Solutions for Fundamentals of Condensed Matter Physics 1st Edition by Cohen

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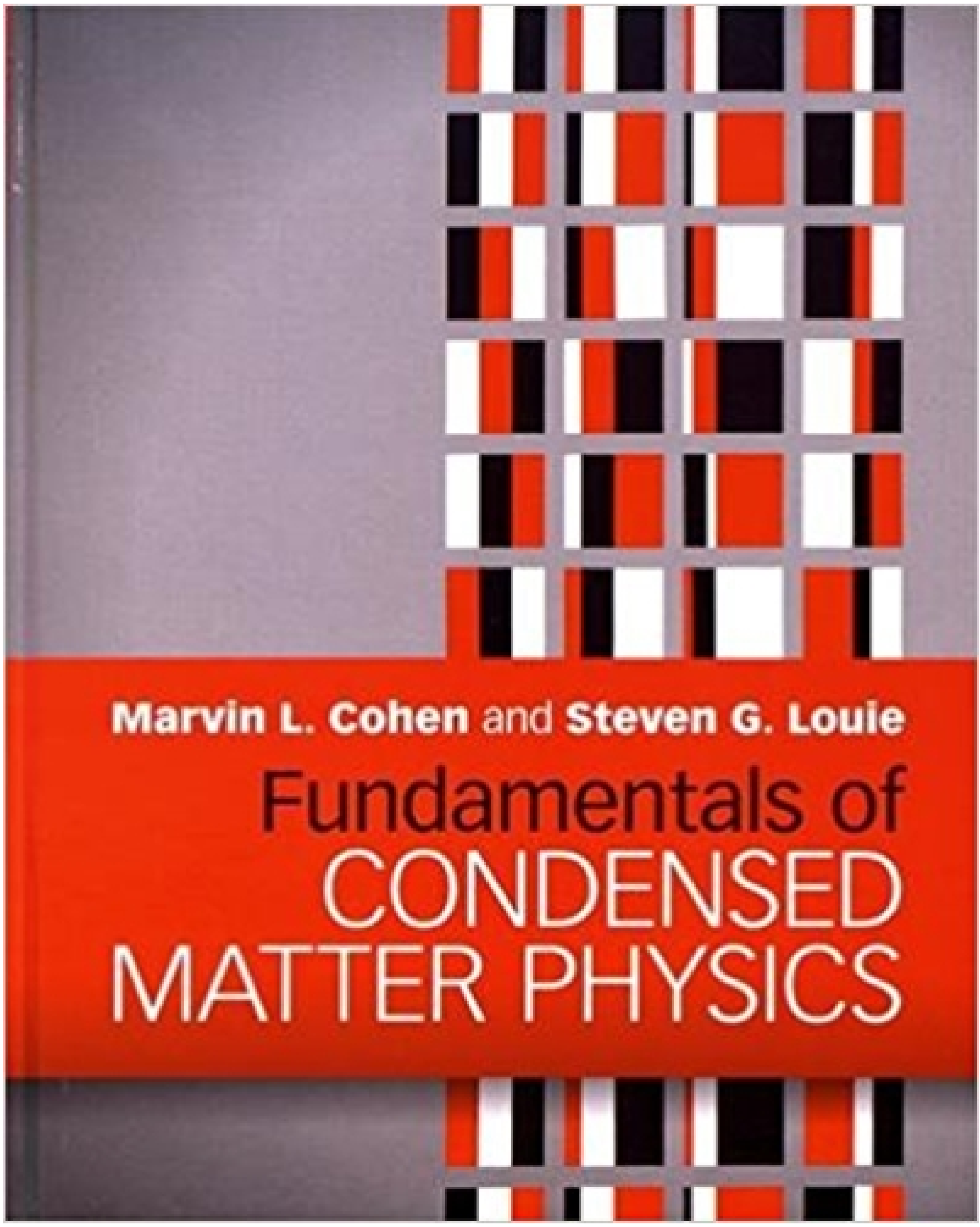

Solutions

Because $\langle n|x|n\rangle = 0$

$$\overline{x_n} = \frac{C}{\hbar\omega}\frac{1}{n'-n}(\langle n|x|n'\rangle\langle n'|x^3|n\rangle + \langle n|x^3|n'\rangle\langle n'|x|n\rangle) \tag{188}$$

Using$\langle n|a|n'\rangle = \sqrt{n'}\delta_{n,n'-1}$, $\langle n|a^\dagger|n'\rangle = \sqrt{n'+1}\delta_{n,n'+1}$

$$\langle n|x|n'\rangle = \frac{1}{2}\left(\frac{2\hbar}{m\omega}\right)^{(1/2)}\left(\sqrt{n'}\delta_{n,n'-1} + \sqrt{n'+1}\delta_{n,n'+1}\right) \tag{189}$$

So only $n' = n+1$ and $n' = n-1$ contribute. The only relevant terms in x^3 are $a^\dagger a^\dagger a, a^\dagger a a, a^\dagger, a$

$$\langle n|a^\dagger a^\dagger a|n'\rangle = n'\sqrt{n'+1}\delta_{n,n'+1} \tag{190}$$

$$\langle n|a^\dagger a a|n'\rangle = (n'-1)\sqrt{n'}\delta_{n,n'-1} \tag{191}$$

This gives

$$\langle n|x^3|n'\rangle = \frac{3}{8}\left(\frac{2\hbar}{m\omega}\right)^{(3/2)}\left[n\sqrt{n}\delta_{n,n'+1} + (n+1)\sqrt{n+1}\delta_{n,n'-1}\right] \tag{192}$$

$$\overline{x}_n = \frac{2C}{\hbar\omega}\frac{1}{2}\left(\frac{2\hbar}{m\omega}\right)^{(1/2)}\frac{3}{8}\left(\frac{2\hbar}{m\omega}\right)^{(3/2)}\left[(n+1)^2 - n^2\right] \tag{193}$$

$$= \frac{3}{2}C\frac{\hbar}{m^2\omega^3}(2n+1) \tag{194}$$

As a result, the mean position of the particle depends on the number of phonons excited. That is, the mean position depends on the temperature. This is thermal expansion.

Sec. II

II.1. Wannier functions.

