Lecture 8

Introduction to electron-phonon interaction

Contents

1 Dielectric function, screening

We will use the molecule-field method to treat the long-range Coulomb interaction, and apply it to a purely electron system first. Define $\chi_e^0(\mathbf{q},\omega)$ as the density-response function of electron before taking into account Coulomb interaction, i.e., it is due to density-response for the kinetic energy dispersion and Fermi liquid corrections. For example, $\chi_e^0(\mathbf{q},\omega)$ takes the Lindhardt function for spherical Fermi surface as

$$\chi_e^0(\mathbf{q},\omega) = -2\int \frac{d^3\mathbf{k}}{2\pi}\frac{n_f(\epsilon_k)-n_f(\epsilon_{k+q})}{\omega-(\epsilon_{k+q}-\epsilon_k)+i\eta}. \tag{1}$$

In the long wavelength limit $q\to 0$, it is approximated as

$$\chi_e^0(\mathbf{q},\omega) = N_0\Big(1-\frac{s}{2}\ln|\frac{1+s}{1-s}|\Big)+i\frac{\pi}{2}N_0\theta(1-|s|), \tag{2}$$

where $s=\omega/(v_f q)$, N_0 is the density of states at the Fermi surface, and $\theta(x)$ is the step function which equals 1 and 0 at $x>0$ and <0, respectively. If further consider the limit of $s\to 0$ and take into account the Fermi liquid correction, we have

$$\lim_{q\to 0}\lim_{\omega\to 0}\chi_e^0(\mathbf{q},\omega) = \frac{N_0}{1+F_0^s}, \tag{3}$$

where F_0^s is the Fermi liquid parameter is the density channel.

Now we further consider the renormalization from the long-range Coulomb interaction. Suppose that we apply an external electric potential $\phi_{ex}(q,\omega)$ in the limit of $q\to 0$ and $\omega/q\to 0$. ϕ_{ex} changes electric density distribution by $\delta\rho_{el}$, which in turn also generates an induced potential ϕ_{ind} via the Poisson equation $-\nabla^2\phi_{ind} = 4\pi\delta\rho_{el}$, or,

$$\phi_{ind}(\mathbf{q},\omega) = \frac{4\pi}{q^2}\delta\rho_{el}(\mathbf{q},\omega). \tag{4}$$

Then the total electric potential $\phi_{tot} = \phi_{ex} + \phi_{ind}$. Since ϕ_{tot} already takes care of the long-range nature of the Coulomb potential, we can directly use $\chi_e^0(q,\omega)$ to obtain the change of electron density. Hence, this is a feedback process as shown in the Fig 1, as captured by the following equations

$$\begin{aligned}\delta\rho_{el}(\mathbf{q},\omega) &= -e\chi_{el}^0(\mathbf{q},\omega)(e\phi_{tot}(\mathbf{q},\omega)) = -e^2\chi_{el}^0(\mathbf{q},\omega)\Big(\phi_{ex}(\mathbf{q},\omega) + \phi_{ind}(\mathbf{q},\omega)\Big\}\\ &= -e^2\chi_{el}^0(\mathbf{q},\omega)\Big(\phi_{ex}(\mathbf{q},\omega) + \frac{4\pi}{q^2}\delta\rho_{el}(\mathbf{q},\omega)\Big).\end{aligned} \tag{5}$$

Hence,

$$\delta\rho_{el}(\mathbf{q},\omega) = -\frac{e^2\chi_{el}^0(\mathbf{q},\omega)}{\epsilon_e(\mathbf{q},\omega)}\phi_{ex}, \tag{6}$$

where ϵ_e is the dielectric function from electron-electron interactions

$$\epsilon_e(\mathbf{q},\omega) = 1 + \frac{4\pi e^2}{q^2}\chi_{el}^0(\mathbf{q},\omega). \tag{7}$$

