Lect 12: Electron-phonon interaction in metals

Mahan chap 6.4

We consider the coupling between electrons and lattice ions.

$$H_{0e} = \sum_i \frac{\vec{P}_i^2}{2m} + \sum_{i,\alpha} V_{ei}(\vec{r}_i - R_\alpha^{(0)}) + \frac{1}{2}\sum_{ij} \frac{e^2}{|r_i - r_j|},$$

This part is the electron Hamiltonian in the absence of phonons, ($R_\alpha^{(0)}$ is the equilibrium position of lattice ions.) We will neglect the lattice structure for electrons and approximate them as in the Jellium model.

$$H_{op} = \sum_i \frac{\vec{P}_\alpha}{2M} + \frac{1}{2}\sum_{\alpha\beta}\frac{1}{2}(Q_\alpha - Q_\beta)_\mu (Q_\alpha - Q_\beta)_\nu \Phi_{\mu\nu}(R_\alpha^0 - R_\beta^0)$$

describes the bare-phonon Hamiltonian. These are phonons without electron-phonon and electron-electron interaction. The ions are not charge neutral. If we treat electrons as rigid background, the ion phonon (bare) mode is just the plasma oscillation of ions at $q \to 0$

$$\Omega_{ip}^2 = \frac{4\pi e^2 Z^2 n}{M} \approx Z^2 \left(\frac{m_e}{M}\right) \omega_p^2 << \omega_p^2 \leftarrow \text{electron plasma frequency}$$

we know in real metal, phonons have linear dispersion relation. This is due to the screening of electrons.

We introduce the ion collective coordinate (phonons) $\vec{Q}_k$,

$$\vec{Q}_\alpha = \frac{1}{N^{1/2}} \sum_k \vec{Q}_k e^{i\vec{k}\cdot\vec{R}_\alpha^{(0)}},$$ where $\vec{Q}_k$ can be represented

$$\vec{Q}_k = \sum_\lambda \left(\frac{\hbar}{2M\Omega_{k\lambda}}\right)^{1/2} \vec{\xi}_{k\lambda} (a_{k\lambda} + a^\dagger_{-k\lambda}),$$ where λ denotes the polarization.

Now let us consider the electron-phonon interaction

$$\Delta V(r) = -\sum_\alpha \vec{Q}_\alpha \cdot \nabla V_{el}(\vec{r} - \vec{R}_\alpha^{(0)})$$

$$V_{el}(r) = \frac{-1}{V}\sum_q e^{i\vec{q}\cdot\vec{r}}\, V_{el}(\vec{q}) \Rightarrow \nabla V_{el}(\vec{r}-\vec{R}_\alpha^{(0)}) = \frac{1}{V}\sum_q e^{-i\vec{q}\cdot\vec{R}_\alpha^{(0)}}\, i\vec{q}\, e^{i\vec{q}\cdot\vec{r}}\, V_{el}(\vec{q})$$

$$\Rightarrow \Delta V(r) = \frac{-1}{VN^{1/2}}\sum_\alpha\sum_q\sum_{k\lambda} \vec{Q}_k e^{i\vec{k}\cdot\vec{R}_\alpha^{(0)} - i\vec{q}\cdot\vec{R}_\alpha^{(0)}}\, i\vec{q}\, e^{i\vec{q}\cdot\vec{r}}\, V_{el}(\vec{q})$$

$$= \frac{-N^{1/2}}{V}\sum_q i\, e^{i\vec{q}\cdot\vec{r}}\,(\vec{q}\cdot\vec{Q}_q)\, V_{el}(\vec{q})$$

$$= \frac{-N^{1/2}}{V}\sum_{q,\lambda}\left(\frac{\hbar}{2M\Omega_{k\lambda}}\right)^{1/2}(i\vec{q}\cdot\vec{\xi}_{k\lambda})\, V_{el}(\vec{q})\,(a_{q\lambda}+a^+_{-q\lambda})$$

