Chapter 2 Fermi and Bose gases

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Questions

Qu.2.1 Momentum operator

Show that the state $\psi_k(\mathbf{r}) = \exp(i\mathbf{k}\cdot\mathbf{r})$ is an eigenstate of the momentum operator $\hat{\mathbf{p}} = -i\hbar\vec{\nabla}$ and find the eigenvalue.

$$\hat{p}\psi_k(\vec{r}) = -i\hbar\vec{\nabla}e^{i\vec{k}\cdot\vec{r}}$$

$$= -i\hbar\frac{\partial}{\partial\vec{r}}e^{i\vec{k}\cdot\vec{r}} = -i\hbar\left(\frac{\partial}{\partial x}\hat{x}+\frac{\partial}{\partial y}\hat{y}+\frac{\partial}{\partial z}\hat{z}\right)e^{i(k_x x+k_y y+k_z z)}$$

$$= -i\hbar\left(ik_x e^{i\vec{k}\cdot\vec{r}}\hat{x}+ik_y e^{i\vec{k}\cdot\vec{r}}\hat{y}+ik_z e^{i\vec{k}\cdot\vec{r}}\hat{z}\right)$$

$$= \hbar\vec{k}e^{i\vec{k}\cdot\vec{r}} = \hbar\vec{k}\psi_k(\vec{r}).$$

So, $\psi_k(\vec{r})$ is an eigenstate of $\hat{p}$ with eigenvalue $\hbar\vec{k}$.

Qu.2.2 Density of states for free electrons

(a) What is the fermi wavevector and fermi energy as a function of particle density for a free electron gas in one and two dimensions (define density appropriately)?

(b) Calculate the density of states in energy for free electrons in one and two dimensions. [Answer:$(2m/\pi\hbar^2)\times(\hbar^2/2mE)^{\frac{1}{2}}$, (d=1); $(m/\pi\hbar^2)$, d=2; $(m/\pi^2\hbar^2)\times(2mE/\hbar^2)^{\frac{1}{2}}$, d=3 .]

(c) Show how the 3D density of states can be re-written as

$$(3/2)(n/E_F)(E/E_F)^{\frac{1}{2}}$$

with $n = N/V$.

(a) Consider the allowed states in one dimension with length L.

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) = \varepsilon\psi(x).$$

$$\psi(x) = \frac{1}{\sqrt{L}}e^{ikx}.$$

Apply periodic boundary condition to get

$$k = \frac{2\pi n}{L}. \qquad (n: \text{integer})$$

The density of k space is $\frac{L}{2\pi}$ in 1-D.

Each allowed state in k-space could be occupied by two electrons:

$$2 \cdot \frac{L}{2\pi} \cdot \underbrace{2k_F}_{\uparrow} = N.$$

Volume of k-space. Fermi Line

$$\Rightarrow \quad k_F = \frac{N\pi}{2L} = \frac{\pi n_e}{2}. \qquad \left(n_e : \text{density of electrons}, \ \frac{N}{L}\right)$$

$$\varepsilon_F = \frac{\hbar^2 k_F^2}{2m} = \frac{\hbar^2 \pi^2 n_e^2}{8m}.$$

For the case of 2D, in L^2 space.

$$-\frac{\hbar^2}{2m}\nabla^2\psi = \varepsilon\psi. \quad \Rightarrow \quad \psi = \frac{1}{L}e^{i\vec{k}\cdot\vec{r}}.$$

Apply periodic boundary condition to get

$$k_x = \frac{2\pi n_x}{L}, \quad k_y = \frac{2\pi n_y}{L}.$$

Fermi circle

Then $2 \cdot \left(\frac{L}{2\pi}\right)^2 \cdot \underbrace{\pi k_F^2} = N.$

$$\Rightarrow \quad k_F = \frac{\sqrt{2\pi N}}{L} = \sqrt{2\pi n_e}. \qquad (n_e \cdot L^2 = N).$$

$$\varepsilon_F = \frac{\hbar^2 k_F^2}{2m} = \frac{\pi \hbar^2 n_e^2}{m}.$$

(b) Density of states $g(E)$ is defined as

$$g(E) = \frac{dN}{V\,dE}$$

Number of electron states in unit energy interval in unit volume.

dN could be calculated in k-space:

$$dN = \frac{V}{8\pi^3} \cdot 2 \cdot 4\pi k^2\, dk$$

$$\frac{\sqrt{2m\varepsilon}}{\hbar} = k$$

$$dk = \frac{\sqrt{m}\, d\varepsilon}{\sqrt{2\varepsilon}\,\hbar}$$

$$\xrightarrow{\varepsilon = \frac{\hbar^2 k^2}{2m}} \quad = \frac{V}{\pi^2} \cdot \frac{2m\varepsilon}{\hbar^2} \cdot \frac{\sqrt{m}\, d\varepsilon}{\sqrt{2\varepsilon}\,\hbar}$$

$$= \frac{V}{\pi^2 \hbar^3} \cdot m^{\frac{3}{2}} \cdot (2\varepsilon)^{\frac{1}{2}}\, d\varepsilon.$$

$$\Rightarrow \quad g(\varepsilon) = \frac{m^{\frac{3}{2}} (2\varepsilon)^{\frac{1}{2}}}{\pi^2 \hbar^3}.$$

For the case of 3D.

① In the case of 2D.

$$dN = \frac{L^2}{4\pi^2} \cdot 2 \cdot 2\pi k\, dk$$

$$= \frac{L^2}{\pi} \cdot \frac{\sqrt{\cancel{2}m\cancel{\varepsilon}}}{\hbar} \cdot \frac{\sqrt{m}\, d\varepsilon}{\sqrt{\cancel{2\varepsilon}}\,\hbar} = \frac{L^2 m\, d\varepsilon}{\pi \hbar^2}.$$

$$\Rightarrow \quad g(\varepsilon) = \frac{m}{\pi \hbar^2}. \qquad (2D)$$

② In the case of 1D.

$$dN = \frac{L}{2\pi} \cdot 2 \cdot 2\,dk = \frac{2L}{\pi} \cdot \frac{\sqrt{m}}{\sqrt{2\varepsilon}} \frac{d\varepsilon}{\hbar}.$$

$$\Rightarrow \quad g(\varepsilon) = \frac{\sqrt{2m}}{\sqrt{\varepsilon}\,\pi\hbar}. \qquad (1D)$$

(c) I already derived density of states in 3D as

$$g(\varepsilon) = \frac{m^{\frac{3}{2}}(2\varepsilon)^{\frac{1}{2}}}{\pi^2\hbar^3}.$$

Fermi energy in 3D could be derived as

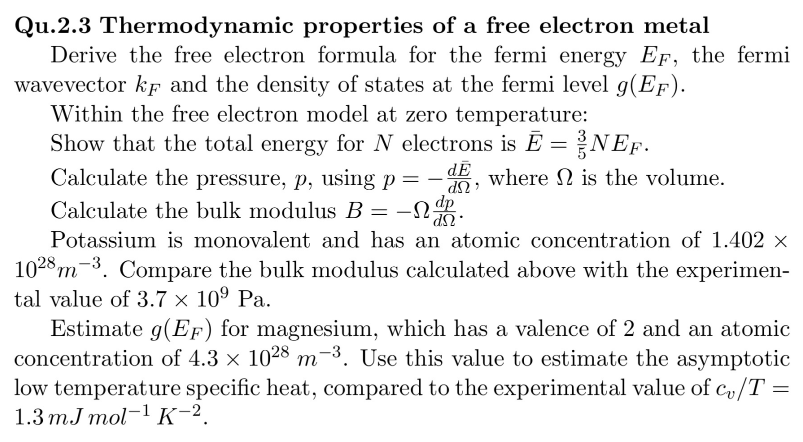
$$2 \cdot \left(\frac{L}{2\pi}\right)^3 \cdot \frac{4}{3}\pi k_F^3 = N.$$

$$\Rightarrow \quad k_F = \frac{(3\pi^2 N)^{\frac{1}{3}}}{L} = (3\pi^2 n)^{\frac{1}{3}}.$$

$$\varepsilon_F = \frac{\hbar^2 k_F^2}{2m} = \frac{\hbar^2 (3\pi^2 n)^{\frac{2}{3}}}{2m}.$$

$$\Rightarrow \quad m = \frac{\hbar^2 (3\pi^2 n)^{\frac{2}{3}}}{2\varepsilon_F}.$$ Plug in to get

$$g(\varepsilon) = \frac{\cancel{\hbar^3} \cdot 3\cancel{\pi^2} n}{(2\varepsilon_F)^{\frac{3}{2}}} \cdot \frac{\sqrt{2\varepsilon}}{\pi^2 \cancel{\hbar^3}} = \frac{3n}{2} \cdot \frac{1}{\varepsilon_F} \cdot \sqrt{\frac{\varepsilon}{\varepsilon_F}}.$$



Qu.2.3 Thermodynamic properties of a free electron metal

Derive the free electron formula for the fermi energy E_F, the fermi wavevector k_F and the density of states at the fermi level $g(E_F)$.

Within the free electron model at zero temperature:

Show that the total energy for N electrons is $\bar{E} = \frac{3}{5}NE_F$.

Calculate the pressure, p, using $p = -\frac{d\bar{E}}{d\Omega}$, where Ω is the volume.

Calculate the bulk modulus $B = -\Omega\frac{dp}{d\Omega}$.

Potassium is monovalent and has an atomic concentration of $1.402 \times 10^{28} m^{-3}$. Compare the bulk modulus calculated above with the experimental value of 3.7×10^9 Pa.

Estimate $g(E_F)$ for magnesium, which has a valence of 2 and an atomic concentration of $4.3 \times 10^{28}\ m^{-3}$. Use this value to estimate the asymptotic low temperature specific heat, compared to the experimental value of $c_v/T = 1.3\,mJ\,mol^{-1}\,K^{-2}$.

1 mol

~

1.3mJ/mol·K

From Qu. 2.2 I got $g(\varepsilon) = \frac{3n}{2\varepsilon_F}\sqrt{\frac{\varepsilon}{\varepsilon_F}}$.

Then $g(\varepsilon_F) = \frac{3n}{2\varepsilon_F}$.

I already derived $E_F = \frac{\hbar^2(3\pi^2 n)^{\frac{2}{3}}}{2m}$, $k_F = (3\pi^2 n)^{\frac{1}{3}}$

For free electron model at 0 K.

$d\varepsilon^{\frac{5}{2}} = \frac{5}{2}\varepsilon^{\frac{3}{2}}d\varepsilon$

$$\bar{\varepsilon} = \int_0^{\varepsilon_F} \varepsilon g(\varepsilon)\, d\varepsilon = \int_0^{\varepsilon_F} \frac{3n}{2\varepsilon_F}\frac{1}{\sqrt{\varepsilon_F}} \cdot \varepsilon^{\frac{3}{2}} d\varepsilon$$

$$= \frac{3n}{2\varepsilon_F}\cdot\frac{1}{\sqrt{\varepsilon_F}}\cdot\frac{2}{5}\varepsilon_F^{\frac{5}{2}} = \frac{3}{5}n\varepsilon_F.$$

$$\Rightarrow \bar{E} = \frac{3}{5}N\varepsilon_F.$$

$$p = -\frac{d\bar{E}}{d\Omega} = -\frac{d}{dV}\left(\frac{3}{5}\cdot\frac{\hbar^2}{2m}\cdot(3\pi^2)^{\frac{2}{3}} N^{\frac{5}{3}} V^{-\frac{2}{3}}\right)$$

$$= \frac{\hbar^2}{5m}(3\pi^2)^{\frac{2}{3}} N^{\frac{5}{3}} V^{-\frac{5}{3}} = \frac{\hbar^2}{5m}(3\pi^2)^{\frac{2}{3}} n^{\frac{5}{3}}.$$

$$B = -\Omega \frac{dp}{d\Omega} = -\Omega \cdot \frac{\hbar^2}{5m}(3\pi^2)^{\frac{2}{3}} N^{\frac{5}{3}} \cdot \left(-\frac{5}{3}\right) V^{-\frac{8}{3}}$$

$$= \frac{\hbar^2}{3m}(3\pi^2)^{\frac{2}{3}} N^{\frac{5}{3}} \Omega^{-\frac{5}{3}} = \frac{\hbar^2}{3m}(3\pi^2)^{\frac{2}{3}} n^{\frac{5}{3}}.$$

Plug in $n_e = 1.402 \times 10^{28}\, m^{-3}$, $m = m_e$.

$$B_{Potassium} = 3174943582 = 3.17 \times 10^{9}\ Pa.$$

The bulk modulus I got is close to, but smaller than 3.7×10^{9} Pa.

$$g(E_F) = \frac{3n}{2E_F} = \frac{3nm}{\hbar^2}(3\pi^2 n)^{-\frac{2}{3}} = \frac{3m}{\hbar^2}(3\pi^2)^{-\frac{2}{3}} n^{\frac{1}{3}}.$$

Plug in $n = 2 \times 4.3 \times 10^{28}\, m^{-3} = 8.6 \times 10^{28}\, m^{-3}$ to get

$$g(E_F)_{Mg} = 1.133 \times 10^{47}.$$

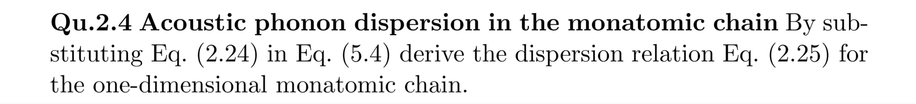
This term stands for the mol volume of Mg.

I will not derive, but just use the formula:

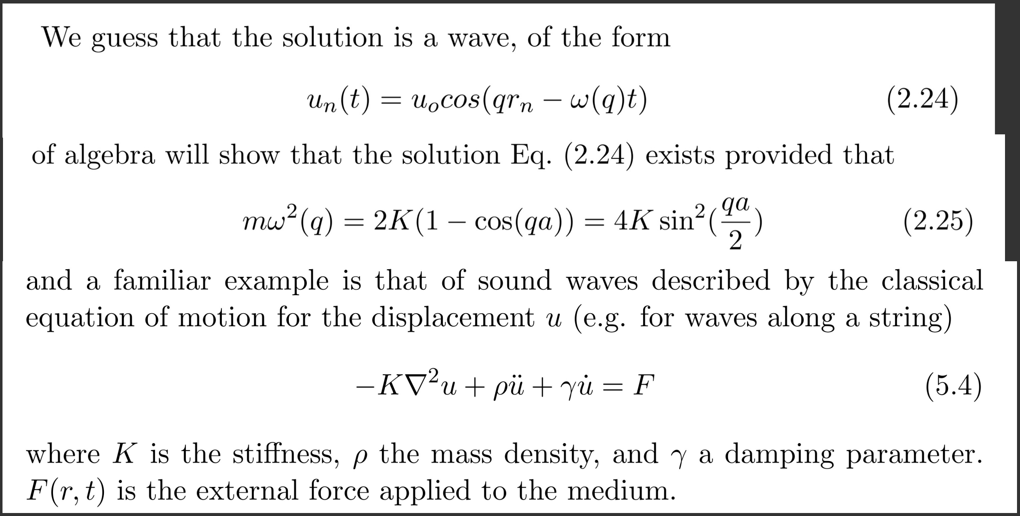
$$\frac{C_v}{T} = \frac{\pi^2}{3} k_B^2\, g(E_F) \cdot \frac{N_A}{\underline{n_{Mg}}} = \frac{\pi^2}{3} k_B^2 \cdot \frac{3m}{\hbar^2}(3\pi^2)^{-\frac{2}{3}} n^{-\frac{2}{3}} \cdot N_A \cdot 2$$

$$= 9.953 \times 10^{-4}\ J/mol\cdot K = 0.995\ mJ/mol\cdot K.$$

This is close to $1.3\ mJ\ mol^{-1} K^{-1}$. still smaller.



Qu.2.4 Acoustic phonon dispersion in the monatomic chain By substituting Eq. (2.24) in Eq. (5.4) derive the dispersion relation Eq. (2.25) for the one-dimensional monatomic chain.



We guess that the solution is a wave, of the form

$$u_n(t) = u_o cos(qr_n - \omega(q)t) \qquad (2.24)$$

of algebra will show that the solution Eq. (2.24) exists provided that

$$m\omega^2(q) = 2K(1 - \cos(qa)) = 4K\sin^2(\frac{qa}{2}) \qquad (2.25)$$

and a familiar example is that of sound waves described by the classical equation of motion for the displacement u (e.g. for waves along a string)

$$-K\nabla^2 u + \rho\ddot{u} + \gamma\dot{u} = F \qquad (5.4)$$

where K is the stiffness, ρ the mass density, and γ a damping parameter. $F(r,t)$ is the external force applied to the medium.

Plug in $u_n(t) = u_0 \cos(qr_n - \omega(q)t)$ into

$$-K\nabla^2 u + \rho\ddot{u} + \gamma\dot{u} = F.$$ to get.

$$-K\nabla^2 u - \rho\omega^2(q)u_0\cos(qr_n - \omega(q)t) - \gamma u_0 \omega(q)\sin(qr_n - \omega(q)t) = F.$$

↳ without friction $\gamma = 0$.

$$\frac{\partial u}{\partial x} = -u_0 q \cdot \frac{x}{r_n}\sin(qr_n - \omega(q)t).$$

$$\frac{\partial^2 u}{\partial x^2} = -u_0 q^2 \frac{x^2}{r_n^2}\cos(qr_n - \omega(q)t) - u_0 q \cdot \frac{r_n^2 - x^2}{r_n^3}\sin(qr_n - \omega(q)t)$$

$$\frac{\partial^2 u}{\partial y^2} = -u_0 q^2 \frac{y^2}{r_n^2}\cos(qr_n - \omega(q)t) - u_0 q\frac{r_n^2 - y^2}{r_n^3}\sin(qr_n - \omega(q)t)$$

$$\Rightarrow \nabla^2 u = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \quad (2D)$$

$$= -u_0 q^2 \cos(q r_n - w(q)t) - u_0 \frac{q}{r_n} \sin(q r_n - w(q)t).$$

$$\Rightarrow K u_0 q^2 \cos(q r_n - w(q)t) + K u_0 \frac{q}{r_n} \sin(q r_n - w(q)t)$$

$$- \rho w^2(q) u_0 \cos(q r_n - w(q)t) = F.$$

Got stuck here. should fix later.

Qu.2.5 Acoustic and optic phonons in the diatomic chain

This question involves somewhat messy algebra to derive the dispersion relation for the diatomic chain.

In the diatomic chain, we take the unit cell to be of length a, and take x_A and x_B to be the coordinates of the A and B atoms within the unit cell. Hence, in the n^{th} cell,

$$r_{n,A} = na + x_A; \qquad r_{n,B} = na + x_B \quad . \tag{2.46}$$

In the equations of motionEq. (2.30), look for solutions of the form

$$u_{n,\alpha} = e_\alpha(q) \exp i(qr_{n,\alpha} - \omega(q)t) + e^*_\alpha(q) \exp i(-qr_{n,\alpha} + \omega(q)t) \tag{2.47}$$

where $\alpha = A$ or B, and e_α are complex numbers that give the amplitude and phase of the oscillation of the two atoms.

Separating out the terms that have the same time dependence, show that (for equal masses, $m_A = m_B = m$)

$$\begin{aligned} m\omega^2(q)e_A(q) &= D_{AA}(q)e_A(q) + D_{AB}(q)e_B(q) \\ m\omega^2(q)e_B(q) &= D_{BA}(q)e_A(q) + D_{BB}(q)e_B(q) \end{aligned} \tag{2.48}$$

where

$$D_{AA}(q) = D_{BB}(q) = K + K' \quad , \tag{2.49}$$

$$\begin{aligned} -D_{AB}(q) &= K \exp iq(r_{n,B} - r_{n,A}) + K' \exp iq(r_{n-1,B} - r_{n,A}) \\ -D_{BA}(q) &= K \exp iq(r_{n,A} - r_{n,B}) + K' \exp iq(r_{n+1,A} - r_{n,B}) \end{aligned} \tag{2.50}$$

Check that $D_{AB} = D^*_{BA}$.

The 2x2 matrix equation can have a non-trivial solution if the determinant vanishes:

$$\begin{vmatrix} D_{AA}(q) - m\omega^2(q) & D_{AB}(q) \\ D_{BA}(q) & D_{BB}(q) - m\omega^2(q) \end{vmatrix} = 0 \tag{2.51}$$

Hence show that the frequencies of the modes are given by

$$m\omega^2(q) = K + K' \pm [(K+K')^2 - 4KK' \sin^2(\frac{qa}{2})]^{1/2} \quad . \tag{2.52}$$

Sketch the dispersion relations when $K/K' = 2$.

Discuss what happens if $K = K'$.

masses and two different spring constants (see Fig. 2.3). We can now write down two equations of motion, one for each type of atom:

$$\begin{aligned} m_A \frac{\partial^2 u_{nA}}{\partial t^2} &= K(u_{nB} - u_{nA}) + K'(u_{n-1,B} - u_{nA}) \\ m_B \frac{\partial^2 u_{nB}}{\partial t^2} &= K'(u_{n+1A} - u_{nB}) + K(u_{n,A} - u_{nB}) \end{aligned} \tag{2.30}$$

Plug (2.47) in (2.30) to get

$$m_A\left[\omega^2(q)\, e_A(q) \exp i\left(q r_{n,A} \underline{- \omega(q) t}\right) + \omega^2(q)\, e_A^*(q) \exp i\left(-q r_{n,A} + \omega(q) t\right)\right]$$

$$+\, e_B(q)\, \underline{\exp(-i\omega(q)t)} \left[K \exp(i q r_{n,B}) + K' \exp(i q r_{n-1,B})\right]$$

$$+\, e_B^*(q) \exp(i\omega(q)t) \left[K \exp(-i q r_{n,B}) + K' \exp(-i q r_{n-1,B})\right]$$

$$-(K+K')\left[e_A(q) \exp\underline{(-i\omega(q)t)} \exp(i q r_{n,A}) + e_A^*(q) \exp(i\omega(q)t) \exp(-i q r_{n,A})\right] = 0. \quad ①$$

$$m_B\left[\omega^2(q)\, e_B(q) \exp i\left(q r_{n,B} \underline{- \omega(q) t}\right) + \omega^2(q)\, e_B^*(q) \exp i\left(-q r_{n,B} + \omega(q) t\right)\right]$$

$$+\, e_A(q) \exp\underline{(-i\omega(q)t)} \left[K \exp(i q r_{n,A}) + K' \exp(i q r_{n+1,A})\right]$$

$$+\, e_A^*(q) \exp(i\omega(q)t) \left[K \exp(-i q r_{n,A}) + K' \exp(-i q r_{n+1,A})\right]$$

$$-(K+K')\left[e_B(q)\, \underline{\exp(-i\omega(q)t)} \exp(i q r_{n,B}) + e_B^*(q) \exp(i\omega(q)t) \exp(-i q r_{n,B})\right] = 0. \quad ②$$

Seperate the terms with same time dependence, in ① : (marked in $\sim$)

$$m_A\, \omega^2(q)\, e_A(q) \exp(i q r_{n,A}) + e_B(q)\left[K \exp(i q r_{n,B}) + K' \exp(i q r_{n-1,B})\right]$$

$$-(K+K')\, e_A(q) \exp(i q r_{n,A}) = 0.$$

$$\Rightarrow$$

$$m_A\, \omega^2(q)\, e_A(q) = \underbrace{(K+K')}_{D_{AA}(q)} e_A(q) + \underbrace{\left[-K \exp\left(iq(r_{n,B}-r_{n,A})\right) - K' \exp\left(iq(r_{n-1,B}-r_{n,A})\right)\right]}_{D_{AB}(q)} e_B(q) = 0.$$

Seperate the terms with same time dependence, in ② : (marked in $\sim\sim$)

$$m_B\,\omega^2(q)\,e_B(q)\exp(iqr_{n,B}) + e_A(q)\left[K\exp(iqr_{n,A}) + K'\exp(iqr_{n+1,A})\right]$$
$$-(K+K')\,e_B(q)\exp(iqr_{n,B}) = 0.$$

$\Rightarrow$

$$m_B\,\omega^2(q)\,e_B(q) = \underbrace{(K+K')}_{D_{BB}(q)}e_B(q) + \underbrace{\left[-K\exp(iq(r_{n,A}-r_{n,B}) - K'\exp(iq(r_{n+1,A}-r_{n,B})\right]}_{D_{BA}(q)}e_B(q) = 0.$$

$$D^*_{BA} = -K\exp(iq(r_{n,B}-r_{n,A})) - K'\exp(iq(\underline{r_{n,B}-r_{n+1,A}}))$$

Since $\quad r_{n,B} - r_{n+1,A} = na + x_B - (n+1)a - x_A = x_B - x_A - a$

$$= r_{n-1,B} - r_{n,A}.$$

$$D^*_{BA} = D_{AB}.$$

Now that the equation becomes

$$\left[D_{AA}(q) - m\omega^2(q)\right]e_A(q) + D_{AB}(q)\,e_B(q) = 0.$$
$$D_{BA}(q)\,e_A(q) + \left[D_{BB}(q) - m\omega^2(q)\right]e_B(q) = 0.$$

From principles in linear algebra we know the solution exists when

$$\begin{vmatrix} D_{AA}(q) - m\omega^2(q) & D_{AB}(q) \\ D_{BA}(q) & D_{BB}(q) - m\omega^2(q) \end{vmatrix} = 0.$$

$$\Rightarrow \quad m^2\omega^4(q) - (D_{AA}+D_{BB})\,m\omega^2(q) + D_{AA}D_{BB} - D_{AB}D_{BA} = 0.$$

$$\Rightarrow \quad m\omega^2(q) = \frac{1}{2}\left(D_{AA} + D_{BB} \pm \sqrt{(D_{AA}-D_{BB})^2 + 4D_{AB}D_{BA}}\right).$$

Plug in to get

$$m\omega^2(q) = K+K' \pm \sqrt{\Delta}.$$

$$\Delta = (D_{AA}-D_{BB})^2 + 4D_{AB}D_{BA}$$

$$-D_{AB} = K\exp(iq(x_B-x_A)) + K'\exp(iq(x_B-x_A-a)).$$

$$-D_{BA} = K\exp(iq(x_A-x_B)) + K'\exp(iq(x_A-x_B+a)).$$

$$\Rightarrow \quad \Delta = 0 + K^2+K'^2 + KK'\cdot\left[\exp(-iqa)+\exp(iqa)\right]$$

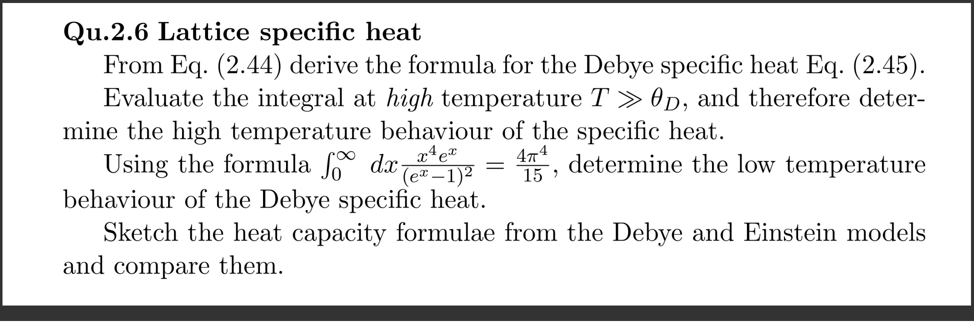
$$= (K+K')^2 + 2KK'\cos qa - 2KK'$$

$$= (K+K')^2 - 4KK'\sin^2\left(\frac{qa}{2}\right).$$

$$\Longrightarrow \quad m\omega^2(q) = K+K' \pm \sqrt{(K+K')^2 - 4KK'\sin^2\left(\frac{qa}{2}\right)}.$$

When $K/K' = 2$, $\quad m\omega^2(q) = 3K' \pm 2K'\sqrt{4-2\sin^2\left(\frac{qa}{2}\right)}$.

If $K=K'$. $\quad m\omega^2(q) = 2K \pm 2K\cos\left(\frac{qa}{2}\right)$.



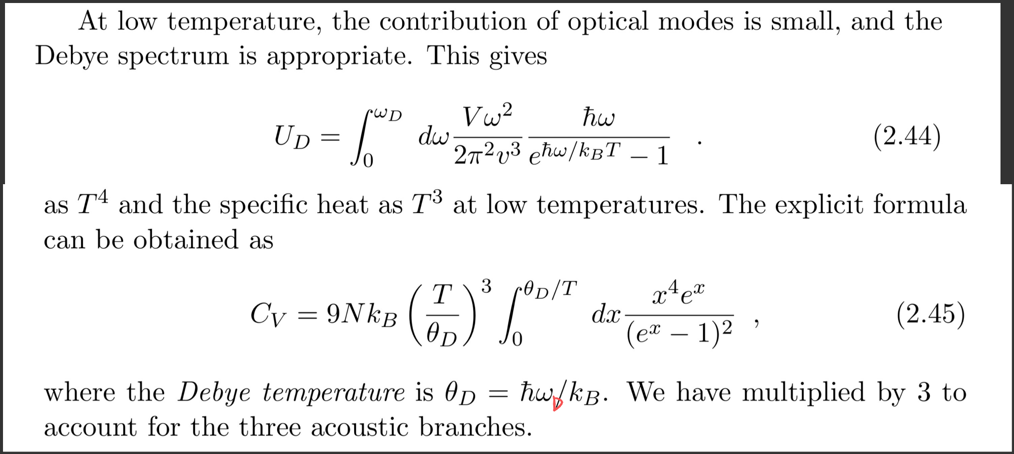
Qu.2.6 Lattice specific heat

From Eq. (2.44) derive the formula for the Debye specific heat Eq. (2.45).

Evaluate the integral at *high* temperature $T \gg \theta_D$, and therefore determine the high temperature behaviour of the specific heat.

Using the formula $\int_0^\infty dx \frac{x^4 e^x}{(e^x-1)^2} = \frac{4\pi^4}{15}$, determine the low temperature behaviour of the Debye specific heat.

Sketch the heat capacity formulae from the Debye and Einstein models and compare them.



