2. INTERAZIONE ELETTRONE-FONONE IN SECONDA QUANTIZZAZIONE

12/10/2015

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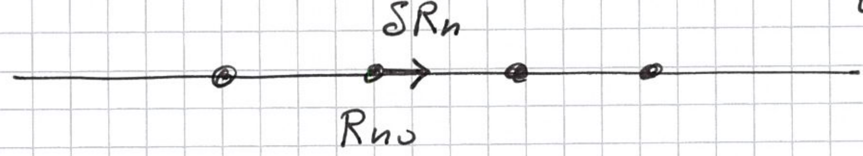
The Electron-Phonon Hamiltonian

§ 1. Second quantization for Phonons

[D. Pines, Elementary Excitations in Solids]



(1d)

$$H = \sum_i \frac{P_i^2}{2M} + \frac{1}{2}\sum_{i\neq j} V(R_i - R_j)$$

$$H = \sum_i \frac{P_i^2}{2M} + \frac{1}{2}\sum_{i\neq j} V(R_{i0} - R_{j0}) + \sum_{i,j} \frac{A_{ij}}{2}\,\delta R_i \delta R_j$$

$$A_{ij} = \frac{\partial^2 V(R_i - R_j)}{\partial R_i \partial R_j}$$

$$A_{ii} = \sum_{\substack{j \\ (j\neq i)}} \frac{\partial^2 V(R_i - R_j)}{\partial R_i^2}$$

The equation of motion for the i-th atom is

$$\dot{P}_i = M\,\delta\ddot{R}_i = -\frac{\partial H}{\partial R_i} = -\sum_j A_{ij}\,\delta R_j$$

Considering oscillatory solutions

$$\delta R_i(t) = e^{-i\omega t}\,\delta R_i$$

$$M\omega^2 \delta R_i = \sum_j A_{ij}\,\delta R_j$$

Considering a Fourier expansion for δR_n

$$\delta R_n = \sum_k q_k\, e^{ikR_{n0}}$$

we obtain a dispersion relation

$$M\omega_k^2 = \sum_j A_{ij}\, e^{ik(R_{j0}-R_{i0})}$$

Introducing normal coordinates (p_k, q_k) in the following way

$$P_i = \sqrt{\frac{M}{N}} \sum_k p_k\, e^{ik\cdot R_{i0}}$$

$$\delta R_i = \frac{1}{\sqrt{NM}} \sum_k q_k\, e^{ikR_{i0}}$$

$$\left[\ q_k = \sqrt{\frac{M}{N}} \sum_i \delta R_i\, e^{-ikR_{i0}}\ \right]$$

From the reality condition of P_i and δR_i we have

$$p_k^+ = p_{-k}$$

$$q_k^+ = -q_{-k}$$

The Hamiltonian can be rewritten as

$$H = \sum_k \frac{p_k^+ p_k}{2} + \omega_k^2 \frac{q_k^+ q_k}{2}$$

Quantization: commutation rules

$$[P_i, \delta R_j] = \frac{\hbar}{i}\delta_{ij}$$

$$[P_i, P_j] = [R_i, R_j] = 0$$

from these we obtain

$$[p_k, q_{k'}] = \frac{\hbar}{i}\delta_{kk'}$$

$$[p_k, p_{k'}] = [q_k, q_{k'}] = 0$$

We now introduce a^+ and a according to the following transformation

$$p_k = i\sqrt{\frac{\hbar\omega_k}{2}}\left(a_k^+ - a_{-k}\right)$$

$$q_k = \sqrt{\frac{\hbar}{2\omega_k}}\left(a_k + a_{-k}^+\right)$$

one can see that

$$a_k^+ = \frac{1}{\sqrt{2\omega_k\hbar}}\left(\omega q_{-k} - i p_k\right) =$$

$$= \frac{1}{\sqrt{2\omega_k\hbar}}\left[\omega_k\sqrt{\frac{\hbar}{2\omega_{-k}}}\left(a_{-k} + a_k^+\right) - i\cdot i\sqrt{\frac{\hbar\omega_k}{2}}\left(a_k^+ - a_{-k}\right)\right]$$

and

$$a_k = \frac{1}{\sqrt{2\omega_k\hbar}}\left(\omega_k q_k + i p_{-k}\right) =$$

$$= \frac{1}{\sqrt{2\omega_k\hbar}}\left[\omega_k\sqrt{\frac{\hbar}{2\omega_{-k}}}\left(a_k + a_{-k}^+\right) + i\cdot i\sqrt{\frac{\hbar\omega_{-k}}{2}}\left(a_{-k}^+ - a_k\right)\right]$$

$$[a_k, a_{k'}^+] = \delta_{kk'}$$

$$[a_k, a_{k'}] = [a_k^+, a_{k'}^+] = 0$$

and we can rewrite the Hamiltonian

$$H = \sum_k \hbar\omega_k \left[a_k^+ a_k + \frac{1}{2}\right]$$

$$N_k^{op} = a_k^+ a_k$$

$$N_k^{op} |n_k\rangle = n_k |n_k\rangle$$

From the properties of the Harmonic oscillator wavefunctions

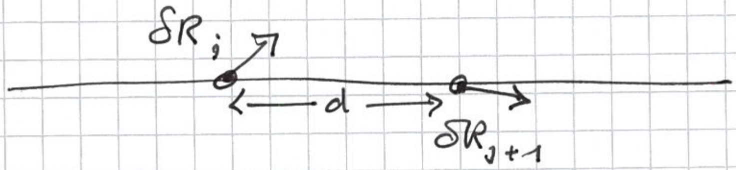
$$(P_k = \sqrt{M} p_k) \quad \langle n_k | P_k | n_k + 1\rangle = -\langle n_k + 1 | P_k | n_k\rangle = -i \left(\frac{n_k + 1}{2}\right)^{1/2}$$

$$\left(Q_k = \frac{q_k}{\sqrt{M}}\right) \quad \langle n_k | Q_k | n_k + 1\rangle = \langle n_k + 1 | Q_k | n_k\rangle = \left(\frac{n_k + 1}{2}\right)^{1/2}$$

