Quantum Condensed Matter Physics Examples

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Topic 1 Lorentz dipole oscillator model, Drude model, Sommerfeld theory, lattices

Problem 1.1 Sapphire

A sapphire crystal doped with titanium absorbs strongly around 500 nm. *Calculate the difference in the refractive index of the doped crystal above and below the mk* 500 *nm absorption band, if the density of absorbing atoms is* 1×10^{25} m^{-3}. *The refractive index of undoped sapphire is* 1.77.

Using the Lorentz oscillator model, assume all the conducting electrons have the same

natural frequency ω,

$$\chi(\omega) = \frac{ne^2}{m\epsilon_0}\frac{1}{\omega_T^2 - \omega^2 - i\omega\gamma}$$

The imaginary part peaks at

$$\omega = \omega_T = \frac{2\pi c}{\lambda}$$

Below the peak where $\omega \ll \omega_T$,

$$\chi_-(\omega) = \frac{ne^2}{m\epsilon_0}\frac{1}{\omega_T^2}$$

Above the peak where $\omega \gg \sqrt{\frac{ne^2}{m\epsilon_0}}$,

$$\chi_+(\omega) = 0$$

so that

$$\Delta\epsilon = \Delta\chi(\omega) = \frac{ne^2}{m\epsilon_0}\frac{1}{\omega_T^2}$$

and use

$$n = \sqrt{\epsilon}$$

$$\text{if } \Delta\epsilon \ll \epsilon \implies \Delta n \approx \frac{1}{2\sqrt{\epsilon}}\Delta\epsilon$$

$$\Delta n \approx \frac{1}{2n_\infty}\frac{n_{(\text{density})}e^2}{m\epsilon_0}\frac{1}{\omega_T^2}$$

$$\Delta n = 6.3 \times 10^{-4}$$

Was the resonance frequency a result of doping?

Problem 1.2 Reflectivity of metals

The phase velocity of light in a conducting medium is c divided by the refractive index $N(\omega) = \epsilon^{1/2}(\omega)$. *Using Drude model results*

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

where ω_p *is the plasma frequency and* $1/\tau \ll \omega_p$ *for a good Drude metal.*

(a) $\omega \ll 1/\tau$

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

$$\begin{aligned} &\approx 1 + i \underbrace{\frac{\omega_p^2}{\omega/\tau}}_{\gg 1} \\ &\approx i\frac{\omega_p^2\tau}{\omega} \\ N(\omega) &\approx \epsilon^{1/2}(\omega) \\ &\approx \sqrt{\frac{\sigma_0}{2\omega\epsilon_0}}(1+i) \end{aligned}$$

where

$$\sigma(\omega) = \frac{\epsilon_0\omega_p^2\tau}{1 - i\omega\tau}$$

N is large and has roughly equal real and imaginary parts.

(b) $1/\tau \ll \omega \ll \omega_p$

$$\begin{aligned} \epsilon(\omega) &= 1 - \frac{\omega_p^2}{\omega^2}\frac{1}{1 + i/\omega\tau} \\ &\approx 1 - \frac{\omega_p^2}{\omega^2}\frac{1}{1 + i/\omega\tau} \\ &\approx 1 - \frac{\omega_p^2}{\omega^2} + \frac{i}{\omega\tau}\frac{\omega_p^2}{\omega^2} \\ &\approx -\frac{\omega_p^2}{\omega^2} + \frac{i}{\omega\tau}\frac{\omega_p^2}{\omega^2} \\ N(\omega) &\approx \left(i + \frac{1}{2\omega\tau}\right)\frac{\omega_p}{\omega} \end{aligned}$$

N is (mostly) imaginary and large.

(c) $\omega > \omega_p$

$$\begin{aligned} \epsilon(\omega) &= 1 - \frac{\omega_p^2/\omega}{\omega + i/\tau} \\ &\approx 1 - \frac{\omega_p^2}{\omega^2} \\ N(\omega) &\approx \sqrt{1 - \frac{\omega_p^2}{\omega^2}} \end{aligned}$$

N is real and < 1.

Consider a light wave with the electric field polarised in the x-direction at normal incidence from the vacuum on a good Drude metal occupying the region $z > 0$. In the vacuum, the

incident E_1 and reflected E_2 waves give rise to a field

$$E_x = E_1 \exp\left(+i\omega(\frac{z}{c} - t)\right) + E_2 \exp\left(-i\omega(\frac{z}{c} + t)\right)$$

In the medium, the electric field is

$$E_x = E_0 \exp\left(+i\omega\left(\frac{z}{c/N(\omega)} - t\right)\right)$$

Matching electric field and magnetic field ($\propto \frac{1}{i\omega}\boldsymbol{\nabla} \times \mathbf{E} = \frac{1}{i\omega}\frac{\partial E_x}{\partial z}\hat{\mathbf{e}}_y$),