At low temperature, the contribution of optical modes is small, and the Debye spectrum is appropriate. This gives

$$U_D = \int_0^{\omega_D} d\omega \frac{V\omega^2}{2\pi^2 v^3} \frac{\hbar\omega}{e^{\hbar\omega/k_BT}-1} \quad . \tag{2.44}$$

as T^4 and the specific heat as T^3 at low temperatures. The explicit formula can be obtained as

$$C_V = 9Nk_B\left(\frac{T}{\theta_D}\right)^3 \int_0^{\theta_D/T} dx \frac{x^4 e^x}{(e^x-1)^2} \quad , \tag{2.45}$$

where the *Debye temperature* is $\theta_D = \hbar\omega_D/k_B$. We have multiplied by 3 to account for the three acoustic branches.

$$C_v = \left(\frac{\partial U_D}{\partial T}\right)_v = \int_0^{\omega_D} d\omega \frac{V\omega^2}{2\pi^2 v^3}\cdot\frac{\hbar\omega}{e^{\hbar\omega/k_BT}-1}\cdot\left(\frac{\hbar\omega}{k_BT^2}\right)\cdot\frac{e^{\frac{\hbar\omega}{k_BT}}}{\left(e^{\frac{\hbar\omega}{k_BT}}-1\right)^2}$$

$$\xrightarrow{\frac{\hbar\omega}{k_BT}=x} \int_0^{\frac{\hbar\omega_D}{k_BT}} \frac{k_BT}{\hbar}dx \, \frac{V\left(\frac{k_BTx}{\hbar}\right)^2}{2\pi^2 v^3}\cdot\frac{\left(\frac{k_BTx}{\hbar}\right)\cdot\hbar}{e^x-1}\cdot\frac{x}{T}\cdot\frac{e^x}{(e^x-1)^2}$$

$$= \int_0^{\frac{\hbar\omega_D}{k_BT}} \left(\frac{k_BT}{\hbar}\right)^4\cdot\frac{V}{2\pi^2 v^3}\cdot\frac{\hbar}{T}\cdot\frac{x^4e^x}{(e^x-1)^2}dx$$

$$\xrightarrow{\theta_D=\frac{\hbar\omega_D}{k_B}} \int_0^{\theta_D/T}\frac{V}{2\pi^2 v^3}\cdot\frac{k_B^4T^3}{\hbar^3}\cdot\frac{x^4e^x}{(e^x-1)^2}dx.$$

$\omega = vk$

Also, for the Debye model

$$g_D(\omega) = \frac{V}{8\pi^3} \cdot 4\pi k^2 \overset{\nearrow \frac{1}{v}}{\frac{dk}{d\omega}} = \frac{V}{2\pi^2} \cdot \frac{\omega^2}{v^3} .$$

$$\int_0^{\omega_D} g_D(\omega)\, d\omega = \int_0^{\omega_D} \frac{V}{2\pi^2 v^3} \omega^2 d\omega = \frac{V\omega_D^3}{6\pi^2 v^3} = N .$$

The Integral becomes

$$\int_0^{\Theta_D/T} \frac{3N\hbar}{\omega_D^3} \cdot \left(\frac{k_B}{\hbar}\right)^4 T^3 \frac{x^4 e^x}{(e^x-1)^2} dx$$

$$= \int_0^{\Theta_D/T} \frac{3N\hbar^4}{(k_B\Theta_D)^3} \cdot \frac{k_B^4}{\hbar^4} T^3 \frac{x^4 e^x}{(e^x-1)^2} dx$$

$$= \int_0^{\Theta_D/T} 3Nk_B \left(\frac{T}{\Theta_D}\right)^3 \frac{x^4 e^x}{(e^x-1)^2} dx$$

$\downarrow$ 3 acoustic branches, multiply by 3

(2.45)

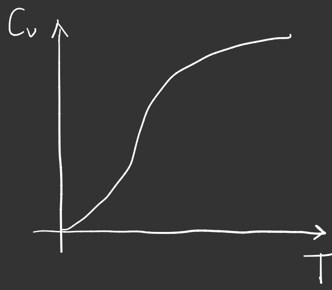
At low temperatures, $\Theta_D/T \to \infty$.

$$C_v = 9Nk_B \left(\frac{T}{\Theta_D}\right)^3 \int_0^\infty \frac{x^4 e^x}{(e^x-1)^2} dx$$

$$= 9Nk_B \left(\frac{T}{\Theta_D}\right)^3 \frac{4\pi^4}{15} = \frac{12\pi^4}{5} Nk_B \left(\frac{T}{\Theta_D}\right)^3 .$$

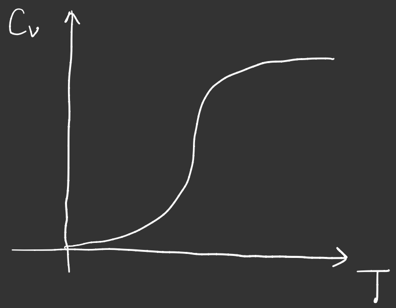
So C_v increase with T^3 at $T \to 0$.

C_v in Debye model:



$$C_v = \int_0^{\Theta_D/T} 3Nk_B \left(\frac{T}{\Theta_D}\right)^3 \frac{x^4 e^x}{(e^x-1)^2}\,dx$$

C_v in Einstein model:



$$C_v = 3Nk_B \left(\frac{\hbar\omega_0}{k_B T}\right)^2 \frac{e^{\frac{\hbar\omega_0}{k_B T}}}{\left(e^{\frac{\hbar\omega_0}{k_B T}}-1\right)^2}.$$

Should plot in Mathematica for further comparision,

might do it later.

Chapter 3 Diffraction Conditions and Brillouin Zones

Qu.3.1 BCC and FCC lattices

Show that the reciprocal lattice of a body centred cubic lattice (BCC) of spacing a is a face centred cubic (FCC) lattice of spacing $4\pi/a$; and that the reciprocal lattice of a FCC lattice of spacing a is a BCC lattice of spacing $4\pi/a$.

The direct lattice could be represented as

$$\vec{R_n} = n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3 .$$

The reciprocal lattice satisfies:

$$\vec{G_h} \cdot \vec{R_n} = 2\pi m . \qquad (m : \text{integer})$$

$$\Rightarrow \vec{G_h} = h_1\vec{b_1} + h_2\vec{b_2} + h_3\vec{b_3} .$$

$$\vec{b_1} = 2\pi \frac{\vec{a_2} \times \vec{a_3}}{\vec{a_1} \cdot (\vec{a_2} \times \vec{a_3})}$$

$$\vec{b_2} = 2\pi \frac{\vec{a_3} \times \vec{a_1}}{\vec{a_1} \cdot (\vec{a_2} \times \vec{a_3})} .$$

$$\vec{b_3} = 2\pi \frac{\vec{a_1} \times \vec{a_2}}{\vec{a_1} \cdot (\vec{a_2} \times \vec{a_3})} .$$

△ For BCC,

$$\vec{a_1} = -\frac{a}{2}\hat{x} + \frac{a}{2}\hat{y} + \frac{a}{2}\hat{z} .$$

$$\vec{a_2} = \frac{a}{2}\hat{x} - \frac{a}{2}\hat{y} + \frac{a}{2}\hat{z} .$$

$$\vec{a_3} = \frac{a}{2}\hat{x} + \frac{a}{2}\hat{y} - \frac{a}{2}\hat{z} .$$

Plug in to get

$$\vec{b}_1 = 2\pi \frac{\frac{a^2}{2}(\hat{y}+\hat{z})}{\frac{1}{2}a^3} = \frac{2\pi}{a}(\hat{y}+\hat{z}).$$

$$\vec{b}_2 = \frac{2\pi}{a}(\hat{z}+\hat{x}).$$

$$\vec{b}_3 = \frac{2\pi}{a}(\hat{x}+\hat{y}).$$

This vector set represents an FCC lattice.

△ For FCC,

$$\vec{a}_1 = \frac{a}{2}(\hat{y}+\hat{z}), \quad \vec{a}_2 = \frac{a}{2}(\hat{z}+\hat{x}), \quad \vec{a}_3 = \frac{a}{2}(\hat{x}+\hat{y}).$$

Plug in to get

$$\vec{b}_1 = 2\pi \cdot \frac{\frac{a^2}{4}(-\hat{x}+\hat{y}+\hat{z})}{\frac{a^3}{4}} = \frac{2\pi}{a}(-\hat{x}+\hat{y}+\hat{z}).$$

$$\vec{b}_2 = \frac{2\pi}{a}(\hat{x}-\hat{y}+\hat{z}). \qquad \vec{b}_3 = \frac{2\pi}{a}(\hat{x}+\hat{y}-\hat{z}).$$

This vector set represent a BCC lattice.

Qu.3.2 Reciprocal lattice cell volume

Show that the volume of the primitive unit cell of the reciprocal lattice is $(2\pi)^3/\Omega_{cell}$, where Ω_{cell} is the volume of the primitive unit cell of the crystal.

The reciprocal lattice could be written as

$$\vec{G}_h = h_1 \vec{b}_1 + h_2 \vec{b}_2 + h_3 \vec{b}_3 .$$

and $\vec{b}_i \cdot \vec{a}_j = 2\pi \delta_{ij}$. $(*)$

Suppose $\vec{b}_1 = \eta \, \vec{a}_2 \times \vec{a}_3$. Plug in $(*)$ to get

$$\eta_1 = \frac{2\pi}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)} .$$

Similarly,

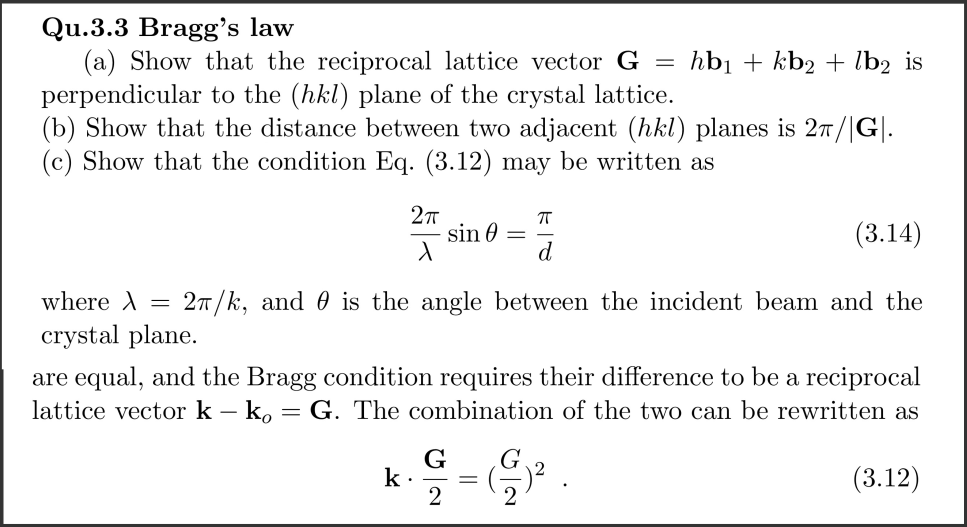
$$\vec{b}_1 = 2\pi \frac{\vec{a}_2 \times \vec{a}_3}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)}$$

$$\vec{b}_2 = 2\pi \frac{\vec{a}_3 \times \vec{a}_1}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)} .$$

$$\vec{b}_3 = 2\pi \frac{\vec{a}_1 \times \vec{a}_2}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)} .$$

So, $\Omega^* = \vec{b}_1 \cdot (\vec{b}_2 \times \vec{b}_3) = \left(\frac{2\pi}{\Omega_{cell}}\right)^3 (\vec{a}_2 \times \vec{a}_3) \cdot \left[(\vec{a}_3 \times \vec{a}_1) \times (\vec{a}_1 \times \vec{a}_2)\right]$

$$= \frac{(2\pi)^3}{\Omega_{cell}} .$$



Qu.3.3 Bragg's law

(a) Show that the reciprocal lattice vector $\mathbf{G} = h\mathbf{b}_1 + k\mathbf{b}_2 + l\mathbf{b}_2$ is perpendicular to the (hkl) plane of the crystal lattice.
(b) Show that the distance between two adjacent (hkl) planes is $2\pi/|\mathbf{G}|$.
(c) Show that the condition Eq. (3.12) may be written as

$$\frac{2\pi}{\lambda}\sin\theta = \frac{\pi}{d} \tag{3.14}$$

where $\lambda = 2\pi/k$, and θ is the angle between the incident beam and the crystal plane.

are equal, and the Bragg condition requires their difference to be a reciprocal lattice vector $\mathbf{k} - \mathbf{k}_o = \mathbf{G}$. The combination of the two can be rewritten as

$$\mathbf{k}\cdot\frac{\mathbf{G}}{2} = \left(\frac{G}{2}\right)^2 . \tag{3.12}$$

(a) Given Miller index (hkl).

We know $\left(\frac{\vec{a}_1}{h} - \frac{\vec{a}_2}{k}\right)$ is a vector inside the plane.

And $\vec{G}\cdot\left(\frac{\vec{a}_1}{h} - \frac{\vec{a}_2}{k}\right) = \vec{b}_1\cdot\vec{a}_1 - \vec{b}_2\cdot\vec{a}_2 = 0$.

So $\vec{G}$ is perpendicular to (hkl) plane.

(b) Distance between two adjacent planes is

$$d = \frac{\vec{a}_1}{h}\cdot\frac{\vec{G}}{|\vec{G}|} = \frac{h\,\vec{a}_1\cdot\vec{b}_1}{h\,|\vec{G}|} = \frac{2\pi}{|\vec{G}|}.$$

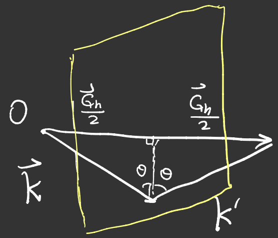
(c) The relationship could be drawn as below

We could see that

$$\vec{k}\cdot\frac{\vec{G}}{2} = \frac{\vec{G}}{2}\cdot\frac{\vec{G}}{2} = \left(\frac{G}{2}\right)^2.$$

The yellow part is crystal plane, and $\vec{k}$ the incident beam,

We have $k\sin\theta = \frac{G}{2}$.



Also $|\vec{G}| = \frac{2n\pi}{d}$, $k = \frac{2\pi}{\lambda}$,

$$\Rightarrow \frac{2\pi}{\lambda}\sin\theta = \frac{n\pi}{d}.$$

$$\Rightarrow n\lambda = d\sin\theta.$$

Chapter 4 Electronic Structure Theory

Qu.4.1 Bloch's theorem Prove Bloch's theorem by operating with the translation operator on $H\psi$ and using the periodic symmetry of the potential. Show furthermore that $T_{\mathbf{R}}T_{\mathbf{R}'} = T_{\mathbf{R}'}T_{\mathbf{R}} = T_{\mathbf{R}+\mathbf{R}'}$; the translation operators commute with themselves.

We have translation operator $\hat{T}_{\vec{R}} f(\vec{r}) = f(\vec{r}+\vec{R})$.

From the periodic symmetry of potential we know the Hamiltonian also have the periodic symmetry:

$$\hat{H}(\vec{r}+\vec{R}) = \hat{H}(\vec{r}).$$

For that $\hat{T}_{\vec{R}}\hat{H}\psi(\vec{r}) = \hat{H}(\vec{r}+\vec{R})\psi(\vec{r}+\vec{R})$

$$= \hat{H}(\vec{r})\hat{T}_{\vec{R}}\psi(\vec{r}).$$

We have $\hat{T}_{\vec{R}}\hat{H} = \hat{H}\hat{T}_{\vec{R}}$.

Suppose $\hat{T}_{R}, \hat{H}$ have simultaneous eigenfunction $\psi(\vec{r})$.

$$\Rightarrow \quad \hat{T}_{\vec{R}}\psi(\vec{r}) = \lambda_{\vec{R}}\psi(\vec{r}) = \psi(\vec{r}+\vec{R}).$$

$$\Rightarrow |\lambda_{\vec{R}}| = 1. \quad \lambda_{\vec{R}} = e^{i\beta_{\vec{R}}}.$$

△ That is, $\psi(\vec{r}+\vec{R}) = e^{i\beta_{\vec{R}}}\psi(\vec{r})$.

$$\hat{T}_{\vec{R}}\hat{T}_{\vec{R}'}\psi(\vec{r}) = \hat{T}_{\vec{R}}\lambda_{\vec{R}'}\psi(\vec{r}) = \lambda_{\vec{R}}\lambda_{\vec{R}'}\psi(\vec{r}) = \hat{T}_{\vec{R}'}\hat{T}_{\vec{R}}\psi(\vec{r}).$$

$\hat{T}_{\vec{R}}\hat{T}_{\vec{R}'} = \hat{T}_{\vec{R}+\vec{R}'}$. (Continuity of Translation).

That is $T_{\vec{R}}T_{\vec{R}'} = T_{\vec{R}'}T_{\vec{R}} = T_{\vec{R}+\vec{R}'}$.

Qu.4.2 Another proof of Bloch's theorem

A more elegant way to prove Bloch's theorem is to note that the translation operator can be written

$$T_{\mathbf{R}} = e^{-i\hat{\mathbf{P}}\cdot\mathbf{R}/\hbar},$$

where $\hat{\mathbf{P}}$ is the momentum operator. (If you don't know how to do this, make the replacement $\hat{\mathbf{P}} = -i\hbar\nabla$, and check that the operator generates the infinite Taylor series expansion of $f(\mathbf{r}+\mathbf{R})$.) By multiplying by the ket $<\mathbf{k}|$ (an eigenfunction of momentum), show that either $<\mathbf{k}|\psi>= 0$, or $c(\mathbf{R}) = e^{-i\mathbf{k}\cdot\mathbf{R}}$.

We should show that $\hat{T}_{\vec{R}} f(\vec{r}) = f(\vec{r}+\vec{R})$.

$$e^{-i\vec{P}\cdot\vec{R}/\hbar} f(\vec{r}) = e^{-\vec{\nabla}\cdot\vec{R}} f(\vec{r}) \qquad \times$$

$$= e^{-\left(\frac{\partial R_x}{\partial x}+\frac{\partial R_y}{\partial y}+\frac{\partial R_z}{\partial z}\right)} f(\vec{r}).$$

$$f(\vec{r}+\vec{R}) = \sum_{n=0}^{\infty}\frac{1}{n!}\left[(\vec{r}+\vec{R})-\vec{r}\right]^n \left.\frac{d^n f(\vec{r}+\vec{R})}{d(r+R)^n}\right|_{\vec{r}+\vec{R}=\vec{r}}$$

$$= \sum_{n=0}^{\infty}\frac{1}{n!}\vec{R}^n\frac{d^n}{d\vec{r}^n}f(\vec{r})$$

$$= \sum_{n=0}^{\infty}\frac{1}{n!}\left(\frac{i\vec{R}}{\hbar}\cdot\underline{\frac{\hbar}{i}\frac{d}{d\vec{r}}}\right)^n f(\vec{r}) = \sum_{n=0}^{\infty}\frac{1}{n!}\left(\frac{i\vec{R}\cdot\vec{P}}{\hbar}\right)^n f(\vec{r})$$

$$= e^{i\vec{R}\cdot\vec{P}/\hbar} f(\vec{r}) = \hat{T}_{\vec{R}} f(\vec{r}).$$

Also, $\hat{T}_{\vec{R}}\, |\psi\rangle = c(\vec{R})\, |\psi\rangle .$

$|\psi\rangle : |\psi(\vec{r})\rangle .$

$$\Rightarrow \quad e^{i\vec{R}\cdot\vec{P}/\hbar}\, |\psi\rangle = c(\vec{R})|\psi\rangle$$

$$\langle k|\, e^{i\vec{R}\cdot\vec{P}/\hbar}\, |\psi\rangle = c(\vec{R})\, \langle \vec{k}|\psi\rangle$$

$$\langle k|\left(e^{i\vec{R}\cdot\vec{P}}|\psi\rangle - c(\vec{R})\,|\psi\rangle\right) = 0$$

$$\Rightarrow \langle k|\psi\rangle\cdot\left(e^{i\vec{R}\cdot\vec{P}} - c(\vec{R})\right) = 0 .$$

$$\Rightarrow \langle k|\psi\rangle = 0 \quad \text{or} \quad c(\vec{R}) = e^{i\vec{k}\cdot\vec{R}} .$$

$$(\vec{P} = \hbar\vec{k})$$

Qu.4.3 One-dimensional band

Consider a one-dimensional system which is filled up to the first Brillouin zone boundary at $k = \pi/a$, and assume that there is a small gap produced by a single Fourier component of the lattice potential $U = U_{K=2\pi/a}$ (small meaning that $U/E^0_{\frac{1}{2}K} \ll 1$). Consider momenta close to the zone boundary, show that a good approximation for the energy dispersion of the bands is

$$E = E_0\left(1 \pm \sqrt{\frac{U^2}{E_0^2} + 4x^2}\right)$$

where $E_0 = E^0_{\frac{1}{2}K}$ and $k = (\pi/a)(1+x)$, with $x \ll 1$.

Evaluate the change in electronic energy for a small gap (at zero temperature)

$$E_{elec} = \sum_{k\ occupied} [E(k;U) - E(k;U=0)]$$

to leading order in U/E_0. (Hint: the result is non-analytic - **don't** try a Taylor series in U.)

We shall be using this result later to understand the Peierls instability of a one-dimensional system.

With $U/E^{0}_{\frac{1}{2}k} << 1$ we apply perturbation theory:

$$H = H_0 + U.$$

We already have $\psi_k^{(0)}(x) = \frac{1}{\sqrt{2a}} e^{ikx}.$

$$\varepsilon_k^{(0)} = \frac{\hbar^2 k^2}{2m}.$$

For first-order approximation

$$\psi_k(x) = \psi_k^{(0)}(x) + \psi_k^{(1)}(x).$$

$$= \frac{1}{\sqrt{2a}} e^{ikx} + \sum_{k'}{}' \frac{H_{kk'}}{\varepsilon_k^0 - \varepsilon_{k'}^0} \psi_{k'}^{(0)}(x)$$

$$H_{kk'} = \langle k'|U|k\rangle = \frac{1}{2a}\int_{-a}^{a} e^{-i(k-k')x}\, U\, dx$$

And $\varepsilon_k^{(1)} = H'_{kk} = \langle k|U|k\rangle = 0.$

$$\varepsilon_k^{(2)} = \sum_{k'} \frac{|H'_{kk'}|^2}{\varepsilon_k^{(0)} - \varepsilon_{k'}^{(0)}}.$$

For momenta close to zone boundary, $k = \frac{\pi}{a}(1+x).$

Let $k' = -\frac{\pi}{a}(1-x).$ $\quad H'_{kk} = U\cdot\frac{1}{2a}\int_{-a}^{a} e^{-\frac{2\pi i}{a}x}\, dx = U.$

$$\varepsilon_k^{(0)} - \varepsilon_{k'}^{(0)} = \frac{\hbar^2}{2m}\frac{\pi^2}{a^2}\left[(1+x)^2 - (1-x)^2\right] \longrightarrow 0.$$

So we should apply non-degenerate perturbation

$$\psi(x) = a\psi_k^{(0)}(x) + b\psi_{k'}^{(0)}(x).$$

Plug in $(H_0 + U)\psi = \varepsilon\psi.$

Also $\quad H_0\psi_k^{(0)} = \varepsilon_k^{(0)}\psi_k^{(0)}. \quad H_0\psi_{k'}^{(0)} = \varepsilon_{k'}^{(0)}\psi_{k'}^{(0)}.$

$$\Rightarrow \quad a\varepsilon_k^{(0)}\psi_k^{(0)} + b\varepsilon_{k'}^{(0)}\psi_{k'}^{(0)} + aU\psi_k^{(0)} + bU\psi_{k'}^{(0)} = a\varepsilon\psi_k^{(0)} + b\varepsilon\psi_{k'}^{(0)}.$$

$$a\left(\varepsilon_k^{(0)} - \varepsilon + U\right)\psi_k^{(0)} + b\left(\varepsilon_{k'}^{(0)} - \varepsilon + U\right)\psi_{k'}^{(0)} = 0.$$

$$\xrightarrow{\cdot\, \psi_k^{(0)*}} \qquad a\left(\varepsilon_k^{(0)} - \varepsilon\right) + bU = 0.$$

$$\xrightarrow{\cdot\, \psi_{k'}^{(0)*}} \qquad aU + b\left(\varepsilon_{k'}^{(0)} - \varepsilon\right) = 0.$$

The solution exists when

$$\begin{vmatrix} \varepsilon_k^{(0)} - \varepsilon & U \\ U & \varepsilon_{k'}^{(0)} - \varepsilon \end{vmatrix} = 0.$$

$$\Rightarrow \quad \varepsilon = \frac{\varepsilon_k^{(0)} + \varepsilon_{k'}^{(0)}}{2} \pm \frac{1}{2}\sqrt{\left(\varepsilon_k^{(0)} - \varepsilon_{k'}^{(0)}\right)^2 + 4U^2}$$

For momenta close to zone boundary, $k = \frac{\pi}{a}(1+x)$.

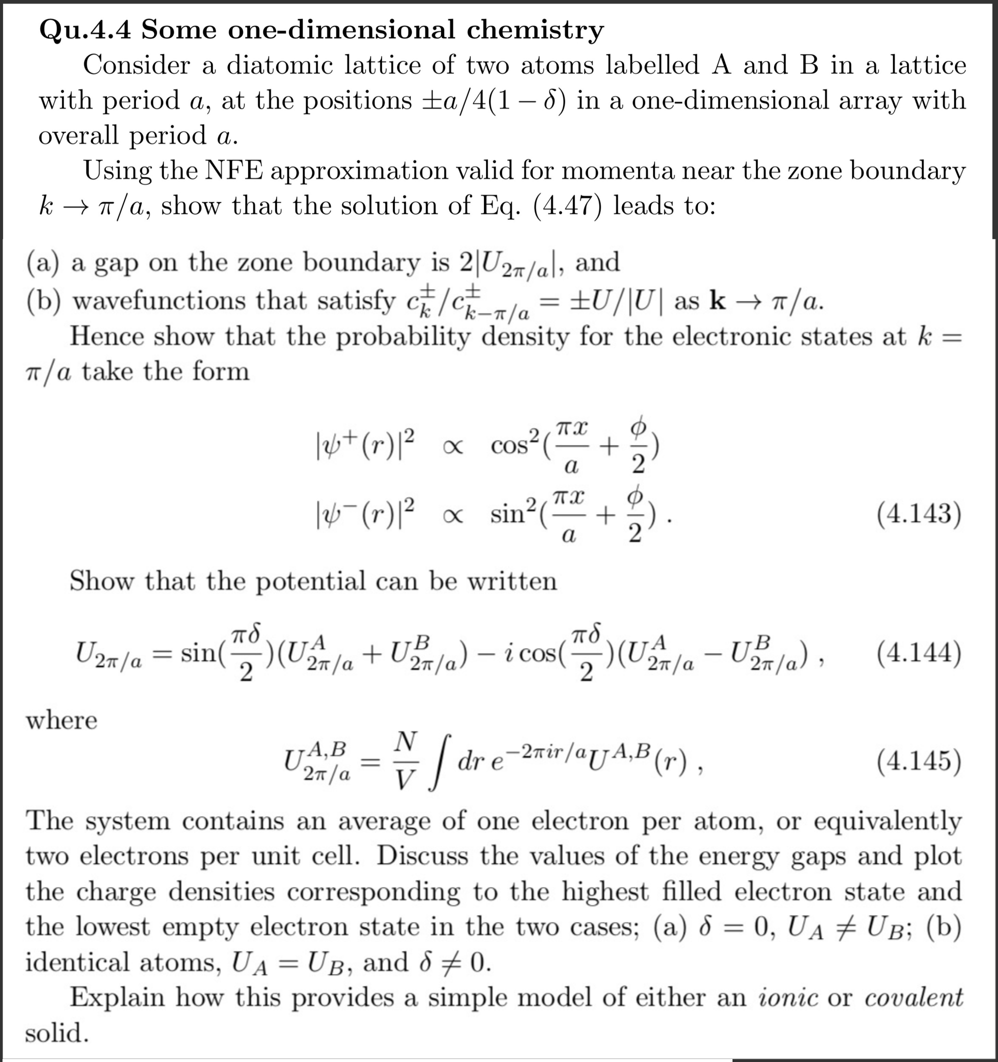
$$\varepsilon = \frac{\hbar^2 k^2}{2m} \pm \sqrt{\left(\frac{2\hbar^2\pi^2 x}{ma^2}\right)^2 + 4U^2}$$

$$= \frac{\hbar^2\pi^2}{2ma^2} \pm \sqrt{\left(\frac{\hbar^2\pi^2}{2ma^2}\cdot 4x\right)^2 + 4U^2}$$

$$= E_0\left(1 \pm \sqrt{\frac{U^2}{E_0^2} + 4x^2}\right).$$

$$E_{elec} = \sum_{k \text{ occupied}} \left[E(k;U) - E(k;U=0) \right]$$

$$= \sum_k \sum_{k'} \frac{|H_{kk'}|^2}{\varepsilon_k^{(0)} - \varepsilon_{k'}^{(0)}} = \sum_k \sum_n \frac{|\langle \overset{\overset{k+\frac{2\pi n}{a}}{\downarrow}}{k'} | U | k \rangle|^2}{\frac{\hbar^2}{2m}\left[k^2 - \left(k + \frac{2\pi n}{a}\right)^2\right]}$$



Qu.4.4 Some one-dimensional chemistry

Consider a diatomic lattice of two atoms labelled A and B in a lattice with period a, at the positions $\pm a/4(1-\delta)$ in a one-dimensional array with overall period a.

Using the NFE approximation valid for momenta near the zone boundary $k \to \pi/a$, show that the solution of Eq. (4.47) leads to:

(a) a gap on the zone boundary is $2|U_{2\pi/a}|$, and
(b) wavefunctions that satisfy $c_k^{\pm}/c_{k-\pi/a}^{\pm} = \pm U/|U|$ as $\mathbf{k} \to \pi/a$.