(a) Wannier function is defined as,

$$W_n(\boldsymbol{r} - \boldsymbol{R}_l) = \frac{1}{\sqrt{N}}\sum_{\boldsymbol{k}} e^{-i\boldsymbol{k}\cdot\boldsymbol{R}_l} u_{n\boldsymbol{k}}(\boldsymbol{r}) \tag{195}$$

Use planewaves as an approximation for the band states, and use a cubic cell with dimension a,

$$\psi_{n\boldsymbol{k}}(\boldsymbol{r}) = \frac{1}{\sqrt{V}}e^{i\boldsymbol{k}\cdot\boldsymbol{r}} \tag{196}$$

and therefore,

$$W_n(\boldsymbol{r} - \boldsymbol{R}_l) = \frac{1}{\sqrt{NV}}\sum_{\boldsymbol{k}\in BZ} e^{-i\boldsymbol{k}\cdot\boldsymbol{R}_i} e^{i\boldsymbol{k}\cdot\boldsymbol{r}}$$

$$= \sqrt{\frac{V}{N}}\int fracd\boldsymbol{k}(2\pi)^3 e^{i\boldsymbol{k}\cdot(\boldsymbol{r}-\boldsymbol{R}_l)} = \sqrt{\frac{V}{N}}\frac{1}{\pi^3}\frac{\sin(\frac{\pi}{a}(x - R_{lx}))}{x - R_{lx}}\frac{\sin(\frac{\pi}{a}(y - R_{ly}))}{y - R_{ly}}\frac{\sin(\frac{\pi}{a}(z - R_{lz}))}{z - R_{lz}} \tag{197}$$

(b)

$$\begin{aligned}\langle W_n(\boldsymbol{R}_i)|\hat{H}|W_m(\boldsymbol{R}_j)\rangle &= \int d\boldsymbol{r}\frac{1}{\sqrt{N}}\sum_{\boldsymbol{k}_1} e^{i\boldsymbol{k}_1\cdot\boldsymbol{R}_i}\psi^*_{n\boldsymbol{k}_1}(\boldsymbol{r})\hat{H}\frac{1}{\sqrt{N}}\sum_{\boldsymbol{k}_2} e^{-i\boldsymbol{k}_2\cdot\boldsymbol{R}_j}\psi_{m\boldsymbol{k}_2}(\boldsymbol{r}) \\ &= \frac{1}{N}\sum_{\boldsymbol{k}_1\boldsymbol{k}_2} e^{i\boldsymbol{k}_1\cdot\boldsymbol{R}_i}e^{-i\boldsymbol{k}_2\cdot\boldsymbol{R}_j}\langle\psi_{n\boldsymbol{k}_1}|\hat{H}|\psi_{m\boldsymbol{k}_2}\rangle = \frac{1}{N}\sum_{\boldsymbol{k}_1\boldsymbol{k}_2} e^{i\boldsymbol{k}_1\cdot\boldsymbol{R}_i}e^{-i\boldsymbol{k}_2\cdot\boldsymbol{R}_j}E_{n\boldsymbol{k}_1}\delta_{mn}\delta_{\boldsymbol{k}_1\boldsymbol{k}_2} \\ &= \delta_{mn}\frac{1}{N}\sum_{\boldsymbol{k}_1} e^{i\boldsymbol{k}_1\cdot(\boldsymbol{R}_i-\boldsymbol{R}_j)}E_{n\boldsymbol{k}_1}\end{aligned} \tag{198}$$

(c) If we allow mixing of different bands, the Wannier function with band index n at cell $\boldsymbol{R}$ is defined by,

$$w_{n\boldsymbol{R}}(\boldsymbol{x}) = \sqrt{\frac{V}{(2\pi)^3}}\int_{BZ} d\boldsymbol{k}e^{-i\boldsymbol{k}\cdot\boldsymbol{R}}\left[\sum_m U^{(\boldsymbol{k})}_{mn}\psi_{mk}(\boldsymbol{x})\right] \tag{199}$$

Note that the unit of Bloch wavefunction is $[\psi(\boldsymbol{x})] = L^{-3/2}$, $\boldsymbol{U}$ is dimensionless, and therefore we also require that $w(\boldsymbol{x})$ be of the same unit with $\psi(\boldsymbol{x})$.

After we get the Wannier functions, we can calculate the hopping parameters between these MLWFs, which are exactly the Hamiltonian matrix elements between these Wannier functions.

$$\begin{aligned}\langle w_{m\boldsymbol{R}_1}|\hat{H}|w_{n\boldsymbol{R}_2}\rangle &= \frac{V}{(2\pi)^3}\int d\boldsymbol{x}\left[\int d\boldsymbol{k}_1 e^{-i\boldsymbol{k}_1\cdot\boldsymbol{R}_1}\sum_{m'} U^{(\boldsymbol{k}_1)}_{m'm}\psi_{m'\boldsymbol{k}_1}(\boldsymbol{x})\right]\hat{H}(\boldsymbol{x})\left[\int d\boldsymbol{k}_2 e^{-i\boldsymbol{k}_2\cdot\boldsymbol{R}_2}\sum_{n'} U^{(\boldsymbol{k}_2)}_{n'n}\psi_{n'\boldsymbol{k}_2}(\boldsymbol{x})\right] \\ &= \frac{V}{(2\pi)^3}\sum_{m'n'}\int d\boldsymbol{k}_1 d\boldsymbol{k}_2 e^{i\boldsymbol{k}_1\cdot\boldsymbol{R}_1}e^{-i\boldsymbol{k}_2\cdot\boldsymbol{R}_2}U^{(\boldsymbol{k}_1)*}_{m'm}U^{(\boldsymbol{k}_2)}_{n'n}\int d\boldsymbol{x}\psi^*_{m'\boldsymbol{k}_1}(\boldsymbol{x})\hat{H}(\boldsymbol{x})\psi_{n'\boldsymbol{k}_2}(\boldsymbol{x}) \\ &= \frac{V}{(2\pi)^3}\sum_{m'n'}\int d\boldsymbol{k}_1 d\boldsymbol{k}_2 e^{i\boldsymbol{k}_1\cdot\boldsymbol{R}_1}e^{-i\boldsymbol{k}_2\cdot\boldsymbol{R}_2}U^{(\boldsymbol{k}_1)*}_{m'm}U^{(\boldsymbol{k}_2)}_{n'n}\delta_{\boldsymbol{k}_1\boldsymbol{k}_2}\delta_{m'n'}E_{m'\boldsymbol{k}_1} \\ &= \frac{V}{(2\pi)^3}\int d\boldsymbol{k}_1 e^{i\boldsymbol{k}_1\cdot(\boldsymbol{R}_1-\boldsymbol{R}_2)}\sum_{m'} U^{(\boldsymbol{k}_1)*}_{m'm}U^{(\boldsymbol{k}_1)}_{m'n}E_{m'\boldsymbol{k}_1} \\ &= \frac{V}{(2\pi)^3}\int d\boldsymbol{k}_1 e^{i\boldsymbol{k}_1\cdot(\boldsymbol{R}_1-\boldsymbol{R}_2)}\sum_{m'} E_{m'\boldsymbol{k}_1}U^{(\boldsymbol{k}_1)\dagger}_{mm'}U^{(\boldsymbol{k}_1)}_{m'n} \\ &= \langle w_{m(\boldsymbol{R}_1-\boldsymbol{R}_2)}|\hat{H}|w_{n\boldsymbol{0}}\rangle\end{aligned} \tag{200}$$

which depends only upon $(\boldsymbol{R}_1 - \boldsymbol{R}_2)$.