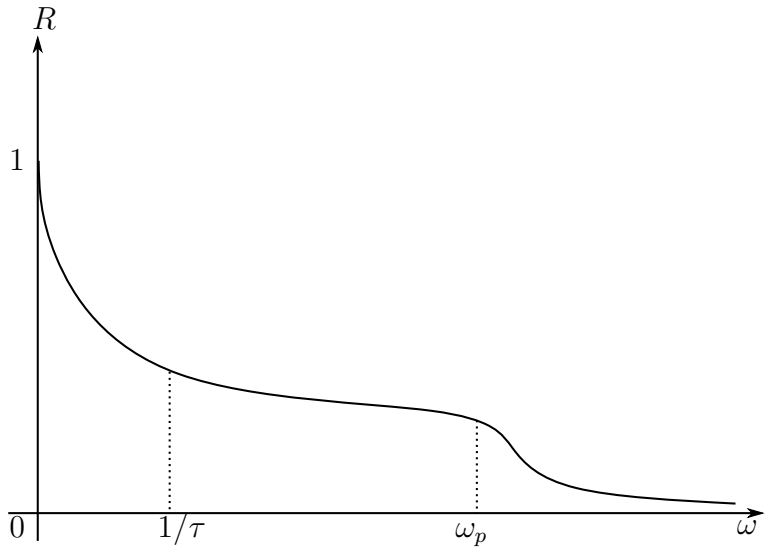
$$E_1 + E_2 = E_0$$
$$E_1 - E_2 = E_0 N(\omega)$$

Thence

$$\frac{2E_2}{2E_1} = \frac{E_0 - E_0 N}{E_0 + E_0 N}$$
$$R \equiv \left|\frac{E_2}{E_1}\right|^2 = \left|\frac{1-N}{1+N}\right|^2$$

Using the Drude results above

$$R \approx \begin{cases} 1 - \frac{4\,\mathrm{Re}(N)}{|N|^2} \approx 1 - 2\sqrt{\frac{2\epsilon_0\omega}{\sigma_0}} & \omega \ll 1/\tau \\ 1 - \frac{4\,\mathrm{Re}(N)}{|N|^2} \approx 1 - \frac{4\omega}{2\omega\tau\omega_p} = 1 - \frac{2}{\omega_p\tau} & 1/\tau \ll \omega \ll \omega_p \\ \left(\frac{1-(1-\frac{\omega_p^2}{2\omega^2})}{1+(1-\frac{\omega_p^2}{2\omega^2})}\right)^2 \approx \frac{\omega_p^2}{2\omega^2}^2 \frac{1}{2^2} = \frac{\omega_p^4}{16\omega^4} & \omega \gg \omega_p \end{cases}$$



Problem 1.3 Optical properties of solids

At optical frequencies

- glass is transparent because it is an insulator with a filled valence band and large band gap which forbids electron interaction with photon.
- silver is shiny because metals have a typically low skin depth which makes them reflective.
- graphite is a semiconductor with narrow bandgap, so its electrons are easily excited to the conduction band by photon absorption, making it absorptive.
- powdered sugar is very transmittal just like glass, but the powder form randomises the direction of incident light and makes sugar appear white.

Problem 1.4 Static conductivity tensor

In the Drude model, the equation of motion for $\mathbf{j}$ in a solid of relaxation time τ is

$$\left(\frac{\partial}{\partial t}+\frac{1}{\tau}\right)\mathbf{j}=\frac{nq}{m}\mathbf{F}(t)$$

In the presence of a magnetic field $\mathbf{B}$ along the z-axis, the force on charge carrier is

$$\begin{aligned}\mathbf{F}&=q(\mathbf{E}+\mathbf{v}\times\mathbf{B})\\ F_i&=q\big(E_i+\epsilon_{ij3}B_z v_j\big)\\ F_i&=qE_i+\frac{1}{n}\epsilon_{ij3}B_z j_j\end{aligned}$$

Looking for static solution such that $\frac{\partial}{\partial t}=0$ and denote cyclotron frequency $\omega_c=qB/m$

$$\begin{aligned}\frac{1}{\tau}j_i&=\frac{nq^2}{m}E_i+\frac{qB_z}{m}\epsilon_{ij3}j_j\\ \big(\delta_{ij}-\omega_c\tau\epsilon_{3ij}\big)j_j&=\frac{nq^2\tau}{m}E_i\\ \begin{pmatrix}1 & -\omega_c\tau & \\ +\omega_c\tau & 1 & \\ & & 1\end{pmatrix}\mathbf{j}&=\sigma_0\mathbf{E}\\ \mathbf{j}&=\frac{\sigma_0}{1+(\omega_c\tau)^2}\begin{pmatrix}1 & +\omega_c\tau & \\ -\omega_c\tau & 1 & \\ & & 1+(\omega_c\tau)^2\end{pmatrix}\mathbf{E}\end{aligned}$$

where the matrix was inverted block-diagonally and m should be interpreted as effective mass. In the limit $\omega_c\tau \gg 1$, we have

$$\sigma_{xy} = \sigma_{yx} = \frac{\sigma_0}{\omega_c\tau} = \frac{nq^2\tau/m}{(qB/m)\tau} = \frac{nq}{B}$$

Problem 1.5 Density of states of free electrons

(a)

The total number of occupied states in the Fermi sphere is

$$N = 2\frac{1}{(2\pi/L)^n}\int_{|\mathbf{k}|\leq k_F} \mathrm{d}^n\mathbf{k}$$

where L is the dimension of the box. Fermi energy and Fermi wave vector are related by

$$\epsilon_F = \frac{\hbar^2 k_F^2}{2m}$$

In 1D, Fermi wavevector is

$$N = \frac{1}{\pi}L2k_F \qquad \Longrightarrow \qquad n = \frac{N}{L} = \frac{2}{\pi}k_F \qquad \Longrightarrow \qquad k_F = \frac{\pi}{2}n$$

In 2D,

$$N = \frac{2}{4\pi^2}L^2\pi k_F^2 \qquad \Longrightarrow \qquad n = \frac{N}{L^2} = \frac{1}{2\pi}k_F^2 \qquad \Longrightarrow \qquad k_F = \sqrt{2\pi n}$$

(b)