Hence show that the probability density for the electronic states at $k = \pi/a$ take the form

$$\begin{aligned} |\psi^+(r)|^2 &\propto \cos^2\left(\frac{\pi x}{a} + \frac{\phi}{2}\right) \\ |\psi^-(r)|^2 &\propto \sin^2\left(\frac{\pi x}{a} + \frac{\phi}{2}\right) . \end{aligned} \tag{4.143}$$

Show that the potential can be written

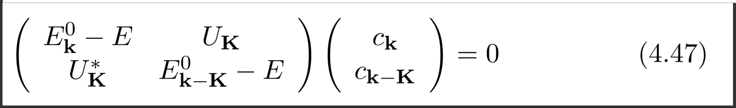
$$U_{2\pi/a} = \sin\left(\frac{\pi\delta}{2}\right)(U^A_{2\pi/a} + U^B_{2\pi/a}) - i\cos\left(\frac{\pi\delta}{2}\right)(U^A_{2\pi/a} - U^B_{2\pi/a}) , \tag{4.144}$$

where

$$U^{A,B}_{2\pi/a} = \frac{N}{V}\int dr\, e^{-2\pi i r/a} U^{A,B}(r) , \tag{4.145}$$

The system contains an average of one electron per atom, or equivalently two electrons per unit cell. Discuss the values of the energy gaps and plot the charge densities corresponding to the highest filled electron state and the lowest empty electron state in the two cases; (a) $\delta = 0$, $U_A \neq U_B$; (b) identical atoms, $U_A = U_B$, and $\delta \neq 0$.

Explain how this provides a simple model of either an *ionic* or *covalent* solid.



$$\begin{pmatrix} E^0_{\mathbf{k}} - E & U_{\mathbf{K}} \\ U^*_{\mathbf{K}} & E^0_{\mathbf{k}-\mathbf{K}} - E \end{pmatrix} \begin{pmatrix} c_{\mathbf{k}} \\ c_{\mathbf{k}-\mathbf{K}} \end{pmatrix} = 0 \tag{4.47}$$

(a) The solution exists when

$$\begin{vmatrix} E^0_{\vec{k}} - E & U_{\vec{k}} \\ U^*_{\vec{k}} & E^0_{\vec{k}-\vec{K}} - E \end{vmatrix} = 0$$

$$\Rightarrow E = \frac{E^0_{\vec{k}} + E^0_{\vec{k}-\vec{K}}}{2} \pm \sqrt{\left(\frac{E^0_{\vec{k}} - E^0_{\vec{k}-\vec{K}}}{2}\right)^2 + U^2_{\vec{k}}} \qquad (*)$$

on the zone boundary we have gap

$$E_+ - E_- = 2|U_{\vec K}| = 2|U_{2\pi/a}|.$$

(b) Plug (*) back to equations

$$(E^0_{\vec k} - E)C_{\vec k} + U_{\vec K} C_{\vec k-\vec K} = 0$$

$$U^*_{\vec K} C_{\vec k} + (E^0_{\vec k-\vec K} - E)C_{\vec k-\vec K} = 0$$

We get $C_{\vec k}/C_{\vec k-\vec K} = \dfrac{U_{\vec K}}{E - E^0_{\vec k}} = \dfrac{U_{\vec K}}{\underline{\frac{E^0_{\vec k-\vec K} - E^0_{\vec k}}{2}} \pm \sqrt{\left(\underline{\frac{E^0_{\vec k} - E^0_{\vec k-\vec K}}{2}}\right)^2 + U_{\vec K}^2}}$

as $\vec k \to \pi/a$, $C^\pm_{\vec k}/C^\pm_{\vec k-\frac{\pi}{a}} = \pm U/|U|$.

For that $\psi_{\vec k}(\vec r) = \sum_{\vec K} C_{\vec k-\vec K}\, e^{i(\vec k-\vec K)\cdot\vec r}$. when $\vec k \to \pi/a$.

$$\psi^+(\vec r) \propto C_{\vec k}\, e^{i\vec k\cdot\vec r} + C_{\vec k-\vec K}\, e^{-i\vec k\cdot\vec r}$$

$$\propto C_k\left(e^{i\vec k\cdot\vec r} + e^{-i\vec k\cdot\vec r}\right) \propto C_k\cdot\cos(kr) \propto C_k\cdot\cos\left(\tfrac{1}{2}\vec K\cdot\vec r\right).$$

$$\psi^-(\vec r) \propto C_{\vec k}\, e^{i\vec k\cdot\vec r} + C_{\vec k-\vec K}\, e^{-i\vec k\cdot\vec r}$$

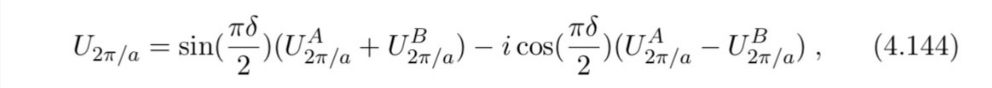
$$\propto C_k\left(e^{i\vec k\cdot\vec r} - e^{-i\vec k\cdot\vec r}\right) \propto C_k\cdot\sin(kr) \propto C_k\cdot\sin\left(\tfrac{1}{2}\vec K\cdot\vec r\right).$$

$\Rightarrow \quad |\psi^+(\vec r)|^2 \propto \left|\cos^2\left(\tfrac{1}{2}\vec K\cdot\vec r\right)\right|. \qquad E = E_+.$

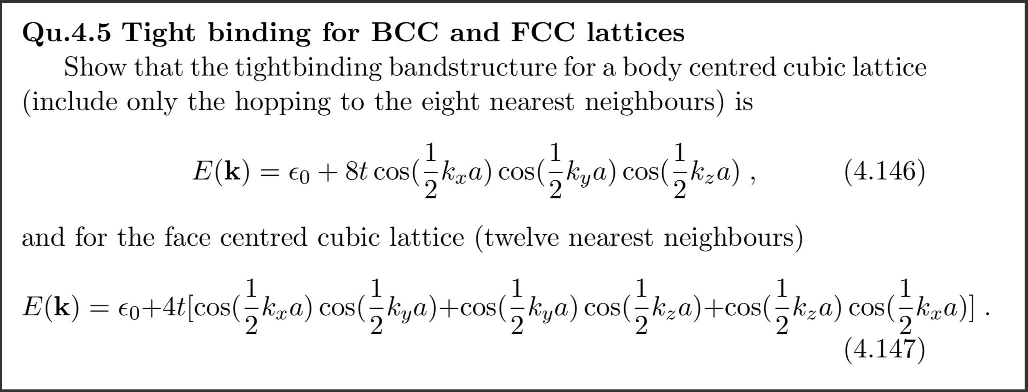
$|\psi^-(\vec r)|^2 \propto \left|\sin^2\left(\tfrac{1}{2}\vec K\cdot\vec r\right)\right|. \qquad E = E_-.$

$$U^{A,B}_{2\pi/a} = \frac{N}{V}\int dr\, e^{-2\pi i r/a}\, U^{A,B}(r) ,$$

A, B at positions $\pm a/4(1-\delta)$.



$$U_{2\pi/a} = \sin(\frac{\pi\delta}{2})(U^A_{2\pi/a} + U^B_{2\pi/a}) - i\cos(\frac{\pi\delta}{2})(U^A_{2\pi/a} - U^B_{2\pi/a}) , \qquad (4.144)$$



Qu.4.5 Tight binding for BCC and FCC lattices

Show that the tightbinding bandstructure for a body centred cubic lattice (include only the hopping to the eight nearest neighbours) is

$$E(\mathbf{k}) = \epsilon_0 + 8t\cos(\frac{1}{2}k_xa)\cos(\frac{1}{2}k_ya)\cos(\frac{1}{2}k_za)\,, \tag{4.146}$$

and for the face centred cubic lattice (twelve nearest neighbours)

$$E(\mathbf{k}) = \epsilon_0 + 4t[\cos(\frac{1}{2}k_xa)\cos(\frac{1}{2}k_ya) + \cos(\frac{1}{2}k_ya)\cos(\frac{1}{2}k_za) + \cos(\frac{1}{2}k_za)\cos(\frac{1}{2}k_xa)]\,. \tag{4.147}$$

The tight binding model shows that:

$$E(\vec{k}) = \mathcal{E}_n - J(0) - \sum_{n.n} J(\vec{R}_s)\, e^{i\vec{k}\cdot\vec{R}_s} \, .$$

(consider s orbital)

nearest neighbour

For BCC we have $\vec{R_s} = \left(\pm\frac{a}{2}, \pm\frac{a}{2}, \pm\frac{a}{2}\right)$.

$$\begin{aligned} E(\vec{k}) = \mathcal{E}_n - J(0) - J_1 \Big(& e^{\frac{i}{2}k_xa} e^{\frac{i}{2}k_ya} e^{\frac{i}{2}k_za} + e^{-\frac{i}{2}k_xa} e^{\frac{i}{2}k_ya} e^{\frac{i}{2}k_za} \\ & + e^{\frac{i}{2}k_xa} e^{-\frac{i}{2}k_ya} e^{\frac{i}{2}k_za} + e^{-\frac{i}{2}k_xa} e^{-\frac{i}{2}k_ya} e^{\frac{i}{2}k_za} \\ & + e^{\frac{i}{2}k_xa} e^{\frac{i}{2}k_ya} e^{-\frac{i}{2}k_za} + e^{-\frac{i}{2}k_xa} e^{\frac{i}{2}k_ya} e^{-\frac{i}{2}k_za} \\ & + e^{\frac{i}{2}k_xa} e^{-\frac{i}{2}k_ya} e^{-\frac{i}{2}k_za} + e^{-\frac{i}{2}k_xa} e^{-\frac{i}{2}k_ya} e^{-\frac{i}{2}k_za} \Big) \end{aligned}$$

$$\begin{aligned} = \mathcal{E}_n - J(0) - 2J_1 \Big[& \cos\frac{k_xa}{2}\left(e^{\frac{i}{2}k_ya} e^{\frac{i}{2}k_za} + e^{-\frac{ik_y}{2}a} e^{\frac{i}{2}k_za}\right) \\ & + \cos\frac{k_xa}{2}\left(e^{\frac{i}{2}k_ya} e^{-\frac{i}{2}k_za} + e^{-\frac{ik_y}{2}a} e^{\frac{i}{2}k_za}\right)\Big] \end{aligned}$$

$$= \mathcal{E}_n - 8J_1 \cos\frac{k_xa}{2} \cos\frac{k_ya}{2} \cos\frac{k_za}{2} \, .$$

For FCC we have

$$\vec{R}_s = \left(\pm\frac{a}{2}, 0, \pm\frac{a}{2}\right), \left(\pm\frac{a}{2}, \pm\frac{a}{2}, 0\right), \left(0, \pm\frac{a}{2}, \pm\frac{a}{2}\right).$$

$$E(\vec{k}) = \varepsilon_n - J(0) - J_1\Big(e^{\frac{ik_x a}{2}} e^{\frac{ik_z}{2}a} + e^{-\frac{ik_x}{2}a} e^{\frac{ik_z}{2}a} + e^{\frac{ik_x}{2}a} e^{-\frac{ik_z}{2}a}$$

$$+ e^{-\frac{ik_x a}{2}} e^{-\frac{ik_z}{2}a} + \cdots \Big)$$

$$= \varepsilon_n - 4J_1\left(\cos\frac{k_x a}{2}\cos\frac{k_z a}{2} + \cos\frac{k_x a}{2}\cos\frac{k_y a}{2} + \cos\frac{k_y a}{2}\cos\frac{k_z a}{2}\right).$$

Qu.4.6 Pseudopotential

Show that $< \chi|f_n >= 0$ if we choose $\beta_n =< f_n|\mathbf{k} >$.

The pseudopotential is not unique. Show that the valence eigenvalues of a Hamiltonian $H + V_R$ are the same for any operator of the form

$$V_R\phi = \sum_n < F_n|\phi > f_n \ ,$$

where the F_n are **arbitrary** functions.

$$|\vec{\chi}> = |\vec{k}> - \sum_n \beta_n |f_{n\vec{k}}>$$

$$= |\vec{k}> - \sum_n <f_{n\vec{k}}|\vec{k}>|f_{n\vec{k}}>$$

$$<f_{n\vec{k}}|\vec{\chi}> = <f_{n\vec{k}}|\vec{k}> - \sum_n <f_{n\vec{k}}|\vec{k}><f_{n\vec{k}}|f_{n\vec{k}}>$$

$$= 0 = <\vec{\chi}|f_{n\vec{k}}>.$$

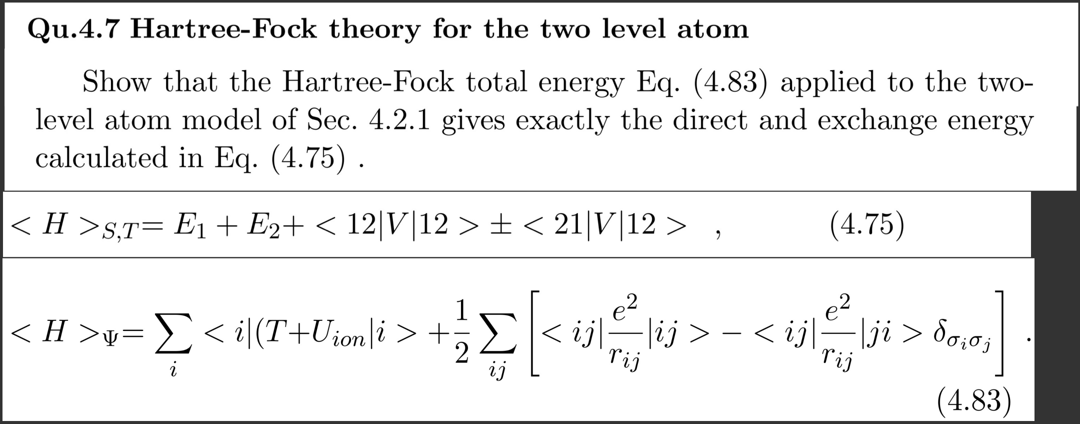
$$(H+V_R)|\psi> = E|\psi>$$

$$|\psi> = |\phi> - \sum_n <f_n|\phi>|f_n>.$$

$$\Rightarrow (H+V_R)|\phi> + \sum_n (E-E_n)<f_n|\phi>|f_n> = E|\phi>.$$

$$\Rightarrow H|\phi> + \sum_n \left[(E-E_n)<f_n|\phi> + <F_n|\phi>\right]|f_n> = E|\phi>.$$

We could take advantage of $<\chi|f_{n\vec{k}}>$ in the proof.



Qu.4.7 Hartree-Fock theory for the two level atom

Show that the Hartree-Fock total energy Eq. (4.83) applied to the two-level atom model of Sec. 4.2.1 gives exactly the direct and exchange energy calculated in Eq. (4.75) .

$$< H >_{S,T}= E_1 + E_2+ < 12|V|12 > \pm < 21|V|12 > \quad , \qquad (4.75)$$

$$< H >_{\Psi}= \sum_i < i|(T+U_{ion}|i > +\frac{1}{2}\sum_{ij}\left[< ij|\frac{e^2}{r_{ij}}|ij > - < ij|\frac{e^2}{r_{ij}}|ji > \delta_{\sigma_i\sigma_j}\right] . \qquad (4.83)$$

For singlet states, $S=0$

$$\frac{|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle}{\sqrt{2}}, \qquad S_z = 0 .$$

$$\psi_s(\vec r_1, \vec r_2) = \left(\psi_1(\vec r_1)\psi_2(\vec r_2) + \psi_2(\vec r_1)\psi_1(\vec r_2)\right)/\sqrt{2}$$

$$= \left(|12\rangle + |21\rangle\right)/\sqrt{2} .$$

$$\langle H\rangle_\Psi = \langle 1|T+U_{ion}|1\rangle + \langle 2|T+U_{ion}|2\rangle$$

$$+ \frac{1}{2}\left[\langle 12|\frac{e^2}{r_{12}}|12\rangle \underset{\sim}{+} \langle 12|\frac{e^2}{r_{12}}|21\rangle \right.$$

$$\left. + \langle 21|\frac{e^2}{r_{21}}|21\rangle \underset{\sim}{+} \langle 21|\frac{e^2}{r_{21}}|12\rangle\right]$$

$S_z = 0.$

$\delta_{\sigma_i\sigma_j} = 0.$

$$= \langle 1|T+U_{ion}|1\rangle + \langle 2|T+U_{ion}|2\rangle$$

$$+ \int d\vec r\, d\vec r'\, |\psi_1(\vec r)|^2 \frac{e^2}{|\vec r - \vec r'|} |\psi_2(\vec r')|^2 + \int d\vec r\, d\vec r'\, \psi_2^*(\vec r)\psi_1^*(\vec r') \frac{e^2}{|\vec r - \vec r'|} \psi_1(\vec r)\psi_2(\vec r') .$$

$$= E_1 + E_2 + \langle 12|V|12\rangle + \langle 21|V|12\rangle .$$

For Triplet states, $S = 1$.

$$|\uparrow\uparrow\rangle. \qquad S_z = 1.$$

$$(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)/\sqrt{2}. \qquad S_z = 0.$$

$$|\downarrow\downarrow\rangle. \qquad S_z = -1.$$

$$\psi_T(\vec{r}_1, \vec{r}_2) = (\psi_1(\vec{r}_1)\psi_2(\vec{r}_2) - \psi_2(\vec{r}_1)\psi_1(\vec{r}_1))/\sqrt{2}.$$

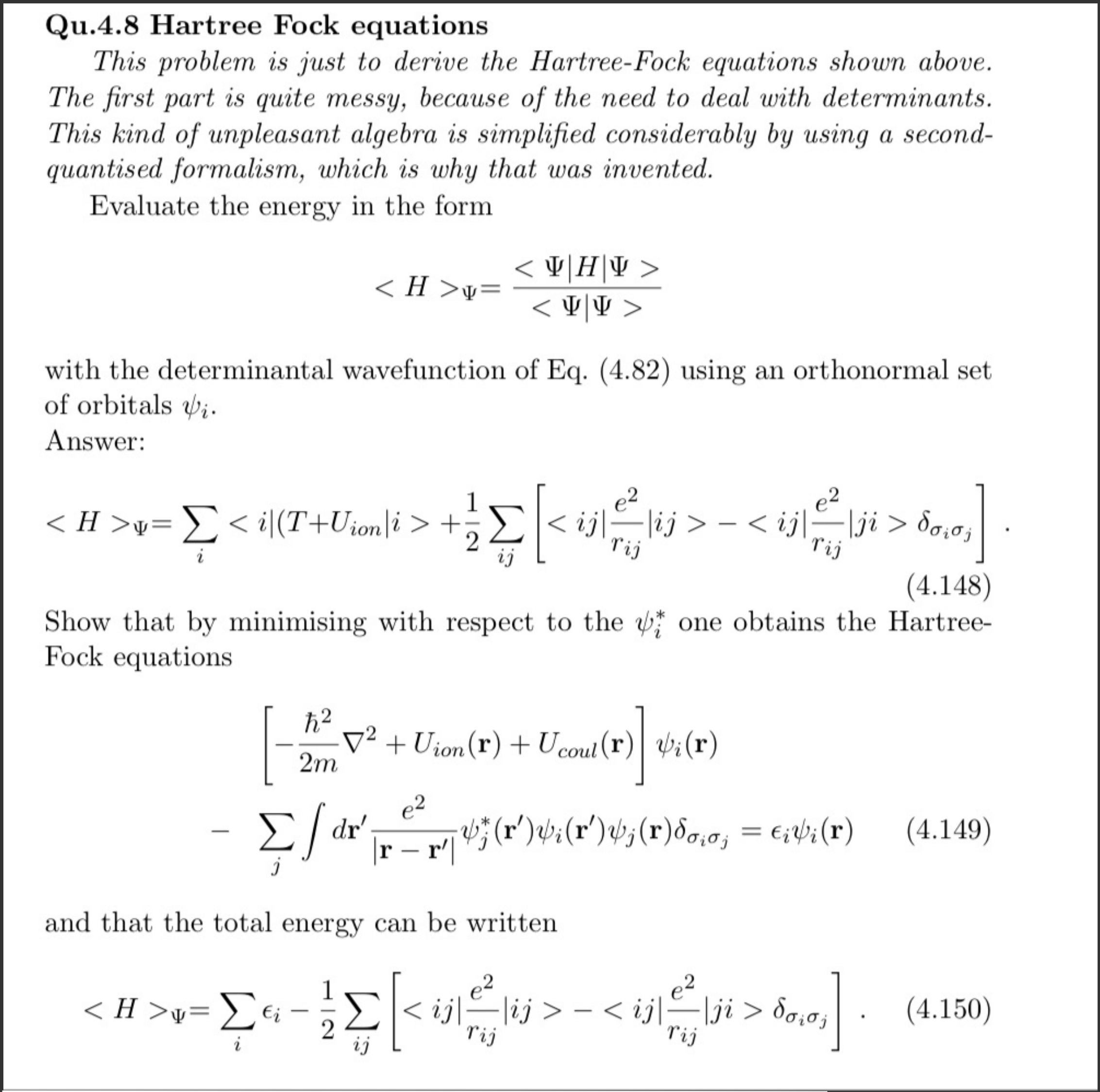
$$= (|12\rangle - |21\rangle)/\sqrt{2}.$$

$$\langle H \rangle_{\psi_T} = \langle 1|T + U_{ion}|1\rangle + \langle 2|T + U_{ion}|2\rangle$$

$$+ \frac{1}{2}\left[\langle 12|\frac{e^2}{r_{12}}|12\rangle - \langle 12|\frac{e^2}{r_{12}}|21\rangle\right.$$

$$\left. + \langle 21|\frac{e^2}{r_{21}}|21\rangle - \langle 21|\frac{e^2}{r_{21}}|12\rangle\right]$$

$$= E_1 + E_2 + \langle 12|V|12\rangle - \langle 21|V|12\rangle.$$



Qu.4.8 Hartree Fock equations

This problem is just to derive the Hartree-Fock equations shown above. The first part is quite messy, because of the need to deal with determinants. This kind of unpleasant algebra is simplified considerably by using a second-quantised formalism, which is why that was invented.

Evaluate the energy in the form

$$< H >_\Psi = \frac{< \Psi|H|\Psi >}{< \Psi|\Psi >}$$

with the determinantal wavefunction of Eq. (4.82) using an orthonormal set of orbitals ψ_i.

Answer:

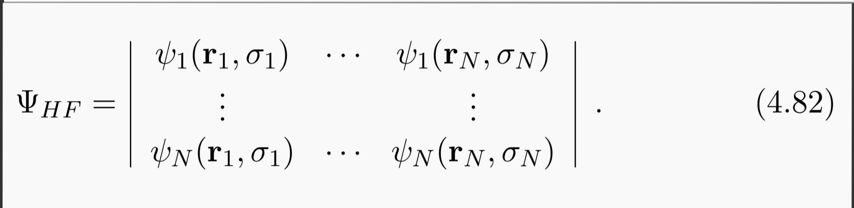
$$< H >_\Psi = \sum_i < i|(T+U_{ion}|i > + \frac{1}{2}\sum_{ij}\left[< ij|\frac{e^2}{r_{ij}}|ij > - < ij|\frac{e^2}{r_{ij}}|ji > \delta_{\sigma_i\sigma_j}\right] . \tag{4.148}$$

Show that by minimising with respect to the ψ_i^* one obtains the Hartree-Fock equations

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + U_{ion}(\mathbf{r}) + U_{coul}(\mathbf{r})\right]\psi_i(\mathbf{r}) - \sum_j \int d\mathbf{r}' \frac{e^2}{|\mathbf{r}-\mathbf{r}'|}\psi_j^*(\mathbf{r}')\psi_i(\mathbf{r}')\psi_j(\mathbf{r})\delta_{\sigma_i\sigma_j} = \epsilon_i\psi_i(\mathbf{r}) \tag{4.149}$$

and that the total energy can be written

$$< H >_\Psi = \sum_i \epsilon_i - \frac{1}{2}\sum_{ij}\left[< ij|\frac{e^2}{r_{ij}}|ij > - < ij|\frac{e^2}{r_{ij}}|ji > \delta_{\sigma_i\sigma_j}\right] . \tag{4.150}$$



$$\Psi_{HF} = \begin{vmatrix} \psi_1(\mathbf{r}_1,\sigma_1) & \cdots & \psi_1(\mathbf{r}_N,\sigma_N) \\ \vdots & & \vdots \\ \psi_N(\mathbf{r}_1,\sigma_1) & \cdots & \psi_N(\mathbf{r}_N,\sigma_N) \end{vmatrix} . \tag{4.82}$$

$$\langle H \rangle_{\Psi} = \frac{\langle \Psi | H | \Psi \rangle}{\langle \Psi | \Psi \rangle}.$$

$$\Psi_{HF} = \frac{1}{\sqrt{N!}} \begin{vmatrix} \psi_1(\vec{r}_1, \sigma_1) & \cdots & \psi_1(\vec{r}_N, \sigma_N) \\ \vdots & & \vdots \\ \psi_N(\vec{r}_N, \sigma_1) & \cdots & \psi_N(\vec{r}_N, \sigma_N) \end{vmatrix}$$

$$= \frac{1}{\sqrt{N!}} \sum_{n=1}^{N!} (-1)^{P_n} P_n \left\{ \psi_1(1)\psi_2(2)\cdots\psi_N(N) \right\}.$$

Also, $$H_{elec} = \sum_{n=1}^{N} \left[-\frac{\hbar^2}{2m} \nabla_i^2 + U_{ion}(\vec{r}_i) \right] + \frac{1}{2} \sum_{i \neq j} \frac{e^2}{|\vec{r}_i - \vec{r}_j|}$$

$$= \sum_{n=1}^{N} \underline{\left[-\frac{\hbar^2}{2m} \nabla_i^2 + U_{ion}(\vec{r}_i) \right]} + \sum_{i=1}^{N} \sum_{j>i}^{N} \underline{\frac{e^2}{r_{ij}}}$$

$$= \sum_{i=1}^{N} h_1(i) + \sum_{i=1}^{N} \sum_{j>i}^{N} h_2(i,j).$$

For h_1,

$$\langle \psi | h_1(1) | \psi \rangle = \frac{1}{N!} \sum_{i}^{N!} \sum_{j}^{N!} (-1)^{P_i} (-1)^{P_j} \int d\vec{r}_1 d\vec{r}_2 \cdots d\vec{r}_N$$

$$\times P_i \left\{ \psi_1^*(1)\psi_2^*(2)\cdots\psi_N^*(N) \right\} h_1 P_j \left\{ \psi_1(1)\psi_2(2)\cdots\psi_N(N) \right\}.$$

$$= \frac{1}{N!} \sum_{i}^{N!} \int d\vec{r}_1 d\vec{r}_2 \cdots d\vec{r}_N \times P_i \left\{ \psi_1^*(1)\psi_2^*(2)\cdots\psi_N^*(N) \right\} h_1 P_i \left\{ \psi_1(1)\psi_2(2)\cdots\psi_N(N) \right\}.$$

(N-1)! ways

$$= \frac{(N-1)!}{N!} \sum_{i=1}^{N} \int d\vec{r}_1 \, \psi_i^*(\vec{r}_1) h_1(1) \psi_i(\vec{r}_1)$$

$$= \frac{1}{N} \sum_{i=1}^{N} \langle i | h_1 | i \rangle.$$

For h_2,

$$\langle \Psi | \sum_{i=1}^{N} \sum_{j>i}^{N} h_2(i,j) | \Psi \rangle = C_n^2 \langle \Psi | h_2(1,2) | \Psi \rangle$$

$$= \frac{N(N-1)}{2} \cdot \frac{1}{N!} \sum_{i}^{N!} \sum_{j}^{N!} (-1)^{P_i} (-1)^{P_j} \int d\vec{r}_1 \, d\vec{r}_2 \cdots d\vec{r}_N$$

$$\times \; P_i \{ \psi_1^*(1) \psi_2^*(2) \cdots \psi_N^*(N) \} \, h_2(1,2) \, P_j \{ \psi_1(1) \psi_2(2) \cdots \psi_N(N) \}$$

$$= \frac{1}{2(N-2)!} \cdot (N-2)! \sum_{m=1}^{N} \sum_{n \neq m}^{N} \int d\vec{r}_1 \, d\vec{r}_2$$

$$\times \; \psi_m^*(1) \, \psi_n^*(2) \, h(1,2) \left[\chi_m(1) \chi_n(2) - \chi_m(2) \chi_n(1) \right]$$

$$= \frac{1}{2} \sum_{m=1}^{N} \sum_{n \neq m}^{N} \langle mn | h_2(1,2) | mn \rangle - \langle mn | h_2(1,2) | nm \rangle$$

$$= \frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} \langle ij | h_2(1,2) | ij \rangle - \langle ij | h_2(1,2) | ji \rangle$$

Then $\langle \Psi | H | \Psi \rangle = \langle \Psi | \sum_{i=1}^{N} h_1 | \Psi \rangle + \langle \Psi | \sum_{i=1}^{N} \sum_{j>i}^{N} h_2 | \Psi \rangle$

$$= \sum_{i=1}^{N} \langle i | h_1 | i \rangle + \frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} \langle ij | h_2 | ij \rangle - \langle ij | h_2 | ji \rangle$$

$$= \sum_{i=1}^{N} \langle i | -\frac{\hbar^2}{2m} \nabla_i^2 + U_{ion}(\vec{r}_i) | i \rangle + \frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} \left[\langle ij | \frac{e^2}{r_{ij}} | ij \rangle - \langle ij | \frac{e^2}{r_{ij}} | ji \rangle \right]$$

$$= \sum_{i} \langle i | T + U_{ion} | i \rangle + \frac{1}{2} \sum_{ij} \left[\langle ij | \frac{e^2}{r_{ij}} | ij \rangle - \langle ij | \frac{e^2}{r_{ij}} | ji \rangle \, \delta_{\sigma_i \sigma_j} \right].$$

Qu.4.9 Band structure in the Hartree-Fock approximation

Using Eq. (4.91), calculate the density of states near the Fermi energy to leading order in $(E - E_F)/E_F$. If this result were physically correct what would be the temperature-dependence of the electronic specific heat at low temperature?