II.2. Band structure and dynamics of electrons.

(a) (i) The group velocity $v = \frac{d\omega}{dk} = \frac{1}{\hbar}\frac{d\epsilon}{dk} = \frac{a(E_2-E_1)}{2\hbar}\sin(ka)$.

(ii) The effective mass $\frac{1}{m^*} = \frac{1}{\hbar^2}\frac{d^2\epsilon}{dk^2}$.

$$m^* = \frac{2\hbar^2}{a(E_2-E_1)}\frac{1}{\cos(ka)} \tag{201}$$

(iii) Bloch oscillation,

$$\begin{aligned} k(t) &= k(0) + \frac{eE}{\hbar}t \qquad (202)\\ v(k) &= \frac{a(E_2 - E_1)}{2\hbar}\sin(ka) \qquad (203)\\ x(t) &= \int v(k(t))dt \qquad (204)\\ &= \frac{(E_2 - E_1)}{2eE}\left(\cos(\frac{aeE}{\hbar}t) - 1\right) + x(0) \qquad (205) \end{aligned}$$

So the period is $T = \frac{2\pi\hbar}{aeE}$, range of distance is $\frac{(E_2-E_1)}{eE}$.

(b) In Wannier representation,

$$\left[E_n(-i\frac{\partial}{\partial R_x}, -i\frac{\partial}{\partial R_y}) + V(R_x, R_y)\right]\psi(R_x, R_y, t) = i\hbar\frac{\partial}{\partial t}\psi(R_x, R_y, t) \qquad (206)$$

In Bloch representation,

$$\left[E_n(k_x, k_y) + V(i\frac{\partial}{\partial k_x}, i\frac{\partial}{\partial k_y})\right]\psi(k_x, k_y, t) = i\hbar\frac{\partial}{\partial t}\psi(k_x, k_y, t) \qquad (207)$$

II.3. Electrons in an electric field.

(a) The group velocity is

$$v = \frac{1}{\hbar}\frac{d\epsilon}{dk} = -\frac{aE_0}{\hbar}\sin(ka) \qquad (208)$$

(b)

$$\begin{aligned} \hbar\frac{dk}{dt} &= -eE \qquad (209)\\ k(t) &= k(0) - \frac{eE}{\hbar}t \qquad (210) \end{aligned}$$

(c)

$$\begin{aligned} x(t) &= \int v(k(t))dt \qquad (211)\\ &= -\frac{E_0}{eE}\left(\cos(\frac{aeE}{\hbar}t) - 1\right) + x(0) \qquad (212) \end{aligned}$$

Because $x(0) = 0$,

$$x(t) = -\frac{E_0}{eE}\left(\cos(\frac{aeE}{\hbar}t) - 1\right) \qquad (213)$$

II.4. Velocity and effective mass of crystal electrons.

The group velocity $v = \frac{1}{\hbar}\frac{d\epsilon}{dk} = -\frac{aE_0}{\hbar}\sin(ka)$. The effective mass $m^* = -\frac{\hbar^2}{E_0a^2\cos(ka)}$.

(a) $v = -\frac{E_0a^2}{\hbar}\delta k, m^* = -\frac{\hbar^2}{E_0a^2}$.

(b) $v = -\frac{E_0 a^2}{\hbar}\delta k, m^* = -\frac{\hbar^2}{E_0 a^2}$.

(c) $v = -\frac{E_0 a}{\hbar}, m^* = -\frac{\hbar^2}{E_0 \delta k a^3}$.

(d) $v = -\frac{E_0 a}{\hbar}, m^* = \frac{\hbar^2}{E_0 \delta k a^3}$.

II.5. Electron Dynamics.

(a)

$$\epsilon(\boldsymbol{k}) = -2\tau\left[\cos\frac{a}{2}(k_x+k_y) + \cos\frac{a}{2}(k_x-k_y) + \cos\frac{a}{2}(k_x+k_z)\right. \tag{214}$$

$$\left. + \cos\frac{a}{2}(k_x-k_z) + \cos\frac{a}{2}(k_y+k_z) + \cos\frac{a}{2}(k_y-k_z)\right] \tag{215}$$

(b) (i)

$$v_x = \frac{1}{\hbar}\frac{\partial\epsilon}{\partial k_x} \tag{216}$$

$$= \frac{a\tau}{\hbar}\left[\sin\frac{aet}{2\hbar}(\epsilon_x+\epsilon_y) + \sin\frac{aet}{2\hbar}(\epsilon_x-\epsilon_y)\right. \tag{217}$$

$$\left. + \sin\frac{aet}{2\hbar}(\epsilon_x+\epsilon_z) + \sin\frac{aet}{2\hbar}(\epsilon_x-\epsilon_z)\right] \tag{218}$$

so

$$x(t) = \int v(t)dt = \frac{2\tau}{e(\epsilon_x+\epsilon_y)}\left[\cos\frac{ae(\epsilon_x+\epsilon_y)t}{2\hbar} - 1\right] + \text{other similar terms} \tag{219}$$

$$= \frac{2\tau}{e}\left[\frac{1}{\epsilon_x+\epsilon_y}(\cos A(\epsilon_x+\epsilon_y)t - 1) + \frac{1}{\epsilon_x-\epsilon_y}(\cos A(\epsilon_x-\epsilon_y)t - 1)\right. \tag{220}$$

$$\left. + \frac{1}{\epsilon_x+\epsilon_z}(\cos A(\epsilon_x+\epsilon_z)t - 1) + \frac{1}{\epsilon_x-\epsilon_z}(\cos A(\epsilon_x-\epsilon_z)t - 1)\right] \tag{221}$$

(ii)

$$x(t) = y(t) = z(t) = \frac{2\tau}{e\epsilon}(\cos\frac{ae\epsilon}{\hbar} - 1) \tag{222}$$

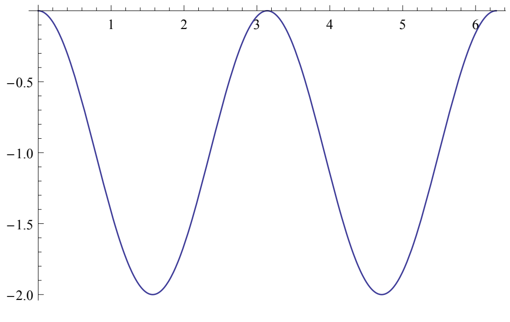

Figure 18: Sketch

(iii) For the estimation, let's take $\tau \cong 5$ eV, and not worry about counting nearest neighbours. The amplitude,

$$\frac{4\tau}{e\epsilon} = \frac{4\sqrt{3} \times 5\text{eV}}{1\text{eV}/mm} \tag{223}$$

for $\epsilon \approx 1$ V/mm. This is roughly 5 mm.