Density of states in energy are defined by

$$g(E) \equiv \frac{\mathrm{d}n}{\mathrm{d}E}$$

Use the results from *(a)* to calculate. For 1D, this is

$$g(E) = \frac{\mathrm{d}}{\mathrm{d}E}\left(\frac{2}{\pi}\frac{\sqrt{2mE}}{\hbar}\right)$$

$$g(E) = \frac{\sqrt{2m}}{\hbar\pi\sqrt{E}}$$

Similarly in 2D

$$g(E) = \frac{\mathrm{d}}{\mathrm{d}E}\left(\frac{1}{2\pi}\frac{2mE}{\hbar^2}\right)$$

$$g(E) = \frac{m}{\pi\hbar^2}$$

(c)

In 3D, repeat the calculations analogously

$$N(k) = \frac{2L^3}{8\pi^3}\frac{4\pi k^3}{3}$$
$$n(k) = n(E) = \frac{k^3}{3\pi^2} = \frac{\sqrt{8m^3}}{3\pi^2\hbar^3}E^{3/2}$$
$$g(E) = \frac{\sqrt{8m^3}}{3\pi^2\hbar^3}\frac{3}{2}\sqrt{E} = \frac{3}{2}\frac{n}{\epsilon_F^{3/2}}\sqrt{E} = \frac{3}{2}\frac{n}{\epsilon_F}\sqrt{\frac{E}{\epsilon_F}}$$

where in the last line n denotes $n(k_F) = \frac{N}{V}$.

Problem 1.6 Thomas-Fermi screening

The charge density and potential of the screening cloud of electrons induced by the presence of a fixed external potential V_{ext} are related by

$$\nabla^2\delta V = -\frac{\delta\rho}{\epsilon_0}$$

Assuming the electron number density is uniform in a region, satisfying

$$n = \int^{E_f} g(E)\,\mathrm{d}E$$

Upon a small perturbation of E_f, electron number density changes

$$\delta n = g(E_f)\delta E_f = -\frac{\delta\rho}{e}$$

where δE_f can be calculated from fixed chemical potential

$$\mu = E_f - eV_{tot} \implies \delta E_f = e\delta V_{tot} = e(V_{\text{ext}} + \delta V)$$

Taking laplacian on both sides of δn equation

$$eg(E_F)\nabla^2(\delta V + V_{\text{ext}}) = -\frac{1}{e}\nabla^2\delta\rho$$
$$g(E_f)\frac{e^2}{\epsilon_0}\delta n + eg(E_f)\nabla^2 V_{\text{ext}} = \nabla^2\delta n$$
$$g(E_f)\frac{e^2}{\epsilon_0}\delta n(q) + q^2\delta n(q) = eq^2 g(E_f)V_{\text{ext}}(q)$$
$$\delta n(q) = \frac{q^2}{q^2 + q_{TF}^2}eg(E_f)V_{\text{ext}}$$

$$\delta n(q) = \frac{q^2}{1 + q^2/q_{TF}^2} \frac{\epsilon_0}{e} V_{\text{ext}}(q)$$

where $q_{TF}^2 \equiv \frac{e^2 g(E_f)}{\epsilon_0}$. In 3D

$$q_{TF}^2 = \frac{e^2}{\epsilon_0} \left[2 \frac{4\pi k_F^2}{2\pi^3} \frac{\mathrm{d}k_f}{\mathrm{d}E_f} \frac{m k_F}{\pi^2 \hbar^2} \right] = \frac{m e^2 k_F}{\pi^2 \epsilon_0 \hbar^2}$$

For $V_{\text{ext}} = \frac{Q}{4\pi\epsilon_0 r}$

$$\begin{aligned}
V_{\text{ext}}(q) &= \frac{Q}{4\pi\epsilon_0} \lim_{\mu \to 0} \int \mathrm{d}\phi \int \mathrm{d}r\, r^2 \int \sin\theta \, \mathrm{d}\theta \, \frac{e^{-\mu r - iqr\cos\theta}}{r} \\
V_{\text{ext}}(q) &= \frac{Q}{4\pi\epsilon_0} \lim_{\mu \to 0} 2\pi \int \mathrm{d}r\, r^2 \frac{e^{-\mu r}\left(e^{iqr} - e^{-iqr}\right)}{iqr^2} \\
V_{\text{ext}}(q) &= \frac{Q}{4\pi\epsilon_0} \lim_{\mu \to 0} 4\pi \int_0^\infty \mathrm{d}r \, \frac{e^{-\mu r}\sin(qr)}{q} = \frac{Q}{\epsilon_0} \lim_{u \to 0} \frac{1}{\mu^2 + q^2} \\
n_{\text{ind}}(q) &= \frac{\epsilon_0}{e} \frac{q^2}{1 + q^2/q_{TF}^2} V_{\text{ext}}(q) \\
n_{\text{ind}}(q) &= \frac{Q q_{TF}^2}{e} \frac{1}{q_{TF}^2 + q^2} \\
n_{\text{ind}} &= \frac{q_{TF}^2}{4\pi} \frac{Q}{e} \frac{\exp(-q_{TF} r)}{r}
\end{aligned}$$

Where in the last line we have simply used the result from the forward FT but set $\frac{1}{\xi} = \mu = q_{TF}$.

Problem 1.7 Diatomic molecule

We restrict the basis of states to just the ground state of each atom in isolation, whereas of course an accurate solution would require a complete set of states that of necessity would include all the excited states of the atoms. The basis set consists of two states $|a\rangle$ and $|b\rangle$ that satisfy

$$\begin{aligned}
H_a |a\rangle &= E_a |a\rangle \\
H_b |b\rangle &= E_b |b\rangle
\end{aligned}$$

and we look for solutions

$$|\psi\rangle = \alpha |a\rangle + \beta |b\rangle$$

Neglecting the direct matrix elements $\langle a|b\rangle$ for simplicity (these are easily included if necessary), derive the matrix equation for the wavefunctions and eigenvalues.