$$\Rightarrow H_{ep} = \int dr\, \psi^+(r)\psi(r)\,\Delta V(r)$$

$$= -i\sum_k\sum_{q,\lambda}\frac{1}{V}\left(\frac{N\hbar}{2M\Omega_{k\lambda}}\right)^{1/2} V_{el}(\vec{q})\,(\vec{\xi}_{k\lambda}\cdot\vec{q})\,(a_{q\lambda}+a^+_{-q\lambda})\, C^+_{k+q} C_k$$

in considering Umklapp process, we consider the scattering between C^+_{k+q+G} and C^+_k

$$H_{ep} = \frac{-i}{\sqrt{V}}\sum_{\substack{k,q,\lambda\\ G}}\left(\frac{N\hbar}{2MV\Omega_{k\lambda}}\right)^{1/2} V_{el}(\vec{q}+\vec{G})\,[\vec{\xi}_{k\lambda}\cdot(\vec{q}+\vec{G})]\,(a_{q\lambda}+a^+_{-q\lambda})\, C^+_{k+q+G,\sigma} C_{k,\sigma}$$

Now let us neglect Umklapp

$$\boxed{H_{ep} = \frac{1}{\sqrt{V}}\sum_{kq\lambda} M_\lambda(q)\, C^+_{k+q,\sigma} C_{k\sigma}\,(a_{q\lambda}+a^+_{-q\lambda})}$$

where $M_\lambda(q) = -i\left(\frac{N\hbar}{2MV\Omega_{q\lambda}}\right)^{1/2} V_{el}(\vec{q})\,(\vec{\xi}_{q\lambda}\cdot\vec{q}) \Rightarrow \boxed{M^*_\lambda(q) = M_\lambda(-q) \text{ if phonon has T.R sym}}$

we define the phonon Green's function as

$$D(q\lambda;t-t') = -i \langle | T A_{q\lambda}(t) A^{+}_{q\lambda}(t') | \rangle, \quad \text{where } A_{q\lambda} = a_{q\lambda} + a^{+}_{-q\lambda}.$$

at zero temperature and free phonon

$$D^{(0)}(q, t-t') = -i\left[\theta(t-t')\, e^{-i\omega_q(t-t')} + \theta(t'-t)\, e^{i\omega_q(t-t')}\right]$$

$$D^{(0)}(q,\omega) = \frac{1}{\omega-\omega_q+i\eta} - \frac{1}{\omega+\omega_q-i\eta} = \frac{2\omega_q}{\omega^2-\omega_q^2+i\eta}$$

$\Longrightarrow$ Matsubara $\quad D(q\lambda;\tau-\tau') = -\langle T_\tau A(q,\tau) A(-q,\tau') \rangle$

$$\Rightarrow D^0(q,\tau) = -\theta(\tau)\left[(N_q+1)\, e^{-\tau\omega_q} + N_q\, e^{\tau\omega_q}\right] - \theta(-\tau)\left[N_q\, e^{-\tau\omega_q} + (N_q+1)\, e^{\tau\omega_q}\right]$$

$$\rightarrow \boxed{D^0(q,i\omega_n) = \frac{1}{i\omega_n-\omega_q} - \frac{1}{i\omega_n+\omega_q} = \frac{2\omega_q}{(i\omega_n)^2-\omega_q^2}\ .}$$

§ Renormalization of phonon frequency:

intuitive method: — molecular field method. We define $\chi_e^0(k,\omega)$ and $\chi_{ion}^0(k,\omega)$ as the density-density response function of electrons and ions without taking into account the long-range Coulomb interaction.

$\chi_e^0(k,\omega)$ is the density response of band electron + Fermi liquid,

$\chi_{ion}^0(k,\omega)$ is the density response of the short-range part of interactions between ions. For $\chi_e^0(k,\omega)$, we approximate the lindhard response + FL correction

$$\chi_e^0(k,\omega) = \frac{N_0}{1+F_0^s}\ .$$

(we take the limit $\omega \ll v_F q$ because $\Omega_p \ll v_F q$ for most phonon wavevector q).