II.6. Berry phase in the spin dynamics of an electron in a magnetic field.

(a)

$$H = \frac{e\hbar}{2mc}\boldsymbol{\sigma} \cdot \mathbf{B}(t) \tag{224}$$

$$= \frac{e\hbar|\mathbf{B}(t)|}{2mc} \begin{pmatrix} \cos(\theta) & e^{-i\phi}\sin(\theta) \\ e^{i\phi}\sin(\theta) & -\cos(\theta) \end{pmatrix} \tag{225}$$

We use a trial eigenfunction (in unit of $\frac{e\hbar|\mathbf{B}(t)|}{2mc}$)

$$H \begin{pmatrix} \cos(\theta/2) \\ e^{i\phi}\sin(\theta/2) \end{pmatrix} = \begin{pmatrix} \cos(\theta)\cos(\theta/2) + \sin(\theta)\sin(\theta/2) \\ e^{i\phi}(\sin(\theta)\cos(\theta/2) - \cos(\theta)\sin(\theta/2)) \end{pmatrix} \tag{226}$$

$$= \begin{pmatrix} \cos(\theta/2) \\ e^{i\phi}\sin(\theta/2) \end{pmatrix} \tag{227}$$

(b)

$$\boldsymbol{A}(\theta,\phi) = i\chi_{\uparrow}^{\dagger}(\theta,\phi)\nabla\chi_{\uparrow}(\theta,\phi) \tag{228}$$

$$\nabla\chi_{\uparrow}(\theta,\phi) = \frac{1}{|\boldsymbol{B}|}\begin{pmatrix} -\frac{1}{2}\sin(\theta/2) \\ \frac{1}{2}e^{i\phi}\cos(\theta/2) \end{pmatrix}\hat{\theta} + \frac{1}{|\boldsymbol{B}|\sin(\theta)}\begin{pmatrix} 0 \\ ie^{i\phi}\sin(\theta/2) \end{pmatrix}\hat{\phi} \tag{229}$$

which leads to,

$$\boldsymbol{A}(\theta,\phi) = \frac{-\sin^2(\theta/2)}{|\boldsymbol{B}|\sin(\theta)}\hat{\phi} \tag{230}$$

and therefore,

$$\boldsymbol{\Omega}(\theta,\phi) = \nabla \times \boldsymbol{A}(\theta,\phi) = \frac{1}{2|\boldsymbol{B}|^2}\hat{B} \tag{231}$$

(c)

$$\gamma_{\uparrow} = \int d\boldsymbol{S}\cdot\boldsymbol{\Omega} = -\frac{1}{2}\int \frac{|\boldsymbol{B}|^2}{|\boldsymbol{B}|^2}d\boldsymbol{\omega} \tag{232}$$

$$= -\frac{1}{2}\Delta \tag{233}$$

II.7. Hartree-Fock approximation for ferromagnetic electron gas.

(a) When we go from a paramagnetic to a ferromagnetic ground state, the r_s parameter doesn't change, but the spin degeneracy factor g_s changes from 2 to 1. Alternatively, we can write the ground-state energy E solely in terms of the Fermi wavevector without any reference to g_s, i.e., $E = E(r_s, g_s) = E_k(k_F)$. Now, all we have to do is to relate the Fermi wave vector from paramagnetic case to the ferromagnetic case. We know that,

$$r_s = \left(\frac{3}{4\pi}\right)^{1/3} \left(\frac{1}{n}\right)^{1/3}, \quad n = N/\Omega_{\text{xtal}} \tag{234}$$

Also,

$$\begin{aligned} N &= g_s \sum_k^{k_F} (1) = \frac{g_s \Omega_{\text{xtal}}}{6\pi^2} k_F^3 \\ k_F &= \left(\frac{1}{g_s}\right)^{1/3} \frac{1}{r_s} \end{aligned} \tag{235}$$

The relationship between the paramagnetic and ferromagnetic Fermi wavevector is $k_F^F = 2^{1/3}\, k_F^P$. So, the total energy is given by

$$\begin{aligned} E^P &= E_k(k_F^P) = E^P(r_s) \\ E^F &= E_k(k_F^F) = E_k(2^{1/3}\, k_F^P) = E^F(r_s) \end{aligned} \tag{236}$$

We can rewrite the the ferromagnetic ground-state energy in terms of the paramagnetic one,

$$E^F(r_s) = E_k(2^{1/3}\, k_F^F) = E^P(2^{-1/3}\, r_s) \tag{237}$$

Within the Hartree-Fock approximation,

$$\begin{aligned} E^P(r_s) &= \frac{2.21}{r_s^2} - \frac{0.916}{r_s} \\ E^F(r_s) &= \frac{3.51}{r_s^2} - \frac{1.15}{r_s} \end{aligned} \tag{238}$$

(b) The ground-state energy for the two cases is compared in Fig. 19:

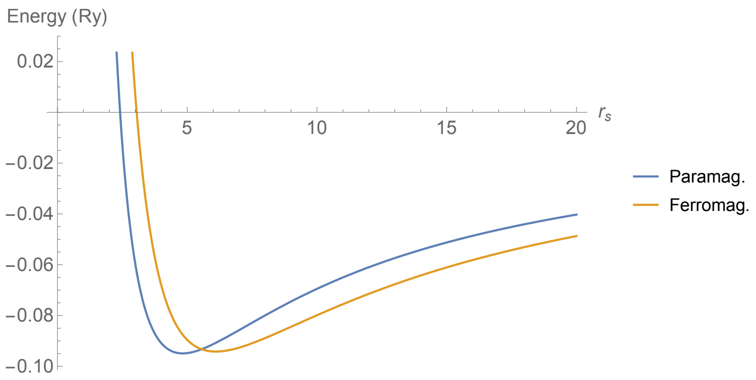

Figure 19: Ground-state energy in FM and AFM cases

Note that the ferromagnetic state is lower in energy than the paramagnetic case for $r_s > 5.56$. This makes sense, as ferromagnetism can be though as a strongly-corollated phenomenum, so it should take place as larger values of r_s.