In the static limit at $q \ll k_f$, it becomes the Thomas-Fermi form as

$$\epsilon_{TF} = 1 + \frac{k_{TF}^2}{q^2}, \quad k_{TF}^2 = 4\pi e^2 N_0/(1+F_s^0), \tag{8}$$

where the k_{TF} is the TF screening wavevector. This renormalizes the long-range Coulomb interaction into the short-ranged Yukawa potential with its Fourier transform as

$$V_{sc}(r) = \frac{e^2}{r}e^{-k_{TF}r} \longrightarrow V_{sc}(q) = \frac{4\pi e^2}{q^2+k_{TF}^2}. \tag{9}$$

2 Phonon-dressed dielectric function

In this part, we consider the lattice ions' contribution to the dielectric function, which also carry charge. We neglect the lattice structure, and pretend the positive ions as a continuum media, i.e., in the viewpoint of the Jellium model. But now the positive charges are mobile, and then the electron-ion systems are modeled as a two-component neutral plasma. If the conduction electrons are frozen, then the ions in metal would exhibit a gapped plasmon frequency

$$\Omega_p^2 = \frac{4\pi n Z^2 e^2}{M} \approx \frac{m_e}{M}Z\omega_p^2, \tag{10}$$

where n is the ion density, $\omega_p^2 = 4\pi n_e e^2/m_e$ is electron plasmon frequency with $n_e = Zn$. Typically, Ω_p is at the order of Debye frequency, say, $10^{13}Hz$, or, at the room temperature. Actually, the phonons in metals are gapless, which is a consequence of screening from mobie electrons, and the electron dielectric function diverges as $q \to \infty$. Overall, the electron-ion systems are neutral, hence, the low energy excitations should be linear like sound waves in the same class of phonons. Below we will show how to derive the renormalized phonon dispersion based on a 2-component plasma model. Certainly, only the longitudinal acoustic phonons can be obtained via this effective method. Due to the hydrodynamic nature of this method, the transverse phonon modes cannot be obtained.

Next step, we use the molecular field method again to include the additional channel from ions and its long-range Coulomb potential. We define $\chi^0_{ion}(\mathbf{k},\omega)$ as the density-density response function before taking into account the Coulomb interaction, which is due to the short range interactions among ions. Suppose an external perturbation $\phi_{ex}(\mathbf{r},t)$ is applied to the systems, and the density fluctuations of electrons and ions are defined as $\delta\rho_{el}$ and $\delta\rho_{ion}$. Then the electron and ion responses are coupled as

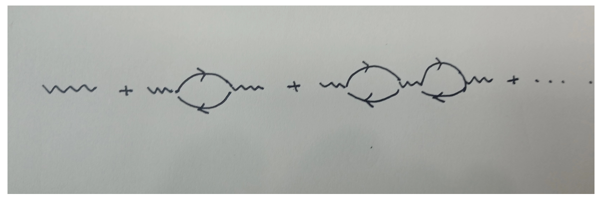


Figure 1: Random phase approximation of dielectric function as a feedback effect of molecular field theory.

$$
\begin{aligned}
\delta\rho_{el} &= -e\chi^0_{el}(e\phi_{tot}) = -e^2\chi^0_{el}(\phi_{ex}+\phi_{ind}),\\
\delta\rho_{ion} &= -Ze\chi^0_{ion}(Ze)\phi_{tot} = -Z^2e^2\chi^0_{el}(\phi_{ex}+\phi_{ind}),\\
\nabla^2\phi_{ind} &= -4\pi(\delta\rho_{el}+\delta\rho_{ion}),
\end{aligned}
\tag{11}
$$

where ρ_{el},ρ_{ion} are charge densities. Transform into the Fourier space, we arrive at