From these relations

$$\langle n_k | a_k | n_k + 1\rangle = \langle n_k + 1 | a_k^+ | n_k\rangle = (n_k + 1)^{1/2}$$

$$\begin{cases} a_k |n_k\rangle = \sqrt{n_k}\, |n_k - 1\rangle \\ a_k^+ |n_k\rangle = \sqrt{n_k + 1}\, |n_k + 1\rangle \\ a_k |0\rangle = 0 \end{cases}$$



$$\delta R_j = \sum_k \sqrt{\frac{\hbar}{2MN\omega_k}} \left(a_k + a_{-k}^+\right) e^{ikR_{j0}}$$

$$\delta R_{j+1} = \sum_k \sqrt{\frac{\hbar}{2MN\omega_k}} \left(a_k + a_{-k}^+\right) e^{i(kR_{j0} + k_x d)}$$

$$\delta R_j - \delta R_{j+1} = \sum_k \sqrt{\frac{\hbar}{2MN\omega_k}} \left(a_k + a_{-k}^+\right)\left(1 - e^{ik_x d}\right)$$

$$\langle |\delta R_j - \delta R_{j+1}|^2 \rangle = \frac{\hbar}{2MN} \sum_{k,k'} \frac{\left(a_k + a_{-k}^+\right)}{\sqrt{\omega_k}} \left(1 - e^{-ik_x d}\right) \times$$

$$\times \frac{\left(a_{k'} + a_{-k'}^+\right)}{\sqrt{\omega_{k'}}} \left(1 - e^{ik'_x d}\right)$$

Taking the thermal average we have

$$\left\langle |\delta R_j - \delta R_{j+1}|^2 \right\rangle = \frac{\hbar}{2MN} \frac{\langle a_k^+ a_k \rangle + \langle a_{-k} a_{-k}^+ \rangle}{\omega_k} \times \left(1 - \cos k_x d\right) =$$

$$= \frac{\hbar}{MN} \sum_k \frac{n(k) + 1/2}{\omega_k} \left(1 - \cos k_x d\right)^{2}$$

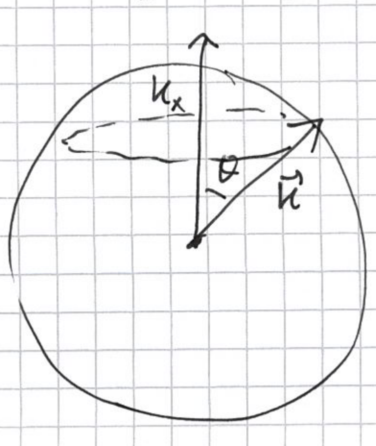
$$n(k) = \frac{1}{e^{\hbar\omega_k/k_B T} - 1} \qquad \text{Bose Einstein distribution}$$

$$\langle |\delta R_j - \delta R_{j+1}|^2 \rangle \simeq \frac{k_B T}{MN} \sum_k \frac{\left(1 - \cos k_x d\right)^{2}}{\omega_k^2}$$

having taken the high T limit

$$k_B T \gg \hbar\omega_k \longrightarrow n(k) \simeq \frac{k_B T}{\hbar\omega_k} \gg 1$$

$$k_x = |\vec{k}| \cos\theta \qquad |\vec{k}| = k$$



$$\sum_{\vec{k}} \frac{k_x^2}{\omega_k^2} = \int^{\pi} \cos^2\theta \sin\theta \, d\theta \int_0^{k_{max}} dk \frac{k^2}{\omega_k^2}$$

For acoustic modes $\omega_k \sim v k$

Considering an isotropic $\cancel{3}$D $\overset{\text{dimensional}}{\vphantom{x}}$ system

$$\langle |\delta R_j|^2 \rangle = \frac{k_B T}{MN} \sum_k \frac{1}{\omega_k^2}$$

3D $$\langle |\delta R_j|^2 \rangle = \frac{k_B T}{MNv^2} \int_0^{k_{MAX}} \frac{k^2 dk}{k^2} \simeq \frac{k_B T}{MNv^2} k_{MAX} \quad \underline{\underline{\text{finite}}}$$

1D $$\sum_k \sim \int_0^{k_{MAX}} dk$$

$$\langle |\delta R_j|^2 \rangle \sim \int_0^{k_{MAX}} \frac{dk}{k^2} \rightarrow \infty \sim N \quad \left(k_{min} = \frac{2\pi}{N} \right)$$

2D $$\langle |\delta R_j|^2 \rangle \sim \int_0^{k_{MAX}} \frac{dk}{k} \rightarrow \infty \sim \log N$$

$\rightarrow$ <u>Mermin & Wagner Theorem</u>

2. Second Quantization for Electrons

Electron density response to an applied field
Electronic Hamiltonian

$$H_0 = H_{el} = \sum_k \varepsilon_k b_k^+ b_k$$

when the fermion operators satisfy the anticommutation relations

$$\begin{cases} [b_k^+, b_{k'}^+]_+ = b_k^+ b_{k'}^+ + b_{k'}^+ b_k^+ = 0 \\ [b_k, b_{k'}]_+ = 0 \\ [b_k^+, b_{k'}] = \delta_{k,k'} \end{cases}$$

and ε_k is the energy band for the state k

Consider now a scalar potential $\phi(x)$ [in which we consider the term $(-e)$ included into ϕ].
The corresponding Hamiltonian is

$$H' = \sum_j \phi(x_j) = \int \phi(x) \{ \sum_j \delta(x - x_j) \} dx$$

where x_j is the position of the j-th electron.

$$\rho(x) = \sum_j \delta(x - x_j)$$

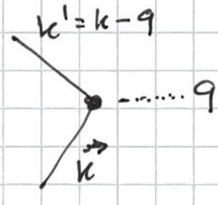
The field operators to create and destroy an electron at position x are

$$\begin{cases} \psi^+(x) = \frac{1}{\sqrt{L}} \sum_k b_k^+ e^{-ikx} \\ \psi(x) = \frac{1}{\sqrt{L}} \sum_k b_k e^{ikx} \end{cases}$$

The density operator is then

$$\rho(x) = \psi^{+}(x)\psi(x) = \frac{1}{L}\sum_{k,k'} b^{+}_{k'} b_k \, e^{i(k-k')x} =$$

$$= \frac{1}{L}\sum_q \rho_q \, e^{-iqx}$$



where

$$\rho_q = \sum_k b^{+}_{k-q} b_k$$

and $q = k - k'$

We can write

$$\phi(x) = \frac{1}{L}\sum_k \phi_k \, e^{ikx}$$

and therefore

$$H' = \int dx\, \phi(x)\rho(x) = \int dx \frac{1}{L}\sum_{k'} e^{ik'x}\phi_{k'} \frac{1}{L}\sum_q e^{iqx}\rho_q =$$

$$= \frac{1}{L^2}\int dx \sum_{k',q} e^{i(k'+q)x}\phi_{k'}\rho_q$$

Since

$$\frac{1}{L}\int dx\, e^{i(k'+q)} = \delta(k'+q)$$

we obtain

$$H' = \frac{1}{L}\sum_{k,q}\phi_{k'}\rho_q \, \delta(k'+q) = \sum_q \phi_{-q}\rho_q$$