II.8. Exchange-correlation hole

(a) (i) There are 2 atoms per cell, so $n = \frac{2}{a^3}$. In Rydberg units, $a = 7.94\, a_0$, so $n = \frac{2}{7.94^3}$, and $r_s = \left(\frac{3}{4\pi}\right)^{1/3} \frac{7.94}{2^{1/3}} = 3.91$.

(ii) We can estimate the exchange-correlation hole from the correlation function $g_{\uparrow\uparrow}(\mathbf{r}, 0) = \frac{1}{2}\left[1 - (f(r))^2\right]$, where $f(r) = \frac{3}{rk_F} j_1(rk_F)$. The first zero of the spherical Bessel function j_1 is at $rk_F = 4.5 = r\frac{1.92}{r_s}$. So, the size of the xc hole is $r \sim 1.97\, a_0$.

(b) (i) The energy is roughly the Coulomb potential between the xc hole and the electron, so it's

$$\epsilon_{xc} = -\frac{e^2}{z^2} = -\frac{2}{z^2}, \quad \text{in Ry} \tag{239}$$

(ii) If we use the correct exchange-correlation hole, the charge density associated to the hole would be farther away, so ϵ_{xc} would be larger (i.e., less negative).

II.9. Wigner electron crystal.

(a) In a Wigner sphere (radius $R = a_0 r_s$), ion charge is evenly distributed, and we can get the electric field by using Gauss's law,

$$\varphi(\boldsymbol{r}) = \int_r^\infty \boldsymbol{E} \cdot d\boldsymbol{l} = \begin{cases} \frac{1}{4\pi\epsilon_0}\left(\frac{3Q}{2R} - \frac{Qr^2}{2R^3}\right), & r < R \\ \frac{Q}{4\pi\epsilon_0 r}, & r > R \end{cases} \tag{240}$$

In the sphere, electrons feel the electric potential,

$$(-e)V(\boldsymbol{r}) = \frac{1}{4\pi\epsilon_0}\left(-\frac{3e^2}{2R} + \frac{e^2 r^2}{2R^3}\right) \tag{241}$$

with $R = a_0 r_s$ and $a_0 = \frac{4\pi\epsilon_0\hbar^2}{me^2}$. In atomic units, we get,

$$V(\boldsymbol{r}) = -\frac{3}{r_s} + \frac{r^2}{r_s^3} \tag{242}$$

(b) In a harmonic model Hamiltonian of electron in a Wigner sphere,

$$\begin{aligned} H &= -\frac{\hbar^2}{2m}\nabla^2 - \frac{1}{4\pi\epsilon_0}\left(\frac{3e^2}{2R} - \frac{e^2r^2}{2R^3}\right) \\ &= E_0 + \left(-\frac{\hbar^2}{2m}\nabla^2 + \frac{e^2}{8\pi\epsilon_0 R^3}r^2\right) = E_0 + \left(\frac{p^2}{2m} + \frac{1}{2}m\omega^2 r^2\right) \end{aligned} \tag{243}$$

where $\omega = \sqrt{\frac{e^2}{4\pi\epsilon_0 m R^3}}$. Using Virial theorem, we know that $E_k = E_p = \frac{1}{2}E$. And the kinetic energy E_k from the zero-point motion is given by,

$$\begin{aligned} E_k &= \frac{1}{2}E = \frac{1}{2}\frac{3}{2}\hbar\omega = \frac{3}{4}\sqrt{\frac{e^2\hbar^2}{4\pi\epsilon_0 m R^3}} \\ &= \frac{3}{2}r_s^{-3/2}(\text{Ry}) \end{aligned} \tag{244}$$

(c) Total energy: $E = -\frac{1.8}{r_s} + \frac{3}{2r_s^{3/2}}$. At equilibrium,

$$\frac{\partial E}{\partial r_s} = 0 \Rightarrow r_s = \frac{25}{16} \tag{245}$$

Then the volume per electron is $V_e = \frac{4\pi}{3} r_s^3 = 15.98$ in units of a_0^3. The bulk modulus is then given by,

$$B = -V \left. \frac{\partial^2 E}{\partial V^2} \right|_{r_s = \frac{25}{16}} = 4.005 \times 10^{-3} \tag{246}$$

II.10. Kramers-Kronig relations.

Assume $\mathbf{E}(t) = \mathbf{E_0}\delta(t)$ is a pulse of electric field at $t = 0$. Then the dielectric function is defined as,

$$\begin{aligned} \mathbf{D}(t) &= \int dt' \epsilon(t') \mathbf{E}(t - t') && (247) \\ &= \epsilon(t)\mathbf{E_0} && (248) \end{aligned}$$

Because $\mathbf{D}(t)$ must vanish for $t < 0$,

$$\epsilon(t) = 0 \qquad for \qquad t < 0 \tag{249}$$

so

$$\epsilon(t) = \int_0^\infty dt e^{i\omega t} \epsilon(t) \tag{250}$$

$e^{i\omega t}$ decays exponentially as a function of t when the imaginary part of ω is greater than zero. By Cauchy's theorem:

$$\epsilon(\omega) = \oint \frac{d\omega'}{2\pi i} \frac{\epsilon(\omega')}{\omega' - \omega - i\eta} \tag{251}$$

assuming η is very small. In order for the Cauchy's theorem to be valid, the function $\epsilon(\omega)$ must drop off faster than ω' for large ω'. Therefore,

$$\epsilon(\omega) - \epsilon^\infty = \oint \frac{d\omega'}{2\pi i} \frac{\epsilon(\omega') - \epsilon^\infty}{\omega' - \omega - i\eta} \tag{252}$$

$-\epsilon^\infty$ is the value of ϵ as ω goes to infinity. Now we can separate the equation into real and imaginary parts.