Approximating the spatially separate orbitals as being orthogonal, the Hamiltonian eigenvalue equation spanned in the basis stated above is

$$\hat{H}\begin{pmatrix}\alpha\\ \beta\end{pmatrix} = E\begin{pmatrix}\alpha\\ \beta\end{pmatrix}$$

The matrix elements are derived from the diatomic Hamiltonian

$$H = T + V_a + V_b$$
$$H_{aa} = \langle a|\left(T + V_a + V_b\right)|a\rangle = \langle a|E_a|a\rangle + \langle a|V_b|a\rangle = E_a + \langle a|V_b|a\rangle = \tilde{E}_a$$
$$H_{ab} = \langle a|\left(T + V_a + V_b\right)|b\rangle = t$$
$$0 = \begin{pmatrix}H_{aa} - E & H_{ab}\\ H_{ba} & H_{bb} - E\end{pmatrix}\begin{pmatrix}\alpha\\ \beta\end{pmatrix}$$

The energy eigenvalues satisfy

$$0 = \tilde{E}_a\tilde{E}_b - t^2 - E(\tilde{E}_a + \tilde{E}_b) + E^2$$
$$E = \frac{1}{2}\left(\tilde{E}_a + \tilde{E}_b \pm \sqrt{(\tilde{E}_a - \tilde{E}_b)^2 + 4t^2}\right)$$

The wavefunctions are then

$$\begin{pmatrix}-\frac{1}{2}\left(-\tilde{E}_a + \tilde{E}_b \pm \sqrt{(\tilde{E}_a - \tilde{E}_b)^2 + 4t^2}\right) & t\\ t & -\frac{1}{2}\left(\tilde{E}_a - \tilde{E}_b \pm \sqrt{(\tilde{E}_a - \tilde{E}_b)^2 + 4t^2}\right)\end{pmatrix}\begin{pmatrix}\alpha\\ \beta\end{pmatrix} = 0$$
$$|\psi\rangle = \begin{pmatrix}\alpha\\ \beta\end{pmatrix} = \gamma\begin{pmatrix}2t\\ \pm\sqrt{\Delta E^2 + 4t^2} - \Delta E\end{pmatrix}$$

where $\Delta E = \tilde{E}_a - \tilde{E}_b$.

(a) covalent bonding

In the case of identical atoms $\tilde{E}_a = \tilde{E}_b$,

$$E = \frac{1}{2}\left(\tilde{E}_a + \tilde{E}_b \pm |2t|\right)$$
$$|\psi\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\ \mp 1\end{pmatrix}$$

The LCAOs have equal contributions from either atom.

(b) ionic bonding

In the strong ionic limit $\Delta E \gg |t|$,

$$E = \frac{1}{2}\Big(\tilde{E}_a + \tilde{E}_b \pm \Delta E\Big)$$
$$E_+ = \max(E_a, E_b); \qquad E_- = \min(E_a, E_b)$$
$$|\psi_\pm\rangle = |a\rangle\,, |b\rangle$$

The energy levels and orbitals remain in their form before hybridisation.

Problem 1.8 BCC and FCC

The lattice sites of a body centred cubic lattice are

$$\text{Ш}_a[\mathbf{r}] + \text{Ш}_a\left[\mathbf{r} + \frac{a}{2}(\mathbf{i}+\mathbf{j}+\mathbf{k})\right]$$

where Ш denotes the 3D Dirac comb (conventionally cyril shah letter). Its fourier transform is

$$\text{Ш}_{\frac{2\pi}{a}}(q)\left[1 + \exp\left(i\frac{a}{2}(q_x+q_y+q_z)\right)\right]$$

The square bracket term vanishes for any

$$q_x + q_y + q_z = \frac{2\pi}{a}(2n+1) \qquad \forall n \in \mathbb{Z}$$

This is a description of the FCC of spacing $\frac{4\pi}{a}$. The properties of FT trivially shows *vice versa*.

Problem 1.9 Reciprocal lattice cell volume

The reciprocal lattice vectors $\{\mathbf{a}_i\}$, by definition, satisfy

$$\mathbf{a}_i \cdot \mathbf{b}_j = 2\pi\delta_{ij}$$

where $\{\mathbf{b}_i\}$ are real lattice vectors. Therefore we can write

$$\Big(\mathbf{a}_1,\, \mathbf{a}_2,\, \mathbf{a}_3\Big)\Big(\mathbf{b}_1,\, \mathbf{b}_2,\, \mathbf{b}_3\Big) = 2\pi \begin{pmatrix} 1 & & \\ & 1 & \\ & & 1 \end{pmatrix}$$
$$\det(\mathbf{a}_1,\, \mathbf{a}_2,\, \mathbf{a}_3)\det(\mathbf{b}_1,\, \mathbf{b}_2,\, \mathbf{b}_3) = (2\pi)^3$$
$$\Omega_{\mathbf{k}} = \det(\mathbf{a}_1,\, \mathbf{a}_2,\, \mathbf{a}_3) = \mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3) = \frac{(2\pi)^3}{\det(\mathbf{b}_1,\, \mathbf{b}_2,\, \mathbf{b}_3)} = \frac{(2\pi)^3}{\mathbf{b}_1 \cdot (\mathbf{b}_2 \times \mathbf{b}_3)} = \frac{(2\pi)^3}{\Omega_{\mathbf{r}}}$$

where $\Omega_{\mathbf{k}}$ is reciprocal space cell volume and $\Omega_{\mathbf{r}}$ is real space cell volume.