$$
\begin{aligned}
\delta\rho_{el}(\mathbf{q},\omega) &= -e^2\chi^0_{el}(\mathbf{q},\omega)\Big[\phi_{ex} - \frac{4\pi}{q^2}(\delta\rho_{el}(\mathbf{q},\omega)+\delta\rho_{ion}(\mathbf{q},\omega))\Big]\\
\delta\rho_{ion}(\mathbf{q},\omega) &= -(Ze)^2\chi^0_{ion}(\mathbf{q},\omega)\Big[\phi_{ex} - \frac{4\pi}{q^2}(\delta\rho_{el}(\mathbf{q},\omega)+\delta\rho_{ion}(\mathbf{q},\omega))\Big],
\end{aligned}
\tag{12}
$$

and then we have

$$
\begin{aligned}
\delta\rho_{el}(\mathbf{q},\omega) = -e^2\chi^0_{el}(\mathbf{q},\omega)\frac{\phi_{ex}(\mathbf{q},\omega)}{\epsilon(q,\omega)},\\
\delta\rho_{ion}(\mathbf{q},\omega) = -(Ze)^2\chi^0_{ion}(\mathbf{q},\omega)\frac{\phi_{ex}(\mathbf{q},\omega)}{\epsilon(q,\omega)},
\end{aligned}
\tag{13}
$$

where the dielectric function becomes

$$
\epsilon_{ep}(\mathbf{q},\omega) = 1 + \frac{4\pi e^2}{q^2}\Big(\chi^0_{el}(\mathbf{q},\omega) + Z^2\chi^0_{ion}(\mathbf{q},\omega)\Big). \tag{14}
$$

The first term in the parenthesis is the contribution from electrons at the RPA level, which equals k_{TF}^2/q^2 in the static limit under the Thomas-Fermi approxiation, and the 2nd one is from the positive ions.

How about the ion response? Ions are heavy, and we use the hydrodynamic method to describe their response.

$$\frac{\partial \rho_{ion}}{\partial t} = -\nabla \cdot \vec{j}_{ion}, \quad \frac{\partial \vec{j}_{ion}}{\partial t} = -\frac{n}{m} \nabla V_{ex}. \tag{15}$$

For the ion's Jellium model, there is no other forces than the Coulomb force, which has been taken in the above self-consistent molecule field theory, and, hence, should not be taken into account again. We have

$$\begin{aligned} -i\omega\delta\rho_{ion}(q,\omega) &= -\mathbf{q} \cdot \mathbf{J}(q,\omega) \\ -i\omega J(q,\omega) &= -\frac{n}{m} iqV_{ex}(q,\omega), \end{aligned} \tag{16}$$

then we have $\delta\rho_{ion}(q,\omega) = nq^2/(m\omega^2)V_{ex}(q,\omega)$, hence,

$$\chi^0_{ion}(q,\omega) = -\frac{nq^2}{M\omega^2}. \tag{17}$$

Hence, the total express of $\epsilon(q,\omega)$ is

$$\epsilon(\mathbf{q},\omega) = 1 - \frac{\Omega_p^2}{\omega^2} + \frac{k_{TF}^2}{q^2}. \tag{18}$$

3 Renormalized phonon spectra

The screening due to electrons significantly changes the phonon spectra from a gapped plasmon type excitation to gapless sound-like excitation at $q \to 0$. It also leads to Peierls instability at $q \to 2k_f$.

3.1 Bohm-Staver formula

We extract the phonon dispersion from the pole of the the response function of ions,

$$\chi_{ion}(\mathbf{q},\omega) = \frac{-nq^2/(M\omega^2)}{1 + \frac{k_{TF}^2}{q^2} - \frac{\Omega_p^2}{\omega^2}} \approx \frac{-nq^2/(M\omega^2)}{\frac{k_{TF}^2}{q^2} - \frac{\Omega_p^2}{\omega^2}} = -\frac{q^2}{k_{TF}^2} \frac{nq^2/M}{\omega^2 - c^2q^2}, \tag{19}$$

where $\omega_{ph} = cq$ and $c = \frac{\Omega_p}{k_{TF}}$. The sound velocity c is much smaller than the Fermi velocity as

$$\frac{c}{v_f} = \frac{\Omega_p}{v_f k_{TF}} = \Big(\frac{4\pi e^2 Z^2 n_{ion}}{M} \frac{1+F_0^s}{4\pi e^2 N_0 v_f^2}\Big). \tag{20}$$