We notice that when η goes to zero, the pole will move to the real axis, so we need to change our contour to include a half-circuit around the pole at $\omega = \omega'$ which passes below the pole. The half-circuit part in the contour contributes half to the contour integral as there is only one pole inside. If we want to discard the contribution from the half-circuit to make it a Cauchy principle value, we must include a factor of 2 in the RHS to keep the equity .

$$\epsilon(\omega) - \epsilon^\infty = P \oint \frac{d\omega'}{\pi i} \frac{\epsilon(\omega') - \epsilon^\infty}{\omega' - \omega} \tag{253}$$

Therefore, using ϵ_1 and ϵ_2 for the real and imaginary part of ϵ we have

$$\epsilon_1(\omega) - \epsilon^{\infty} = P\oint \frac{2\omega' d\omega'}{\pi} \frac{\epsilon_2(\omega')}{\omega'^2 - \omega^2} \tag{254}$$

$$\epsilon_2(\omega) = -P\oint \frac{2\omega' d\omega'}{\pi} \frac{\epsilon_1(\omega') - \epsilon^{\infty}}{\omega'^2 - \omega^2} \tag{255}$$

II.11. Sum rules of dielectric function.

(a) In Drude model,

$$\begin{aligned} \epsilon_1(\omega) &= 1 - \frac{\omega_p^2 \tau^2}{1 + \omega^2\tau^2} \\ \epsilon_2(\omega) &= \frac{\omega_p^2 \tau}{\omega(1 + \omega^2\tau^2)} \end{aligned} \tag{256}$$

For $\tau \to \infty$, $\epsilon_1(\omega) \to 1 - \frac{\omega_p^2}{\omega^2}$ and $\epsilon_2(\omega) = \frac{\omega_p^2}{\omega}\frac{\tau^{-1}}{\tau^{-2}+\omega^2}$.
Use the identity,

$$\lim_{\varepsilon \to 0} \frac{\varepsilon}{x^2 + \varepsilon^2} = \pi\delta(x) \tag{257}$$

and we will have,

$$\epsilon_2(\omega) = \pi\frac{\omega_p^2}{\omega}\delta(\omega), \quad \text{as } \tau^{-1} \to \infty \tag{258}$$

and

$$\int_0^\infty \omega\epsilon_2(\omega) d\omega = \pi\omega_p^2 \int_0^\infty d\omega\delta(\omega) = \frac{\pi\omega_p^2}{2} \tag{259}$$

(b) Take inverse of dielectric function,

$$\epsilon^{-1}(\omega) = \frac{1}{\epsilon_1 + i\epsilon_2} = \frac{\epsilon_1 - i\epsilon_2}{\epsilon_1^2 + \epsilon_2^2} \Rightarrow \text{Im}[\frac{1}{\epsilon}] = -\frac{\epsilon_2}{\epsilon_1^2 + \epsilon_2^2} \tag{260}$$

Use the Kramers-Krönig relation for ϵ^{-1},

$$\text{Re}[\frac{1}{\epsilon(\omega)}] - 1 = \frac{2}{\pi}P\int_0^\infty d\omega' \frac{\omega'\text{Im}[1/\epsilon(\omega')]}{\omega'^2 - \omega^2} \tag{261}$$

Consider the limit $\omega \to \infty$,

$$\text{Re}[1/\epsilon] - 1 = -\frac{2}{\pi\omega^2}P\int_0^\infty d\omega'\, \omega'\text{Im}[1/\epsilon(\omega')] \tag{262}$$

With $\tau \to \infty$ and $\omega \neq 0$, we have $\epsilon_2(\omega) \to 0$, which means,

$$\frac{1}{\epsilon(\omega)} = \frac{1}{\epsilon_1 + i\omega_2} \approx \frac{1}{\epsilon_1} = \frac{1}{1 - \frac{\omega_p^2}{\omega^2}} \tag{263}$$

Here we take $\omega \to \infty$,

$$\text{Re}[1/\epsilon(\omega)] - 1 \approx \frac{\omega_p^2}{\omega^2} \tag{264}$$

which leads to,

$$\begin{aligned} \frac{\omega_p^2}{\omega^2} &= -\frac{2}{\pi\omega^2}P\int_0^\infty d\omega'\, \omega'\text{Im}[1/\epsilon(\omega)] \\ \Rightarrow \int_0^\infty d\omega\, \omega\text{Im}[1/\epsilon(\omega)] &= -\frac{\pi\omega_p^2}{2} \end{aligned} \tag{265}$$

II.12. Induced charge in a metal.

Consider an impurity in a metal. Since there is no oscillation, we take $\omega = 0$. We have Lindhard dielectric function as,

$$\epsilon(q, \omega = 0) = 1 + \frac{k_s^2 F(q/2k_F)}{q^2}, \quad F(q/2k_F) = \frac{1}{2}\frac{1 - (q/2k_F)^2}{4(q/2k_F)} \ln\left|\frac{1 + q/2k_F}{1 - q/2k_F}\right| \tag{266}$$

And $\epsilon_2(\boldsymbol{q}, \omega = 0) = 0$. In this way, $\epsilon(\boldsymbol{q}) = \epsilon_1(\boldsymbol{q}) \in \mathbb{R}$.

From Maxwell's equations,

$$\begin{aligned} \nabla \cdot \boldsymbol{D}(\boldsymbol{r}) &= 4\pi\rho_i(\boldsymbol{r}) \\ \nabla \cdot \boldsymbol{E}(\boldsymbol{r}) &= 4\pi(\rho_i(\boldsymbol{r}) + \rho_s(\boldsymbol{r})) \end{aligned} \tag{267}$$

where ρ_i is impurity charge density and ρ_s is induced charge density.

With Fourier transform, we have,

$$\begin{aligned} i\boldsymbol{q} \cdot \boldsymbol{D}(\boldsymbol{q}) &= 4\pi\rho_i(\boldsymbol{q}) \\ i\boldsymbol{q} \cdot \boldsymbol{E}(\boldsymbol{q}) &= 4\pi(\rho_i(\boldsymbol{q}) + \rho_s(\boldsymbol{q})) \end{aligned} \tag{268}$$

Impurity charge can be treated as a point charge in large r limit,

$$\begin{aligned} \rho_i(\boldsymbol{r}) &= Q\delta(\boldsymbol{r}) \\ \rho_i(\boldsymbol{q}) &= \int \rho_i(\boldsymbol{r}) e^{-i\boldsymbol{q}\cdot\boldsymbol{r}} d\boldsymbol{q} = Q \end{aligned} \tag{269}$$

The dielectric function is defined as,

$$\epsilon(\boldsymbol{q}) = \lim_{\rho_i \to 0} \frac{P(\boldsymbol{q})}{E(\boldsymbol{q})} = \lim_{\rho_i \to 0} \frac{\rho_i(\boldsymbol{q})}{\rho_i(\boldsymbol{q}) + \rho_s(\boldsymbol{q})} = \frac{Q}{Q + \rho_s(\boldsymbol{q})} \Rightarrow \rho_s(\boldsymbol{q}) = \frac{1 - \epsilon(\boldsymbol{q})}{\epsilon(\boldsymbol{q})} Q \tag{270}$$

