Na^*$ ($1s^1 2s^2 2p^6 3s^2$; neutral), because the lowest available orbital is 3s

The valence electronic structure of Na* ($1s^1 2s^2 2p^6 3s^2$), with a nuclear charge of Z and a 1s hole, is very similar to that of Mg ($1s^2 2s^2 2p^6 3s^2$), with a nuclear charge of Z + 1.

Can replace Na* by a Mg impurity in the calculation: Z + 1 approximation.

Conclusion: the screening length for Na^+ is very short (~ radius of the 3s orbital).