for $\chi^\circ_{ion}(q,\omega)$, we use the jellium model ← no other force other than Coulumb, (taking into account by molecular field)

$$\partial n_{ion}/\partial t = -\nabla\cdot\vec{j}_{ion}, \qquad \frac{\partial \vec{j}_{ion}}{\partial t} = -\frac{n_{ion}}{M}\nabla V_{ext}$$

$$\Rightarrow -i\omega\,\delta n(q,\omega) = -i\vec{q}\cdot\vec{J}(q,\omega)$$

$$-i\omega\,\vec{j}(q,\omega) = -\frac{n}{M}(iq\,V_{ex}(q,\omega))$$

keep the leading order of average density

$$\Rightarrow \delta n(q,\omega) = \frac{n}{M}\frac{q^2}{\omega^2}V_{ex}(q,\omega) \Rightarrow \boxed{\chi^\circ_{ion}(q,\omega) = -\frac{nq^2}{M\omega^2}}$$

Now suppose an external field $\varphi_{ex}(r,t) \longrightarrow$ response $\delta\rho_{el}$ and $\delta\rho_{ion}$

$$\Rightarrow \delta\rho_{el} = -e^2\chi^\circ_{el}\,\varphi_{tot} = -e^2\chi^\circ_{el}(\varphi_{ex}+\varphi_{induced})$$

$$\delta\rho_{ion} = -(Ze)^2\chi^\circ_{ion}\,\varphi_{tot} = -(Ze)^2\chi^\circ_{ion}(\varphi_{ex}+\varphi_{induced})$$

$$\vec{\nabla}^2\varphi_{induced} = -4\pi\,[\delta\rho_{el}+\delta\rho_{ion}]$$

$$\Rightarrow \delta\rho_{el}(q,\omega) = -e^2\chi^0_{el}(q,\omega)\left[\varphi_{ex} - \frac{4\pi}{q^2}\left(\delta\rho_{el}(q,\omega)+\delta\rho_{ion}(q,\omega)\right)\right]$$

$$\delta\rho_{ion}(q,\omega) = -(Ze)^2\chi^0_{ion}(q,\omega)\left[\varphi_{ex} - \frac{4\pi}{q^2}\left(\delta\rho_{el}(q,\omega)+\delta\rho_{ion}(q,\omega)\right)\right]$$

$$\Rightarrow \delta\rho_{el}(q,\omega) = -\frac{e^2\chi^\circ_{el}(q,\omega)\,\varphi_{ex}}{1+\frac{4\pi e^2}{q^2}\left[\chi^\circ_{el}(q\omega)+Z^2\chi^\circ_{ion}(q\omega)\right]}$$

$$\delta\rho_{ion}(q,\omega) = \frac{-(Ze)^2\chi^\circ_{ion}(q,\omega)\,\varphi_{ex}}{1+\frac{4\pi e^2}{q^2}\left[\chi^\circ_{el}(q\omega)+Z^2\chi^\circ_{ion}(q\omega)\right]}$$

$$\Rightarrow \quad \varepsilon(q,\omega) = 1 + \frac{4\pi e^2}{q^2}\left[\chi^0_{el}(q,\omega) + z^2\chi^0_{ion}(q,\omega)\right]$$

$$= 1 - \frac{4\pi n z^2}{M\omega^2} + \frac{4\pi e^2}{q^2}\,\frac{N_0}{1+F_0^s} =$$

$$\boxed{\varepsilon(q,\omega) = 1 - \frac{\Omega^2_{p,ion}}{\omega^2} + \frac{k^2_{TF}}{q^2}}$$

quasi-static for electrons

dynamic for ions.

$$k^2_{TF} = \frac{4\pi e^2}{1+F_0^s} N_0$$

F_0^s ← FL correction

Bohm - Stauer formula

$$\chi_{ion} = \frac{-nq^2/M\omega^2}{1 + \frac{k^2_{TF}}{q^2} - \frac{\Omega^2_{p,ion}}{\omega^2}} \approx \frac{-nq^2/M\omega^2}{\frac{k^2_{TF}}{q^2} - \frac{\Omega^2_{p,ion}}{\omega^2}}$$