Plug in $N_0 = \frac{3n_e}{m^* v_f}$ and $n_e = nZ$, we have

$$\frac{c}{v_f} = (\frac{m^* Z(1+F_0^s)}{3M})^{\frac{1}{2}} \sim (m^*/M)^{\frac{1}{2}} \sim 10^{-2}. \tag{21}$$

Here we should not take Z as the actual atomic number, since the inner core electrons screen the nuclear charge. Z remains at the order of 1 for outer shell electrons.

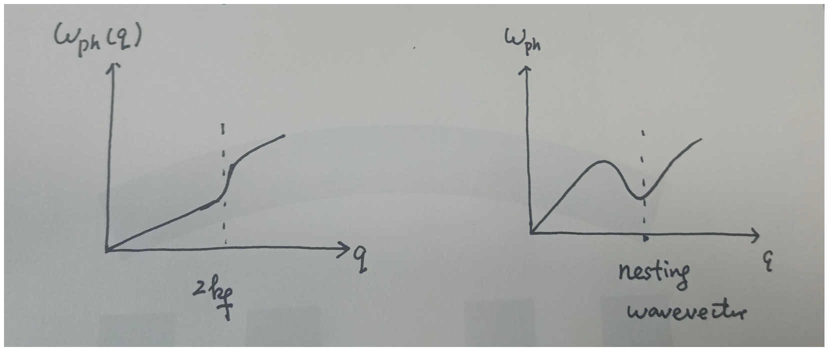


Figure 2: Phonon frequency renormalization due to electron-electron interaction

3.2 Kohn's anomaly

The static limit of the Lindhardt response function can be solved as

$$\begin{aligned} \epsilon(q,\omega=0) &= 1+\frac{k_{TF}^2}{q^2}\Big(\frac{1}{2}+\frac{1}{4x}(1-x^2)\ln|\frac{1+x}{1-x}|\Big), \\ &\longrightarrow 1+\frac{k_{TF}^2}{8k_f^2}\Big(1-(1-x)\ln|\frac{1-x}{2}|\Big) \quad \text{as} \quad (x\to 1) \end{aligned} \tag{22}$$

where $x=\frac{q}{2k_f}$. It has an infinite negative slope at $q=2k_f$, leading to

$$\frac{\partial\epsilon}{\partial q}\sim \ln|1-x| \to -\infty, \tag{23}$$

hence, the phonon dispersion $\frac{\partial\omega_{ph}(q)}{\partial q}$ also has logarithmic divergence in its slope at $q=2k_f$ as shown in Fig. 2.

On the other hand, if there exist Fermi surface nesting at $q=2k_f$, then $\epsilon(q=2k_f,0)$ is enhanced, and in this case phonon is softened. For example, in 1D polyacetylene polymers, $\epsilon(q,0)$ diverges logarithmically as $q\to 2k_f$ leading to the condensation of phonons at $q=2k_f$, and this is the Peierls instability.

4 Effective electron-electron interaction

Taking into account the phonon dressing, the screened Coulomb interaction is qualitatively changed as

$$\begin{aligned} V_{eff}(\mathbf{q},\omega) &= \frac{4\pi e^2/q^2}{1+\frac{k_{TF}^2}{q^2}-\frac{\Omega_p^2}{\omega^2}} = \frac{4\pi e^2}{q^2+k_{TF}^2}\Big(1+\frac{q^2\Omega^2/\omega^2}{q^2+k_{TF}^2-q^2\Omega^2/\omega^2}\Big) \\ &\approx \frac{4\pi e^2}{q^2+k_{TF}^2}\Big(1+\frac{\frac{\Omega_p^2}{k_{TF}^2}q^2}{\omega^2-\frac{\Omega_p^2}{k_{TF}^2}q^2}\Big) \\ &= V_{sc}(q)(1+\frac{\omega_{ph}^2(q)}{\omega^2-\omega_{ph}^2(q)}). \end{aligned} \tag{24}$$

The 2nd term is due to electron-phonon interaction, which generates an attractive interaction at $\omega < \omega_{ph}(q)$.