For a sinusoidal potential we have therefore

$$H' = \phi_q \rho_{-q} + \phi_{-q}\rho_q$$

We study now the effect of this potential on the electron number density. Consider the electron hole pair of momentum $-\hbar q$ described by the operator

$$\rho_{kq} = b^{+}_{k-q}\, b_k$$

The equation of motion for ρ_{kq} is

$$i\hbar\, \dot{\rho}_{kq} = [\rho_{k,q}, H]_- = [\rho_{kq}, H_0] + [\rho_{k,q}, H'] \neq$$

$$[\rho_{kq}, H_0] = b^{+}_{k-q}\, b_k \sum_{k'} \varepsilon_{k'}\, b^{+}_{k'} b_{k'} - \sum_{k'} \varepsilon_{k'} b^{+}_{k'}\, b_{k'}\, b^{+}_{k+q}\, b_k =$$

$$= \sum_{k'} \varepsilon_{k'} \{ b^{+}_{k-q}\, \underbrace{b_k\, b^{+}_{k'}}\, b_{k'} - b^{+}_{k'} \underbrace{b_{k'}\, b^{+}_{k-q}}\, b_k \}$$

Now we can write from the commutators

$$\begin{cases} b_k b^{+}_{k'} = \delta_{kk'} - b^{+}_{k'}\, b_k \\ b_{k'}\, b^{+}_{k-q} = \delta_{k';k-q} - b^{+}_{k-q}\, b_{k'} \end{cases}$$

and therefore

$$[\rho_{k,q}, H_0] = \sum_{k'} \varepsilon_{k'} \{ \delta_{kk'}\, b^{+}_{k-q}\, b_{k'} - b^{+}_{k-q} b^{+}_{k'}\, b_k b_{k'} -$$

$$- \delta_{k';k-q}\, b_{k'} b_k + b^{+}_{k'}\, b^{+}_{k-q}\, b_{k'} b_k \} =$$

$$= (\varepsilon_k - \varepsilon_{k-q})\, \rho_{kq}$$

For the perturbing Hamiltonian we have

$$[\rho_{kq}, H'] = \phi_q \left(b^+_{k-q} b_k \sum_{k'} b^+_{k'+q} b_{k'} - \sum_{k'} b^+_{k+q} b_{k'} b^+_{k-q} b_k \right) +$$

$$+ \phi_{-q} \left(b^+_{k-q} b_k \sum_{k'} b^+_{k'-q} b_{k'} - \sum_{k'} b^+_{k'-q} b_{k'} b^+_{k-q} b_k \right) =$$

$$= \phi_q \left(b^+_{k-q} b_{k-q} - b^+_k b_k \right) + \phi_{-q} \left(b^+_{k-q} b_{k+q} - b^+_{k-2q} b_k \right)$$

The linear response can be computed by taking the thermodynamic average $\langle \cdots \rangle$ of the various terms and considering that for a static potential

$$\langle \dot{\rho}_{kq} \rangle = 0$$

This gives

$$(\varepsilon_k - \varepsilon_{k-q}) \langle \rho_{kq} \rangle + \left[\langle b^+_{k-q} b_{k-q} \rangle - \langle b^+_k b_k \rangle \right] \phi_q = 0$$

and since

$$\rho_q = \sum_k \rho_{kq}$$

we obtain for the density response

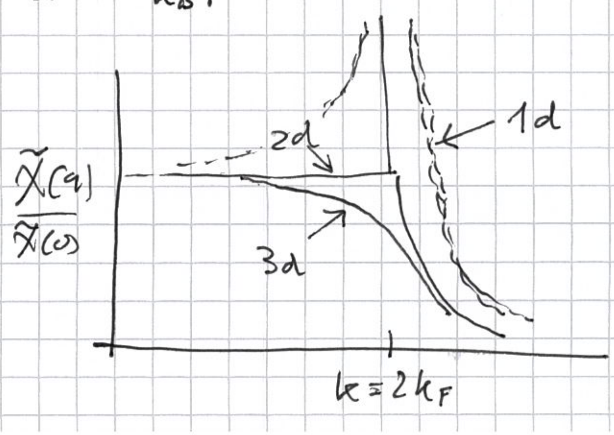
$$\tilde{\chi}(q) = \frac{\langle \rho_q \rangle}{\phi_q} = \sum_k \left[\frac{f_{k-q} - f_k}{\varepsilon_{k-q} - \varepsilon_k} \right] = \sum_k \left(\frac{f_{k+q} - f_k}{\varepsilon_{k+q} - \varepsilon_k} \right)$$

when f_k is the Fermi function

[* Compare Thomas Fermi]

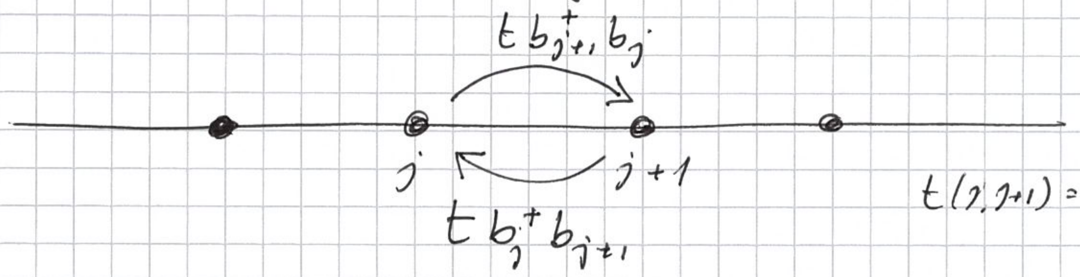
$$f_k = \langle b^+_k b_k \rangle = \frac{1}{\left[\exp\left(\frac{\varepsilon_k - \varepsilon_F}{k_B T} \right) + 1 \right]}$$