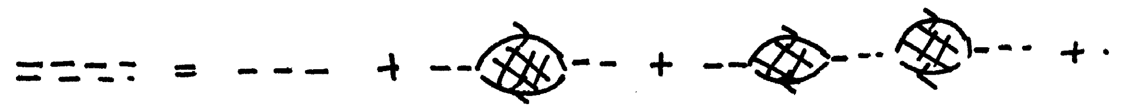
$$\approx -\frac{q^2}{k^2_{TF}} \cdot \frac{nq^2/M}{\omega^2 - c^2q^2} \quad \text{where} \quad c = \frac{\Omega_p}{k_{TF}}$$

$n_{el} = nZ$ (ion density: n)

$$\Rightarrow \quad \frac{c}{v_F} = \frac{\Omega_p}{k_F v_F} = \left[\frac{4\pi e^2 Z^2 n}{M}\,\frac{(1+F_0^s)}{4\pi e^2 N_0 v_F^2}\right]^{1/2}, \qquad N_0 = \frac{3nZ}{m^* v_F^2}$$

$$\boxed{\frac{c}{v_F} = \left[\frac{Z^2(1+F_0^s)\,v_F^2}{M N_0}\right]^{1/2} = \left[\frac{m^* Z(1+F_0^s)}{3M}\right]^{1/2} \sim \underbrace{\left(\frac{m^*}{M}\right)^{1/2}}_{\sim 10^{-2}}}$$

§ Phonon frequency Renormalization ← Green's function



$$D(q,\omega) = \frac{D^0(q,\omega)}{1 - D^0_{(q\omega)}\Pi'(q\omega)},$$ where $\Pi'(q,\omega)$ is electron

bubble dressed by columb line $\Pi'(q,\omega) = \dfrac{\Pi^0(q,\omega)\,|M_\lambda(q,\omega)|^2}{1 - V_q\,\Pi^0(q,\omega)}$

and combined with electron-phone vertex

$$\boxed{\begin{array}{c}\Pi^0 = -\chi_0(q,\omega)\\ \text{lindhard}\end{array}}$$

$$\Rightarrow D(q,\omega) = \frac{D^0(q,\omega)}{1 - |M_\lambda(q,\omega)|^2\, D^0(q,\omega)\,\Pi^0(q,\omega)/\varepsilon(q,\omega)}$$ ← screening of electron gas

plug in $D^0(q,\omega) = \dfrac{2\Omega_{p,ion}}{\omega^2 - \Omega^2_{p,ion} + i\eta}$

$$\Rightarrow D(q,\omega) = \frac{2\Omega_{p,ion}}{\omega^2 - \Omega^2_{p,ion} - 2\Omega_{p,ion}\,|M_\lambda|^2\,\Pi^0/\varepsilon(q\omega)}$$

$$M_\lambda \rightarrow q\left(\frac{\hbar\; N/V}{2M\,\Omega_{p,ion}}\right)^{1/2} \frac{4\pi e^2 z}{q^2}$$

this factor is canceled by perturbation power

$$\Rightarrow 2\,\Omega_{p,ion}\,|M_\lambda|^2 \rightarrow q^2\,\frac{\hbar}{M}\left(\frac{4\pi e^2 z}{q^2}\right)^2 = \frac{4\pi e^2}{q^2}\;\frac{4\pi e^2 z^2 n}{M}$$