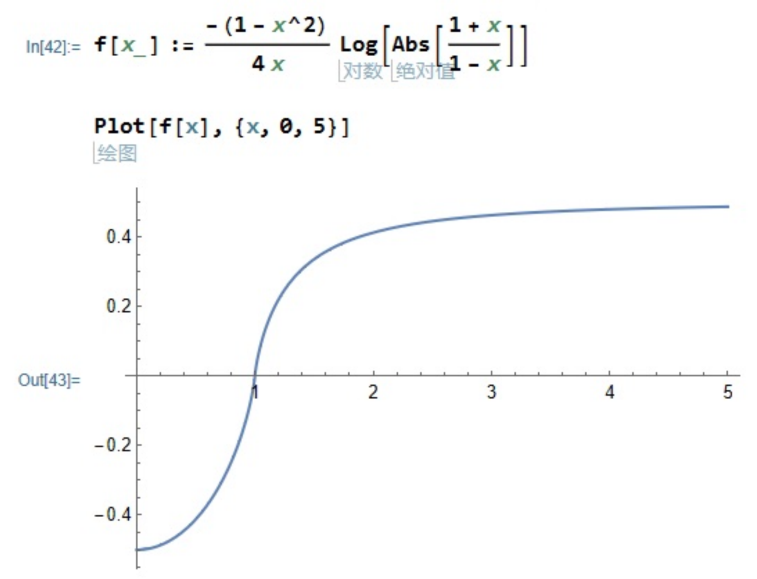
The logarithmic singularity you found is not found in better theories than Hartree-Fock. It arises mathematically from the long-range Coulomb interaction (and in particular the k^{-2} *divergence) which vanishes when we allow for processes to screen the interaction and make it short-range.*

$$\epsilon(\mathbf{k}) = \frac{\hbar^2 k^2}{2m} - \int_{k'<k_F} \frac{d\mathbf{k}'}{(2\pi)^3} \frac{4\pi e^2}{|\mathbf{k}-\mathbf{k}'|^2} \qquad F(x) = \frac{1}{2} + \frac{1-x^2}{4x} \ln\left|\frac{1+x}{1-x}\right| .$$

$$= \frac{\hbar^2 k^2}{2m} - \frac{2e^2 k_F}{\pi} F(k/k_F) , \tag{4.91}$$

$$\varepsilon(\vec{k}) = \frac{\hbar^2 k^2}{2m} - \frac{2e^2 k_F}{\pi}\left(\frac{1}{2} + \frac{1-x^2}{4x}\ln\left|\frac{1+x}{1-x}\right|\right). \qquad x = \frac{k}{k_F}$$

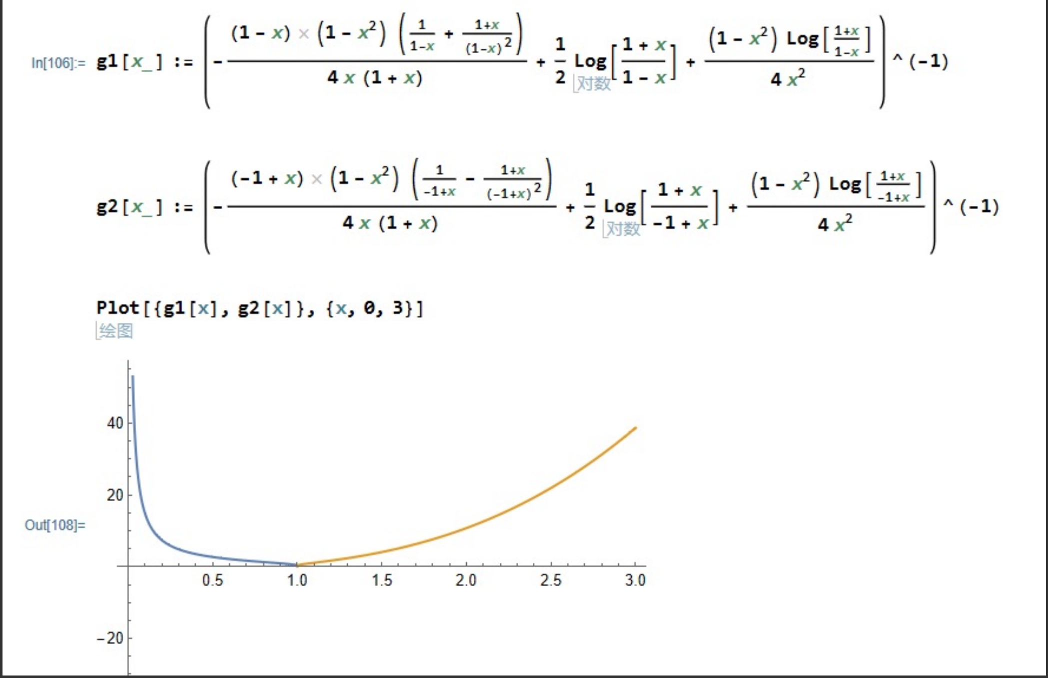
$$g(\varepsilon_F) = \frac{1}{V}\cdot\left(\frac{dN}{d\varepsilon}\right)_{\varepsilon_F} \propto \left(\frac{\partial k}{\partial E}\right)_{E_F}.$$



```
In[42]:= f[x_] := -(1 - x^2)/(4 x) Log[Abs[(1 + x)/(1 - x)]]

Plot[f[x], {x, 0, 5}]

Out[43]=
```

$$\left(\frac{\partial k}{\partial E}\right)_{E_F} = \left[-\frac{(1-x)\times(1-x^2)\left(\frac{1}{1-x}+\frac{1+x}{(1-x)^2}\right)}{4x(1+x)} + \frac{1}{2}\ln\left(\frac{1+x}{1-x}\right) + \frac{(1-x^2)\ln\left(\frac{1+x}{1-x}\right)}{4x^2}\right]^{-1}.$$

(x>1)



In[106]:=

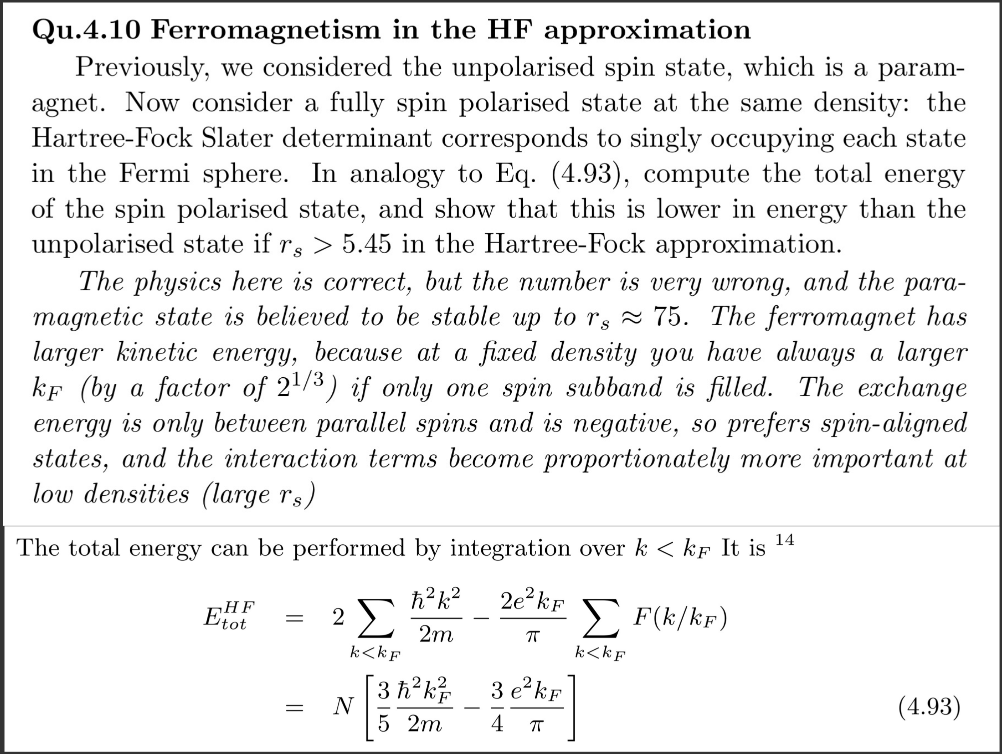
$$\text{g1}[x\_] := \left(-\frac{(1-x)\times(1-x^2)\left(\frac{1}{1-x}+\frac{1+x}{(1-x)^2}\right)}{4x(1+x)} + \frac{1}{2}\,\text{Log}\left[\frac{1+x}{1-x}\right] + \frac{(1-x^2)\,\text{Log}\left[\frac{1+x}{1-x}\right]}{4x^2}\right)\text{\^{}}(-1)$$

$$\text{g2}[x\_] := \left(-\frac{(-1+x)\times(1-x^2)\left(\frac{1}{-1+x}-\frac{1+x}{(-1+x)^2}\right)}{4x(1+x)} + \frac{1}{2}\,\text{Log}\left[\frac{1+x}{-1+x}\right] + \frac{(1-x^2)\,\text{Log}\left[\frac{1+x}{-1+x}\right]}{4x^2}\right)\text{\^{}}(-1)$$

```
Plot[{g1[x], g2[x]}, {x, 0, 3}]
```

Out[108]=

$C_v = \left(\frac{\partial U}{\partial T}\right)_v$, at low temperature



Qu.4.10 Ferromagnetism in the HF approximation

Previously, we considered the unpolarised spin state, which is a paramagnet. Now consider a fully spin polarised state at the same density: the Hartree-Fock Slater determinant corresponds to singly occupying each state in the Fermi sphere. In analogy to Eq. (4.93), compute the total energy of the spin polarised state, and show that this is lower in energy than the unpolarised state if $r_s > 5.45$ in the Hartree-Fock approximation.

The physics here is correct, but the number is very wrong, and the paramagnetic state is believed to be stable up to $r_s \approx 75$. The ferromagnet has larger kinetic energy, because at a fixed density you have always a larger k_F (by a factor of $2^{1/3}$) if only one spin subband is filled. The exchange energy is only between parallel spins and is negative, so prefers spin-aligned states, and the interaction terms become proportionately more important at low densities (large r_s)

The total energy can be performed by integration over $k < k_F$ It is [14]

$$\begin{aligned} E^{HF}_{tot} &= 2\sum_{k<k_F} \frac{\hbar^2 k^2}{2m} - \frac{2e^2 k_F}{\pi} \sum_{k<k_F} F(k/k_F) \\ &= N\left[\frac{3}{5}\frac{\hbar^2 k_F^2}{2m} - \frac{3}{4}\frac{e^2 k_F}{\pi}\right] \end{aligned} \tag{4.93}$$

The assumption in (4.93) is that every occupied one-electron orbital level be two electrons of opposite spin. Now we fill one-electron level with $k < k_\uparrow, k_\downarrow$.

We have $E_\uparrow = N_\uparrow \left(\frac{3}{5}\frac{\hbar^2 k_\uparrow^2}{2m} - \frac{3}{4}\frac{e^2 k_\uparrow}{\pi}\right)$

$$E_\downarrow = N_\downarrow \left(\frac{3}{5}\frac{\hbar^2 k_\downarrow^2}{2m} - \frac{3}{4}\frac{e^2 k_\downarrow}{\pi}\right)$$

And $E = E_\uparrow + E_\downarrow$.

$$\frac{k_\uparrow^3}{6\pi^2} + \frac{k_\downarrow^3}{6\pi^2} = \frac{k_F^3}{3\pi^2}$$

For fully polarized spins $N_\downarrow = N$, $N_\uparrow = 0$.

$$\Rightarrow \quad E = E_\downarrow . \quad k_\downarrow = 2^{\frac{1}{3}} k_F .$$

$$E = N\left(\frac{3}{5}\cdot\frac{\hbar^2 k_F^2 \cdot 2^{\frac{2}{3}}}{2m} - \frac{3}{4}\cdot\frac{2^{\frac{1}{3}} e^2 k_F}{\pi}\right).$$

Compare to E_{tot}^{HF},

$$E - E_{tot}^{HF} = N\cdot\left[\frac{3}{5}\frac{\hbar^2 k_F^2}{2m}\left(2^{\frac{2}{3}}-1\right) - \frac{3}{4}\frac{e^2 k_F}{\pi}\left(2^{\frac{1}{3}}-1\right)\right].$$

Condition of $E = E_{tot}^{HF}$ is

$$k_F = \frac{5}{2}\frac{me^2}{\pi\hbar}\cdot\frac{2^{\frac{1}{3}}-1}{2^{\frac{2}{3}}-1} . \approx$$

That is $r_s = 5.45$.

For $r_s > 5.45$, $E < E_{tot}^{HF}$.

Qu.4.11 Thomas-Fermi screening

Check the formulae in Eq. (4.133) and Eq. (4.134). Suppose that the potential $v_{ext} = Q/r$, show that the induced charge density is then of the form

$$\delta n(r) \propto \frac{e^{-r/\xi}}{r}$$

and identify the screening length ξ.

$$\delta n(\mathbf{q}) = -\frac{v_{ext}(\mathbf{q})}{\frac{4\pi e^2}{q^2}\left[1 + \frac{q^2}{q_{TF}^2}\right]}\,, \tag{4.133}$$

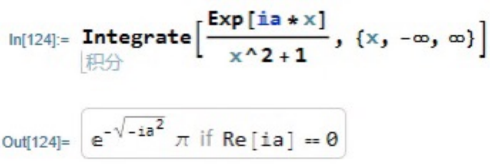
$$q_{TF}^2 = \frac{4}{\pi}\frac{me^2}{\hbar^2}k_F = \frac{4}{\pi}\frac{k_F}{a_B} = (\frac{2.95}{r_s^{\frac{1}{2}}}\text{Å}^{-1})^2\,. \tag{4.134}$$

$$V_{ext} = \frac{Q}{r} = \frac{4\pi Q}{q^2}.$$

Inside metal

$$V(\vec{q}) = \frac{V_{ext}(\vec{q})}{\varepsilon_{TF}(\vec{q})} = \frac{\frac{4\pi Q}{q^2}}{1 + \frac{q_{TF}^2}{q^2}}.$$

$$V(\vec{r}) = \int \frac{d\vec{q}}{(2\pi)^3}\, e^{i\vec{q}\cdot\vec{r}}\, \underbrace{\frac{4\pi Q}{q^2 + q_{TF}^2}} \qquad \tilde{\Phi}(\vec{q})$$



```
In[124]:= Integrate[Exp[ia*x]/(x^2+1), {x, -∞, ∞}]
           积分
Out[124]= e^(-√(-ia^2)) π if Re[ia] == 0
```

$$= \frac{Q}{r}\, e^{-\vec{q}_{TF}\cdot\vec{r}}$$

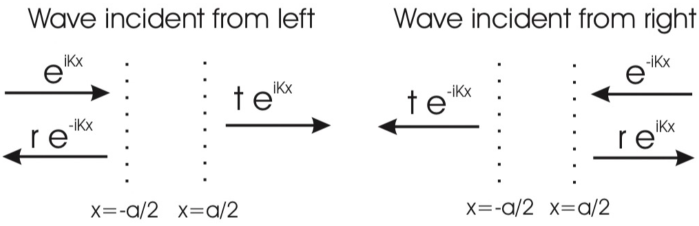
$$\therefore\ \delta n(\vec{q}) \propto \frac{e^{-r/\xi}}{r},$$

$$\xi = \frac{1}{q_{TF}} = \frac{1}{2}\sqrt{\frac{\pi a_B}{k_F}} = \frac{\sqrt{r_s}}{2.95}\ \text{Å}.$$

Qu.4.12 Generalised one-dimensional band theory

Many of the general features of electron bands in a periodic solid can be appreciated without recourse to a detailed model of the lattice potential. In this problem the scattering from the lattice potential is treated in a general way by describing it in terms of wave relfection and transmission. The algebra in the first two parts is messy - but the answer given in section (b) can be used to answer section (c).

Consider a 1D solid, lattice constant a, made of "building blocks" $(-a/2 < x < a/2)$ that scatter plane waves with a reflection coefficient r and transmission coefficient t $(|r|^2 + |t|^2 = 1)$ as shown.


Wave incident from left

Wave incident from right

The energy of the plane wave is written as $\epsilon = \hbar^2 K^2/2m$. In the solid, the building blocks are stacked together indefinitely in the x-direction.

(a) Write the solution to the Schrödinger equation in the solid $\psi(x)$, as a linear combination of $\psi_r(x)$ and $\psi_l(x)$ and use Bloch's theorem to relate the wavefunction at each side of the building block (the same theorem applies to the gradient ψ').

$$\psi(x+a) = e^{ika}\psi(x) \quad ; \psi'(x+a) = e^{ika}\psi'(x)$$

Hence, show

$$\cos(ka) = \frac{t^2 - r^2}{2t} e^{iKa} + \frac{1}{2t} e^{-iKa}$$

.

(b) If the transmission coefficient is $t = |t|e^{i\delta}$, it can be shown that $r = \pm i|r|e^{i\delta}$ (it is relatively easy to demonstrate this graphically for the special case when the scattering is localised at $x = 0$ and one can match ψ at the origin). Use this result to eliminate r and show

$$\frac{\cos(ka + \delta)}{|t|} = \cos ka \quad .$$

(c) Since $|t| < 1$, this result shows there are values of K (and hence ϵ) for which no Bloch states exist. Demonstrate this by sketching the left-hand side as a function of K (or preferably ϵ) Use your sketch to illustrate the behaviour for: (i) strong scattering; (ii) weak scattering.

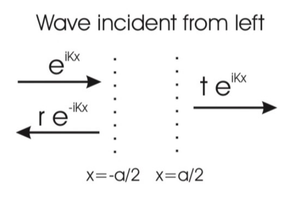
Explain why, in general, electron bands tend to get wider and their gaps narrower as the electron energy increases.

(a) The "building blocks" are solutions of single barrier potential.

within $-\frac{a}{2} \leqslant x \leqslant \frac{a}{2}$ we have

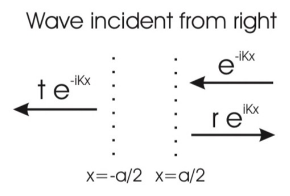
$$\psi(x) = A\psi_l(x) + B\psi_r(x).$$

Of which



$$\psi_l(x) = e^{ikx} + re^{-ikx} \quad (x \leqslant -\tfrac{a}{2})$$

$$= te^{ikx}. \quad (x \geqslant \tfrac{a}{2})$$



$$\psi_r(x) = te^{-ikx} \quad (x \leqslant -\tfrac{a}{2})$$

$$= e^{-ikx} + re^{ikx}. \quad (x \geqslant \tfrac{a}{2})$$

From Bloch theory we have

$$\psi(x+a) = e^{ika}\psi(x).$$

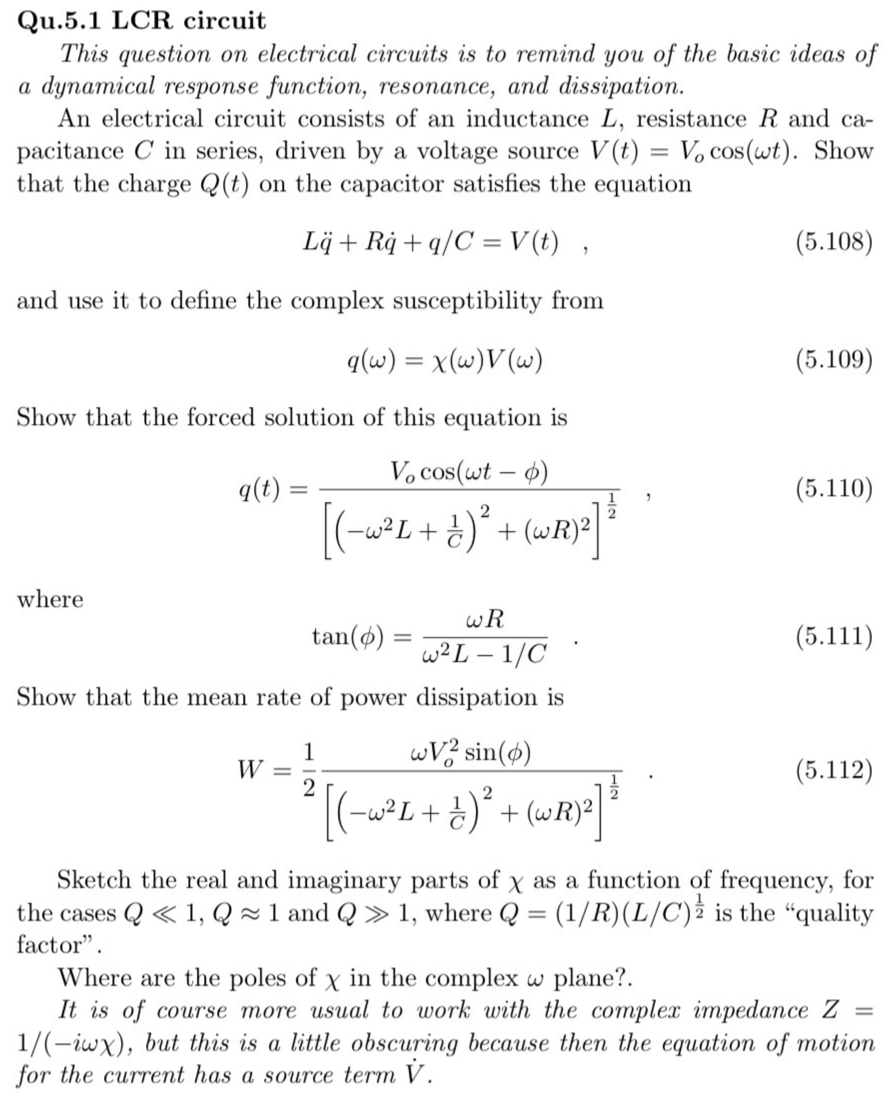
$$\psi'(x+a) = e^{ika}\psi'(x).$$

at $x = -\frac{a}{2}$,

$$\psi(\tfrac{a}{2}) = e^{ika}\psi(-\tfrac{a}{2}), \quad \psi'(\tfrac{a}{2}) = e^{ika}\psi(-\tfrac{a}{2}).$$

$$\Rightarrow Ate^{ik\frac{a}{2}} + B(e^{-ik\frac{a}{2}} + re^{ik\frac{a}{2}})$$

$$= e^{ika}\left[A(e^{-ik\frac{a}{2}} + re^{ik\frac{a}{2}}) + Bte^{ik\frac{a}{2}}\right]$$



Qu.5.1 LCR circuit

This question on electrical circuits is to remind you of the basic ideas of a dynamical response function, resonance, and dissipation.

An electrical circuit consists of an inductance L, resistance R and capacitance C in series, driven by a voltage source $V(t) = V_o \cos(\omega t)$. Show that the charge $Q(t)$ on the capacitor satisfies the equation

$$L\ddot{q} + R\dot{q} + q/C = V(t) \quad , \tag{5.108}$$

and use it to define the complex susceptibility from

$$q(\omega) = \chi(\omega)V(\omega) \tag{5.109}$$

Show that the forced solution of this equation is

$$q(t) = \frac{V_o \cos(\omega t - \phi)}{\left[\left(-\omega^2 L + \frac{1}{C}\right)^2 + (\omega R)^2\right]^{\frac{1}{2}}} \quad , \tag{5.110}$$

where

$$\tan(\phi) = \frac{\omega R}{\omega^2 L - 1/C} \quad . \tag{5.111}$$

Show that the mean rate of power dissipation is

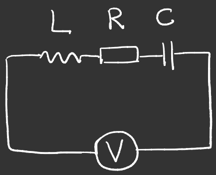
$$W = \frac{1}{2}\frac{\omega V_o^2 \sin(\phi)}{\left[\left(-\omega^2 L + \frac{1}{C}\right)^2 + (\omega R)^2\right]^{\frac{1}{2}}} \quad . \tag{5.112}$$

Sketch the real and imaginary parts of χ as a function of frequency, for the cases $Q \ll 1$, $Q \approx 1$ and $Q \gg 1$, where $Q = (1/R)(L/C)^{\frac{1}{2}}$ is the "quality factor".

Where are the poles of χ in the complex ω plane?.

It is of course more usual to work with the complex impedance $Z = 1/(-i\omega\chi)$, *but this is a little obscuring because then the equation of motion for the current has a source term* $\dot{V}$.

$I = \dot{q}$.



$V = V_0 \cos \omega t$

$$L\frac{dI}{dt} + RI + \frac{q}{C} = V(t).$$

$$\Rightarrow \quad L\ddot{q} + R\dot{q} + \frac{q}{C} = V(t).$$

From $q(\omega) = \chi(\omega) V(\omega)$.

Suppose $q = Ae^{i\omega t}$.

$$-\omega^2 L A e^{i\omega t} + i\omega A R e^{i\omega t} + \frac{Ae^{i\omega t}}{C} = V_0 \cos\omega t.$$

$$\Rightarrow A = \frac{V_0\cos\omega t}{\left(\frac{1}{C}-\omega^2 L\right) + i\omega R} \cdot e^{-i\omega t}$$

$\cot\varphi = -\tan\phi$.

$$= \frac{V_0\cos\omega t}{\left(\frac{1}{C}-\omega^2 L\right)^2 + \omega^2 R^2} \cdot \left[\left(\frac{1}{C}-\omega^2 L\right) - i\omega R\right] e^{-i\omega t}$$

$$= \frac{V_0\cos\omega t}{\sqrt{\left(\frac{1}{C}-\omega^2 L\right)^2 + \omega^2 R^2}} \cdot \underbrace{\frac{\left(\frac{1}{C}-\omega^2 L\right) - i\omega R}{\sqrt{\left(\frac{1}{C}-\omega^2 L\right)^2 + \omega^2 R^2}}}_{-e^{-i\phi}} e^{-i\omega t}$$

$\varphi = \phi + \pi$

$$= \frac{-V_0\cos\omega t}{\sqrt{\left(\frac{1}{C}-\omega^2 L\right)^2 + \omega^2 R^2}} e^{-i(\omega t+\phi)}$$

$$q = Ae^{i\omega t} = \frac{-V_0\cos\omega t}{\sqrt{\left(\frac{1}{C}-\omega^2 L\right)^2 + \omega^2 R^2}} e^{-i\phi}.$$

Should be $e^{i(\omega t-\phi)}$?

Extract the real part to get $q = \dfrac{V_0\cos(\omega t-\phi)}{\sqrt{\left(\frac{1}{C}-\omega^2 L\right)^2 + \omega^2 R^2}}$.