Now let us use a 2nd quantization method to formulate electron-phonon interaction. Write the electron-photon interaction Hamiltonian as

$$H_{eph} = \sum_{kq,\sigma} g(k,q) c^\dagger_{k+q,\sigma} c_{k,\sigma} (a^\dagger_q + a_{-q}).$$

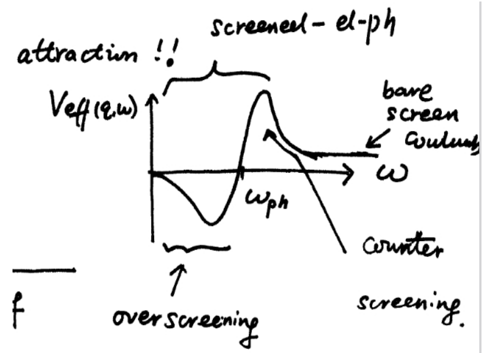


Figure 3: The plot of retarded electron-electron interaction renormalized by electron-phonon interaction

Consider the process that in the initial state $|i\rangle$ of an electron pair with momenta $\mathbf{k}$ and $-\mathbf{k}$ scattering to the final state $|f\rangle$ of another electron pair with momenta $\mathbf{k}+\mathbf{q}$ and $-\mathbf{k}-\mathbf{q}$ via exchanging a phonon. There are two possible processes of scattering: 1) The electron $\mathbf{k}$ first emits a phonon of $-\mathbf{q}$ and its momentum changes to $\mathbf{k}+\mathbf{q}$, then the electron $-\mathbf{k}$ absorbs that phonon and changes to $-\mathbf{k}-\mathbf{q}$. The intermediate state energy is $E_{m1} = \epsilon(k+q) + \epsilon(-k) + \hbar\omega_{-q}$. 2) The electron $-\mathbf{k}$ first emits a phonon of $\mathbf{q}$ and its momentum changes to $-\mathbf{k}-\mathbf{q}$, then the electron $\mathbf{k}$ absorbs that phonon and changes to $\mathbf{k}+\mathbf{q}$. The intermediate state energy is $E_{m2} = \epsilon(k) + \epsilon(-k-q) + \hbar\omega_{-q}$. The energies of the initial and final states are $E_i = \epsilon(k) + \epsilon(-k)$ and $E_f = \epsilon(k+q) + \epsilon(-k-q)$. The scattering matrix elements become

$$\begin{aligned}
\langle f|H_{eph}|i\rangle &= \sum_{i=1,2} \langle f|H_{eph}|m_i\rangle\langle m_i|H_{eph}|i\rangle \frac{1}{2}\Big(\frac{1}{E_i - E_{m_i}} + \frac{1}{E_f - E_{m_i}}\Big) \\
&= \frac{|g(k,q)|^2}{2\hbar}\Big(\frac{1}{\epsilon_k - \epsilon_{k+q} - \hbar\omega_{-q}} + \frac{1}{\epsilon_{-k-q} - \epsilon_{-k} - \hbar\omega_{-q}} \\
&+ \frac{1}{\epsilon_{-k} - \epsilon_{-k-q} - \hbar\omega_{-q}} + \frac{1}{\epsilon_{k+q} - \epsilon_k - \hbar\omega_{-q}}\Big) \\
&= |g(k,q)|^2 \frac{2\hbar\omega_q}{(\epsilon_k - \epsilon_{k+q})^2 - (\hbar\omega_q)^2}.
\end{aligned} \tag{25}$$

By comparing with Eq. 24 and identifying $\hbar\omega = \epsilon_k - \epsilon_{k+q}$, we arrive at

$$|g(k,q)|^2 = \frac{2\pi e^2}{q^2 + k_{TF}^2}\hbar\omega_q \approx \frac{1}{2}\Big(\frac{\partial n}{\partial \mu}\Big)^{-1}\hbar\omega_q \propto q \tag{26}$$

in the long wavelength limit.