$$= v_q\,\Omega^2_{p,ion}$$

⇒ the denominater

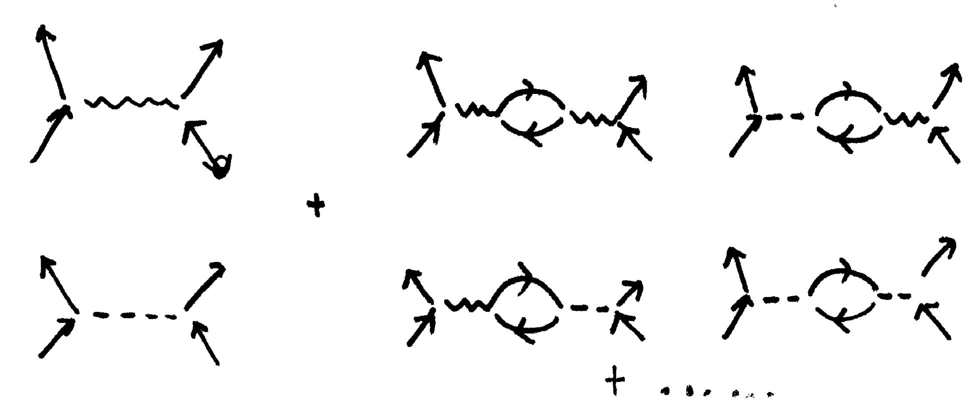
$$= \omega^2 - \Omega^2_{p,ion} - \frac{v_q\,\Pi^0}{\varepsilon(q,\omega)}\,\Omega^2_{p,ion} = \omega^2 - \Omega^2_{p,ion} + \frac{(\varepsilon - 1)}{\varepsilon}\,\Omega^2_{p,ion}$$

$$\Rightarrow D(q,\omega) = \frac{2\,\Omega_{p,ion}}{\omega^2 - \Omega_{p,ion}^2 / \varepsilon(q,\omega)}$$ ← responce from electron gas

by using $\varepsilon(q,\omega) = 1 + \frac{k_{TF}^2}{q^2}$, we get the same result as before

$$\Rightarrow \boxed{\frac{c}{v_F} \sim \left(\frac{m_e^*}{M}\right)^{1/2} < 0.01}$$

§ Effective electron - electron interaction



$$V_{eff} = \frac{V_q + V_{ph}}{1 - (V_q + V_{ph})\Pi}$$

where $V_{ph} = |M_q|^2 D^0(q,\omega)$

I can seperate into two part

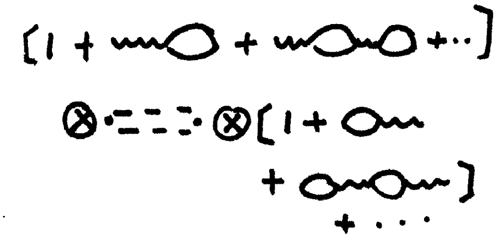
$$V_{eff} = \frac{V_q}{\varepsilon(q,\omega)} + V_{sc\text{-}ph}(q,\omega)$$

$\frac{V_q}{\varepsilon(q,\omega)}$ ← purely screen Coulumb; $V_{sc\text{-}ph}(q,\omega)$ ← screened el-ph

$$V_{sc\text{-}ph}(q,\omega) = \frac{V_q + V_{ph}}{1-(V_q+V_{ph})\Pi} - \frac{V_q}{1 - V_q\Pi} = \frac{V_{ph}}{(1-V_q\Pi)\,(1-(V_q+V_{ph})\Pi)}$$

the denominator $= \varepsilon\,(\varepsilon - V_{ph}\Pi) = \varepsilon^2\left(1 - \frac{V_{ph}P}{\varepsilon}\right)$

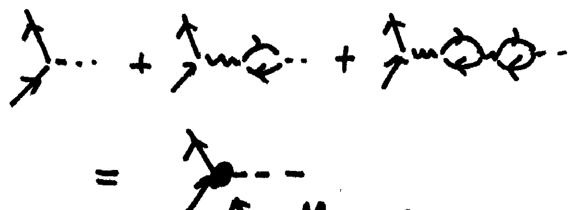
$$\Rightarrow \quad V_{sc\text{-}ph}(q,\omega) = \frac{V_{ph}}{\varepsilon^2\,(1 - V_{ph}\Pi/\varepsilon)}$$



$$\Rightarrow \quad V_{eff}(q,\omega) = \frac{V_q}{\varepsilon(q,\omega)} + \frac{M_q^2}{\varepsilon^2(q,\omega)}\, D(q,\omega)$$

where $D(q,\omega) = \dfrac{2\,\Omega_{p.ion}}{\omega^2 - \Omega_{p.ion}^2/\varepsilon(q,\omega)}$.