$\tilde{\chi}(q)$ Lindhard response function



3. The Electron - Phonon Interaction

Consider a tight binding Hamiltonian in second quantization



$t(j,j+1) = t$

$x_{j+1} - x_j = d = \frac{L}{N}$

$$H = -\sum_j t(j,j+1)\left\{ b^+_j b_{j+1} + b^+_{j+1} b_j \right\}$$

$$\begin{cases} b^+_j = \frac{1}{\sqrt{N}} \sum_k e^{-ikx_j}\, b^+_k \\ b_j = \frac{1}{\sqrt{N}} \sum_k e^{ikx_j}\, b_k \end{cases}$$

$$H = -\sum_j t \left\{ \frac{1}{N} \sum_k e^{-ikx_j}\, b^+_k \sum_{k'} e^{ik'x_{j+1}}\, b_{k'} + \right.$$

$$\left. + \frac{1}{N} \sum_k e^{-ikx_{j+1}}\, b^+_k \sum_{k'} e^{ikx_j}\, b_{k'} \right\} =$$

$$= -t \sum_k \left\{ e^{ikd}\, b^+_k b_k + e^{-ikd}\, b^+_k b_k \right\} =$$

$$= \sum_k \varepsilon_k\, b^+_k b_k \quad ; \quad \varepsilon_k = (-2t) \cos kd$$

$$k = 2\pi n / L$$

$$-\frac{\pi}{d} \leq k \leq \frac{\pi}{d}$$

$$t(j,j+1) = \langle \phi_A(r - R_{j+1}) | V_{j,j+1} | \phi_A(r - R_j) \rangle$$

$$t(j,j+1) \simeq t^0 + t^{(1)}(u_{j+1} - u_j)$$

$$t^{(1)} = \frac{dt}{d(\delta u)}$$

$$H^{(1)} = -\sum_j t^{(1)} (u_{j+1} - u_j) \{ b_j^+ b_{j+1} + b_{j+1}^+ b_j \}$$

$$u_j = \frac{1}{\sqrt{N}} \sum_q Q_q e^{iqR_j} = \sum_q \sqrt{\frac{\hbar}{2mN\omega_q}} (a_q + a_{-q}^+) e^{iqR_j}$$

$$u_{j+1} - u_j = \sum_q \underbrace{\sqrt{\frac{\hbar}{2mN\omega_q}} (a_q + a_{-q}^+)(e^{iqd} - 1)}_{B_q} e^{iqR_j}$$

$$-\sum_j t^{(1)} (u_{j+1} - u_j)\, b_j^+ b_{j+1} =$$

$$= -\sum_j t^{(1)} \sum_q B_q e^{iqR_j} \frac{1}{N} \sum_{k'} e^{-ik'R_j} b_{k'}^+ \sum_k e^{ikR_{j+1}} b_k =$$

$$= -\frac{1}{N} t^{(1)} \sum_q B_q \sum_{kk'} \underbrace{\sum_j e^{i(q-k'+k)R_j}}_{N\delta_{k',k+q}} e^{ikd}\, b_{k'}^+ b_k =$$

$$= -t^{(1)} \sum_{k,q} B_q e^{ikd} b_{k+q}^+ b_k =$$

$$= -t^{(1)} \sum_{k,q} \sqrt{\frac{\hbar}{2mN\omega_q}} \left[e^{i(k+q)d} - e^{ikd} \right] b_{k+q}^+ b_k (a_q + a_{-q}^+)$$

The second term is analogous

$$-\sum_j t^{(1)} (u_{j+1} - u_j)\, b_{j+1}^+ b_j =$$

$$= -t^{(1)} \sum_{k,q} \sqrt{\frac{\hbar}{2mN\omega_q}} \left[-e^{-i(k+q)d} + e^{-ikd} \right] b_{k+q}^+ b_k (a_q + a_{-q}^+)$$

The sum gives

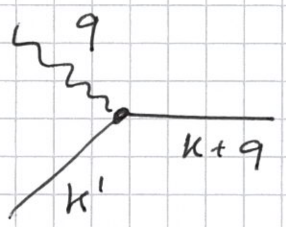
$$H_{el\text{-}ph} = \frac{1}{\sqrt{N}} \sum_{k,q} g(k,q)\, b^{+}_{k+q} b_k \left(a_q - a^{+}_{-q}\right)$$

$$g(k,q) = i\, t^{(1)} \sqrt{\frac{2\hbar}{m\omega_q}} \left[\sin(kd) - \sin(k+q)d\right]$$

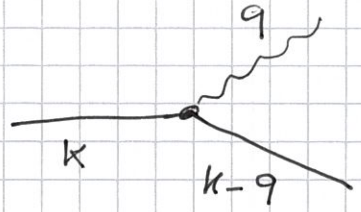
Approximating $g(k,q) \simeq g \simeq \text{const}$

$$H_{el\text{-}ph} = \frac{g}{\sqrt{N}} \sum_q \rho_{-q} \left(a_q + a_{-q}\right)$$

$b^{+}_{k+q} b_k a_q$



$b^{+}_{k+q} b_k a^{+}_{-q}$



Expanding the matrix element beyond first order one can obtain higher order terms

$b^{+}_{k+q+q'} b_k a_q a^{+}_{q'}$

etc.

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Electrical resistivity in a normal metal

Bloch theorem $\quad V(r)$ = periodic potential

$V(r) = 0 \qquad \psi_k = A\, e^{ikr}$

$V(\vec{r}) = V(\vec{r} + \vec{a}) \longrightarrow \psi_k \simeq u_k\, e^{ikr}$

* No scattering from a perfectly periodic potential (quantum effect)

Drude model: quasi free particles $\rightarrow$ Ohm's law

$\vec{J} = \sigma \vec{E} \qquad \vec{E} = \rho \vec{J}$

n = cond. el. density $(-e, m)$

$J_x = -n e v_x = \sigma E_x$

$\frac{\partial}{\partial t} v_x \Big|_{field} = -\frac{e}{m} E_x$

$\frac{\partial}{\partial t} v_x \Big|_{scattering} = -\frac{v_x}{\tau} \qquad \tau$ = relaxation time

$v_x(t) = v_x(0)\, e^{-t/\tau}$

$\frac{\partial v_x}{\partial t}\Big|_{field} + \frac{\partial v_x}{\partial t}\Big|_{scatt.} = 0$