That is,

$$\begin{aligned} \rho_s(\boldsymbol{r}) &= \int \frac{d\boldsymbol{q}}{(2\pi)^3} \rho_s(\boldsymbol{q}) e^{i\boldsymbol{q}\cdot\boldsymbol{r}} = \frac{Q}{(2\pi)^2} \int_0^\infty q^2 dq (-1) \frac{1 - \epsilon(q)}{\epsilon(q)} \frac{e^{iqr} - e^{-iqr}}{iqr} \\ &= \frac{Q}{(2\pi)^2} \frac{1}{ir} \int_{-\infty}^\infty q dq \frac{1 - \epsilon(q)}{\epsilon(q)} e^{iqr} \end{aligned} \tag{271}$$

Define $f(q) = \frac{Q}{(2\pi)^2} q \frac{1 - \epsilon(q)}{\epsilon(q)}$, and we will have,

$$\rho_s(\boldsymbol{r}) = \frac{1}{ir} \int_{-\infty}^\infty f(q) e^{iqr} dq = \frac{Q}{4\pi^2 r} \int_{-\infty}^\infty dq\, q \sin(qr) \left(\frac{q^2}{q^2 + k_s^2 F(q/2k_F)} - 1 \right) \tag{272}$$

The residue at the singular point $z = ik_s$ is proportional to $e^{-k_s r}/r$. But we only consider $r \to \infty$, so it decays to zero.

With two branch cuts, $x_1 = \pm 1 \Leftrightarrow q = \pm 2k_F$, define two contours: $\mathcal{C}_1 = \{(x, y) | x = -2k_F, y \in (+\infty, \eta) \cup (-\eta, -\infty)\}$ and $\mathcal{C}_2 = \{(x, y) | x = 2k_F, y \in (+\infty, +\eta) \cup (-\eta, -\infty)\}$.

$$\begin{aligned} \rho_s(\boldsymbol{r}) &= \frac{Q}{4\pi^2 r} \lim_{\eta \to 0} \left(\int_{\mathcal{C}_1} + \int_{\mathcal{C}_2} \right) q dq\, \sin(qr) \left[\frac{q^2}{q^2 + k_s^2 F(q/2k_F)} - 1 \right] \\ &= \frac{Q}{4\pi^2 r^2} \frac{\pi k_s^2}{4k_F} \frac{8k_F^3}{(4k_F^2 + \frac{1}{2}k_s^2)^2} \lim_{\eta \to 0} \left[e^{-2ik_F} i \int_\eta^\infty du\, e^{-ur} + e^{2ik_F} i \int_\eta^\infty v dv\, e^{-vr} \right] \\ &= \frac{Q}{\pi} \frac{k_s^2/k_F^2}{(4 + k_s^2/(2k_F^2))^2} \frac{\cos(2k_F r)}{r^3} \propto r^{-3} \cos(2k_F r) \end{aligned} \tag{273}$$

II.13. Zeros and poles of dielectric function.

The interaction of light with a medium can be described by the dielectric function $\epsilon(\boldsymbol{k},\omega)$, and the Maxwell equations (in a non-magnetic medium):

$$\begin{aligned} \nabla\cdot(\epsilon\boldsymbol{E}) &= 4\pi\rho_{ext} && (274)\\ \nabla\times\boldsymbol{E} &= -\frac{1}{c}\frac{\partial\boldsymbol{B}}{\partial t} && (275)\\ \nabla\cdot\boldsymbol{B} &= 0 && (276)\\ \nabla\times\boldsymbol{B} &= \frac{4\pi}{c}\boldsymbol{J}_{ext}+\frac{1}{c}\frac{\partial}{\partial t}(\epsilon\boldsymbol{E}) && (277)\end{aligned}$$

Inside the medium there are no external sources, so $\rho_{ext}=\boldsymbol{J}_{ext}=0$. If we Fourier analyze the fields we get,

$$\begin{aligned} \boldsymbol{k}\cdot(\epsilon\boldsymbol{E}) &= 0 && (278)\\ \boldsymbol{k}\cdot\boldsymbol{B} &= 0 && (279)\\ \boldsymbol{k}\times\boldsymbol{E} &= \frac{\omega}{c}\boldsymbol{B} && (280)\\ \boldsymbol{k}\times\boldsymbol{B} &= -\frac{\omega}{c}(\epsilon\boldsymbol{E}) && (281)\end{aligned}$$

In general there are no longitudinal modes because,

$$\boldsymbol{k}\cdot(\epsilon\boldsymbol{E})=0\Longrightarrow\boldsymbol{E}=0 \qquad (282)$$

except when $\epsilon=0$. Therefore, longitudinal modes are only allowed for $(\omega,\boldsymbol{k})\in\epsilon(\omega,\boldsymbol{k})=0$.

Combine Eqn. (279) and (281), one gets the dispersion relationship for the transverse mode:

$$\frac{\omega^2}{k^2}=\frac{c^2}{\epsilon(\boldsymbol{k},\omega)} \qquad (283)$$

At high frequencies $\epsilon\approx 1$ then $\omega^2/k^2=c^2$ is just the free space dispersion, i.e. at high frequencies the light does not interact strongly with the medium. There are also low frequency solutions to Eqn. (283), which are the transverse normal modes of the medium. Since ω^2 is small and c^2 is large, Eqn. (283) is satisfied only if $\epsilon(\boldsymbol{k},\omega)$ is very large, which occurs near the poles of ϵ. For practical purposes, we can say that the transverse normal modes occur at the poles of ϵ.

II.14. Polar insulators.

(a) See *Ashcraft&Mermin* Chap. 27 for detailed derivation.

(b) If $\epsilon(\omega)<0$, then $n=i\sqrt{-\epsilon}$, and $R=1$. Also note that,

$$R(0)=\left|\frac{\sqrt{\epsilon_0}-1}{\sqrt{\epsilon_0}+1}\right|^2,\quad R(\infty)=\left|\frac{\sqrt{\epsilon_\infty}-1}{\sqrt{\epsilon_\infty}+1}\right|^2 \qquad (284)$$

And we can plot the frequency-dependent reflectivity as Fig. 20,

(c) R close to 1 in the polariton region.

(d) For the LO mode there is an additional restoring force coming from the dipole field.