Problem 1.10 Bragg's law

(a)

For all three $\mathbf{r} = x\mathbf{a}_1, y\mathbf{a}_2, z\mathbf{a}_3$ on the (hkl) plane,

$$xh = yk = zl = \text{integer} \implies \mathbf{r} \cdot (h\mathbf{b}_1 + k\mathbf{b}_2 + l\mathbf{b}_3) = 2\pi \times \text{integer}$$

Therefore $\mathbf{G}$ is normal to the (hkl) plane.

(b)

Two adjacent (hkl) planes $\mathbf{r}_1$ and $\mathbf{r}_2$ are related by

$$\begin{aligned}\mathbf{r}_1 \cdot \mathbf{G} &= 2\pi \times (\text{integer}) \\ \mathbf{r}_2 \cdot \mathbf{G} &= 2\pi \times (\text{integer} \pm 1)\end{aligned}$$

Their distance is

$$d = \frac{\big|(\mathbf{r}_1 - \mathbf{r}_2) \cdot \mathbf{G}\big|}{|\mathbf{G}|} = \frac{2\pi}{|G|}$$

(c)

The condition

$$\frac{1}{2}\mathbf{k} \cdot \mathbf{G} = \frac{G^2}{4}$$

is equivalent to

$$\begin{aligned}2k\cos\left(\frac{\pi}{2} - \theta\right) &= G \\ \frac{2\pi}{\lambda}\sin(\theta) = \frac{G}{2} &= \frac{\pi}{d}\end{aligned}$$

where d is as defined in *(b)* and $\frac{\pi}{2} - \theta$ is the angle between the normal of the plane and the k.

Problem 1.11 Acoustic phonon dispersion in the monatomic chain

$$\begin{aligned}u_n &= u_0\cos(qr_n - \omega t) \\ \ddot{u_n} &= -\omega^2 u_0\cos(qr_n - \omega t) \\ K(u_{n+1} + u_{n-1} - 2u_n) &= u_n\big[\cos(qa) + \cos(-qa) - 2\big] - u_0\sin(qr_n - \omega t)\big[\sin(qa) + \sin(-qa)\big] \\ m\omega^2 &= 2K\big[1 - \cos(qa)\big] = 4K\sin^2\left(\frac{qa}{2}\right)\end{aligned}$$

Problem 1.12 Heat capacity of a metal

The metal heat capacity consists of electron heat capacity and phonon heat capacity. Electron obeys Fermi-Dirac statistics. At low temperatures, chemical potential varies weakly with temperature such that $\mu \approx E_f$

$$f(E) = \frac{1}{\exp\left(\frac{E-E_f}{k_B T}\right) + 1}$$

Using Problem 1.5.*(c)*, we have

$$\begin{aligned}
U &= \int_0^\infty g(E) f(E) E \, \mathrm{d}E \\
U &= \int_0^\infty \frac{3n}{2E_f^{3/2}} f(E) E^{3/2} \, \mathrm{d}E \\
U_{E>E_f} &= \frac{3nk_B T}{2} \int_0^\infty \frac{1}{e^u + 1} \left(\frac{E_f + uk_B T}{E_f} \right)^{3/2} \mathrm{d}u \\
U_{E>E_f} &= g(E_f) E_f k_B T \int_0^\infty \frac{1}{e^u + 1} \left(1 + \frac{uk_B T}{E_f} \right)^{3/2} \mathrm{d}u \\
n &= \int_0^\infty g(E) f(E) \, \mathrm{d}E \\
n_{E>E_f} &= g(E_f) k_B T \int_0^\infty \frac{1}{e^u + 1} \left(1 + \frac{uk_B T}{E_f} \right)^{1/2} \mathrm{d}u
\end{aligned}$$

Let's assume E_f only varies weakly with T, such that U can be spanned like

$$U_{E>E_f} = E_f n_{E>E_f} + g(E_f) k_B^2 T^2 \int_0^\infty \frac{u}{e^u + 1} \, \mathrm{d}u + O(T^3)$$

Similarly (in a way that is more or less equally hand wavy as taking $g(E) = g(E_f)$ in the notes)

$$\begin{aligned}
U_{E<E_f} &= E_f n_{E<E_f} + g(E_f) k_B^2 T^2 \int_0^\infty \frac{u}{e^u + 1} \, \mathrm{d}u + O(T^3) \\
C_V &\approx 4 g(E_f) k_B^2 T \int_0^\infty \frac{u}{e^u + 1} \, \mathrm{d}u
\end{aligned}$$

where the total number density is conserved.

Phonons obey Bose-Einstein statistics with zero chemical potential. At low temperatures there are only N_A acoustic modes per mole because optical modes are forbidden by band

gap.

$$N_A = \int_0^{\omega_D} D(\omega)\,\mathrm{d}\omega$$

The density of states $D(k)$ is proportional to $4\pi k^2$ and hence

$$D(\omega) \propto k^2 \frac{\mathrm{d}k}{\mathrm{d}\omega} = \frac{\omega^2}{v^3} \implies \omega_D^3 \propto v^3 N_A$$