Equivilant to screened el-ph vertex



$= \quad M_q/\varepsilon(q,\omega)$

For our purpose, the screened Coulumb potential

$$V(q,\omega) \simeq \frac{4\pi e^2}{q^2 + k_{TF}^2}\,, \quad \text{which is positive}$$

but the screened el-ph

using $2|M_q|^2\,\Omega_{p,ion} = \Omega_{p,ion}^2$

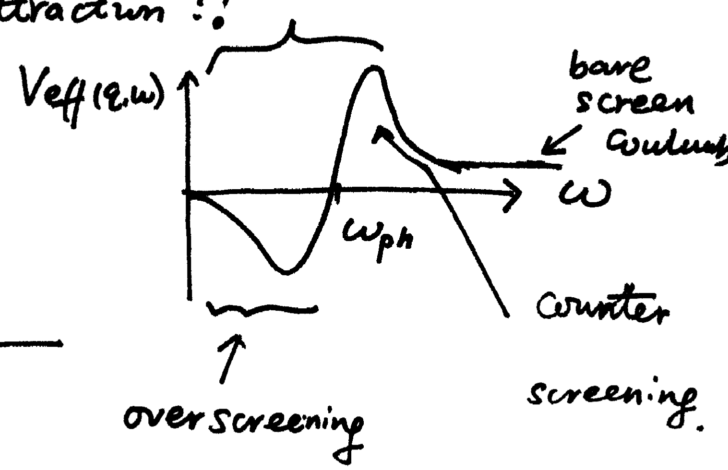
$$V_{sc\text{-}ph}(q,\omega) = \frac{2M_q^2\,\Omega_{p,ion}/\varepsilon^2(q,\omega)}{\omega^2 - \Omega_{p,ion}^2/\varepsilon(q,\omega)} = \frac{v_q\,\Omega_{p,ion}^2/\varepsilon^2(q,\omega)}{\omega^2 - \omega_{ph}^2(q,\omega)}$$

renormalized phonon

$$= \frac{v_q}{\varepsilon(q,\omega)}\;\frac{\omega_{ph}^2(q,\omega)}{\omega^2 - \omega_{ph}^2(q,\omega)}$$

$$\Rightarrow \quad \boxed{\frac{v_q}{\varepsilon(q,\omega)}\left[1 + \frac{\omega_{ph}^2(q,\omega)}{\omega^2 - \omega_{ph}^2(q,\omega)}\right] = V_{eff}(q,\omega)}$$

clearly as $\omega < \omega_{ph}(q,\omega)$, the screen el-ph interaction gives negative contribution $\Rightarrow$ attraction !!



how to understand this result ?

Let us review the classic theory of disperse relation in media:

incidenet E-M field $E_0 e^{-i\omega t}$; the total field $E e^{-i\omega t}$ and the induced $E_{ind} e^{-i\omega t}$, where

$$\boxed{\begin{array}{l} E_{ind} = -4\pi \quad P \\ P = \chi E \quad \text{and } E = E_0 + E_{ind} \end{array}}$$

Suppose in the media, ions are bound with an frequency ω_0

$$\Rightarrow \quad m\ddot{x} + m\omega_0^2 x \overset{+\gamma\dot{x}}{=} eE e^{-i\omega t} \Rightarrow x(\omega) = \frac{eE}{m(\omega_0^2 - \omega^2 - i\omega\gamma)}$$

$$P(\omega) = en\,x(\omega) = \frac{ne^2/m}{\omega_0^2 - \omega^2 - i\omega\gamma} E \Rightarrow \chi = \frac{\frac{1}{4\pi}\omega_p^2}{\omega_0^2 - \omega^2 - i\omega\gamma}$$