$W = \frac{1}{2}\mathrm{Re}(\tilde{U}\tilde{I}^*)$. $Z = R + \frac{1}{i\omega C} + i\omega L = \frac{1}{i\omega}\sqrt{\left(\frac{1}{C}-\omega^2 L\right)^2 + \omega^2 R^2}\, e^{i\phi}$.

$$W = \frac{1}{2}\mathrm{Re}(\tilde{U}\tilde{I}^*) = \frac{1}{2}\mathrm{Re}\left(Z|\tilde{I}|^2\right) = \frac{1}{2}\mathrm{Re}\left[\frac{V_0^2\omega^2}{\sqrt{\left(\frac{1}{C}-\omega^2 L\right)^2 + \omega^2 R^2}} \cdot \frac{e^{i\phi}}{i\omega}\right]$$

$$= \frac{1}{2}\frac{V_0^2\omega\sin\phi}{\sqrt{\left(\frac{1}{C}-\omega^2 L\right)^2 + \omega^2 R^2}}.$$

$$\chi = \frac{q(\omega)}{V(\omega)} = \frac{V_0 \cos(\omega t - \phi)}{\sqrt{\left(\frac{1}{C} - \omega^2 L\right)^2 + \omega^2 R^2}} \Big/ V_0 \cos \omega t$$

$$= \frac{\cos(\omega t - \phi)/\cos \omega t}{\sqrt{\left(\frac{1}{C} - \omega^2 L\right)^2 + \omega^2 R^2}} = \frac{\cos\phi + \sin\phi \tan \omega t}{\omega R \sqrt{1 + \frac{\omega^2 L^2}{R^2}\left(1 - \frac{\omega_0^2}{\omega^2}\right)^2}} . \qquad \omega_0 = \frac{1}{\sqrt{LC}} . \qquad Q = \frac{1}{R}\sqrt{\frac{L}{C}} .$$

$$= \frac{\omega^2 L - \frac{1}{C} + \omega R \tan \omega t}{\omega^2 R^2 \left[1 + \omega^2 LCQ^2 \left(1 - \frac{\omega_0^2}{\omega^2}\right)^2\right]} = \frac{\omega^2 L - \frac{1}{C} + \omega R \tan \omega t}{\omega^2 R^2 \left[1 + \frac{\omega^2}{\omega_0^2} Q^2 \left(1 - \frac{\omega_0^2}{\omega^2}\right)^2\right]}$$

$$= \frac{\frac{1}{C}\left(\frac{\omega^2}{\omega_0^2} - 1\right) + \omega R \tan \omega t}{\omega^2 R^2 \left[1 + \frac{\omega^2}{\omega_0^2} Q^2 \left(1 - \frac{\omega_0^2}{\omega^2}\right)^2\right]} = \frac{\omega_0 Q\left(\frac{\omega^2}{\omega_0^2} - 1\right) + \omega \tan \omega t}{\omega^2 R \left[1 + \frac{\omega^2}{\omega_0^2} Q^2 \left(1 - \frac{\omega_0^2}{\omega^2}\right)^2\right]} .$$

$$= \frac{\left(\frac{\omega^2}{\omega_0^2} - 1\right) + \frac{\omega}{\omega_0 Q} \tan \omega t}{\frac{\omega^2 R}{\omega_0 Q}\left[1 + \frac{\omega^2}{\omega_0^2} Q^2 \left(1 - \frac{\omega_0^2}{\omega^2}\right)^2\right]} .$$

$$Q = \frac{1}{\omega_0 RC}$$

$$\omega_0 = \frac{1}{\sqrt{LC}}$$

X

$$q(\omega) = \frac{V_0 e^{i(\omega t - \phi)}}{\sqrt{\left(\frac{1}{C} - \omega^2 L\right)^2 + \omega^2 R^2}} .$$

$$\chi = \frac{q(\omega)}{V(\omega)} = \frac{e^{-i\phi}}{\sqrt{\left(\frac{1}{C} - \omega^2 L\right)^2 + \omega^2 R^2}} .$$

$$\chi = \frac{q(\omega)}{V(\omega)} = \frac{e^{-i\phi}}{\sqrt{\left(\frac{1}{C}-\omega^2 L\right)^2+\omega^2R^2}}\,.$$

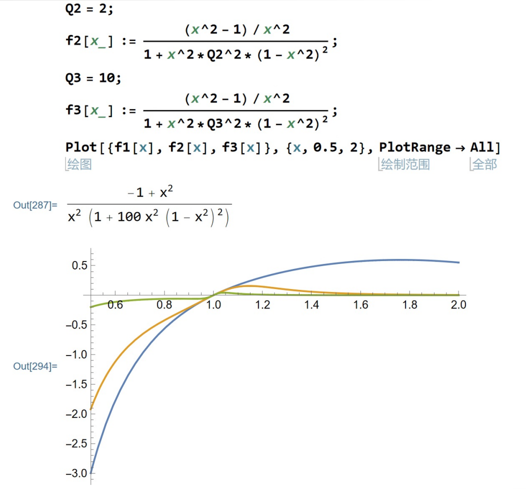
$$= \frac{e^{-i\phi}}{\sqrt{\left(\frac{1}{C}-\omega^2 L\right)^2+\omega^2R^2}} = \frac{\cos\phi + i\sin\phi}{\omega R\sqrt{1+\frac{\omega^2L^2}{R^2}\left(1-\frac{\omega_0^2}{\omega^2}\right)}}\,. \qquad \omega_0 = \frac{1}{\sqrt{LC}}\,. \qquad Q = \frac{1}{R}\sqrt{\frac{L}{C}}\,.$$

$$= \frac{\omega^2L-\frac{1}{C}+i\omega R}{\omega^2R^2\left[1+\omega^2LCQ^2\left(1-\frac{\omega_0^2}{\omega^2}\right)^2\right]} = \frac{\omega^2L-\frac{1}{C}+i\omega R}{\omega^2R^2\left[1+\frac{\omega^2}{\omega_0^2}Q^2\left(1-\frac{\omega_0^2}{\omega^2}\right)^2\right]}$$

$$= \frac{\frac{1}{C}\left(\frac{\omega^2}{\omega_0^2}-1\right)+i\omega R}{\omega^2R^2\left[1+\frac{\omega^2}{\omega_0^2}Q^2\left(1-\frac{\omega_0^2}{\omega^2}\right)^2\right]} = \frac{\omega_0Q\left(\frac{\omega^2}{\omega_0^2}-1\right)+i\omega}{\omega^2R\left[1+\frac{\omega^2}{\omega_0^2}Q^2\left(1-\frac{\omega_0^2}{\omega^2}\right)^2\right]}\,.$$

$$= \frac{\left(\frac{\omega^2}{\omega_0^2}-1\right)+\frac{i\omega}{\omega_0Q}}{\frac{\omega^2R}{\omega_0Q}\left[1+\frac{\omega^2}{\omega_0^2}Q^2\left(1-\frac{\omega_0^2}{\omega^2}\right)^2\right]}\,.$$

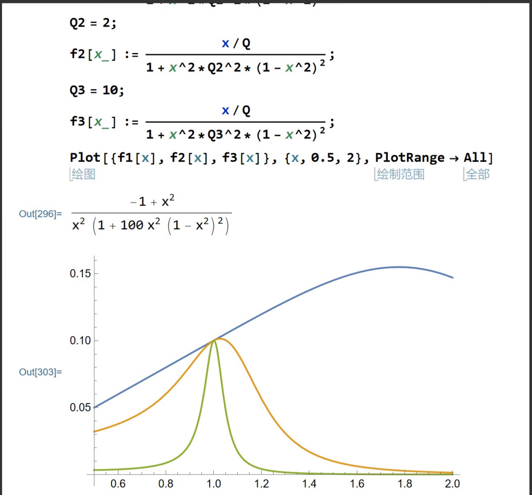
poles of χ: $\omega = \frac{1}{3}\left(1\pm\sqrt{1-\frac{3}{Q^2}}\right).$



```
Q2 = 2;
f2[x_] := ((x^2 - 1) / x^2) / (1 + x^2 * Q2^2 * (1 - x^2)^2);
Q3 = 10;
f3[x_] := ((x^2 - 1) / x^2) / (1 + x^2 * Q3^2 * (1 - x^2)^2);
Plot[{f1[x], f2[x], f3[x]}, {x, 0.5, 2}, PlotRange → All]
```

Out[287]= $\frac{-1+x^2}{x^2\left(1+100\,x^2\left(1-x^2\right)^2\right)}$

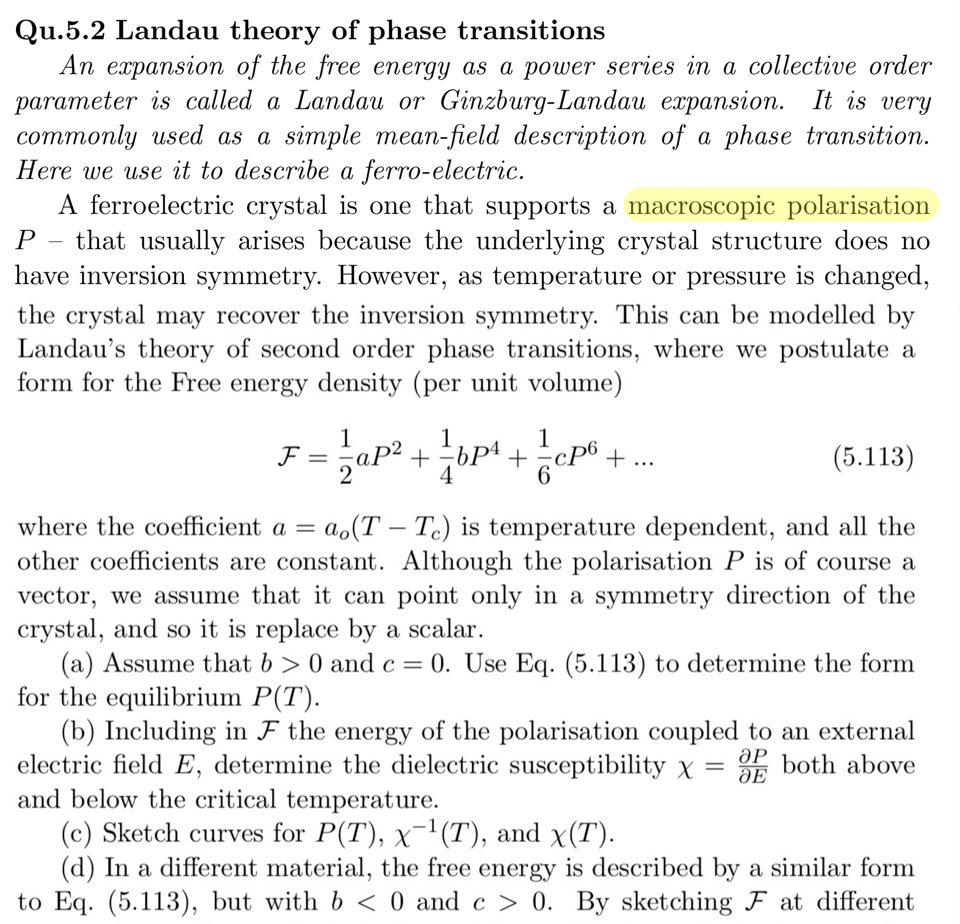
Out[294]=



```
Q2 = 2;
f2[x_] := (x / Q) / (1 + x^2 * Q2^2 * (1 - x^2)^2);
Q3 = 10;
f3[x_] := (x / Q) / (1 + x^2 * Q3^2 * (1 - x^2)^2);
Plot[{f1[x], f2[x], f3[x]}, {x, 0.5, 2}, PlotRange → All]
```

Out[296]= $\frac{-1+x^2}{x^2\left(1+100\,x^2\left(1-x^2\right)^2\right)}$

Out[303]=



Qu.5.2 Landau theory of phase transitions

An expansion of the free energy as a power series in a collective order parameter is called a Landau or Ginzburg-Landau expansion. It is very commonly used as a simple mean-field description of a phase transition. Here we use it to describe a ferro-electric.

A ferroelectric crystal is one that supports a macroscopic polarisation P – that usually arises because the underlying crystal structure does no have inversion symmetry. However, as temperature or pressure is changed, the crystal may recover the inversion symmetry. This can be modelled by Landau's theory of second order phase transitions, where we postulate a form for the Free energy density (per unit volume)

$$\mathcal{F} = \frac{1}{2}aP^2 + \frac{1}{4}bP^4 + \frac{1}{6}cP^6 + ... \tag{5.113}$$

where the coefficient $a = a_o(T - T_c)$ is temperature dependent, and all the other coefficients are constant. Although the polarisation P is of course a vector, we assume that it can point only in a symmetry direction of the crystal, and so it is replace by a scalar.

(a) Assume that $b > 0$ and $c = 0$. Use Eq. (5.113) to determine the form for the equilibrium $P(T)$.

(b) Including in $\mathcal{F}$ the energy of the polarisation coupled to an external electric field E, determine the dielectric susceptibility $\chi = \frac{\partial P}{\partial E}$ both above and below the critical temperature.

(c) Sketch curves for $P(T)$, $\chi^{-1}(T)$, and $\chi(T)$.

(d) In a different material, the free energy is described by a similar form to Eq. (5.113), but with $b < 0$ and $c > 0$. By sketching $\mathcal{F}$ at different temperatures, discuss the behaviour of the equilibrium polarisation and the linear susceptibility, contrasting the results with those found in (c).

(a) $\mathcal{F} = \frac{1}{2}aP^2 + \frac{1}{4}bP^4$.

$= \frac{1}{2}a_o(T-T_c)P^2 + \frac{1}{4}bP^4$.

For equilibrium $\left(\frac{\partial \mathcal{F}}{\partial P}\right) = 0$, $\left(\frac{\partial^2 \mathcal{F}}{\partial P^2}\right) > 0$.

$\Rightarrow \quad a_o(T-T_c)P + bP^3 = 0$.

$\Rightarrow P = 0$ or $P = \pm\sqrt{\frac{a_o(T_c-T)}{b}}$.

(b) (c) Including energy of polarization F has the form

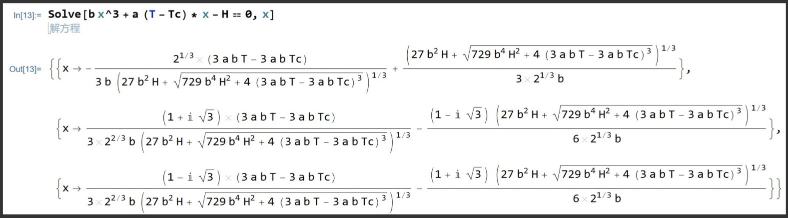
$$F = \frac{1}{2}aP^2 + \frac{1}{4}bP^4 - PE.$$

$$\left(\frac{\partial F}{\partial P}\right) = 0 \Rightarrow a_0(T-T_c)P + bP^3 - E = 0. \qquad (*)$$

$$\Rightarrow a(T-T_c)\frac{\partial P}{\partial E} + 3bP^2\left(\frac{\partial P}{\partial E}\right) - 1 = 0.$$

$$\Rightarrow \chi = \frac{\partial P}{\partial E} = \frac{1}{a(T-T_c) + 3bP^2}.$$

From (*) solve for P:



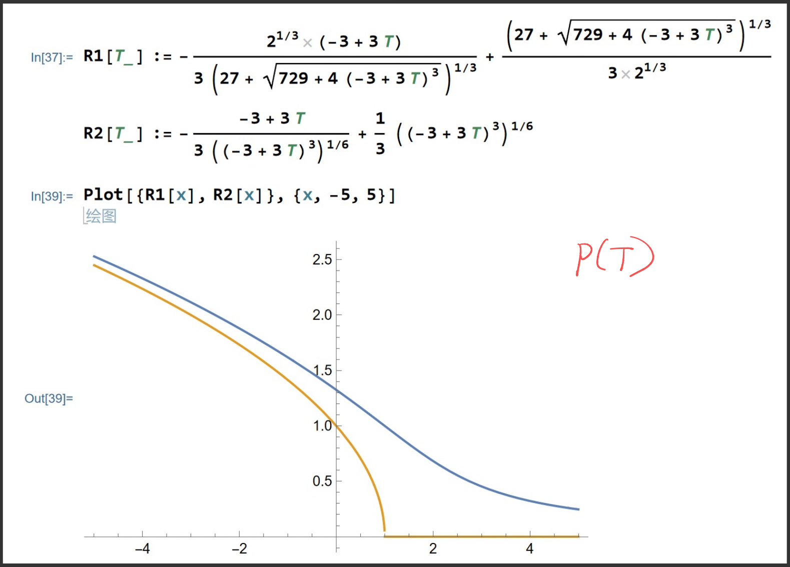
```
In[13]:= Solve[b x^3 + a (T - Tc) * x - H == 0, x]
         解方程
```

Out[13]=

$$\left\{\left\{x \to -\frac{2^{1/3}\times(3\,a\,b\,T - 3\,a\,b\,Tc)}{3\,b\left(27\,b^2 H + \sqrt{729\,b^4 H^2 + 4\,(3\,a\,b\,T - 3\,a\,b\,Tc)^3}\right)^{1/3}} + \frac{\left(27\,b^2 H + \sqrt{729\,b^4 H^2 + 4\,(3\,a\,b\,T - 3\,a\,b\,Tc)^3}\right)^{1/3}}{3\times 2^{1/3}\,b}\right\},\right.$$

$$\left\{x \to \frac{(1 + i\sqrt{3})\times(3\,a\,b\,T - 3\,a\,b\,Tc)}{3\times 2^{2/3}\,b\left(27\,b^2 H + \sqrt{729\,b^4 H^2 + 4\,(3\,a\,b\,T - 3\,a\,b\,Tc)^3}\right)^{1/3}} - \frac{(1 - i\sqrt{3})\left(27\,b^2 H + \sqrt{729\,b^4 H^2 + 4\,(3\,a\,b\,T - 3\,a\,b\,Tc)^3}\right)^{1/3}}{6\times 2^{1/3}\,b}\right\},$$

$$\left.\left\{x \to \frac{(1 - i\sqrt{3})\times(3\,a\,b\,T - 3\,a\,b\,Tc)}{3\times 2^{2/3}\,b\left(27\,b^2 H + \sqrt{729\,b^4 H^2 + 4\,(3\,a\,b\,T - 3\,a\,b\,Tc)^3}\right)^{1/3}} - \frac{(1 + i\sqrt{3})\left(27\,b^2 H + \sqrt{729\,b^4 H^2 + 4\,(3\,a\,b\,T - 3\,a\,b\,Tc)^3}\right)^{1/3}}{6\times 2^{1/3}\,b}\right\}\right\}$$



In[37]:=

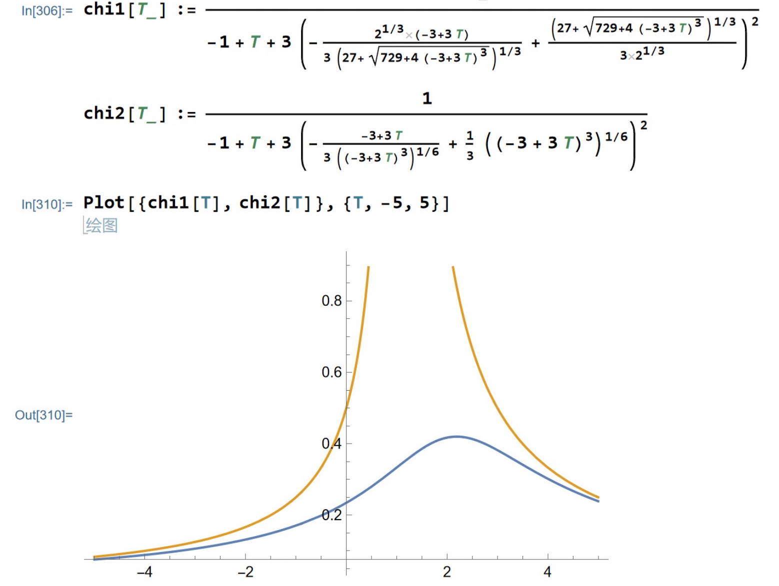
$$R1[T\_] := -\frac{2^{1/3}\times(-3 + 3\,T)}{3\left(27 + \sqrt{729 + 4\,(-3 + 3\,T)^3}\right)^{1/3}} + \frac{\left(27 + \sqrt{729 + 4\,(-3 + 3\,T)^3}\right)^{1/3}}{3\times 2^{1/3}}$$

$$R2[T\_] := -\frac{-3 + 3\,T}{3\left((-3 + 3\,T)^3\right)^{1/6}} + \frac{1}{3}\left((-3 + 3\,T)^3\right)^{1/6}$$

```
In[39]:= Plot[{R1[x], R2[x]}, {x, -5, 5}]
         绘图
```

Out[39]=

$\chi(T)$:



In[306]:= chi1[T_] :=

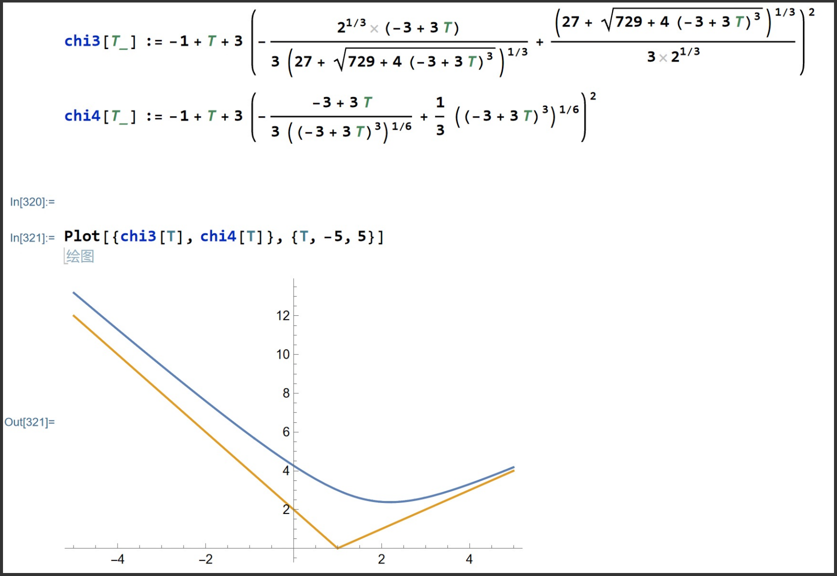
$$\frac{1}{-1+T+3\left(-\frac{2^{1/3}\times(-3+3T)}{3\left(27+\sqrt{729+4(-3+3T)^3}\right)^{1/3}}+\frac{\left(27+\sqrt{729+4(-3+3T)^3}\right)^{1/3}}{3\times 2^{1/3}}\right)^2}$$

chi2[T_] :=

$$\frac{1}{-1+T+3\left(-\frac{-3+3T}{3\left((-3+3T)^3\right)^{1/6}}+\frac{1}{3}\left((-3+3T)^3\right)^{1/6}\right)^2}$$

```
In[310]:= Plot[{chi1[T], chi2[T]}, {T, -5, 5}]
```

$\chi^{-1}(T)$:



chi3[T_] :=

$$-1+T+3\left(-\frac{2^{1/3}\times(-3+3T)}{3\left(27+\sqrt{729+4(-3+3T)^3}\right)^{1/3}}+\frac{\left(27+\sqrt{729+4(-3+3T)^3}\right)^{1/3}}{3\times 2^{1/3}}\right)^2$$

chi4[T_] :=

$$-1+T+3\left(-\frac{-3+3T}{3\left((-3+3T)^3\right)^{1/6}}+\frac{1}{3}\left((-3+3T)^3\right)^{1/6}\right)^2$$

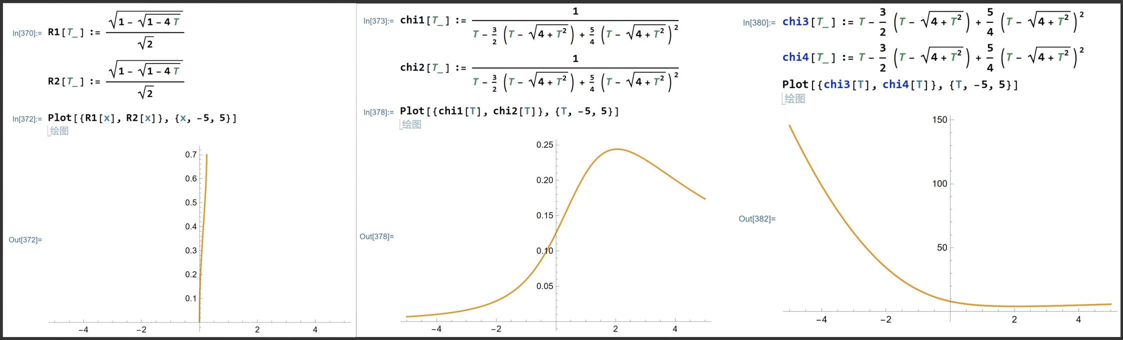
```
In[320]:=

In[321]:= Plot[{chi3[T], chi4[T]}, {T, -5, 5}]
```

(d) $F = \frac{1}{2}aP^2 + \frac{1}{4}bP^4 + \frac{1}{6}cP^6 - PE.$

Let $f = \frac{1}{2}TP^2 - \frac{1}{4}P^4 + \frac{1}{6}P^6 - PE.$

$$TP - P^3 + P^5 - E = 0.$$

$$\chi = \frac{1}{T - 3P^2 + 5P^4}.$$



In[370]:= $\text{R1}[T\_] := \frac{\sqrt{1-\sqrt{1-4T}}}{\sqrt{2}}$

$\text{R2}[T\_] := \frac{\sqrt{1-\sqrt{1-4T}}}{\sqrt{2}}$

```
In[372]:= Plot[{R1[x], R2[x]}, {x, -5, 5}]
```

In[373]:= $\text{chi1}[T\_] := \frac{1}{T - \frac{3}{2}\left(T - \sqrt{4+T^2}\right) + \frac{5}{4}\left(T - \sqrt{4+T^2}\right)^2}$

$\text{chi2}[T\_] := \frac{1}{T - \frac{3}{2}\left(T - \sqrt{4+T^2}\right) + \frac{5}{4}\left(T - \sqrt{4+T^2}\right)^2}$

```
In[378]:= Plot[{chi1[T], chi2[T]}, {T, -5, 5}]
```

In[380]:= $\text{chi3}[T\_] := T - \frac{3}{2}\left(T - \sqrt{4+T^2}\right) + \frac{5}{4}\left(T - \sqrt{4+T^2}\right)^2$

$\text{chi4}[T\_] := T - \frac{3}{2}\left(T - \sqrt{4+T^2}\right) + \frac{5}{4}\left(T - \sqrt{4+T^2}\right)^2$

```
Plot[{chi3[T], chi4[T]}, {T, -5, 5}]
```

$P(T)$ $\chi(T)$ $\chi^{-1}(T)$

The tendancy is different for each quantity and we expect to see different behaviors for given b.c.

Qu.5.3 Reflectivity of metals

The phase velocity of light in a conducting medium is the speed of light divided by the complex dielectric constant $N(\omega) = \epsilon(\omega)^{1/2}$ where we may use for ϵ the Drude result

$$\epsilon(\omega) = 1 - \frac{\omega_p^2}{\omega^2 + i\omega/\tau} \quad . \tag{5.114}$$

In a good Drude metal, we have $1/\tau \ll \omega_p$.

Sketch curves of

(a) $\Re\sigma(\omega)$,
(b) $\Re\epsilon(\omega)$,
(c) $\Im(1/\epsilon(\omega)$.

Consider a light wave with the electric field polarised in the $x-$direction at normal incidence from the vacuum on a good Drude metal (with $1/\tau \ll \omega_p$) occupying the region $z > 0$. In the vacuum ($z < 0$), the incident E_1 and reflected E_2 waves give rise to a field

$$E_x = E_1 \exp(i\omega[z/c - t]) + E_2 \exp(-i\omega[z/c + t]) \quad , \tag{5.115}$$

whereas in the medium, the electric field is

$$E_x = E_0 \exp(i\omega[N(\omega)z/c - t]) \quad . \tag{5.116}$$

Matching the electric and magnetic fields on the boundary, show that

$$\begin{aligned} E_0 &= E_1 + E_2 \quad , & (5.117)\\ NE_0 &= E_1 - E_2 \quad , & (5.118) \end{aligned}$$

and hence show that the reflection coefficient satisfies

$$R = \left|\frac{E_2}{E_1}\right|^2 = \left|\frac{1-N}{1+N}\right|^2 \quad . \tag{5.119}$$

Using the Drude formula above, show that

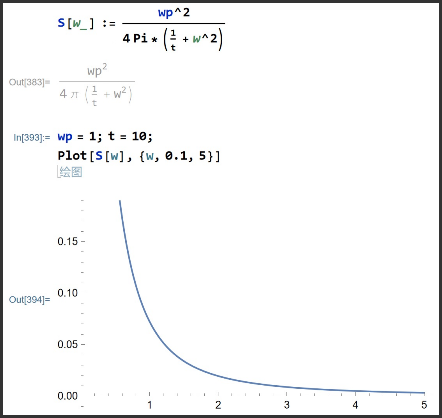
$$\begin{aligned} R &\approx 1 - 2\left(\frac{\omega}{2\pi\sigma(0)}\right)^{1/2} && \text{for } \omega \ll 1/\tau & (5.120)\\ &\approx 1 - \frac{2}{\omega_p\tau} && \text{for } 1/\tau \ll \omega \ll \omega_p & (5.121)\\ &\approx 0 && \text{for } \omega_p \ll \omega & (5.122) \end{aligned}$$

and sketch the reflectivity $R(\omega)$.

Deducing the complex conductivity by measuring the reflectivity is a standard experimental technique. To get both real and imaginary parts from a measurement of only $|R|$ (rather than the complex R) requires employment of the Kramers-Krönig relations.

(a) $$\sigma(\omega) = \frac{\omega_p^2}{4\pi\left(\frac{1}{\tau} - i\omega\right)}.$$

$$\mathrm{Re}\left[\sigma(\omega)\right] = \frac{\left(\frac{1}{\tau}+i\omega\right)\omega_p^2}{4\pi\left(\frac{1}{\tau^2}+\omega^2\right)}.$$



```
S[w_] := wp^2/(4 Pi * (1/t + w^2))
```

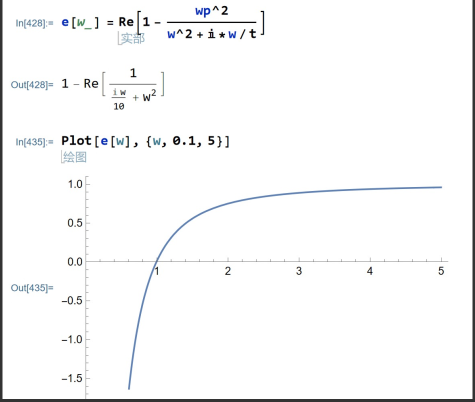
```
Out[383]= wp^2/(4 π (1/t + w^2))
```

```
In[393]:= wp = 1; t = 10;
          Plot[S[w], {w, 0.1, 5}]
          绘图
Out[394]=
```

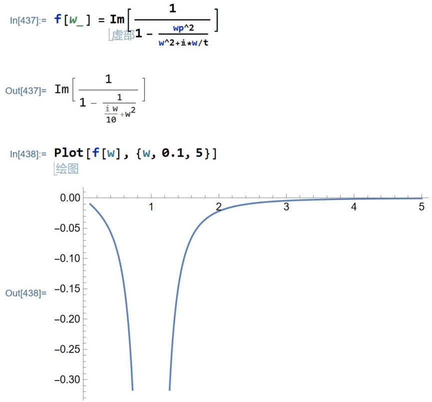
$$\epsilon(\omega) = 1 - \frac{\omega_p^2}{\omega^2 + i\omega/\tau}.$$

Plot $\mathrm{Re}\left[\epsilon(\omega)\right]$.

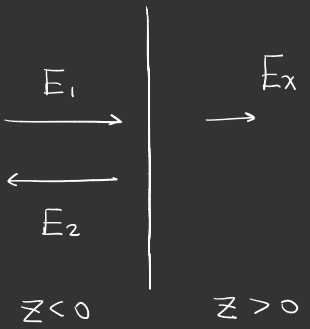
Plot $\mathrm{Im}\left[\frac{1}{\epsilon(\omega)}\right]$.



```
In[428]:= e[w_] = Re[1 - wp^2/(w^2 + i * w / t)]
                 实部
Out[428]= 1 - Re[1/(i w/10 + w^2)]
In[435]:= Plot[e[w], {w, 0.1, 5}]
          绘图
Out[435]=
```



```
In[437]:= f[w_] = Im[1/(1 - wp^2/(w^2+i*w/t))]
                 虚部
Out[437]= Im[1/(1 - 1/(i w/10 + w^2))]
In[438]:= Plot[f[w], {w, 0.1, 5}]
          绘图
Out[438]=
```



$$E_x(z\leq 0)\big|_{z=0} = E_x(z\geq 0)\big|_{z=0}.$$

$$\Rightarrow E_1 e^{-i\omega t} + E_2 e^{-i\omega t} = E_0 e^{-i\omega t}.$$

$$E_1 + E_2 = E_0.$$

$$H(z\leq 0)\big|_{z=0} = H(z\geq 0)\big|_{z=0}$$

Also $H = \sqrt{\frac{\varepsilon}{\mu_0}}\,E$.

$$\Rightarrow \quad \sqrt{\varepsilon}\,E_0 = \sqrt{\varepsilon_0}\,(E_1 - E_2).$$

$$N(\omega)\,E_0 = E_1 - E_2.$$

Solve to get

$$R = \left|\frac{E_2}{E_1}\right|^2 = \left|\frac{1-N}{1+N}\right|^2.$$

$$R = \left|\frac{1-\varepsilon^{\frac{1}{2}}}{1+\varepsilon^{\frac{1}{2}}}\right|^2.$$

and

$$\epsilon(\omega) = 1 - \frac{\omega_p^2}{\omega^2 + i\omega/\tau}$$

$$= 1 - \frac{1}{\frac{\omega^2}{\omega_p^2} + i\frac{\omega}{\omega_p}\cdot\frac{1}{\omega_p\tau}}$$

For $\omega \gg \omega_p$, $\epsilon(\omega) \to 1$. $R \to 0$.