Integrating this with the distribution and energy per mode $\hbar\omega$

$$\begin{aligned} U &= \int_0^{\omega_D} \frac{D(\omega)\hbar\omega}{\exp\big(\hbar\omega/k_B T\big) - 1}\,\mathrm{d}\omega \\ U &\propto \int_0^{\omega_D} \frac{\hbar\omega^3/v^3}{\exp\big(\hbar\omega/k_B T\big) - 1}\,\mathrm{d}\omega \\ U &\propto \frac{k_B^4 T^4}{\hbar^3 v^3} \int_0^{\theta_D/T} \frac{u^2}{e^u - 1}\,\mathrm{d}u \\ U &\propto \frac{k_B T^4}{\theta_D^3} N_A \int_0^{\theta_D/T} \frac{u^2}{e^u - 1}\,\mathrm{d}u \end{aligned}$$

At low temperatures $\theta_D \gg T$ the integral on the right may be approximated as constant with T. Therefore

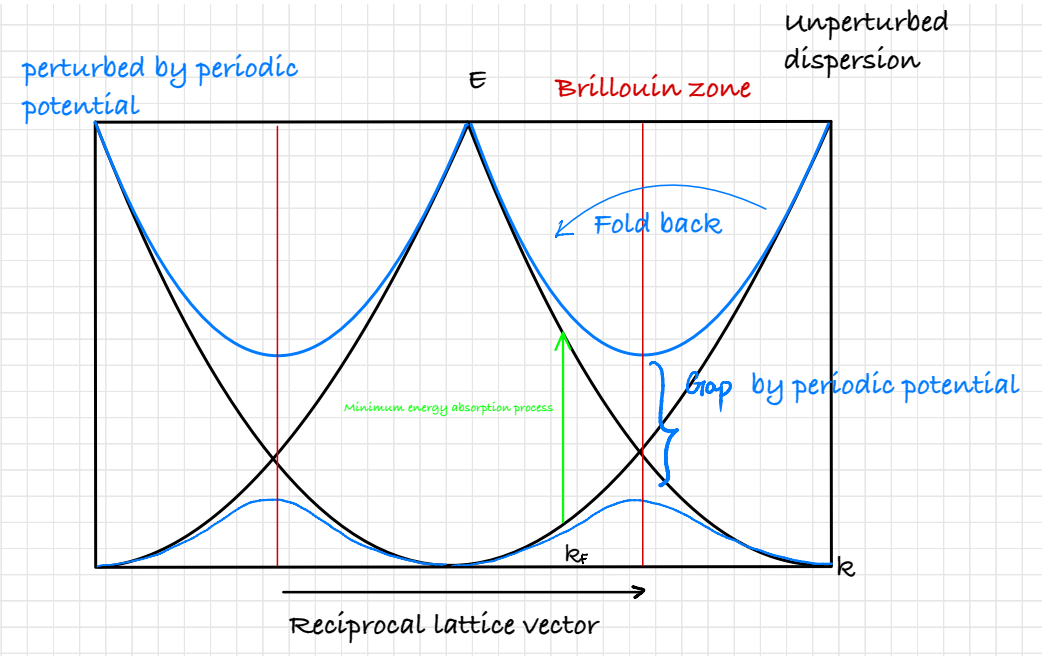
$$C_V = \frac{\partial U}{\partial T} \propto k_B \theta_D^{-3} N_A T^3$$

The two components together yield

$$C = \gamma T + \beta T^3$$

Topic 2 Band structure

Problem 2.1



In the first Brillouin zone of a body centred cubic (BCC) crystal, the shortest distance from the zone centre to the zone boundary is $\sqrt{2}\pi/a$. In every BCC unit cell, there are two atoms each with one valence electron. Taking into account spin, the radius of the Fermi sphere of a monovalent metal satisfies

$$2 \cdot \frac{4\pi}{3} k_F^3 = 2 \cdot \left(\frac{2\pi}{a}\right)^3 \implies k_F = \left(\frac{6}{\pi}\right)^{1/3} \frac{\pi}{a}$$

Using $\frac{6}{\pi} < 2 < 2^{3/2} \implies \left(\frac{6}{\pi}\right)^{1/3} < \sqrt{2}$, we get that the Fermi sphere is entirely contained within the first Brillouin zone.

The minimum energy E_0 required for a photon absorption process is approximately

$$\begin{aligned} E_0 &\approx E\left(\frac{2\sqrt{2}\pi}{a} - k_F\right) - E(k_F) \\ &\approx \left[\left(2\sqrt{2} - \left(\frac{6}{\pi}\right)^{1/3}\right)\left(\frac{\pi}{6}\right)^{1/3}\right]^2 E_f - E_F \\ &\approx 0.638\, E_f \end{aligned}$$

Alkali metals have a BCC structure. The lattice constants a of Na, K, Rb are in increasing order. The broad peaks arising from interband optical absorption are observed at increasing frequencies with higher peaks higher up the periodic table.

Down the table, increasing lattice constants mean lower $k_F \implies$ lower $E_f \implies$ lower E_0. Qualitatively, this is consistent with features of observed data.