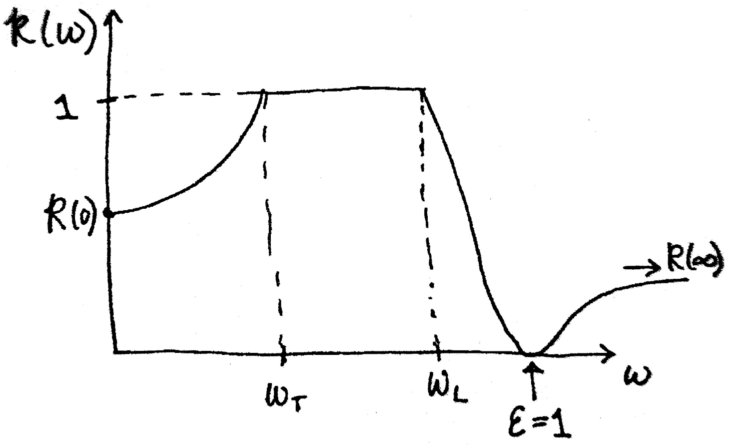

Figure 20: Frequency-dependent reflectivity

II.15. Density functional theory.

Within the Kohn-Sham formalism, we write the energy of the system as a function of the charge density and Kohn-Sham orbitals as

$$\begin{aligned}
E[\rho] &= E_{\text{ext}}[\rho] + T[\{\phi\}] + E_{ee}[\rho] + E_{\text{xc}}[\rho] \\
E_{\text{ext}} &= \int \mathrm{d}^3r\, v_{\text{ext}}(\mathbf{r})\rho(\mathbf{r}) \\
T &= -\frac{1}{2}\sum_i n_i \int \mathrm{d}^3r\, \phi_i^*(\mathbf{r})\nabla^2\phi_i(\mathbf{r}) \\
E_{ee} &= \frac{e^2}{2}\int \mathrm{d}^3r\,\mathrm{d}^3r'\,\frac{\rho(\mathbf{r})\rho(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|} \\
E_{\text{xc}} &= \int \mathrm{d}^3r\, v_{\text{xc}}(\mathbf{r})\rho(\mathbf{r}) \\
\rho(\mathbf{r}) &= \sum_i n_i\phi_i^*(\mathbf{r})\phi_i(\mathbf{r})
\end{aligned} \tag{285}$$

Note that

$$\frac{\partial\rho(\mathbf{r})}{\partial n_j} = |\phi_j(\mathbf{r})| \tag{286}$$

So the derivative of each term is

$$\begin{aligned}
\frac{\partial E_{\text{ext}}}{\partial n_j} &= \int \mathrm{d}^3r\, v_{\text{ext}}(\mathbf{r})\phi_j^*(\mathbf{r})\phi_j(\mathbf{r}) \\
\frac{\partial T}{\partial n_j} &= -\frac{1}{2}\int \mathrm{d}^3r\, \phi_j^*(\mathbf{r})\nabla^2\phi_j(\mathbf{r}) \\
\frac{\partial E_{ee}}{\partial n_j} &= e^2\int \mathrm{d}^3r\,\mathrm{d}^3r'\,\frac{\phi_j^*(\mathbf{r})\phi_j(\mathbf{r})\rho(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|} \\
&= e^2\int \mathrm{d}^3r\; v_H(\mathbf{r})\phi_j^*(\mathbf{r})\phi_j(\mathbf{r}) \\
\frac{\partial E_{\text{xc}}}{\partial n_j} &= \int \mathrm{d}^3r\, v_{\text{xc}}(\mathbf{r})\phi_j^*(\mathbf{r})\phi_j(\mathbf{r})
\end{aligned} \tag{287}$$

We recognize the Kohn-Sham Hamiltonian as

$$H^{KS} = -\frac{1}{2}\nabla^2 + v_{\text{ext}}(\mathbf{r}) + v_H(\mathbf{r}) + v_{xc}(\mathbf{r}) \tag{288}$$

So,

$$\frac{\partial E}{\partial n_j} = \int \mathrm{d}^3r\ \phi_j^*(\mathbf{r}) H^{KS} \phi_j(\mathbf{r}) = \epsilon_j^{KS} \tag{289}$$

This result is also known as Janak's theory; a slightly more complete derivation including self-consistent effects is found in PRB 18, 7165 (1978). In principle, this relation shows that there is a connection between the eigenvalues of the Kohn-Sham equations and the energy to add or remove an electron to the system. However, this relation alone is not enough to prove this property, since this relation is only valid for infinitesimal changes in the number of electrons, which is not physical. It can still be shown that, if the exact exchange-correlation is known, then the Kohn-Sham eigenvalues for the highest occupied and lowest orbitals correspond to the ionization potential and electron affinity of the system, respectively. See PRL 49, 1691 (1982).

II.16. Kohn effect.

For a free electron gas model, the Lindhard dielectric function has the form:

$$\epsilon(q,0) = 1 + \frac{4\pi e^2}{q^2} \frac{n}{\frac{2}{3}E_F} \left[\frac{1}{2} + \frac{4k_F^2 - q^2}{8k_F q} \ln \left| \frac{2k_F + q}{2k_F - q} \right| \right] \tag{290}$$

$\epsilon(q,0)$ is continuous at $q = 2k_F$, but $\frac{\partial \epsilon(q,0)}{\partial q}$ has a logarithmic infinity at $q = 2k_F$. The phonon frequency is determined by the motion of ions. Actually, the potential between ions is screened by the electronic dielectric function. Therefore, there will be some dependence of the phonon frequency on $\epsilon(q)$. As q increase through $2k_F$, the dielectric constant suddenly decrease. Then, it leads to a sudden (small) increase in the frequency ω of a lattice vibration at $q = 2k_F$. This effect influence the longitudinal modes since $\epsilon(q,0)$ above is the longitudinal dielectric constant. For the transverse mode, the influence is not so simple and so large as for longitudinal mode. The detailed effect of the Fermi surface on phonon spectra anomaly is discussed in (PR126, 1693(62) by Kohn et al.).

Sec. III

III.1. Light absorption in InSb.

InSb is a direct band gap semiconductor. We ignore the heavy hole valence band for now. We use the energy and momentum conservation relation in the optical absorption:

$$\frac{p_e^2}{2m_c^*} + \frac{p_h^2}{2m_v^*} = E_{photon} - E_{gap} \tag{291}$$

$$p_e = p_h \tag{292}$$

The electron and hole kinetic energies are 0.309 eV and 0.011 eV, respectively. If the photon momentum is included, we have

$$p_e = p_h + \frac{E_{photon}}{c} \tag{293}$$

The electron and hole momenta differ by approximately 0.8%.

III.2. Exciton.