5 Overscreening

An remarkable feature of the above phonon-dressed screen Coulomb interaction $V_{eff}(q,\omega)$ is that it becomes attractive in the frequency region $\omega < \omega_{ph}(q,\omega)$. How to understand this?

Let us use a simple model for ions as a harmonic oscillator driven by its coupling to electrons. The chemical bonding provides a frequency ω_0, which does not take into account the Coulomb potential. The equation of motion of the ions

$$\ddot{x} + \omega_0^2 x + \gamma \dot{x} = \frac{ZeE}{M} e^{-i\omega t}, \qquad (27)$$

where $Ee^{-i\omega t}$ is the total electric field, and γ is the friction coefficient. According to the E&M theory, we have

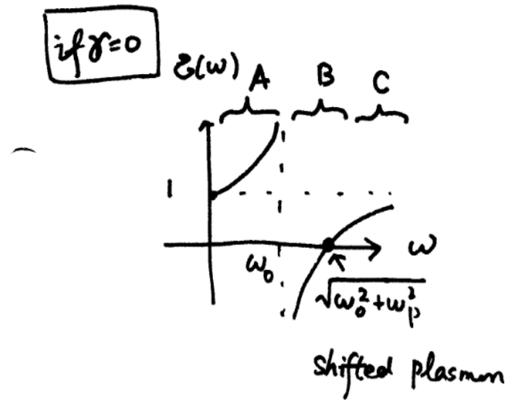


Figure 4: The dielectric function $\epsilon(\omega)$ v.s. ω.

$$P = (Ze)nx = \chi_0 E, \quad E_{ind} = -4\pi P, \quad E = E_0 + E_{ind} = E_0 - 4\pi Zenx. \qquad (28)$$

where P is the polarizations, E_{ind} is the induce field due to polarization, and E_0 is the driving field. The solution of the equation of motion is

$$\begin{aligned} x(\omega) &= \frac{ZeE}{m}\frac{1}{\omega_0^2 - \omega^2 - i\omega\gamma}, \\ \chi_0(\omega) &= \frac{P(\omega)}{E(\omega)} = \frac{Zenx(\omega)}{E(\omega)} = \frac{n(Ze)^2E}{M}\frac{1}{\omega_0^2 - \omega^2 - i\omega\gamma} = \frac{1}{4\pi}\frac{\Omega_P^2}{\omega_0^2 - \omega^2 - i\omega\gamma}, \\ \epsilon(\omega) &= 1 + 4\pi\chi_0(\omega) = 1 + \frac{\Omega_P^2}{\omega_0^2 - \omega^2 - i\omega\gamma}, \\ E_{ind} &= E_0 - E = \frac{\epsilon(\omega) - 1}{\epsilon(\omega)} E_0. \end{aligned} \qquad (29)$$

The actual excitation energy is the determined by the zero of $\epsilon(\omega) = 0$, i.e.,

$$\omega^{\prime,2} = \omega_0^2 + \Omega^2. \qquad (30)$$

This can be understood by the fact that E's dependence on x, i.e.,

$$\ddot{x} + \omega_0^2 x + \gamma x = \frac{ZeE_0}{M} e^{-i\omega t} - 4\pi\frac{(Ze)^2 n}{M} x, = \frac{ZeE_0}{M} e^{-i\omega t} - \Omega^2 x. \qquad (31)$$

According to the behavior of the dielectric function ϵ, we divide the entire frequency into three regions. The relation between E_0, E_{ind}, and E are depicted in Fig. #.