For $\frac{1}{\tau} \ll \omega \ll \omega_p$,

$$1 + i\frac{\omega_p}{\omega}\cdot\omega_p\tau$$

$$\epsilon(\omega) \approx 1 - \frac{1}{\frac{\omega}{\omega_p}\left(\frac{\omega}{\omega_p} + i\frac{1}{\omega_p\tau}\right)} \approx 1 - \frac{\omega_p^2\tau}{i\omega}.$$

$$R \approx \left|1 - \frac{4\varepsilon^{\frac{1}{2}}}{\varepsilon + 1 + 2\varepsilon^{\frac{1}{2}}}\right| = 1 - \left|\frac{2}{1 + \frac{\varepsilon^{\frac{1}{2}} + \varepsilon^{-\frac{1}{2}}}{2}}\right|$$

$$= 1 - \left|\frac{2}{i\omega_p\tau}\right| = 1 - \frac{2}{\omega_p\tau}.$$

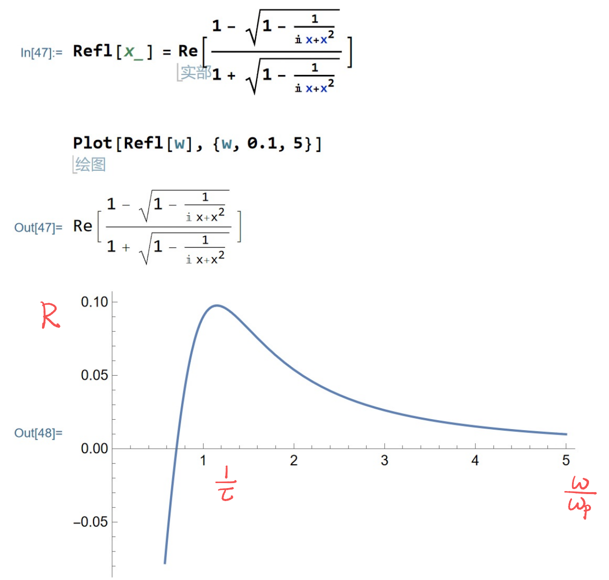
For $\omega \ll \frac{1}{\tau}$.

$$\varepsilon(\omega) = 1 - \frac{1}{\frac{\omega^2}{\omega_p^2} + i\frac{\omega}{\omega_p}\cdot\frac{1}{\omega_p\tau}}, \qquad \sigma(0) = \frac{\omega_p^2\tau}{4\pi}.$$

$$\epsilon(\omega) = 1 - \frac{1}{\frac{\omega^2\tau}{4\pi\sigma(0)} + i\frac{\omega}{4\pi\sigma(0)}} \approx 1 + i\frac{4\pi\sigma(0)}{\omega}.$$

$$R \approx \left|1 - \frac{4\varepsilon^{\frac{1}{2}}}{\varepsilon+1+2\varepsilon^{\frac{1}{2}}}\right| = 1 - \left|\frac{2}{1+\frac{\varepsilon^{\frac{1}{2}}+\varepsilon^{-\frac{1}{2}}}{2}}\right|$$

$$\approx 1 - \left|\frac{2}{\left(i\cdot\frac{4\pi\sigma(0)}{\omega}\right)^{\frac{1}{2}}}\right| = 1 - \left(\frac{\omega}{2\pi\sigma(0)}\right)^{\frac{1}{2}}.$$



In[47]:= $\text{Refl}[x\_] = \text{Re}\left[\frac{1-\sqrt{1-\frac{1}{\mathrm{i}\,x+x^2}}}{1+\sqrt{1-\frac{1}{\mathrm{i}\,x+x^2}}}\right]$

实部

```
Plot[Refl[w], {w, 0.1, 5}]
```

绘图

Out[47]= $\text{Re}\left[\frac{1-\sqrt{1-\frac{1}{\mathrm{i}\,x+x^2}}}{1+\sqrt{1-\frac{1}{\mathrm{i}\,x+x^2}}}\right]$

Out[48]=

Qu.5.4 Phonons

From Eq. (5.8) construct $\Im\chi$ in the limit that $\gamma \to 0$. Use the Kramers Krönig relation to then reconstruct $\Re\chi$ from $\Im\chi$ in the same limit.

$$\chi(\mathbf{q},\omega) = \frac{1}{-\rho\omega^2 + i\gamma\omega + Kq^2} \tag{5.8}$$

$$\begin{aligned}\Re\kappa(\omega) &= \wp\int \frac{d\omega'}{\pi}\frac{\Im\kappa(\omega')}{\omega'-\omega} \\ \Im\kappa(\omega) &= -\wp\int \frac{d\omega'}{\pi}\frac{\Re\kappa(\omega')}{\omega'-\omega}\end{aligned}$$

$$\mathrm{Im}(\chi) = \mathrm{Im}\left[\frac{Kq^2-\rho\omega^2-i\gamma\omega}{(Kq^2-\rho\omega^2)^2+\gamma^2\omega^2}\right] = \frac{-\gamma\omega}{(Kq^2-\rho\omega^2)^2+\gamma^2\omega^2}.$$

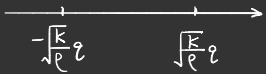
$$\to \frac{-\gamma\omega}{(Kq^2-\rho\omega^2)^2}.$$

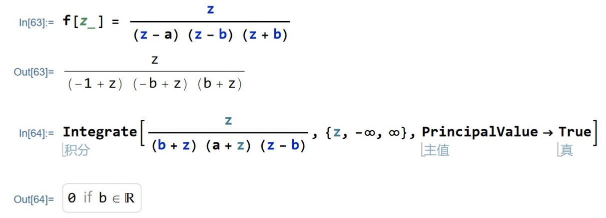
Reconstruct $\mathrm{Re}(\chi)$.

$$\mathrm{Re}(\chi) = \mathcal{P}\int \frac{d\omega'}{\pi}\frac{\mathrm{Im}(\chi(\omega'))}{\omega'-\omega}$$

$$= \mathcal{P}\int \frac{d\omega'}{\pi}\frac{-\gamma\omega'}{(\rho\omega'^2-Kq^2)^2(\omega'-\omega)}$$

$$= \mathcal{P}\int \frac{d\omega'}{\pi}\frac{-\gamma\omega'}{\rho^2\left(\omega'-\sqrt{\frac{K}{\rho}}q\right)\left(\omega'+\sqrt{\frac{K}{\rho}}q\right)(\omega'-\omega)} = 0 \ ?$$





```
In[63]:= f[z_] = z / ((z - a) (z - b) (z + b))

Out[63]= z / ((-1 + z) (-b + z) (b + z))

In[64]:= Integrate[z / ((b + z) (a + z) (z - b)), {z, -∞, ∞}, PrincipalValue → True]
         积分                                                  主值             真

Out[64]= 0 if b ∈ ℝ
```

Qu.5.5 Screened Coulomb interaction

Consider a nucleus of charge Z producing an potential

$$V_{ext}(\mathbf{q}) = -\frac{4\pi Z e^2}{q^2}$$

Using the long-wavelength limit of the dielectric function, show that the screened potential satisfies

$$V_{scr}(\mathbf{q}=0) = -\frac{2}{3}\Omega E_F$$

where Ω is the volume of the unit cell, and E_F is the Fermi energy for Z free electrons per unit cell.

In the long-wavelength limit ($q \to 0$, $\omega \neq 0$)

$$\epsilon^{RPA}(0,\omega) = 1 - \frac{\omega_p^2}{\omega^2} = 1 - \frac{4\pi n e^2}{m\omega^2}.$$

Also, $$\frac{V_{scr}}{V_{ext}} = \frac{1}{\varepsilon(\vec{q},\omega)}.$$

X

$$V_{scr}(\vec{q}=0) = \lim_{q\to 0}\left[\left(1-\frac{\omega_p^2}{\omega^2}\right)\cdot\frac{-4\pi Z e^2}{q^2}\right]$$

We know that

$$V_{ext}(\vec{q}) = -\frac{4\pi Z e^2}{q^2}.$$

$$V_{scr}(\vec{q}) = \frac{1}{\varepsilon(\vec{q})} = \frac{-4\pi Z e^2}{q^2 + k_0^2}.$$

$$V_{scr}(\vec{q}=0) = -\frac{4\pi Z e^2}{k_0^2}.$$

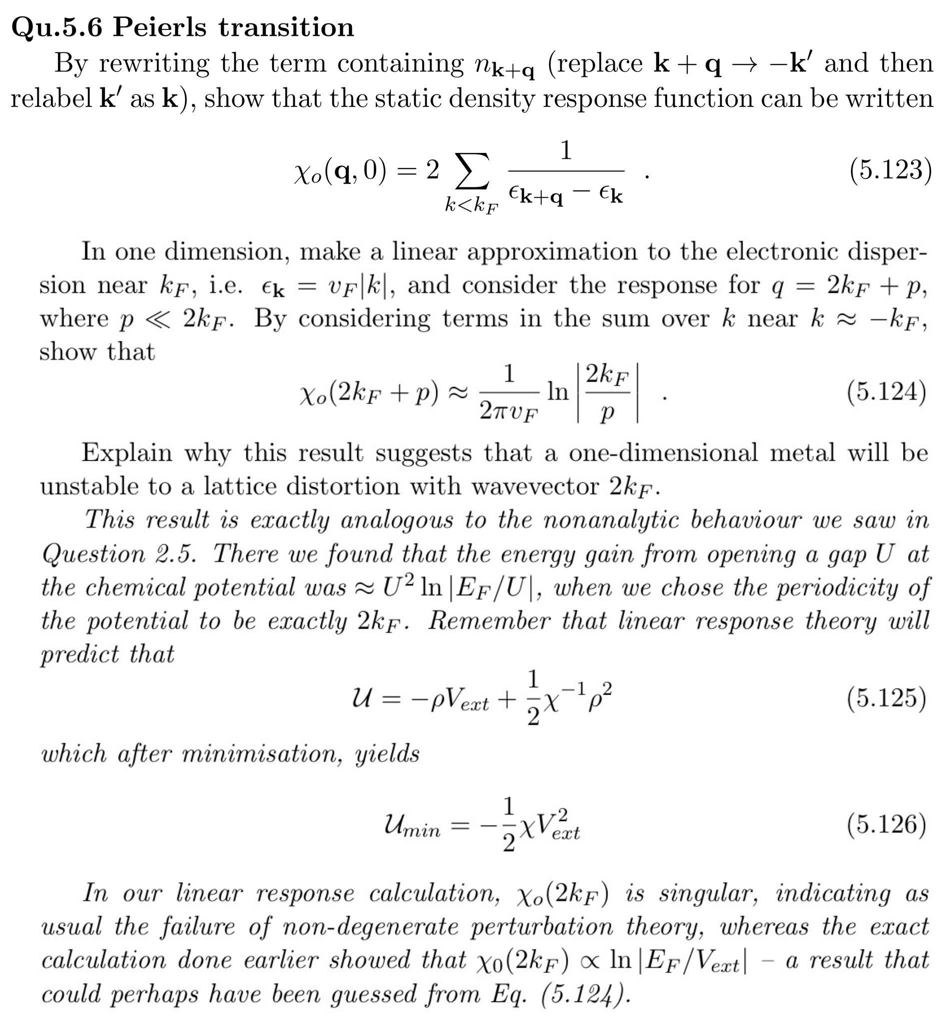
$$k_0^2 = 4\pi e^2 \frac{\partial n_0}{\partial \mu} \xrightarrow{T \ll T_F} 4\pi e^2 g(\varepsilon_F).$$

$$g(\varepsilon_F) = \frac{m\sqrt{2m\varepsilon_F}}{\pi^2 \hbar^3} = \frac{3\cancel{\pi^2}\cancel{\hbar^3} n \cdot \cancel{\sqrt{2}}}{2\cancel{\pi^2}\cancel{\hbar^3}\varepsilon_F \cdot \cancel{\sqrt{2}}} = \frac{3n}{2\varepsilon_F}.$$

$$k_0^2 = 4\pi e^2 \cdot \frac{3n}{2\varepsilon_F}.$$

$$V_{scr}(\vec{q}=0) = -\frac{4\pi Z e^2}{4\pi e^2 \cdot 3n} \cdot 2\varepsilon_F$$

$$= -\frac{2Z\varepsilon_F}{3n} = -\frac{2}{3}\Omega E_F.$$



Qu.5.6 Peierls transition

By rewriting the term containing $n_{\mathbf{k}+\mathbf{q}}$ (replace $\mathbf{k}+\mathbf{q} \to -\mathbf{k}'$ and then relabel $\mathbf{k}'$ as $\mathbf{k}$), show that the static density response function can be written

$$\chi_o(\mathbf{q},0) = 2\sum_{k<k_F} \frac{1}{\epsilon_{\mathbf{k}+\mathbf{q}} - \epsilon_{\mathbf{k}}} \quad . \tag{5.123}$$

In one dimension, make a linear approximation to the electronic dispersion near k_F, i.e. $\epsilon_{\mathbf{k}} = v_F|k|$, and consider the response for $q = 2k_F + p$, where $p \ll 2k_F$. By considering terms in the sum over k near $k \approx -k_F$, show that

$$\chi_o(2k_F + p) \approx \frac{1}{2\pi v_F} \ln\left|\frac{2k_F}{p}\right| \quad . \tag{5.124}$$

Explain why this result suggests that a one-dimensional metal will be unstable to a lattice distortion with wavevector $2k_F$.

This result is exactly analogous to the nonanalytic behaviour we saw in Question 2.5. There we found that the energy gain from opening a gap U at the chemical potential was $\approx U^2 \ln|E_F/U|$, when we chose the periodicity of the potential to be exactly $2k_F$. Remember that linear response theory will predict that

$$\mathcal{U} = -\rho V_{ext} + \frac{1}{2}\chi^{-1}\rho^2 \tag{5.125}$$

which after minimisation, yields

$$\mathcal{U}_{min} = -\frac{1}{2}\chi V_{ext}^2 \tag{5.126}$$

In our linear response calculation, $\chi_o(2k_F)$ is singular, indicating as usual the failure of non-degenerate perturbation theory, whereas the exact calculation done earlier showed that $\chi_0(2k_F) \propto \ln|E_F/V_{ext}|$ – a result that could perhaps have been guessed from Eq. (5.124).

By definition, response function has result:

$$\chi_o(\vec{q},\omega) = \frac{\partial\langle\rho\rangle}{\partial V} = 2\sum_{\vec{k}} \frac{n(\vec{k}) - n(\vec{k}+\vec{q})}{\varepsilon_{\vec{k}+\vec{q}} - \varepsilon_{k} - \hbar\omega - i\eta} .$$

$$\chi_o(\vec{q},0) = 2\sum_{\vec{k}} \frac{n(\vec{k}) - n(\vec{k}+\vec{q})}{\varepsilon_{\vec{k}+\vec{q}} - \varepsilon_{\vec{k}}}$$

$$= 2\sum_{\vec{k}'} \frac{n(-\vec{k}'-\vec{q}) - n(-\vec{k}')}{\varepsilon_{\vec{k}+\vec{q}} - \varepsilon_{\vec{k}}}$$

$$n(\vec{k}) = \begin{cases} 1, & |k| < k_F \\ 0, & \text{other.} \end{cases}$$?

$$\Rightarrow \chi_0(\vec{q}, 0) = 2 \sum_{k<k_F} \frac{1}{\varepsilon_{\vec{k}+\vec{q}} - \varepsilon_{\vec{k}}}.$$

$$\chi_0(2k_F + p) = 2 \sum_{k<k_F} \frac{1}{\varepsilon_{k+2k_F+p} - \varepsilon_k}.$$

near $k \approx -k_F$, $\varepsilon_k = v_F |k|$.

There's plenty of information about Pierels transition.

and Kohn anormalty, I might do the integral later...

$$\chi_0(2k_F + p) = 2 \sum_{k<k_F} \frac{1}{\varepsilon_{k+2k_F+p} - \varepsilon_k}$$

Qu.5.7 Optical properties

Discuss why, at optical frequencies, glass is transparent, and silver is shiny, while graphite appears black, and powdered sugar is white.

$$R = \left| \frac{n+ik-1}{n+ik+1} \right|^2 \text{ (from air)}, \quad T = (1-R)^2 e^{-\alpha L}, \quad \alpha = \frac{4\pi k}{\lambda}.$$

① For glass, $n = 1.5$, $k \approx 0.3$,

$R \approx 0.04$, $T \approx 1$.

Large transmission, small absorption, small reflection → transparent.

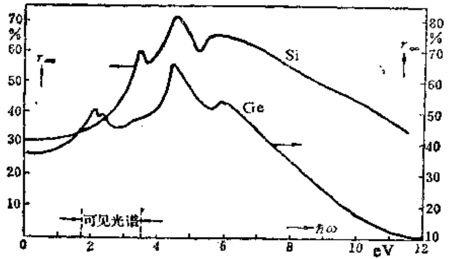
② For silver, $n \approx 0.05$, $k = 3.9$

$R \approx 1$, $T \approx 0$.

$T\downarrow$, $A\uparrow$, $R\uparrow$, shiny.

③ For graphite, $n = 2.7$, $k = 1.5$.

$R \approx 0.5$, $T \approx 0$.



Absorption Spectrum for Si and Ge

图 9-2 硅和锗在室温下的反射系数

Also, semiconductors have small reflection within visible light energy.

Still has reflection, small transmission, high absorption → black

④ For sugar powder, it is a molecular crystal.

Also has diffuse reflection, with large R and T. → white.

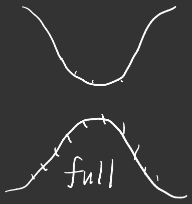
Qu.5.8 Metals and insulators

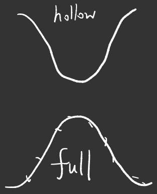
Explain the differences between a metal and an insulator. Your discussion should include reference to: single particle properties; screening of the Coulomb interaction; optical properties; and electrical and thermal properties.

Screening of the Coulomb interaction leads to NFE approximation.

As is discussed in NFE model, using perturbation theroy, we have energy gaps at boundaries of Brillouin zones, and the energy bands are filled with electrons.

When the valence band is full and conduction band half filled, the solid behave like conductor, while valence band full, conduction band not filled, solid behave like insulator.





From Drude result of dielectric constant we know metals has a frequency region with large reflectivity, which leads to their shiny appearence. (Q.5.3)

For insulators, taking into consideration of polarization.

we get $\varepsilon_r \approx 1 + \frac{\omega_p^2}{\omega_0^2 - \omega^2}$. correlate the eigenfrequency of molecules to the optical properties.

Electrical and Thermal Properties:

From $\sigma = \frac{ne^2\tau}{m^*}$, the conductivity is determined by carrier electron density. Conductors have larger n than insulator.

Thermal conductivity: $K = \frac{\pi^2}{3}\left(\frac{k_B}{e}\right)^2 T\sigma$. means that metals also have higher thermal conductivity.

Heat capacity of electron in metal is $C_e = \frac{\pi^2}{2} R \frac{k_B T}{E_F}$.

Chapter 6 Magnetism

Qu.6.1 Exchange

Consider single-particle wavefunctions on two neighbouring identical atoms ψ_A, ψ_B, which may be assumed real. These are to be used as the basis for a two-electron state. Show that the charge density in a singlet (triplet) state made out of the two orbitals is given by

$$\rho(r) = |\psi_A(r)|^2 + |\psi_B(r)|^2 \pm 2 < \psi_A|\psi_B > \psi_A(r)\psi_B(r) \quad . \tag{6.32}$$

Explain why the singlet state will usually be lower in energy.

ψ_A ψ_B

I will follow the explanation in Sakurai's "Advanced Quantum Mechanics". Chapter 7.

The total spin commute with Hamiltonian:

$$[S_{tot}, H] = 0.$$

$$\phi = \underbrace{\psi(\vec{r}_1, \vec{r}_2)}_{\text{spacial}}\underbrace{\chi}_{\text{spin}}.$$

Of which

$$\chi(m_1, m_2) = \begin{cases} \left.\begin{array}{l} \chi_{++}. \\ \frac{1}{\sqrt{2}}(\chi_{+-}+\chi_{-+}) \\ \chi_{--} \end{array}\right\} \text{Triplet} \\ \frac{1}{\sqrt{2}}(\chi_{+-}-\chi_{-+}) \text{ — Singlet} \end{cases}$$

Consider the symmetry of spacial and spin part.

$$\langle \vec{r}_1, m_1; \vec{r}_2, m_2 | \underset{\sim}{P_{12}} | \alpha \rangle = \langle \vec{r}_2, m_2; \vec{r}_1, m_1 | \alpha \rangle. \qquad P_{12} = P_{12}^{\text{spacial}} P_{12}^{\text{spin}}.$$

Fermi–Dirac statics requires that

$$\langle \vec{r}_1, m_1; \vec{r}_2; m_2 | \alpha \rangle = -\langle \vec{r}_2, m_2; \vec{r}_1, m_1 | \alpha \rangle.$$

Then $\quad |\alpha\rangle \longrightarrow P_{12}|\alpha\rangle.$

$$\psi(\vec{r}_1,\vec{r}_2) \longrightarrow \psi(\vec{r}_2,\vec{r}_1), \quad \chi(m_1,m_2) \longrightarrow \chi(m_2,m_1)$$

So we have $\phi = \underset{\text{antisymmetry}}{\psi_A}\;\underset{\text{Triplet}}{\chi_T}$ or $\underset{\text{symmetry}}{\psi_S}\;\underset{\text{Singlet}}{\chi_S}$.

that is

$$\phi(\vec{r}_1,\vec{r}_2) = \begin{cases} \frac{1}{\sqrt{2}}\left(\varphi_1(\vec{r}_1)\varphi_2(\vec{r}_2) + \varphi_1(\vec{r}_2)\varphi_2(\vec{r}_1)\right) & \rightarrow \text{Spin Singlet} \\ \frac{1}{\sqrt{2}}\left(\varphi_1(\vec{r}_1)\varphi_2(\vec{r}_2) - \varphi_1(\vec{r}_2)\varphi_2(\vec{r}_1)\right) & \rightarrow \text{Spin Triplet} \end{cases}$$

The probability density of observing electron 1 around $\vec{r}_1$:

$$\mathcal{P} = \frac{1}{2}\Big(|\varphi_1(\vec{r}_1)|^2 |\varphi_2(\vec{r}_2)|^2 + |\varphi_1(\vec{r}_2)|^2 |\varphi_2(\vec{r}_1)|^2 \pm 2\mathrm{Re}\left[\varphi_1(\vec{r}_1)\varphi_2(\vec{r}_2)\varphi_1^*(\vec{r}_2)\varphi_2^*(\vec{r}_1)\right]\Big)$$

$$\xrightarrow{\text{near neighbour}} = |\varphi_1(\vec{r})|^2 |\varphi_2(\vec{r})|^2 \pm \mathrm{Re}\left[\varphi_1(\vec{r})\varphi_2(\vec{r})\varphi_1^*(\vec{r})\varphi_2^*(\vec{r})\right]$$

$$= |\varphi_1(\vec{r})|^2 |\varphi_2(\vec{r})|^2 \pm \langle \varphi_1(\vec{r}) | \varphi_2(\vec{r}) \rangle \varphi_1(\vec{r})\varphi_2(\vec{r})$$

$\varphi_1(\vec{r}), \varphi_2(\vec{r})$ are solutions to Schrödinger equation:

$$\hat{H} = -\frac{\hbar^2}{2m}(\nabla_1^2 + \nabla_2^2) - \frac{e^2}{r_1} - \frac{e^2}{r_2}. \qquad \hat{H}\psi = E\psi.$$

We have energy:

Singlet $$E_1 = 2E_0 + \frac{e^2}{r} + \frac{K+A}{1+\Delta^2}.$$ (derivation ...)

Triplet $$E_2 = 2E_0 + \frac{e^2}{r} + \frac{K-A}{1-\Delta^2}.$$

$$K = \iint |\varphi_1(\vec{r})|^2 V |\varphi_2(\vec{r})|^2 d\tau_1 d\tau_2$$ Coloumb repelling energy

$$A = \iint \varphi_1^*(\vec{r}) \varphi_2^*(\vec{r}) V \varphi_1(\vec{r}) \varphi_2(\vec{r}) d\tau_1 d\tau_2$$ Coloumb exchange energy

$$V = e^2\left(\frac{1}{r_{12}} - \frac{1}{r_{b1}} - \frac{1}{r_{a2}}\right)$$

$$\Delta = \int \varphi_1(\vec{r}) \varphi_2(\vec{r}) d\tau_1 = \int \varphi_1(\vec{r}) \varphi_2(\vec{r}) d\tau_2$$ overlap integral

So the Singlet state is lower in energy.

Qu.6.2 One-dimensional spin waves

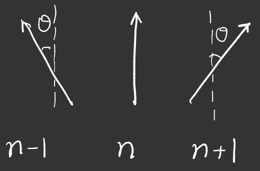
Assume a one-dimensional chain of spins, precessing according to Eq. (6.30). By considering two neighbours of the n^{th} spin, as in Fig. 6.8, each at relative angles θ, show that the rate of precession according to Eq. (6.30) is

$$\omega = \frac{4JS}{\hbar}(1 - \cos\theta) \quad . \tag{6.33}$$

Hence show that for a spin wave of wavevector q, the dispersion is

$$\hbar\omega = 4JS(1 - \cos(qa)) \quad . \tag{6.34}$$

$$\delta\dot{\mathbf{S}}_n = \frac{2JS}{\hbar} \sum_{j=n.n.\ of\ n} (\delta\mathbf{S}_n - \delta\mathbf{S}_j) \wedge \hat{z} \tag{6.30}$$



The interaction energy on the nth spin:

$$E_n = -2J S_n \cdot (S_{n-1} + S_{n+1}).$$

Also $\mu_n = -S_n g \mu_B$.

$$E_n = -\mu_n \cdot \underbrace{\left[-\frac{2J}{g\mu_B}(S_{n-1} + S_{n+1})\right]}_{} .$$ B_{eff}

Eqn of motion:

$$\hbar \frac{dS_n}{dt} = \vec{\mu}_n \times B_{eff} = 2J\left(\vec{S}_n \times \vec{S}_{n-1} + \vec{S}_n \times \vec{S}_{n+1}\right)$$

Component form:

$$\frac{dS_n^x}{dt} = \frac{2J}{\hbar}\left[S_n^y\left(S_{n-1}^z + S_{n+1}^z\right) - S_n^z\left(S_{n-1}^y + S_{n+1}^y\right)\right]$$

$$\Longrightarrow \frac{dS_n^x}{dt} = \frac{2JS}{\hbar}\left(2S_n^y - S_{n-1}^y - S_{n+1}^y\right)$$

$$\frac{dS_n^y}{dt} = -\frac{2JS}{\hbar}\left(2S_n^x - S_{n-1}^x - S_{n+1}^x\right) \qquad \frac{dS_n^z}{dt} = 0.$$

We get solution form:

$$S_n^x = u \exp\left[i(pka - \omega t)\right].$$

$$S_n^y = v \exp\left[i(pka - \omega t)\right].$$

Plug in to get

$$-i\omega u = \frac{2JS}{\hbar}\left(2 - e^{-ika} - e^{ika}\right) v = \frac{4JS}{\hbar}(1-\cos ka)\, v.$$

$$-i\omega v = \frac{2JS}{\hbar}\left(2 - e^{-ika} - e^{ika}\right) u = -\frac{4JS}{\hbar}(1-\cos ka)\, u.$$

The solution exists when

$$\begin{bmatrix} i\omega & \frac{4JS}{\hbar}(1-\cos ka) \\ -\frac{4JS}{\hbar}(1-\cos ka) & i\omega \end{bmatrix} = 0.$$

$$\Rightarrow \quad \hbar\omega = 4JS(1-\cos ka).$$

Is the dispersion relation.

Qu.6.3 Colossal magnetoresistance

This question introduces an active subject of current research: although lengthy, it involves nothing beyond the material discussed in the lectures. In a material like that shown in Fig. 6.10 the magnetism arises from a mechanism called **double exchange**, which is a version of itinerant exchange but involving two types of d-bands. The prototype compound is $La_{1-x}Sr_xMnO_3$, where the valence of La is 3+ and Sr is 2+. This is a cubic (perovskite) crystal structure where the Mn ions are nominally equidistant from six oxygen neighbours in three cartesian directions.

(a) Explain why the valence of Mn in the compound $La_{1-x}Sr_xMnO_3$ is expected to be between 3+ and 4+ and that the occupancy of the d-levels is expected to be $4-x$ electrons per Mn ion.

(b) The degeneracy of the 5 d-levels in the free ion is split by the cubic environment into a low energy three-fold degenerate subset (whose notation is t_{2g}) and a higher energy doubly degenerate orbital set (e_g). Explain why the spin configurations of these levels for the Mn^{3+} and Mn^{4+} ions are expected to be as shown in Fig. 6.12.

(c) The lowest three electron states can be regarded as forming a classical spin $S=\frac{3}{2}$ which has negligible hopping from site to site, whereas the highest state is potentially itinerant. Now consider two neighbouring sites i,j in the solid, each having the same "core" spin S, and sharing a single itinerant e_g electron, that has a tight-binding matrix element

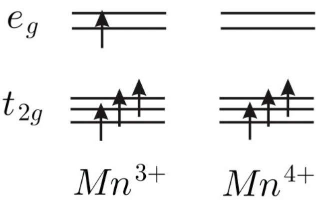


Figure 6.12:

$$t = < \phi_{e_g}(\mathbf{r}-\mathbf{R}_i)|H|\phi_{e_g}(\mathbf{r}-\mathbf{R}_j) > \qquad (6.35)$$

for hopping from site to site.