$-\frac{e}{m} E_x - \frac{v_x}{\tau} = 0 \qquad v_x = -\frac{e\tau}{m} E_x$

$J_x = -n e v_x \qquad \boxed{\sigma = \frac{n e^2 \tau}{m}}$

Cu $(T = 300\,K) \qquad \sigma = 6 \times 10^5\, (\Omega\, cm)^{-1}$

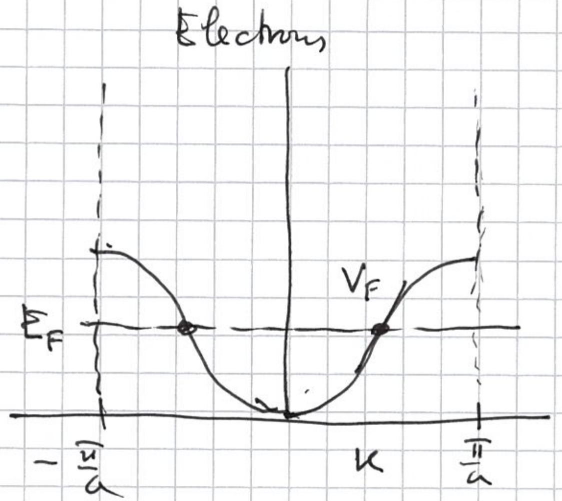
$n = 8.5 \times 10^{22}\, cm^{-3} \qquad \tau \sim 2 \times 10^{-14}\, sec$

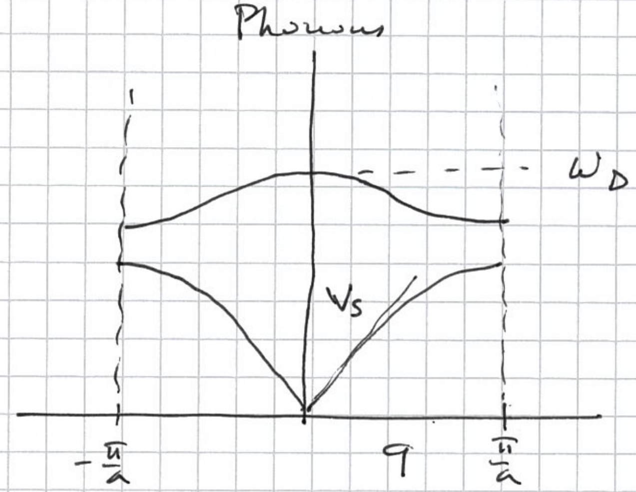
$v_F = 1.6 \times 10^8\, cm/sec \qquad \boxed{\lambda \sim v_F \tau \simeq 300\,Å}$

However: microscopic transport theory is related to the Fermi Surface NOT to the total electron density

Relation between Fermi Surface and n_{el} can be made only for parabolic bands.

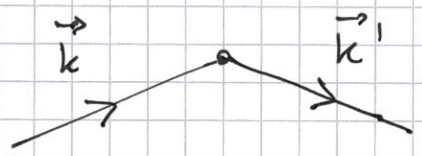
Microscopic theory of resistivity





$$\begin{cases} E_F \simeq 4\,eV \\ V_F \sim 10^8\,cm/sec \end{cases} \qquad \begin{cases} \hbar\omega_D \simeq \cancel{0.1\,eV}\ 0.01-0.1\,eV \\ V_s \sim 10^6\,cm/sec \end{cases}$$

Given that $E_F \gg \hbar\omega_D$ scattering is quasi-elastic



$\longrightarrow \quad \langle \vec{k}' | V | \vec{k} \rangle$

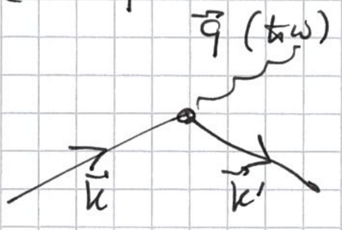
$$P(\vec{k},\vec{k}')\,d\Omega = \frac{2\pi}{\hbar} \left| \langle \vec{k}' | V | \vec{k} \rangle \right|^2 d\Omega$$

Fermionic nature

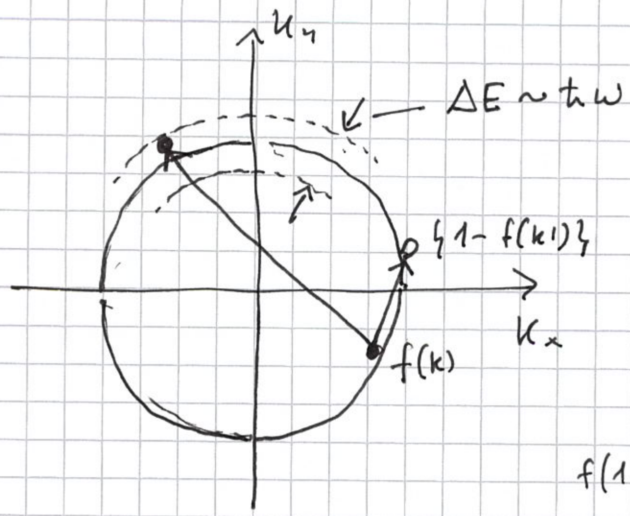
$$P(\vec{k},\vec{k}')\, f(\vec{k}) \{ 1 - f(\vec{k}') \}$$

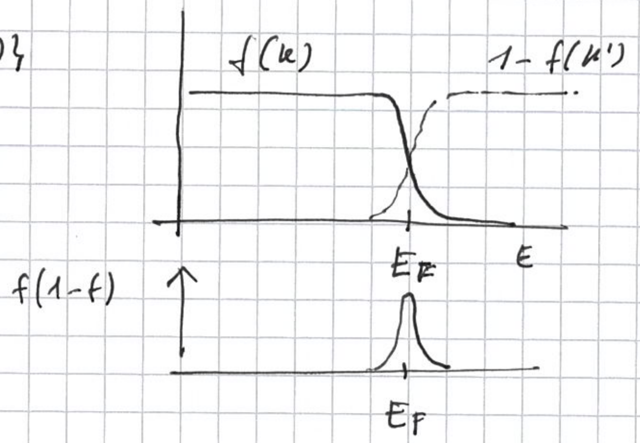
(a) impurities (elastic) $|\vec{k}'| = |\vec{k}|$

(b) phonons



$$\begin{cases} \dfrac{\hbar^2 (\vec{k}')^2}{2m} = \dfrac{\hbar^2 \vec{k}^2}{2m} \pm \hbar\omega_q \\ \vec{k}' = \vec{k} + \vec{q} + \vec{G} \end{cases}$$





Boltzmann transport equation

$f(\vec{k}, r)$

$\frac{2}{8\pi^3} f(\vec{k}, \vec{r})\, d^3k\, d^3r$ # of el. in volume element

$f(\vec{k}, r)$ dependence on t

(a) $v_k = \frac{1}{\hbar} \nabla_k E_k$

(b) $\frac{dk}{dt} = -\frac{e}{\hbar}\left[E + \frac{1}{c} \vec{v}_k \times \vec{B} \right]$