Problem 2.2

Near the zone boundary, the energy perturbation is dominated by nearly degenerate contributions. In the nearly degenerate subspace,

$$H\left|\psi\right\rangle = (T+V)\left|\psi\right\rangle = E\left|\psi\right\rangle$$

$$\frac{\hbar^2}{2m}\begin{pmatrix} k^2 & \\ & \left(k-2\pi/a\right)^2 \end{pmatrix}\left|\psi\right\rangle + \begin{pmatrix} \left\langle k\right|U\left|k\right\rangle & \left\langle k\right|U\left|k-2\pi/a\right\rangle \\ \left\langle k-2\pi/a\right|U\left|k\right\rangle & \left\langle k-2\pi/a\right|U\left|k-2\pi/a\right\rangle \end{pmatrix}\left|\psi\right\rangle = E\left|\psi\right\rangle$$

$$\begin{vmatrix} \frac{\hbar^2k^2}{2m}+U_0-E & U_{2\pi/a} \\ U^*_{2\pi/a} & \frac{\hbar^2(k-2\pi/a)^2}{2m}+U_0-E \end{vmatrix} = 0$$

Setting $U_0 = 0$ because the physics is invariant under constant shift of potential,

$$E^{\pm} = \frac{1}{2}\frac{\hbar^2}{2m}\left[k^2+\left(k-\frac{2\pi}{a}\right)^2\right] \pm \frac{1}{2}\sqrt{\left(\frac{\hbar^2}{2m}\right)^2\left[k^2+\left(k-\frac{2\pi}{a}\right)^2\right]^2 - 4\left(\frac{\hbar^2}{2m}\right)^2k^2\left(k-\frac{2\pi}{a}\right)^2 + 4\left|U_{2\pi/a}\right|^2}$$

$$E^{\pm} = \frac{1}{2}\frac{\hbar^2}{2m}\left[k^2+\left(k-\frac{2\pi}{a}\right)^2\right] \pm \frac{1}{2}\sqrt{\left(\frac{\hbar^2}{2m}\right)^2\left[k^2-\left(k-\frac{2\pi}{a}\right)^2\right]^2 + 4\left|U_{2\pi/a}\right|^2}$$

(a)

On the zone boundary $k = \pi/a$, there is a gap

$$E^{\pm} = \frac{\hbar^2k^2}{2m} \pm \frac{1}{2}\sqrt{4\left|U_{2\pi/a}\right|^2}$$
$$\Delta E = E^+ - E^- = 2\left|U_{2\pi/a}\right|$$

(b)

On the zone boundary, the eigenstates of the energy equation satisfy

$$\begin{pmatrix} \frac{\hbar^2k^2}{2m} & U_{2\pi/a} \\ U^*_{2\pi/a} & \frac{\hbar^2k^2}{2m} \end{pmatrix}\begin{pmatrix} c^{\pm}_k \\ c^{\pm}_{k-\frac{2\pi}{a}} \end{pmatrix} = \left(\frac{\hbar^2k^2}{2m} \pm \left|U_{2\pi/a}\right|\right)\begin{pmatrix} c^{\pm}_k \\ c^{\pm}_{k-\frac{2\pi}{a}} \end{pmatrix}$$

$$\frac{c_k^{\pm}}{c_{k-\frac{2\pi}{a}}^{\pm}} = \pm\frac{U_{2\pi/a}}{\left|U_{2\pi/a}\right|}$$

The probability density for the electronic states at $k = \frac{\pi}{a}$ takes the form

$$\left\langle\psi^{+}\middle|r\right\rangle \propto {U_{2\pi/a}}^{1/2}\exp\left(i\frac{\pi x}{a}\right) + {U_{2\pi/a}^{*}}^{1/2}\exp\left(-i\frac{\pi x}{a}\right) \propto \cos\left(\frac{\pi x}{a}+\frac{\phi}{2}\right)$$

$$\left|\psi^{(1)}(r)\right|^2 = \left|\left\langle\psi^{+}\middle|r\right\rangle\right|^2 \propto \cos^2\left(\frac{\pi x}{a}+\frac{\phi}{2}\right)$$

$$\left\langle\psi^{-}\middle|r\right\rangle \propto {U_{2\pi/a}}^{1/2}\exp\left(i\frac{\pi x}{a}\right) - {U_{2\pi/a}^{*}}^{1/2}\exp\left(-i\frac{\pi x}{a}\right) \propto \sin\left(\frac{\pi x}{a}+\frac{\phi}{2}\right)$$

$$\left|\psi^{(2)}(r)\right|^2 = \left|\left\langle\psi^{-}\middle|r\right\rangle\right|^2 \propto \sin^2\left(\frac{\pi x}{a}+\frac{\phi}{2}\right)$$

where we set $\arg(U_{2\pi/a}) = \phi$.

Now consider diatomic lattice

$$U(g) = \frac{1}{L}\int_{L/2}^{L/2} e^{-igx}\left[U^A\left(-\frac{a}{4}(1-\delta)+x\right) + U^B\left(+\frac{a}{4}(1-\delta)+x\right)\right]$$

$$L\to\infty \qquad U(g) = U^A(g)\exp\left(-\frac{iga(1-\delta)}{4}\right) + U^B(g)\exp\left(\frac{iga(1-\delta)}{4}\right)$$

$$U_{2\pi/a} = U^A_{2\pi/a}\exp\left(-\frac{i2\pi(1-\delta)}{4}\right) + U^B_{2\pi/a}\exp\left(\frac{i2\pi(1-\delta)}{4}\right)$$

$$U_{2\pi/a} = -iU^A_{2\pi/a}\exp\left(\frac{i\pi\delta}{2}\right) + iU^B_{2\pi/a}\exp\left(-\frac{i\pi\delta}{2}\right)$$

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

U_A and U_B can both be assumed to be even in position space, so they are both real after FT.