Explain the origin of the terms

$$H_{int} = -J\sum_i \hat{\mathbf{s}}_i\cdot\mathbf{S}_i + J_x\sum_{ij}\mathbf{S}_i\cdot\mathbf{S_j} \quad , \qquad (6.36)$$

in the total Hamiltonian ($\hat{\mathbf{s}}_i$) is the spin of the e_g electron) and suggest relative magnitudes of U, $J$and J_x.[9]

(a) $3\cdot(1-x) + 2x - 6 = -x-3.$

The valence of Mn will be $x+3$. Since $0 \leqslant x \leqslant 1$.

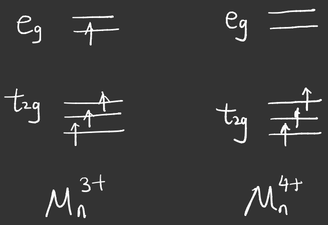
It should be between 3 and 4.

Electron configuration: Electron per Mn in d orbital $4-x$.

La : $[Xe]\,5d^1 6s^2$.

Sr : $[Kr]\,5s^2$.

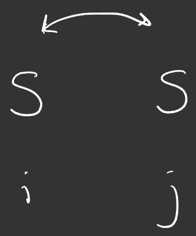
Mn : $[Ar]\,3d^5 4s^2$.



(b) From Q6.1 and Hund's Rule we know that electrons occupy orbitals with same energy singly without being in pairs.

Then we have configuration ↗.

(c) The Hint term originates from the exchange interaction of neighbouring ions and electrons.



$$H_{int} = -J\sum_i \vec{s}_i\cdot\vec{S}_i + J_x\sum_{ij}\vec{S}_i\cdot\vec{S}_j$$

neighbouring electron and ion

neighbouring ions

(d) Consider two neighbouring core spins $\mathbf{S}_i$ $\mathbf{S}_j$ that are at a relative angle θ_{ij}. By considering that the spin wavefunction of the itinerant electron must, for $J \gg t$, be always aligned with the local core spin $\mathbf{S}$, explain why the Schrödinger equation for the itinerant electron can be simplified to one in which the tight-binding hopping matrix element from site i to site j is replaced by

$$t_{eff} = t\cos(\frac{\theta_{ij}}{2}) \quad . \tag{6.37}$$

To do this, you may wish to note that under a rotation by an angle θ, the spin wavefunction transforms as

$$\begin{pmatrix} |\uparrow'> \\ |\downarrow'> \end{pmatrix} = \begin{pmatrix} \cos\frac{\theta}{2} & \sin\frac{\theta}{2} \\ -\sin\frac{\theta}{2} & \cos\frac{\theta}{2} \end{pmatrix} \begin{pmatrix} |\uparrow> \\ |\downarrow> \end{pmatrix} \tag{6.38}$$

(e) Sketch the density of states of the itinerant electrons for different alignments of the core spins $\mathbf{S}$:
ferromagnetic (all core spins aligned),
antiferromagnetic (all neighbouring core spins anti-aligned),
paramagnetic (core spins randomly aligned).
Discuss how the total Free energies of these states differ, and suggest what is the magnetic ground state when $x = 0$; and when $tx > J_x$; give rough estimates of the transition temperatures of the ordered magnetic states toward high temperature paramagnetism.

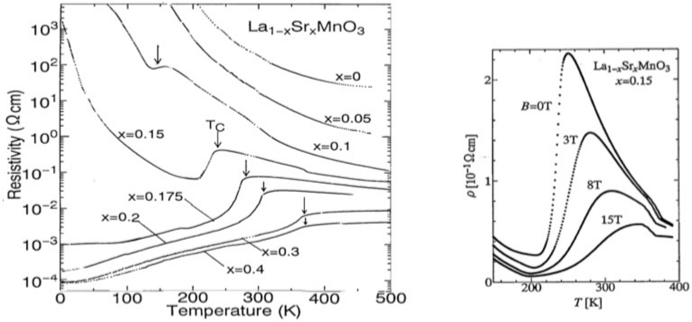


Figure 6.13: Resistivity as a function of temperature and magnetic field for a series of samples of doped manganese oxides with different compositions. The ferromagnetic transition temperatures T_c are marked by the arrows.

(f) Fig. 6.13 shows the resistivity as a function of temperature of several samples of $La_{1-x}Sr_xMnO_3$ with different concentrations x, as well as the magnetic-field-dependence of the resistivity (which gives rise to the label "colossal" magnetoresistance).[10] Discuss this data in light of the results above.

---

[9] In second-quantised notation, the full Hamiltonian can be written as

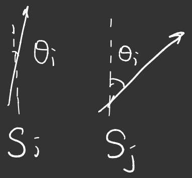
$$H = t \sum_{ij=n.n.,\sigma} \hat{c}^\dagger_{i\sigma}\hat{c}_{j\sigma} + U\sum_i \hat{n}_{i\sigma}\hat{n}_{i-\sigma} - J\sum_i \hat{\mathbf{s}}_i \cdot \mathbf{S}_i + J_x \sum_{ij} \mathbf{S}_i \cdot \mathbf{S}_\mathbf{j} \quad .$$

U is interaction of form

$$U = \frac{e^2}{4\pi\varepsilon_0}\iint |\psi(\vec{r}_1)|^2 \frac{1}{|\vec{r}_1-\vec{r}_2|}|\psi(\vec{r}_2)|^2 \, d\vec{r}_1 d\vec{r}_2 .$$

J_x is a function of $|\vec{r}_1-\vec{r}_2|$.

(d)



$J >> t$.

We want to prove that

$$\mathcal{H} = t\sum_{ij}\hat{c}^\dagger_{i\sigma}\hat{c}_{j\sigma} + U\sum_{j}\hat{n}_{i\sigma}\hat{n}_{i-\sigma} + H_{int}$$

$\downarrow$

$t_{eff} = t\cos\left(\frac{\theta_{ij}}{2}\right)$. for H'.

From the definition of hopping integral:

$$t = \int \varphi_j^*\left[V(r)-v_i(r)\right]\varphi_i \, dr .$$

with $\varphi_j \longrightarrow T(\theta_j)\varphi_j$, $\varphi_i \longrightarrow T(\theta_i)\varphi_i^*$.

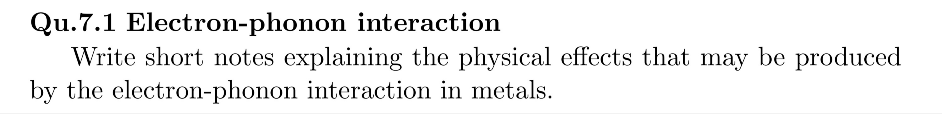
X

$$t' = \int T^*(\theta_j)\varphi_j^*\left[V(r)-v_i(r)\right]T(\theta_i)\varphi_i \, dr$$

$$= T^*(\theta_j)T(\theta_i)\,t = \begin{bmatrix}\cos\frac{\theta_j}{2} & -\sin\frac{\theta_j}{2}\\ \sin\frac{\theta_j}{2} & \cos\frac{\theta_j}{2}\end{bmatrix}\begin{bmatrix}\cos\frac{\theta_i}{2} & \sin\frac{\theta_i}{2}\\ -\sin\frac{\theta_i}{2} & \cos\frac{\theta_i}{2}\end{bmatrix} t$$

$$= t\cos\left(\frac{\theta_i-\theta_j}{2}\right).$$

Chapter 7 Electrons and phonons



Qu.7.1 Electron-phonon interaction

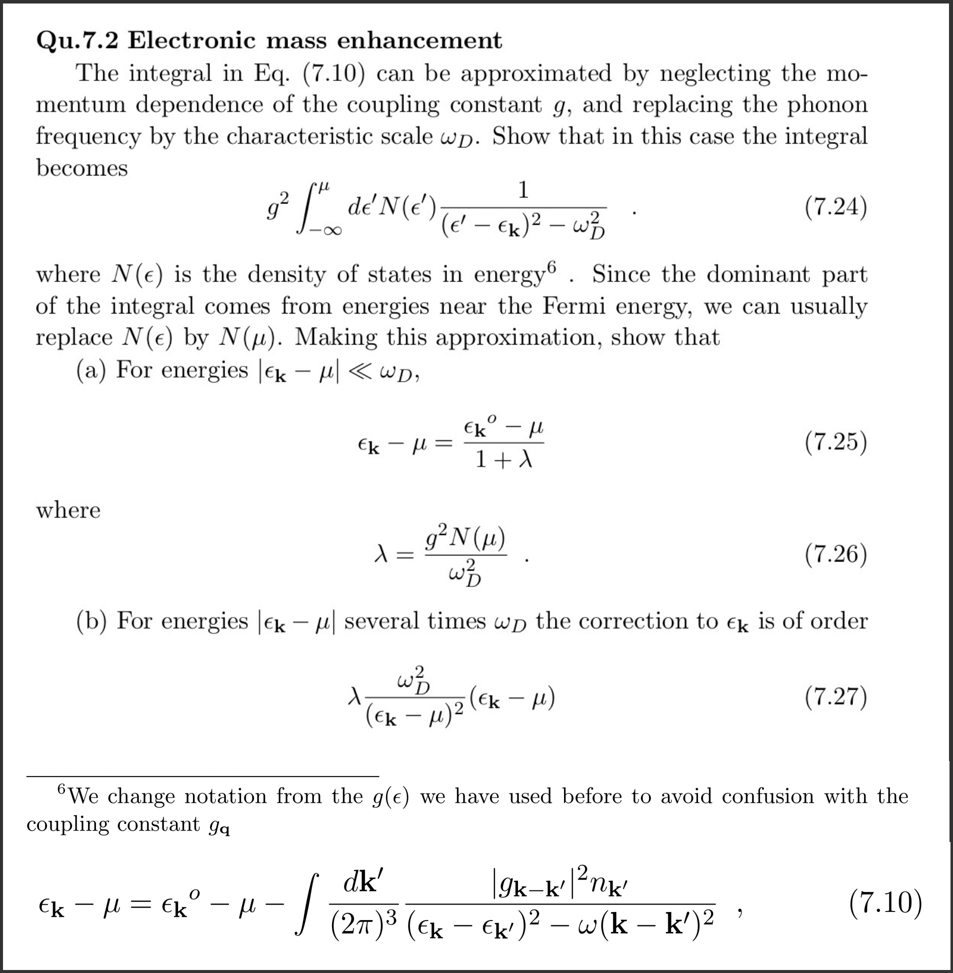
Write short notes explaining the physical effects that may be produced by the electron-phonon interaction in metals.

Phonon is quantized lattice vibration. The scattering of electrons around moving atoms' potential is called electron-phonon interaction.

Electron-phonon interaction will lead to effective interaction between electrons. Since the lattice distortion has longer characteristic time than fluctuations in electron gas, this produces correlation of the electron density waves as if there's an attractive potential between electrons.

There will also be enhancement of effective mass around Fermi surface, since the electron-phonon coupling gives substantial renormalization of the energy spectrum near Fermi surface.

Two electrons near Fermi surface might bind together to form a pair since they have effective attraction. The fermi sea give the possibility that the electron pairs persists even with arbitrary weak interaction.



Qu.7.2 Electronic mass enhancement

The integral in Eq. (7.10) can be approximated by neglecting the momentum dependence of the coupling constant g, and replacing the phonon frequency by the characteristic scale ω_D. Show that in this case the integral becomes

$$g^2 \int_{-\infty}^{\mu} d\epsilon' N(\epsilon') \frac{1}{(\epsilon' - \epsilon_{\mathbf{k}})^2 - \omega_D^2} \quad . \tag{7.24}$$

where $N(\epsilon)$ is the density of states in energy[6] . Since the dominant part of the integral comes from energies near the Fermi energy, we can usually replace $N(\epsilon)$ by $N(\mu)$. Making this approximation, show that

(a) For energies $|\epsilon_{\mathbf{k}} - \mu| \ll \omega_D$,

$$\epsilon_{\mathbf{k}} - \mu = \frac{\epsilon_{\mathbf{k}}{}^{o} - \mu}{1 + \lambda} \tag{7.25}$$

where

$$\lambda = \frac{g^2 N(\mu)}{\omega_D^2} \quad . \tag{7.26}$$

(b) For energies $|\epsilon_{\mathbf{k}} - \mu|$ several times ω_D the correction to $\epsilon_{\mathbf{k}}$ is of order

$$\lambda \frac{\omega_D^2}{(\epsilon_{\mathbf{k}} - \mu)^2} (\epsilon_{\mathbf{k}} - \mu) \tag{7.27}$$

---

[6] We change notation from the $g(\epsilon)$ we have used before to avoid confusion with the coupling constant $g_{\mathbf{q}}$

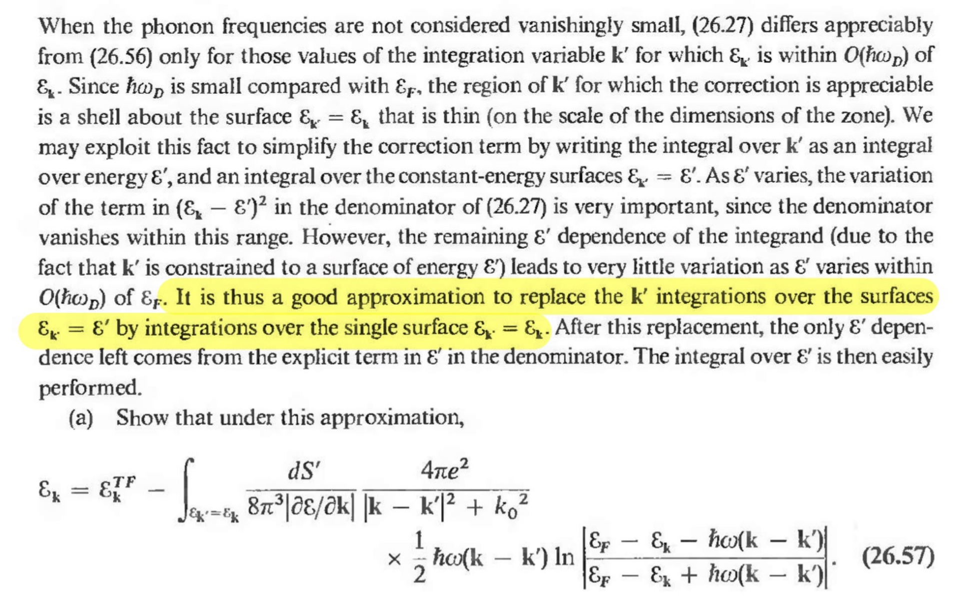
$$\epsilon_{\mathbf{k}} - \mu = \epsilon_{\mathbf{k}}{}^{o} - \mu - \int \frac{d\mathbf{k}'}{(2\pi)^3} \frac{|g_{\mathbf{k}-\mathbf{k}'}|^2 n_{\mathbf{k}'}}{(\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k}'})^2 - \omega(\mathbf{k} - \mathbf{k}')^2} \quad , \tag{7.10}$$

By approximation $g_{\vec{k}-\vec{k}'} \longrightarrow g$, $\omega \longrightarrow \omega_D$.

Integral in (7.10) becomes

$$\int \frac{d\vec{k}'}{(2\pi)^3} \frac{g^2 n_{\vec{k}'}}{(\varepsilon_{\vec{k}} - \varepsilon_{\vec{k}'})^2 - \omega_D(\vec{k}-\vec{k}')^2}$$

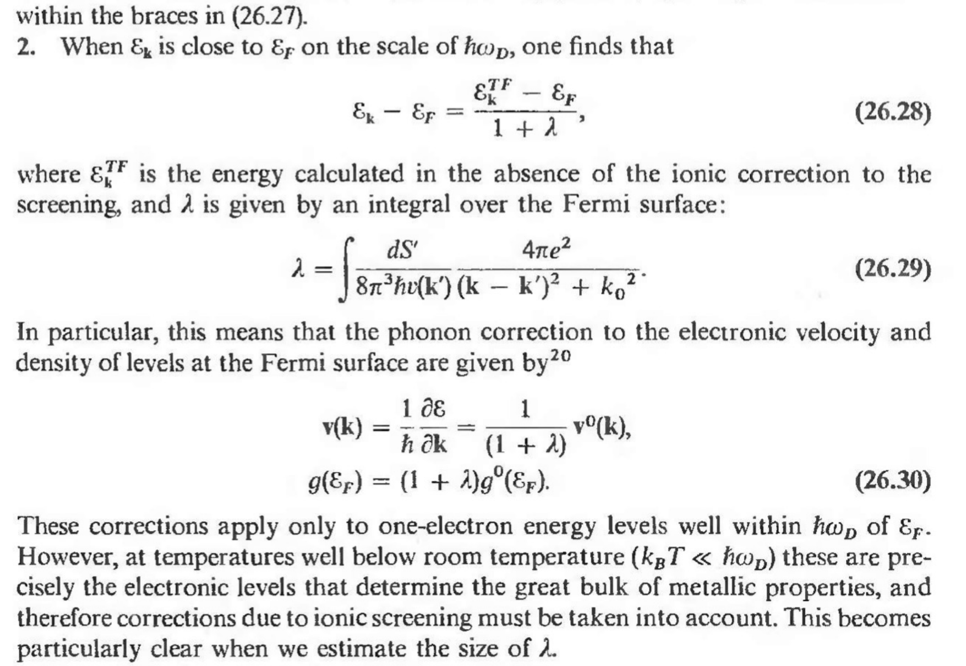
Sorry, I don't think I understand the material. Belew are just some information I found.



When the phonon frequencies are not considered vanishingly small, (26.27) differs appreciably from (26.56) only for those values of the integration variable $\mathbf{k}'$ for which $\mathcal{E}_{\mathbf{k}'}$ is within $O(\hbar\omega_D)$ of $\mathcal{E}_{\mathbf{k}}$. Since $\hbar\omega_D$ is small compared with $\mathcal{E}_F$, the region of $\mathbf{k}'$ for which the correction is appreciable is a shell about the surface $\mathcal{E}_{\mathbf{k}'} = \mathcal{E}_{\mathbf{k}}$ that is thin (on the scale of the dimensions of the zone). We may exploit this fact to simplify the correction term by writing the integral over $\mathbf{k}'$ as an integral over energy $\mathcal{E}'$, and an integral over the constant-energy surfaces $\mathcal{E}_{\mathbf{k}'} = \mathcal{E}'$. As $\mathcal{E}'$ varies, the variation of the term in $(\mathcal{E}_{\mathbf{k}} - \mathcal{E}')^2$ in the denominator of (26.27) is very important, since the denominator vanishes within this range. However, the remaining $\mathcal{E}'$ dependence of the integrand (due to the fact that $\mathbf{k}'$ is constrained to a surface of energy $\mathcal{E}'$) leads to very little variation as $\mathcal{E}'$ varies within $O(\hbar\omega_D)$ of $\mathcal{E}_F$. It is thus a good approximation to replace the $\mathbf{k}'$ integrations over the surfaces $\mathcal{E}_{\mathbf{k}'} = \mathcal{E}'$ by integrations over the single surface $\mathcal{E}_{\mathbf{k}'} = \mathcal{E}_{\mathbf{k}}$. After this replacement, the only $\mathcal{E}'$ dependence left comes from the explicit term in $\mathcal{E}'$ in the denominator. The integral over $\mathcal{E}'$ is then easily performed.

(a) Show that under this approximation,

$$\mathcal{E}_{\mathbf{k}} = \mathcal{E}_{\mathbf{k}}^{TF} - \int_{\mathcal{E}_{\mathbf{k}'}=\mathcal{E}_{\mathbf{k}}} \frac{dS'}{8\pi^3|\partial\mathcal{E}/\partial\mathbf{k}|}\,\frac{4\pi e^2}{|\mathbf{k}-\mathbf{k}'|^2 + k_0{}^2} \times \frac{1}{2}\hbar\omega(\mathbf{k}-\mathbf{k}')\ln\left|\frac{\mathcal{E}_F - \mathcal{E}_{\mathbf{k}} - \hbar\omega(\mathbf{k}-\mathbf{k}')}{\mathcal{E}_F - \mathcal{E}_{\mathbf{k}} + \hbar\omega(\mathbf{k}-\mathbf{k}')}\right|. \tag{26.57}$$



1. The value of $\mathcal{E}_F$ and the shape of the Fermi surface are unaffected by the ionic correction to the screening; i.e., they are correctly given by ignoring the second term within the braces in (26.27).
2. When $\mathcal{E}_{\mathbf{k}}$ is close to $\mathcal{E}_F$ on the scale of $\hbar\omega_D$, one finds that

$$\mathcal{E}_{\mathbf{k}} - \mathcal{E}_F = \frac{\mathcal{E}_{\mathbf{k}}^{TF} - \mathcal{E}_F}{1 + \lambda}, \tag{26.28}$$

where $\mathcal{E}_{\mathbf{k}}^{TF}$ is the energy calculated in the absence of the ionic correction to the screening, and λ is given by an integral over the Fermi surface:

$$\lambda = \int \frac{dS'}{8\pi^3\hbar v(\mathbf{k}')}\,\frac{4\pi e^2}{(\mathbf{k}-\mathbf{k}')^2 + k_0{}^2}. \tag{26.29}$$

In particular, this means that the phonon correction to the electronic velocity and density of levels at the Fermi surface are given by[20]

$$\mathbf{v}(\mathbf{k}) = \frac{1}{\hbar}\frac{\partial\mathcal{E}}{\partial\mathbf{k}} = \frac{1}{(1+\lambda)}\mathbf{v}^0(\mathbf{k}),$$
$$g(\mathcal{E}_F) = (1+\lambda)g^0(\mathcal{E}_F). \tag{26.30}$$

These corrections apply only to one-electron energy levels well within $\hbar\omega_D$ of $\mathcal{E}_F$. However, at temperatures well below room temperature ($k_BT \ll \hbar\omega_D$) these are precisely the electronic levels that determine the great bulk of metallic properties, and therefore corrections due to ionic screening must be taken into account. This becomes particularly clear when we estimate the size of λ.

Qu.7.3 Cooper's problem

For those who want to work out a non-trivial problem using operator techniques, this is Cooper's problem done that way. It is good practice of your operator technique to go through the following manipulations of $H|\psi_C>$, although this is pretty hard. But if you follow the rules, it all works out in about a page of algebra.

The wavefunction of a Cooper pair of electrons added to the Fermi sea is

$$|\psi_C>= \sum_{\mathbf{k}>k_F} g_{\mathbf{k}} \hat{c}^{\dagger}_{\mathbf{k}\uparrow} \hat{c}^{\dagger}_{-\mathbf{k}\downarrow} |FS> \quad , \tag{7.28}$$

where only terms in the sum for $k > k_F$ are allowed.

---

[6] We change notation from the $g(\epsilon)$ we have used before to avoid confusion with the coupling constant $g_{\mathbf{q}}$

We can now test out the pair wavefunction with the Hamiltonian

$$H = \sum_p \epsilon_p \hat{c}_p^\dagger \hat{c}_p + \frac{1}{2} \sum_{pp'q} V_q \hat{c}_p^\dagger \hat{c}_{p'}^\dagger \hat{c}_{p'-q} \hat{c}_{p+q} \quad . \tag{7.29}$$

applied to the two electrons in question, but leaving the fermi sea inert. V_q is here taken to be an *attractive* interaction.

Show that the first term in Eq. (7.29) operating on $|\psi_C>$ is

$$\begin{aligned} H_o|\psi_C> &= \sum_{pk\sigma} \epsilon_p g_k \hat{c}_{p\sigma}^\dagger \hat{c}_{p\sigma} \hat{c}_{k\uparrow}^\dagger \hat{c}_{-k\downarrow}^\dagger |FS> \\ &= \sum_k 2\epsilon_k g_k \hat{c}_{\mathbf{k}\uparrow}^\dagger \hat{c}_{-\mathbf{k}\downarrow}^\dagger |FS> \quad . \end{aligned} \tag{7.30}$$

(Hint: the trick in all of these operator manipulations is to move the anahilation operator to the RHS, so that it can destroy the vacuum state. Along the way, it has to anticommute with the creation operators initially on its right and these anticommutators always generate an extra δ-function. The two terms in the last equation come because we must have either $p = k$, $\sigma =\uparrow$, or $p = -k$, $\sigma =\downarrow$– and $\epsilon_{-p} = \epsilon_p$. Remember that for this toy problem **alone**, we don't apply the Hamiltonian to the Fermi sea.)

Similarly, show that the operation of the second term in Eq. (7.29) gives

$$H_{int}|\psi_C> = \sum_{kpp'q\sigma\sigma'} V_q g_k \hat{c}_{p\sigma}^\dagger \hat{c}_{p'\sigma'}^\dagger \delta_{p+q,k} \delta_{\sigma\uparrow} \delta_{p'-q,-k} \delta_{\sigma'\downarrow} |FS> \tag{7.31}$$

$$= \sum_{kk'>k_F} V_{k-k'} g_{k'} \hat{c}_{k\uparrow}^\dagger \hat{c}_{-k\downarrow}^\dagger |FS> \quad . \tag{7.32}$$

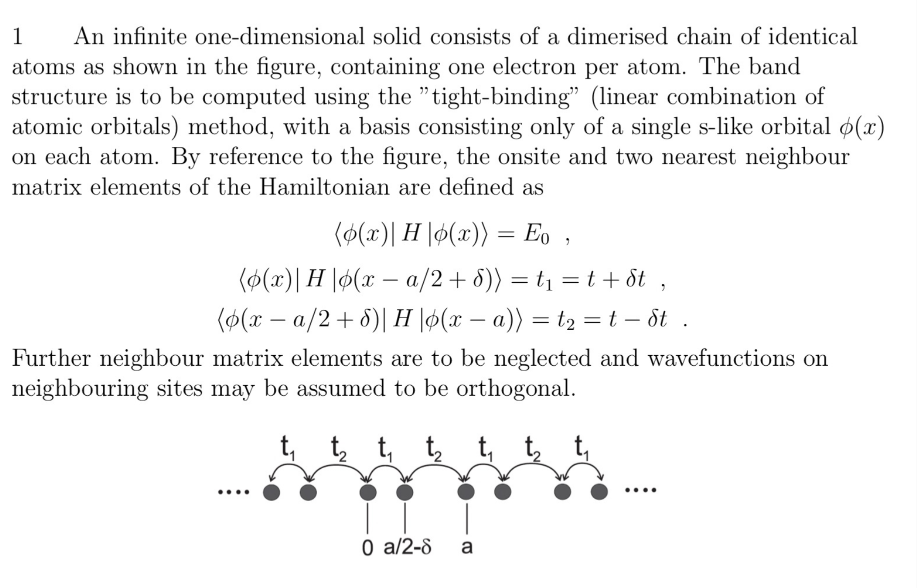
Getting to the final equation involves a little crafty relabelling of the momenta in the sum.

This gets us to the two-particle Schrödinger equation Eq. (7.19).

In the momentum representation, the two particle state can be an eigenstate of energy E if

$$(E - 2\epsilon_k) g_k = \sum_{k'>k_F} V_{k-k'} g_{k'} \quad . \tag{7.19}$$

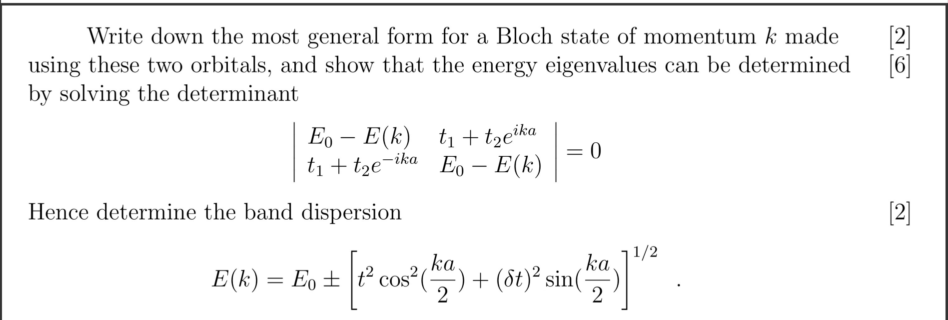
Final exam yuxiang @uchicago.edu



1 An infinite one-dimensional solid consists of a dimerised chain of identical atoms as shown in the figure, containing one electron per atom. The band structure is to be computed using the ”tight-binding” (linear combination of atomic orbitals) method, with a basis consisting only of a single s-like orbital $\phi(x)$ on each atom. By reference to the figure, the onsite and two nearest neighbour matrix elements of the Hamiltonian are defined as

$$\langle\phi(x)|\,H\,|\phi(x)\rangle = E_0 \ ,$$
$$\langle\phi(x)|\,H\,|\phi(x-a/2+\delta)\rangle = t_1 = t+\delta t \ ,$$
$$\langle\phi(x-a/2+\delta)|\,H\,|\phi(x-a)\rangle = t_2 = t-\delta t \ .$$

Further neighbour matrix elements are to be neglected and wavefunctions on neighbouring sites may be assumed to be orthogonal.