(c) scattering $\vec{k} \to \vec{k}'$

Stationary state

$$\boxed{\left.\frac{\partial f(\vec{k}, \vec{r})}{\partial t}\right|_{drift} + \left.\frac{\partial f(\vec{k}, \vec{r})}{\partial t}\right|_{scatt} = 0}$$

$$f^0(k) = \frac{1}{e^{(E_k - E_F)/k_B T} + 1} = f^0(E_k)$$

$$g(\vec{k}, \vec{r}) = f(\vec{k}, \vec{r}) - f^0\{\vec{k}, T(\vec{r})\}$$

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$$J(r) = -e\left(\frac{2}{8\pi^3}\right)\int v_k \overbrace{f(\bar{k},\bar{r})}^{-f^0(\bar{k},\bar{r})} d^3k = -e\frac{2}{8\pi^2}\int v_k\, g(\bar{k},\bar{r})\, d^3k$$

$$(\Delta f)_{\text{diff}} = f(\bar{k},\bar{r},t+\Delta t) - f(k,r,t)$$

if at $(t+\Delta t) \to (k,r)$

then at t $\quad k' = k - \frac{dk}{dk}\Delta t \;;\; r' = r - v_k \Delta t$

$$f(\bar{k},\bar{r},t+\Delta t) = f\left(\bar{k} - \frac{dk}{dt}\Delta t \,;\, \bar{r} - \bar{v}_k\Delta t, t\right) \simeq$$

$$\simeq f(\bar{k},\bar{r},t) - (\nabla_k f)\frac{d\bar{k}}{dt}\Delta t + \cdots$$

$$-(\nabla_k f)\frac{d\vec{k}}{dt} = \frac{e}{\hbar}\left\{\nabla_k f^0 + \nabla_k g\right\}\left\{E + \frac{1}{c}\bar{v}_k \times \bar{B}\right\} \simeq$$

$$\simeq e\frac{\partial f^0}{\partial E_k}\vec{v}_k \cdot \vec{E}$$

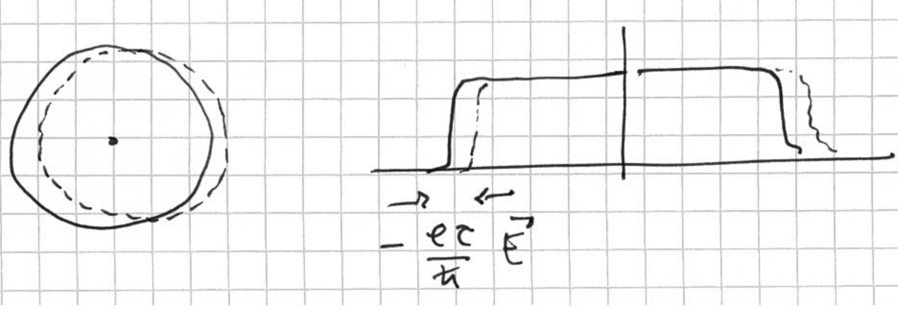
<u>Scattering</u>: $\quad P(\bar{k},\bar{k}') \quad \vec{k} \to \bar{k}'$

$$\left.\frac{\partial g(k)}{\partial t}\right|_{\text{scatt}} = -\frac{g(k)}{\tau} \qquad g_k(t) = g_k(0)e^{-t/\tau}$$

$$\left.\frac{\partial f(k)}{\partial t}\right|_{\text{diff}} + \left.\frac{\partial f(k)}{\partial t}\right|_{\text{scatt.}} = 0$$

$$\boxed{g(k) = e\tau\left(\frac{\partial f^0}{\partial E_k}\right)\vec{v}_k \cdot E}$$

$$f(k) = f^0(k) + \frac{e\tau}{\hbar}\left(\frac{\partial f^0}{\partial E_k}\right)\nabla_k E(\bar{k})\cdot \cancel{E} = f^0\left(k + \frac{e\tau}{\hbar}\vec{E}\right)$$



Conductivity

$$\boxed{\vec{J} = -\frac{e^2}{4\pi^3}\int v_k\, \tau \left(\frac{\partial f^0}{\partial E_k}\right)(\vec{v_k}\cdot\vec{E})\, d^3k = \sigma \vec{E}}$$

If we have $\quad E(k) = \dfrac{\hbar^2 k^2}{2m^*} \quad$ (not so in graphene) 

$$\vec{v}_k = \frac{\hbar \vec{k}}{m^*} \qquad \sigma = \frac{J_x}{E_x} = -\frac{e^2\hbar^2}{4\pi^3 m^{*2}}\int \tau\left(\frac{\partial f^0}{\partial E_k}\right) k_x^2\, d^3k$$

$$\frac{\partial f^0}{\partial E_k} \sim -\delta(E - E_F) \qquad \langle k_x^2\rangle \simeq \frac{1}{3}\langle k^2\rangle$$

$$\sigma = \frac{J_x}{E_x} \simeq \frac{n e^2 \tau_F}{m^*}$$

$$E_F = \left(\frac{\hbar^2}{2m^*}\right)(3\pi^2 n) \qquad$$ NB: only for parabolic bands $\sigma \sim n$

Microscopic transport $\rightarrow$ Fermi Surface ($\neq n$)

$$\sigma \sim \int v_k^2\left(-\frac{\partial f}{\partial E_k}\right)\cdot\tau \sim \underbrace{\underset{\sim k_F}{N(E_F)}\ \underset{k_F^2}{\langle v_F^2\rangle}}_{k_F^3 \,\sim\, n(E_F)}\ \tau$$

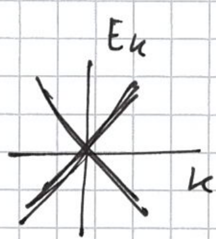
$v_F \sim k_F$

$E_F \sim k_F^2$

$D(E_F) \sim E_F^{1/2} \sim k_F$

$n \sim E_F^3$

But in graphene



$v_F = \text{const}$

$E_F \sim k_F$

...

NB: also τ may depend on v_F etc

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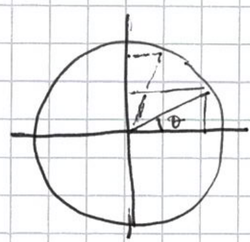
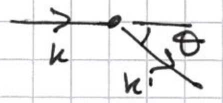
Diffraction model for Resistivity

* What was Omer looking for ($\rho \sim T^5$)?