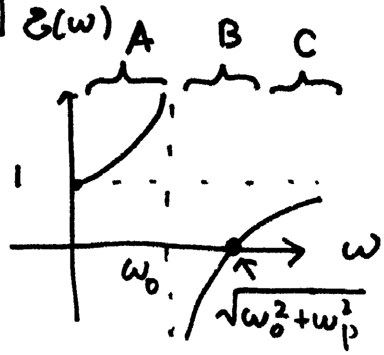
$$\left.\begin{array}{l} \Rightarrow \quad E_{ind} = -\dfrac{\omega_p^2}{\omega_0^2 - \omega^2 - i\omega\gamma} E \\ E = E_0 + E_{ind} \end{array}\right\} \Rightarrow \quad E\left(1 + \frac{\omega_p^2}{\omega_0^2 - \omega^2 - i\omega\gamma}\right) = E_0$$

$$\varepsilon = 1 + \frac{\omega_p^2}{\omega_0^2 - \omega^2 - i\omega\gamma}$$

$$E_{ind} = E_0 - E$$

$$= \left(1 - \frac{1}{\varepsilon}\right) E_0 = \frac{\varepsilon - 1}{\varepsilon} E_0$$

$\boxed{\text{if } \gamma = 0}$



shifted plasmon

$\boxed{E_{ind} \parallel -E}$

Region A:

under-screening, $\chi > 0$

$-E_{ind} \parallel E \parallel E_0$

$\xrightarrow{E_0}$

$\xrightarrow[E]{} \xleftarrow[E_{ind}]{}$, $|E_{ind}| < |E_0|$.

$\varepsilon > 1$, $n = \sqrt{\varepsilon(\omega)}$.
↑ refraction index

Region B: over-screening ($\chi < 0$)

$\xleftarrow{E} \xrightarrow{E_0}$

$\xleftarrow[E_{ind} = -4\pi\chi E]{}$, $E \parallel -E_0$ $\boxed{-4\pi\chi > 1}$ ← $\boxed{E_{ind} \parallel E \text{ and } E_{ind} > E}$

forbiden region for E-M wave!!

$-\infty < \varepsilon < 0 \Rightarrow n = i\sqrt{|\varepsilon|}$

at $\varepsilon = 0$, or $-4\pi\chi = 1 \Rightarrow E = E_{ind}$ & E_0. Intrinsic mode

Region C: Counter-screening ($\chi < 0$, and $0 < -4\pi\chi < 1$)

$\xrightarrow{E_0} \xrightarrow{E_{ind}}$

$\xrightarrow[E]{}$

$\boxed{E_{ind} \parallel E \text{ and } E_{ind} < E}$ ⇒ E is enhanced compared to E_0

$$n = \sqrt{\varepsilon(\omega)} \Rightarrow v_{phase} = \frac{c}{\sqrt{n}} > c.$$

EM-wave can propagate in this regime.

§ Application to our el-ph system:

$$\frac{\pi e^2}{q^2+k_{TF}^2} = \frac{v_q}{\varepsilon(q,\omega)}$$: screening Coulomb potential as input E_0.

↖ low ω for electron gas, but not low for lattice.

For the lattice, in the Jellium mode, the ω_0 is zero. (we think the positive ion as mobie) $\Rightarrow$ $\varepsilon_{ion} = 1 + \frac{\omega^2_{ph}}{-\omega^2} \Rightarrow \frac{1}{\varepsilon_{ion}} = \frac{\omega^2}{\omega^2-\omega_{ph}^2}$

i.e. there's no under-screening regime, but over / counter screening regime.

§ Kohn's anomaly

$$\varepsilon(q, \underbrace{\omega}_{=0}) = 1+ \frac{4\pi e^2}{q^2}N_0 \left[\frac{1}{2} + \frac{1}{4x}(1-x^2)\ln\left|\frac{1+x}{1-x}\right|\right]$$ where $x = \frac{q}{2k_F}$

$$\approx 1 + \frac{4\pi e^2}{4k_F^2}\cdot N_0 \frac{1}{2}\left[1 - (1-x)\ln\left|\frac{1-x}{2}\right|\right]$$ as $x \sim 1$

it has infinite slope at $q = 2k_F$ $\Rightarrow \frac{\partial \varepsilon}{\partial q} \sim \frac{\pi e^2 N_0}{2}\ln|1-x|$

$\Rightarrow \frac{\partial}{\partial q}\omega_{ph}(q)$ has logrith - divergence at $q = 2k_F$.

If Fermi surface has nesting

$\Rightarrow \varepsilon(q=2k_F, \omega=0)$ is greatly enhanced

$\Rightarrow$ phonon is softened!!