(A)Under-screening $\omega < \omega_0$ in which $\epsilon(\omega) > 1$ and $\chi(\omega) > 0$. In this low frequency region, the polarization is in phase with the total E-field – the ions can follow with the driving. We have $\chi_0 > 0$ and $\epsilon > 1$. Suppose that the driving field E_0 is generated by an electron. After its coupling with phonons, E is weakened compared to E_0 by the polarization field E_{ind}. It remains parallel to E_0 and thus still repels the 2nd electron. In this region, the refraction index $n(\omega) = \sqrt{\epsilon(\omega)} > 1$.

(B) Overscreening $\omega_0 < \omega < \omega'$ in which $-\infty < \epsilon(\omega) < 0$ and $\chi(\omega) < 0$. Since the driving frequency ω is closer to the excitation energy, the polarization P increases such that the polarization field E_{ind} overcomes the driving field E_0, such that E is anti-parallel to E_0, hence it becomes to attract the 2nd electron. In this region, $\epsilon = i\sqrt{|\epsilon|}$, and E&M modes cannot propagate.

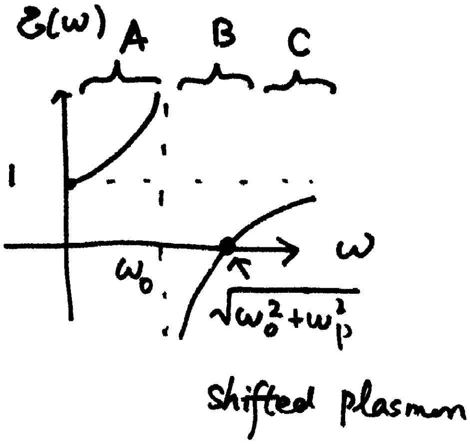
(C) Counter-screening at $\omega > \omega'$, in which $0 < \epsilon(\omega) < 1$ and $\chi < 0$. In this region, the polarization P is has a π-phase difference with E_0, such that the polarization field E_{ind} is parallel to E_0. Hence, it even enhances E_0. In this high frequency region, electrons repel even stronger. The refraction index $0 < n(\omega) < 1$.

For the jellium model of ions, ω_0 is zero. On the other hand, Ω is softened to $\omega_{ph} = q/k_{TF}\Omega$ by the screening from electrons. Hence, we have $\epsilon_{ion} = 1 + \frac{\omega_{ph}^2}{-\omega^2}$. It contributes the factor of

$$\frac{1}{\epsilon_{ion}} = \frac{\omega^2}{\omega^2 - \omega_{ph}^2} \tag{32}$$

in Eq. 24.

if $\gamma = 0$

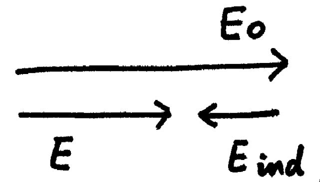


$E_{ind} \parallel -E$

Region A:

under-screening, $\chi > 0$

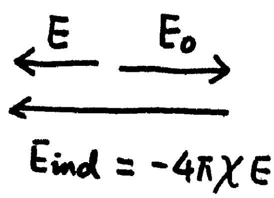
$- E_{ind} \parallel E \parallel E_0$



$|E_{ind}| < |E_0|$.

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

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



$E \parallel -E_0$ ↑ $-4\pi\chi > 1$

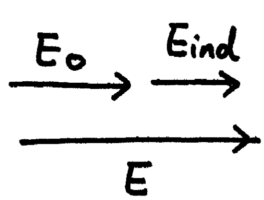
$E_{ind} \parallel E$ and $E_{ind} > E$ ←

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 $0 < -4\pi\chi < 1$)



$E_{ind} \parallel E$ and $E_{ind} < E$ $\Rightarrow$ 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:

$$\frac{\lambda e^2}{q^2+k_{TF}^2} = \frac{v_q}{\varepsilon(q,\omega)}$$: 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.