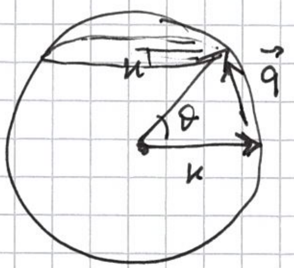
$$\rho = \frac{m}{ne^2}\frac{1}{\tau_F}$$



$$\frac{1}{\tau_F} = \int_{S_F'} P(\vec{k}\to\vec{k}')\underbrace{(1-\cos\theta)}\, dS_F'$$



momentum change



$$\vec{k}' = \vec{k} + \vec{q}$$

$$|\vec{k}| = |\vec{k}'| = |\vec{k}+\vec{q}| = k_F$$

$$\sin\tfrac{1}{2}\theta = q/2k_F$$

$$dS_F' = 2\pi k_F^2 \sin\theta\, d\theta \qquad (0 \le \theta \le 2\pi)$$

$V(\vec{r})$ = potential due to all ions

$$P(\vec{k}\to\vec{k}')\, dS_F' = \frac{2\pi}{\hbar}\left|\langle \vec{k}'|V|\vec{k}\rangle\right|^2 \frac{1}{2}\underbrace{D(E_F)\frac{2\pi k_F^2 \sin\theta\, d\theta}{4\pi k_F^2}}_{\text{density of states associated to } dS_F'}$$

Spin not change in scattering

$$|\vec{k}\rangle = \Omega^{-1/2}\exp(i\vec{k}\cdot\vec{r})$$

$$D(E_F) = \frac{3n\Omega}{2E_F} \qquad \tfrac{1}{2}D(E_F) = D_\uparrow(E_F) = D_\downarrow(E_F)$$

$$\rho = \frac{3\pi m\Omega}{8e^2\hbar E_F}\int_{x=0}^{2}\left|\langle \vec{k}+\vec{q}|V(\vec{r})|\vec{k}\rangle\right|^2 x^3\, dx$$

$d\theta \sin\theta(1-\cos\theta)$

$$0 \le q \le 2k_F$$

$$x = q/2k_F$$

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$$\langle|\langle \bar{k}+\bar{q}|V|\bar{k}\rangle|\rangle = \frac{1}{\Omega}\sum_n e^{i(\bar{k}+\bar{q})\vec{r}}\, v(\bar{r}-\bar{R}_n)\, e^{i\bar{k}\cdot\bar{r}}\, d^3r =$$

$$= \frac{1}{\Omega}\sum_n e^{-i\bar{q}\bar{R}_n}\int e^{-i(\bar{k}+\bar{q})(\bar{r}-\bar{R}_n)}\, v(\bar{r}-\bar{R}_n)\, e^{i\bar{k}(\bar{r}-\bar{R}_n)}\, d^3r =$$

$$= \underbrace{\frac{1}{N}\sum_n e^{-iq\cdot R_n}}_{S(\vec{q})} \cdot \underbrace{\frac{1}{\Omega_0}\int e^{-i(\bar{k}+\bar{q})\cdot r}\, v(r)\, e^{i\bar{k}\cdot\bar{r}}\, d^3r}_{v(\vec{q})}$$

$$= S(\vec{q}) \cdot v(\vec{q}) \qquad \Omega_0 = \frac{\Omega}{N}$$

$v(\bar{r})$ = effective screened pseudopotential acting on cond. el.

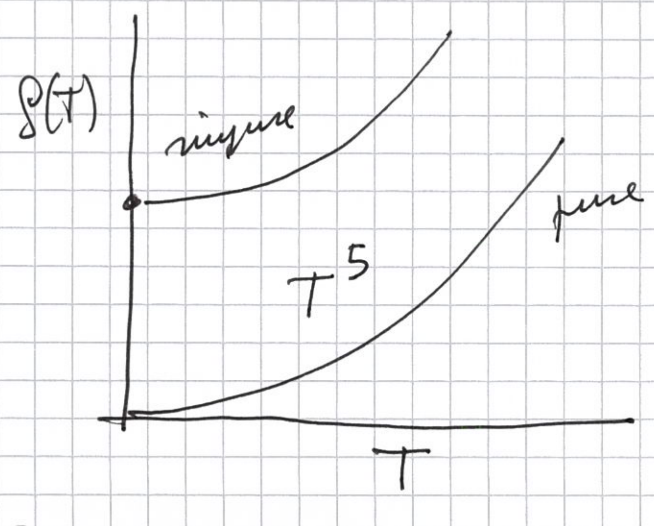
$S(\vec{q})$ = structure factor

<u>Simply periodic case</u> (Bloch theorem)

$$S(\vec{q}) = \frac{1}{N}\sum_n e^{-i\vec{q}\cdot\vec{R}_n} = \delta_{\vec{q},\vec{G}}$$

for a general $\vec{q}$ $\quad S(\vec{q}) = 0 \rightarrow \rho = 0$

<u>Resistivity of Metals</u> (impurities + phonons)



$$\vec{R}_j = \vec{R}_j^\circ + \vec{u}(R_j^\circ)$$

consider a single lattice wave $\vec{Q}$

$$\vec{u}(\vec{R}_j^\circ) = \vec{u}_0\, e^{i\vec{Q}\cdot\vec{R}_j^\circ}$$

$$S(\vec{q}) = \frac{1}{N}\sum_j e^{-i\vec{q}\cdot\vec{R}_j^0}\, e^{-i\vec{q}\cdot\vec{u}(\vec{R}_j^0)} \simeq$$

$$\simeq \frac{1}{N}\sum_j e^{-i\vec{q}\cdot\vec{R}_j^0}\left\{1 - i\vec{q}\cdot\vec{u}(\vec{R}_j^0)\right\} = \qquad |\vec{q}\cdot\vec{u}| \ll 1$$

$$= \frac{1}{N}\sum_j e^{-i\vec{q}\cdot\vec{R}_j^0}\left[1 - i\vec{q}\cdot\vec{u}_0\, e^{i\vec{Q}\cdot\vec{R}_j}\right] =$$

$$= \frac{1}{N}\sum_j e^{-i\vec{q}\cdot\vec{R}_j^0} - \frac{i}{N}\sum_j \vec{q}\cdot\vec{u}_0\, e^{-i(\vec{q}-\vec{Q})\cdot\vec{R}_j^0} =$$

$$= \frac{1}{N} N \delta_{\vec{q},\vec{0}} - \frac{iN}{N}\vec{q}\cdot\vec{u}_0\,\delta_{\vec{q}-\vec{Q},0}$$

Scattering occurs only for $\vec{k}' - \vec{k} = \vec{q} = \vec{Q}$
absorption of a phonon

[The term $e^{-i\vec{Q}\cdot\vec{R}_j^0}$ would correspond to emission]

Ziman formula

$$\rho \sim \int_0^{2k_F} |v(\vec{Q})|^2\, |\vec{Q}\cdot\vec{u}_{0Q}|^2\, Q^3\, dQ$$

<u>NB:</u> Only longitudinal waves $\vec{Q} \parallel \vec{u}_0$ contribute to resistivity. Not transverse waves $\vec{Q} \perp \vec{u}_0$.