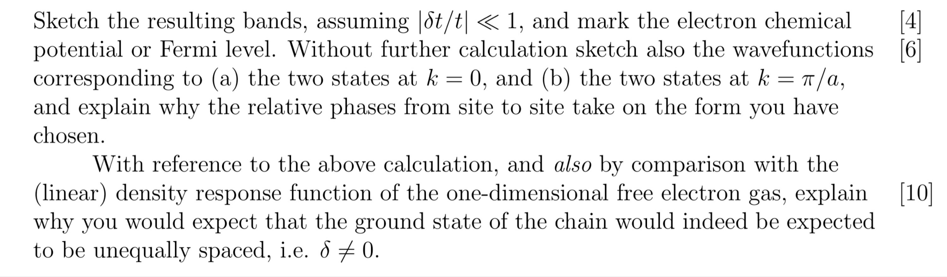


Write down the most general form for a Bloch state of momentum k made using these two orbitals, and show that the energy eigenvalues can be determined by solving the determinant [2] [6]

$$\begin{vmatrix} E_0-E(k) & t_1+t_2e^{ika} \\ t_1+t_2e^{-ika} & E_0-E(k) \end{vmatrix} = 0$$

Hence determine the band dispersion [2]

$$E(k) = E_0 \pm \left[t^2\cos^2(\frac{ka}{2}) + (\delta t)^2\sin(\frac{ka}{2})\right]^{1/2} \ .$$



Sketch the resulting bands, assuming $|\delta t/t| \ll 1$, and mark the electron chemical potential or Fermi level. Without further calculation sketch also the wavefunctions corresponding to (a) the two states at $k=0$, and (b) the two states at $k=\pi/a$, and explain why the relative phases from site to site take on the form you have chosen. [4] [6]

With reference to the above calculation, and *also* by comparison with the (linear) density response function of the one-dimensional free electron gas, explain why you would expect that the ground state of the chain would indeed be expected to be unequally spaced, i.e. $\delta \neq 0$. [10]

We have ansatz for Bloch state in LCAO method:

$$\psi_{n\vec{k}}(\vec{r}) = \frac{1}{\sqrt{N}}\sum_{\vec{R}} e^{i\vec{k}\cdot\vec{R}}\,\phi_n(\vec{r}-\vec{R}).$$

For our case, within a unit

$$\psi_0(r) = \phi(r) + e^{ik\cdot(\frac{a}{2}-\delta)}\phi(r-\tfrac{a}{2}+\delta)$$

Since $\int \phi^* \phi = 1$

Then $$\psi_{nk}(r) = \frac{1}{\sqrt{2N}}\sum_{\vec{R}}\left[e^{ik\cdot R}\phi(r-R) + e^{\overset{R+}{ik\cdot(\frac{a}{2}-\delta)}}\phi(r-\tfrac{a}{2}+\delta-R)\right].$$

Plug in the Schrödinger equation

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(r) - \mathcal{E}(k)\right]\psi = 0.$$

$$\Rightarrow \quad \int \psi^*\left[H - \mathcal{E}(\vec{k})\right]\psi = 0.$$

$$\Rightarrow \quad \mathcal{E}(k) = \langle\phi(r)|H|\phi(r)\rangle + \langle\phi(r)|H|\phi(r-\tfrac{a}{2}+\delta)\rangle e^{ik\cdot(\frac{a}{2}-\delta)}$$

$$+ \langle\phi(r-\tfrac{a}{2}+\delta)|H|\phi(r)\rangle e^{-ik\cdot(\frac{a}{2}-\delta)} + \langle\phi(r-\tfrac{a}{2}+\delta)|H|\phi(r-\tfrac{a}{2}+\delta)\rangle e^{ik\cdot(a-2\delta)}$$

$$= E_0 + e^{ik\cdot(\frac{a}{2}-\delta)}t_1 + e^{-ik\cdot(\frac{a}{2}-\delta)}t_2$$

$$+ \langle\phi(r-\tfrac{a}{2}+\delta)|H|\phi(r-\tfrac{a}{2}+\delta)\rangle e^{ik\cdot(a-2\delta)}$$

✗ does not seem to work.

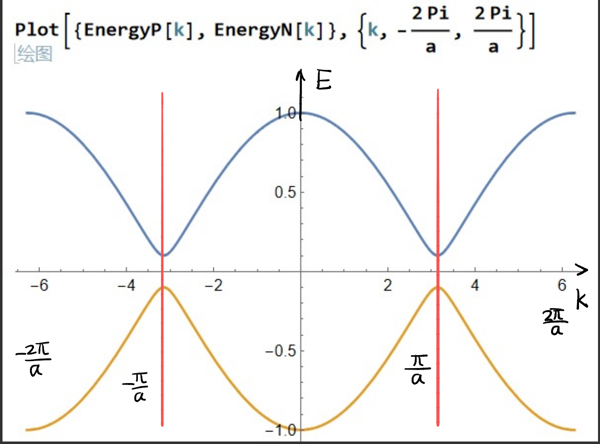
will derive again in next page

We get $$\begin{vmatrix} E - E(k) & t_1 + t_2 e^{ika} \\ t_1 + t_2 e^{-ika} & E - E(k) \end{vmatrix} = 0.$$

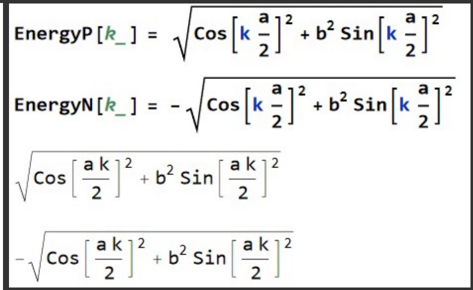
$$\Rightarrow \quad E(k) = E_0 \pm \left[t_1^2 + t_2^2 + t_1 t_2 \left(e^{ika} + e^{-ika}\right)\right]^{\frac{1}{2}}$$

$$= E_0 \pm \left[2t^2 + 2(\delta t)^2 + \left(t^2 - \delta t^2\right) \cdot 2\cos ka\right]^{\frac{1}{2}}$$

$$= E_0 \pm 2\sqrt{t^2 \cos^2 \frac{ka}{2} + (\delta t)^2 \sin^2 \frac{ka}{2}} \; .$$



```
Plot[{EnergyP[k], EnergyN[k]}, {k, -2 Pi/a, 2 Pi/a}]
```



```
EnergyP[k_] = Sqrt[Cos[k a/2]^2 + b^2 Sin[k a/2]^2]
EnergyN[k_] = -Sqrt[Cos[k a/2]^2 + b^2 Sin[k a/2]^2]
Sqrt[Cos[a k/2]^2 + b^2 Sin[a k/2]^2]
-Sqrt[Cos[a k/2]^2 + b^2 Sin[a k/2]^2]
```

$(a = 1, \; b = 0.1)$

Fermi surface

$$\text{(a)} \quad \psi_{n0}(r) = \sum_R \left[c_1 \phi(r) + c_2 \phi\left(r - \frac{a}{2} + \delta\right)\right]$$

$$\psi_{n\frac{\pi}{a}}(r) = \sum_R \left[c_1 e^{i\frac{\pi}{a}R} \phi(r) + c_2 e^{i\frac{\pi}{a}\left(R + \frac{a}{2} - \delta\right)} \phi\left(r - \frac{a}{2} + \delta\right)\right]$$

$$= \sum_R \left[c_1 e^{i\frac{\pi}{a}R} \phi(r) + i c_2 e^{\frac{i\pi R}{a} - \frac{i\pi\delta}{a}} \phi\left(r - \frac{a}{2} + \delta\right)\right]$$

Relative phase

We want to show that the $\delta \neq 0$ state always has lower energy.

From above derivation we know

$$E(\vec{k}) = E_0 \pm 2\sqrt{t^2 \cos^2 \frac{ka}{2} + (\delta t)^2 \sin^2 \frac{ka}{2}} .$$

I got the following derivation from internet.

The energy gain due to gap opening is given by

$$\Delta E_e = \frac{Na}{2\pi} \int_{-\frac{\pi}{2a}}^{\frac{\pi}{2a}} \left[E(\vec{k}) - E_{\text{original}} \right] dk$$

$$= -2t \frac{Na}{2\pi} \int_{-\frac{\pi}{2a}}^{\frac{\pi}{2a}} \left[\sqrt{\cos^2\left(\frac{ka}{2}\right) + \left(\frac{\delta t}{t}\right)^2 \sin^2\left(\frac{ka}{2}\right)} - \cos\left(\frac{ka}{2}\right) \right] dk$$

$$= -2t \frac{N}{\pi} \int_0^{\frac{\pi}{2}} \left[\sqrt{\cos^2\theta + \left(\frac{\delta t}{t}\right)^2 \sin^2\theta} - \cos\theta \right] d\theta$$

$\lambda : \left(\frac{\delta t}{t}\right)^2.$

$$= -\frac{2tN}{\pi} \int_0^{\pi/2} \underline{\left[\sqrt{1 - (1-\lambda)\sin^2\theta}\, d\theta - 1 \right]} .$$

For $\lambda \ll 1$.

$$\approx -\frac{2tN}{\pi} \left[1 + \lambda\left(a_1 - \frac{1}{4}\ln\lambda\right) + O(\lambda^2) \right].$$

Also the energy loss from lattice distortion:

$$\Delta E_l = N \cdot 2\underset{\sim}{k}\,\delta^2 .$$

spring constant

Total energy: $\Delta E = \Delta E_e + \Delta E_\ell$

Find minimum energy from $\frac{d\Delta E}{d\lambda} = 0$.

$$\Rightarrow \quad \Delta E = \frac{Nt}{\pi} \exp\left(-\frac{c+t}{t}\right).$$

As long as t is positive, ΔE is positive.

So the dimerized chain has lower energy. i.e.

The ground state of chain is unequally spaced.

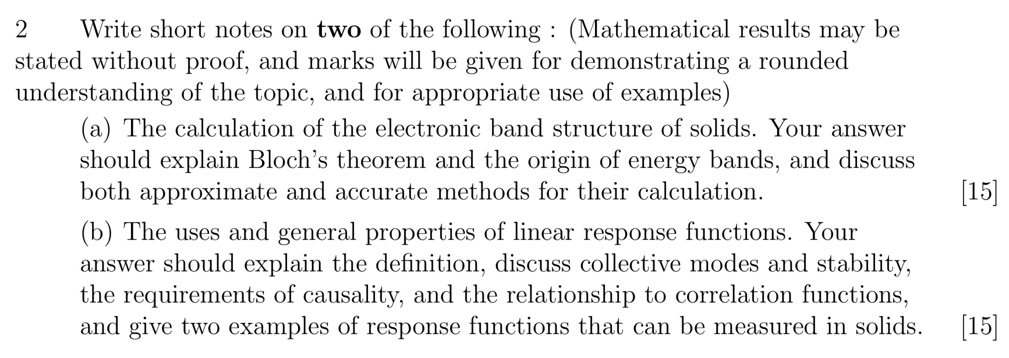
Density response function:

$$\delta\rho(\vec{q},\omega) = \chi(\vec{q},\omega)\, V(\vec{q},\omega).$$

We have charge density wave (CDW) in this case:

$$\rho(x) = \rho_0 + \rho_1 \cos(2k_F x + \varphi).$$

This response persists after displacement δ is present.



2 Write short notes on **two** of the following : (Mathematical results may be stated without proof, and marks will be given for demonstrating a rounded understanding of the topic, and for appropriate use of examples)

(a) The calculation of the electronic band structure of solids. Your answer should explain Bloch's theorem and the origin of energy bands, and discuss both approximate and accurate methods for their calculation. [15]

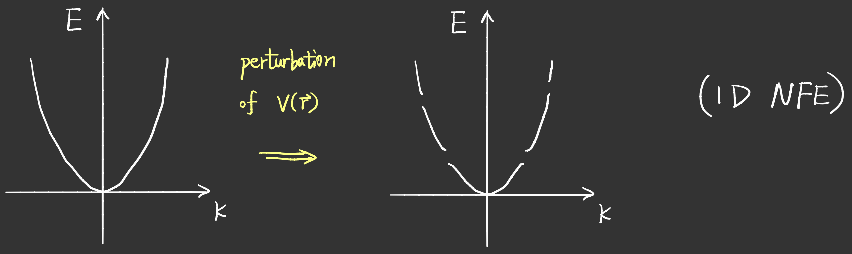
(b) The uses and general properties of linear response functions. Your answer should explain the definition, discuss collective modes and stability, the requirements of causality, and the relationship to correlation functions, and give two examples of response functions that can be measured in solids. [15]

(a) Though Bloch's theorem applies to various kinds of excitations in solids, we will focus on that of electrons.

Without introducing the interaction of electrons and ions, we cannot get insight of Bloch wave function. The electron wave function with translation symmetry originates from the periodicity of lattice potential.

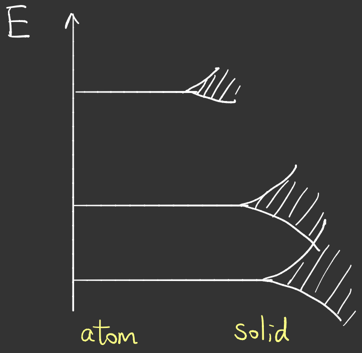
$$\underset{\substack{\downarrow\\ \text{periodic, } V(\vec r+\vec l)=V(\vec r)}}{\left[-\frac{\hbar^2}{2m}\nabla^2+V(\vec r)\right]}\psi = E\psi \Rightarrow \underset{\substack{\Downarrow\\ \text{periodic } |\psi_{\vec k}|^2}}{\psi_{\vec k}(\vec r+\vec l)=\psi_{\vec k}(\vec r)\,e^{i\vec k\cdot\vec l}}$$

NFE Model: One significant result of periodic potential is energy gap at the boundaries of Brillouin zone. The dispersion relation of free electrons has parabolic form, while we apply perturbation method (small V(r) for NFE), and degenerate perturbation method at zone boundary, we get energy gap. The continuous E-k regions and discontinuity regions consists of the total band structure.



The band structure could also be understood from a point of view of scattering of wave functions. The perturbed electron wave function has right and left propagating waves and they have strong scattering at BZ boundaries, which lead to gaps in energy bands.

Tight binding model: When V(r) is strong we apply tight binding model, which give us insight from energy levels of atoms to energy bands of solids.



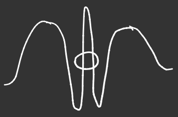
Beyond these rough models, in real calculation we got more reliable methods. They will give fine adjustments of electron wave functions and lattice potential.

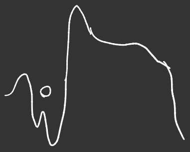
OPW and pseudo potential: Add a Bloch function to the plane wave solution. Atom wave function give suppression to lattice potential.

OPW
$$|\chi_{\vec{k}}\rangle = |\vec{k}\rangle - \sum_{n} \beta_n |f_{n\vec{k}}\rangle.$$

pseudo potential →
$$V_s|\phi\rangle = U|\phi\rangle + \sum_{n}(E-E_n)\langle f_n|\phi\rangle|f_n\rangle.$$

APW: Combine NFE and TBE.


wavefunction


pseudo potential

Above are all methods with single electron approximation. When taking into interaction of electrons, we get more improvements. The interaction of electrons could be simplified as single electron motion in an effective potential——Hartree approximation.

$$E = \frac{\langle \psi | H | \psi \rangle}{\langle \psi | \psi \rangle} .$$

minimum energy

Take into consideration of antisymmetric condition——HF approximation.

DFT: Calculation of electronic structure based on electron density. Get the ground state energy by calculating the variational minimum of n(r).

Combine all the above together: ab initio method.

Accurate method? I think they are all approximation. Relative accurate.

(b) To get information about the physical properties of a given system, we could apply perturbation (fluctuation) to the equilibrium state and learn about its response, so that to gain some insight about the collective modes of excitations present in system from the (linear) response function.

$$u_\alpha(\vec{q},\omega) = \underset{\text{linear response function}}{\chi_{\alpha\beta}(\vec{q},\omega)}\ \underset{\text{applied force}}{F_\beta(\vec{q},\omega)}.$$

The collective modes are waves propagating through the solid. Modes of oscillations in system is described by the pole structures of response function.

Stability: If there exists a curve w=w(q) where response function is divergent, this is a sign of instability. At the critical point there is a continuous phase transition.

Principle of causality: The response functions must be casual or retarded, because it is impossible that we get response before the force is applied. This impose conditions on the response functions in Fourier space.

$$\underset{\text{Principle of casuality}}{K(t-t') = 0 \quad \text{if} \quad t'>t.} \xrightarrow[\text{in upper plane}]{\text{analytical of } \omega} \text{Kramers-Kröniq relations}$$

Correlation function: A classical correlation function for the density relates the density at one point in space and time to a nearby point. The generalized susceptibility could be identified with the correlation function of the observable O(t). The susceptibility is the retarded Green function of the observable.

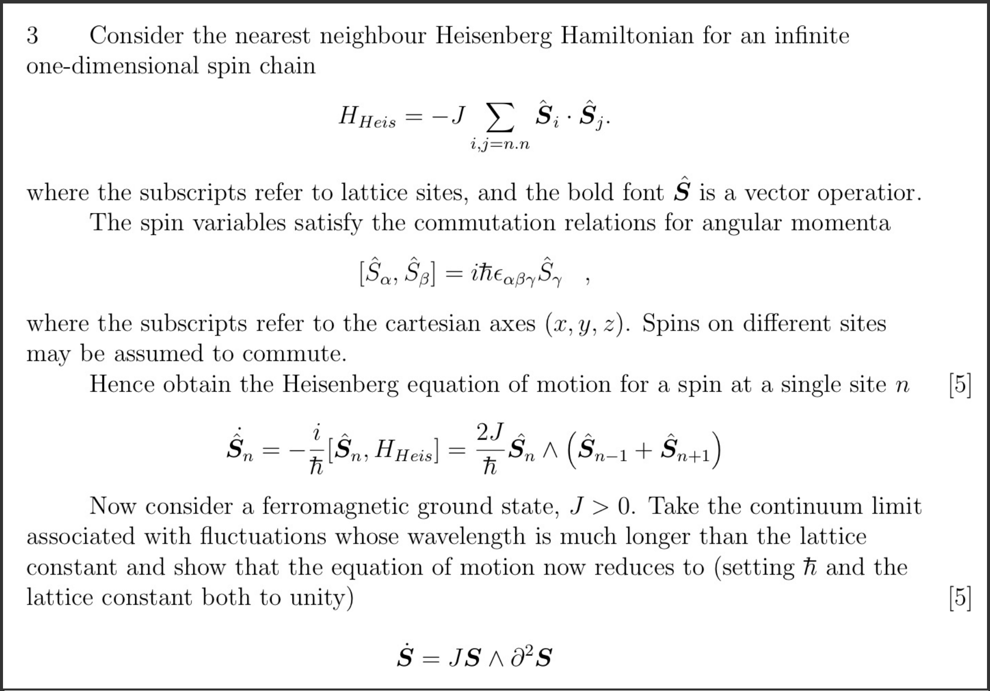
$$g(\vec{r},t;\vec{r}',t') = <\rho(\vec{r},t)\,\rho(\vec{r}',t')> - <\rho^2>.$$

$$\chi(\vec{x},t;x',t') = \underbrace{-\frac{i}{\hbar}\,\theta(t-t')}_{\text{retarded propagator}} <\underset{\substack{\uparrow\\ \text{ground state}}}{G}|\,[\vec{O}(\vec{x},t),\,\vec{O}(\vec{x}',t')]\,|G>.$$

Examples.

1. Dielectric function. Could be measured by conductive/capacitive spectroscopy.

2. Conductivity. Measured by applying electrical current and measure conductivity.



3 Consider the nearest neighbour Heisenberg Hamiltonian for an infinite one-dimensional spin chain

$$H_{Heis} = -J \sum_{i,j=n.n} \hat{\boldsymbol{S}}_i \cdot \hat{\boldsymbol{S}}_j .$$

where the subscripts refer to lattice sites, and the bold font $\hat{\boldsymbol{S}}$ is a vector operatior.

The spin variables satisfy the commutation relations for angular momenta

$$[\hat{S}_\alpha, \hat{S}_\beta] = i\hbar\epsilon_{\alpha\beta\gamma}\hat{S}_\gamma \quad ,$$

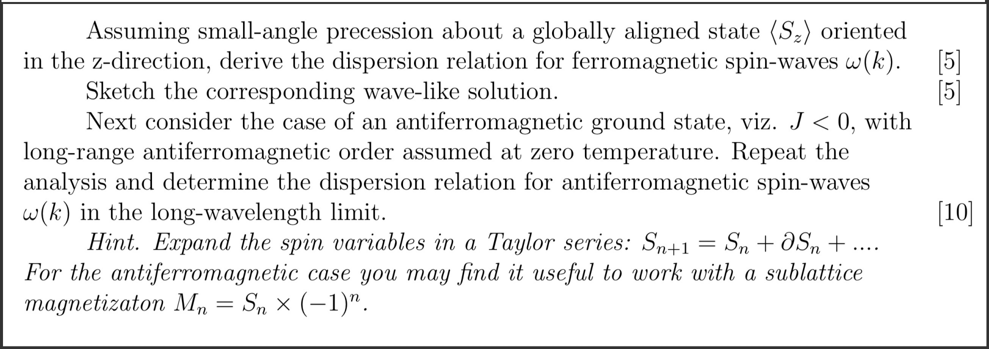
where the subscripts refer to the cartesian axes (x, y, z). Spins on different sites may be assumed to commute.

Hence obtain the Heisenberg equation of motion for a spin at a single site n [5]

$$\dot{\hat{\boldsymbol{S}}}_n = -\frac{i}{\hbar}[\hat{\boldsymbol{S}}_n, H_{Heis}] = \frac{2J}{\hbar}\hat{\boldsymbol{S}}_n \wedge \left(\hat{\boldsymbol{S}}_{n-1} + \hat{\boldsymbol{S}}_{n+1}\right)$$

Now consider a ferromagnetic ground state, $J > 0$. Take the continuum limit associated with fluctuations whose wavelength is much longer than the lattice constant and show that the equation of motion now reduces to (setting $\hbar$ and the lattice constant both to unity) [5]

$$\dot{\boldsymbol{S}} = J\boldsymbol{S} \wedge \partial^2 \boldsymbol{S}$$



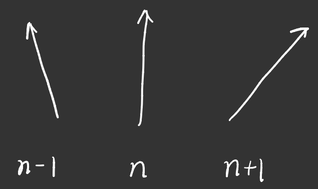
Assuming small-angle precession about a globally aligned state $\langle S_z \rangle$ oriented in the z-direction, derive the dispersion relation for ferromagnetic spin-waves $\omega(k)$. [5]

Sketch the corresponding wave-like solution. [5]

Next consider the case of an antiferromagnetic ground state, viz. $J < 0$, with long-range antiferromagnetic order assumed at zero temperature. Repeat the analysis and determine the dispersion relation for antiferromagnetic spin-waves $\omega(k)$ in the long-wavelength limit. [10]

Hint. Expand the spin variables in a Taylor series: $S_{n+1} = S_n + \partial S_n + \ldots$. *For the antiferromagnetic case you may find it useful to work with a sublattice magnetizaton* $M_n = S_n \times (-1)^n$.

The interaction energy of nth spin:



$$E_n = -2J S_n \cdot (S_{n-1} + S_{n+1}).$$

Also $\mu_n = -g\mu_B S_n$.

$$E_n = -\mu_n \cdot \underbrace{\left[-\frac{2J}{g\mu_B}(S_{n-1} + S_{n+1})\right]}_{B_{eff}}.$$

We gain eqn of motion:

$$\hbar \frac{dS_n}{dt} = \vec{\mu}_n \times \vec{B}_{eff} = 2J\left(\vec{S}_n \times \vec{S}_{n-1} + \vec{S}_n \times \vec{S}_{n+1}\right)$$

That is

$$\dot{S}_n = 2J\,\hat{S}_n \wedge \left(\hat{S}_{n-1} + \hat{S}_{n+1}\right).$$

Could also be derived from

$$\dot{\hat{S}}_n = -\frac{i}{\hbar}\left[\hat{S}_n , H_{Heis}\right]$$

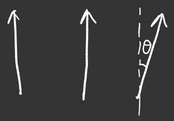
with $H_{Heis} = -J\sum_n \hat{S}_n \hat{S}_{n+1}$.

$$\Rightarrow \quad \dot{\hat{S}}_n = -\frac{2iJ}{\hbar}\left[\hat{S}_n , \hat{S}_n\cdot\left(\hat{S}_{n-1} + \hat{S}_{n+1}\right)\right].$$

$$= 2J\,\hat{S}_n \wedge \left(\hat{S}_{n-1} + \hat{S}_{n+1}\right).$$

In the continuum limit

$\hbar \to 0, \quad S \to \infty, \quad \hbar S = \text{constant}.$



$$\hat{S}_n \hat{S}_{n+1} \approx S^2\cos\theta \approx S^2 - \frac{1}{2}S^2\theta^2.$$

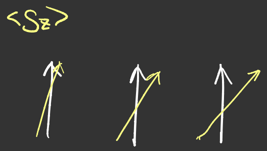
$$\Rightarrow \quad H_{Heis} = -JS^2 \sum_n \theta_{n,n+1}^2 \approx$$

$$\dot{\vec{S}} = J\vec{S} \wedge \partial^2 \vec{S}.$$

Component form:

$$\begin{cases} \dfrac{dS_n^x}{dt} = \dfrac{2J}{\hbar}\left[S_n^y\left(S_{n-1}^z + S_{n+1}^z\right) - S_n^z\left(S_{n-1}^y + S_{n+1}^y\right)\right] \\ \dfrac{dS_n^y}{dt} = \dfrac{2J}{\hbar}\left[S_n^z\left(S_{n-1}^x + S_{n+1}^x\right) - S_n^x\left(S_{n-1}^z + S_{n+1}^z\right)\right] \\ \dfrac{dS_n^z}{dt} = \dfrac{2J}{\hbar}\left[S_n^x\left(S_{n-1}^y + S_{n+1}^y\right) - S_n^y\left(S_{n-1}^x + S_{n+1}^x\right)\right] \end{cases} \Rightarrow \begin{cases} \dfrac{dS_n^x}{dt} = \dfrac{2JS}{\hbar}\left(2S_n^y - S_{n-1}^y - S_{n+1}^y\right) \\ \dfrac{dS_n^y}{dt} = -\dfrac{2JS}{\hbar}\left(2S_n^x - S_{n-1}^x - S_{n+1}^x\right) \\ \dfrac{dS_n^z}{dt} = 0. \end{cases}$$

We get solution form:



$$S_n^x = u \exp\left[i(pka - \omega t)\right].$$

$$S_n^y = v \exp\left[i(pka - \omega t)\right].$$

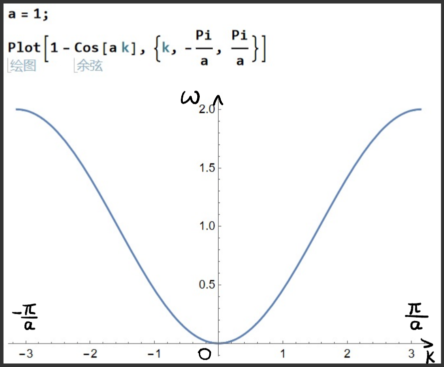
Plug in to get

$$-i\omega u = \frac{2JS}{\hbar}\left(2 - e^{-ika} - e^{ika}\right)v = \frac{4JS}{\hbar}(1-\cos ka)v.$$

$$-i\omega v = \frac{2JS}{\hbar}\left(2 - e^{-ika} - e^{ika}\right)u = -\frac{4JS}{\hbar}(1-\cos ka)u.$$

The solution exists when

$$\begin{bmatrix} i\omega & \dfrac{4JS}{\hbar}(1-\cos ka) \\ -\dfrac{4JS}{\hbar}(1-\cos ka) & i\omega \end{bmatrix} = 0.$$



```
a = 1;
Plot[1 - Cos[a k], {k, -Pi/a, Pi/a}]
```

$$\Rightarrow \qquad \omega = \frac{4JS}{\hbar}(1-\cos ka).$$

Is the dispersion relation of 1D FM chain.

The case of antiferromagnetic

$$\begin{cases} \dfrac{dS_n^x}{dt} = \dfrac{2J}{\hbar}\left[S_n^y\left(S_{n-1}^z + S_{n+1}^z\right) - S_n^z\left(S_{n-1}^y + S_{n+1}^y\right)\right] \\ \dfrac{dS_n^y}{dt} = \dfrac{2J}{\hbar}\left[S_n^z\left(S_{n-1}^x + S_{n+1}^x\right) - S_n^x\left(S_{n-1}^z + S_{n+1}^z\right)\right] \\ \dfrac{dS_n^z}{dt} = \dfrac{2J}{\hbar}\left[S_n^x\left(S_{n-1}^y + S_{n+1}^y\right) - S_n^y\left(S_{n-1}^y + S_{n+1}^x\right)\right] \end{cases} \Rightarrow \begin{cases} \dfrac{dS_n^x}{dt} = (-1)^{n-1} \cdot \dfrac{2JS}{\hbar}\left(2S_n^y + S_{n-1}^y + S_{n+1}^y\right) \\ \dfrac{dS_n^y}{dt} = -(-1)^{n-1} \cdot \dfrac{2JS}{\hbar}\left(2S_n^x + S_{n-1}^x + S_{n+1}^x\right) \\ \dfrac{dS_n^z}{dt} = 0. \end{cases}$$

For even n we have

$\langle S_z \rangle$

↑ ↓ ↑ ↓

$$S_n^x(t) = u e^{i(kna-\omega t)}$$

$$S_n^y(t) = -iu e^{i(kna-\omega t)}$$

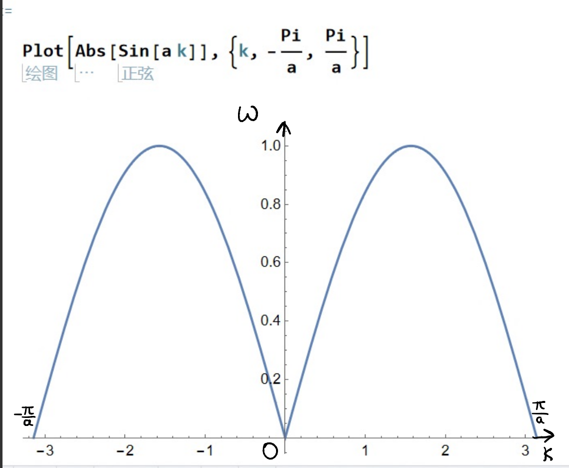
$$S_{n+1}^x(t) = v e^{i(kna-\omega t)}$$

$$S_{n+1}^y(t) = -iv e^{i(kna-\omega t)}$$

Plug in to get

$$i\omega u = \frac{2JS}{\hbar}\left(-2iu - 2iv\cos ka\right)$$

$$i\omega v = -\frac{2JS}{\hbar}\left(-2iv - 2iu\cos ka\right)$$



Plot[Abs[Sin[a k]], {k, -Pi/a, Pi/a}]

The solution exists when

$$\begin{bmatrix} -\omega-1 & -\dfrac{4JS}{\hbar}\cos ka \\ \dfrac{4JS}{\hbar}\cos ka & -\omega+1 \end{bmatrix} = 0.$$

$$\Rightarrow \quad \omega = \frac{4JS}{\hbar}\left|\sin ka\right|.$$

Is the dispersion relation of 1D antiferromagnetic chain.