<u>T dependence</u>

$$\overline{u^2_{0Q}} \propto n_Q = \frac{1}{e^{\hbar\omega_q/k_BT} - 1} \simeq \begin{cases} \dfrac{k_BT}{\hbar\omega_Q} & \text{if } \hbar\omega_Q \ll k_BT \\ 0 & \text{if } \hbar\omega_Q \gg k_BT \end{cases}$$

For $T \gtrsim \Theta_{Debye}$ $\quad \bar{n}_Q \sim T \quad \rightarrow \quad \boxed{\rho \sim T}$

At low T however only $\hbar\omega_Q \lesssim k_B T$ are excited

then $\hbar Q v_s \lesssim k_B T$ or $Q \lesssim k_B T / \hbar v_s$

$$\boxed{\rho \sim T \int_0^{Q_{MAX} \sim T} Q^3 \, dQ \sim T^5}$$

$\rho(T_{room} = 300K) \sim 10^{-6}$ Ω/cm

good metals

$$\rho \sim \int_0^{2k_F} |Q \cdot u_{0Q}|^2 \, Q^3 \, dQ$$

low T $\quad \bar{u}_0^2 \sim \frac{k_B T}{\hbar v_s Q} \quad$ if $Q < \frac{k_B T}{\hbar v_s}$

THOMAS FERMI SCREENING OF THE ELECTRON GAS

$$\nabla^2 \phi_{ext}(r) = -4\pi \rho_{ext}(r)$$

$$\rho_{ext}(r) = \rho_{ext}(q) \cos q \cdot r$$

$$\phi_{ext}(q) = \frac{4\pi}{q^2} \rho_{ext}(q)$$

Screening for ρ_{ind} & ϕ_{ind}

$$\phi(q) = \phi_{ext}(q) + \phi_{ind}(q)$$

$$\varepsilon(q) = \frac{\phi_{ext}(q)}{\phi(q)} = \frac{\rho_{ext}(q)}{\rho(q)}$$

$$\phi_{ind}(q) = -\frac{4\pi e}{q^2} n_{ind}(q)$$

Free electron gas (+ Pauli principle)

$$|\vec{k}\rangle \qquad E^0(k) = \frac{\hbar k^2}{2m}$$

$$n(r) = n_0 + n_{ind}(r) = n_0 + n_{ind}(q) \cos(q \cdot r)$$

$$n_{ind} \ll n_0$$

$$\varepsilon(q) = \frac{\phi_{ex}(q)}{\phi(q)} = 1 - \frac{\phi_{ind}(q)}{\phi(q)} = 1 + \frac{4\pi e}{q^2} \frac{n_{ind}(q)}{\phi(q)}$$

Problem : relation between n_{ind} and ϕ

$$\left[-\frac{\hbar^2}{2m}\nabla^2 - e\phi(r)\right]\psi_k(r) = E_k \psi_k(r)$$

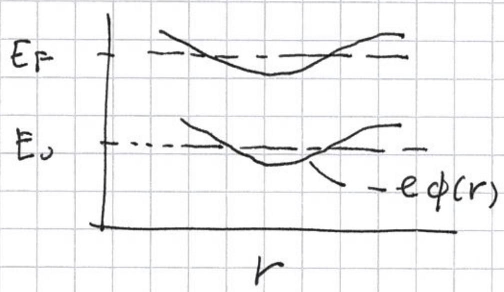
from $\psi_k^* \psi_k \rightarrow n_{ind}$

Assumption : $q \ll k_F$ or $q \cdot a \ll 1$ TF approximation

$\phi(r) \simeq$ const over $\lambda_F \simeq \frac{2\pi}{k_F} \approx 1\,\text{Å}$

We have then simply

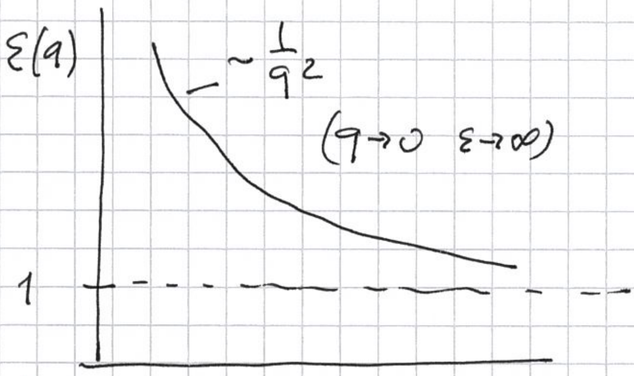
$\phi(r) \sim$ const $\to E(k) \simeq \frac{\hbar^2 k^2}{2m} - e\phi(r)$ (for $k \gg q$)



$n_{ind}(r) = e\phi(r)\, D(E_F)$

$$\boxed{\varepsilon(q) = 1 + \frac{4\pi e^2}{q^2} D(E_F) = 1 + \frac{K_s^2}{q^2}}$$

$K_s^2 = 4\pi e^2 D(E_F) = 4\pi e^2 \frac{3 n_0}{2 E_F}$ $\quad K_s \simeq 10^{-8}\,\text{cm}^{-1} \approx 1\,\text{Å}^{-1}$



$\phi(r) = \frac{1}{r}$

$\phi(r) = \frac{1}{r} e^{-\alpha r} = \sum_q \phi(q) e^{i q \cdot r}$

$\phi(q) = \frac{4\pi}{\Omega(q^2 + \alpha^2)}$

for $\alpha = 0$ $\quad \phi_{ext}(q) = \frac{4\pi e}{\Omega q^2}$

$$\phi(q) = \frac{4\pi e}{\Omega q^2 \varepsilon(q)} = \frac{4\pi e}{(q^2 + k_s^2)}$$

$$\phi(r) = \frac{e}{r} e^{-k_s r}$$