(a) identical atoms

This effectively halves the lattice constant $a \to \frac{a}{2}$. As a result, the first Brillouin zone boundary is at $\frac{\pi}{a/2} = \frac{2\pi}{a}$. The gap there is

$$\Delta E = 2\left|U_{4\pi/a}\right|$$

$\phi = 0$ in this case. The electron charge densities take the form

$$\left|\psi^{(1)}(r)\right|^2 \propto \cos^2\left(\frac{\pi x}{a}\right)$$

$$\left|\psi^{(2)}(r)\right|^2 \propto \sin^2\left(\frac{\pi x}{a}\right)$$

(b) $\delta = 0$

The form of the potential is changed but the zone boundary is still $\frac{\pi}{a}$ which means the energy gap is given by

$$U_{2\pi/a} = -i\Big(U^A_{2\pi/a} - U^B_{2\pi/a}\Big)$$
$$\Delta E = 2\Big|U^A_{2\pi/a} - U^B_{2\pi/a}\Big|$$

Depending on which of A or B is more attractive, $\phi = \mp\frac{\pi}{2}$

$$\Big|\psi^{(1)}(r)\Big|^2 \propto \cos^2\left(\frac{\pi(x \mp a/4)}{a}\right)$$
$$\Big|\psi^{(2)}(r)\Big|^2 \propto \cos^2\left(\frac{\pi(x \pm a/4)}{a}\right)$$

The bands are shifted towards opposite directions by $\frac{\pi}{4}$. Both are periodic over a. Comparing with R_n of a and b, we see the gap is small and the charge densities are centered on top of the atoms, which are ionic features.

(c) $U_A = U_B$

$$U_{2\pi/a} = \Big(U^A_{2\pi/a} + U^B_{2\pi/a}\Big)\sin\left(\frac{\pi\delta}{2}\right)$$

The potential is real at the boundary $\phi = 0$ and the bandgap is large.

$$\Big|\psi^{(1)}(r)\Big|^2 \propto \cos^2\left(\frac{\pi x}{a}\right)$$
$$\Big|\psi^{(2)}(r)\Big|^2 \propto \sin^2\left(\frac{\pi x}{a}\right)$$

The first band resembles a "bonding" state and the second an "antibonding" state of covalent lattices.

Problem 2.3 NFE approximation for a square lattice

(a)

In the nearly free electron approximation, each wavefunction labeled by $\mathbf{k}$ is a superposition of all the states that could be labeled by $\mathbf{k}$, that is, the free electron states related to $\mathbf{k}$ by any reciprocal lattice vector.

$$|\psi_{\mathbf{k}}\rangle = \sum_{\mathbf{G}} c_{\mathbf{k}-\mathbf{G}}\,|\mathbf{k}-\mathbf{G}\rangle$$

Consider only degenerate states which dominate the energy perturbation.

The reciprocal lattice vectors of the 2D square crystal of side a are

$$\mathbf{b}_1 = \frac{2\pi}{a}(1,0) \qquad \mathbf{b}_2 = \frac{2\pi}{a}(0,1)$$

At $\mathbf{k}_0 = \frac{2\pi}{a}(0,0) = \mathbf{0}$, there is no $\mathbf{G} \neq 0$ that has the same energy as $|\mathbf{0}\rangle$.

$$|\psi_{\mathbf{k}_0}\rangle = |\mathbf{0}\rangle$$

At $\mathbf{k}_1 = \frac{2\pi}{a}\left(\frac{1}{2}, 0\right)$,

$$E^{(0)}_{\mathbf{k}_1-\mathbf{b}_1} = E^{(0)}_{\mathbf{k}_1}$$

so

$$|\psi_{\mathbf{k}_1}\rangle = c_{\mathbf{k}_1}\left|\frac{1}{2}\mathbf{b}_1\right\rangle + c_{\mathbf{k}_1-\mathbf{b}_1}\left|-\frac{1}{2}\mathbf{b}_1\right\rangle$$

At $\mathbf{k}_2 = \frac{2\pi}{a}\left(\frac{1}{2}, \frac{1}{2}\right)$,

$$E^{(0)}_{\mathbf{k}_1-\mathbf{b}_1} = E^{(0)}_{\mathbf{k}_1-\mathbf{b}_2} = E^{(0)}_{\mathbf{k}_1-\mathbf{b}_1-\mathbf{b}_2} = E^{(0)}_{\mathbf{k}_1}$$

where $\mathbf{b}_2 = \frac{2\pi}{a}(0,1)$. so

$$|\psi_{\mathbf{k}_2}\rangle = c_{\mathbf{k}_2}\left|\frac{1}{2}\mathbf{b}_1 + \frac{1}{2}\mathbf{b}_2\right\rangle + c_{\mathbf{k}_2-\mathbf{b}_1}\left|-\frac{1}{2}\mathbf{b}_1 + \frac{1}{2}\mathbf{b}_2\right\rangle + c_{\mathbf{k}_2-\mathbf{b}_2}\left|\frac{1}{2}\mathbf{b}_1 - \frac{1}{2}\mathbf{b}_2\right\rangle + c_{\mathbf{k}_2-\mathbf{b}_1-\mathbf{b}_2}\left|-\frac{1}{2}\mathbf{b}_1 - \frac{1}{2}\mathbf{b}_2\right\rangle$$

(b)

Given

$$V(x,y) = -2V_0\left[\cos\left(\frac{2\pi x}{a}\right) + \cos\left(\frac{2\pi y}{a}\right)\right]$$

$$\tilde{V}(k_x,k_y) = -V_0\Big[\delta(k_x - b)\delta\big(k_y\big) + \delta(k_x + b)\delta\big(k_y\big) + \delta\big(k_y - b\big)\delta(k_x) + \delta\big(k_y + b\big)\delta(k_x)\Big]$$

where $b = |\mathbf{b}_1| = |\mathbf{b}_2|$. The shifts of delta functions indicate the difference $\mathbf{k}_1 - \mathbf{k}_2$ for the matrix element $V_{\mathbf{k}_1,\mathbf{k}_2}$ to be nonzero.

The energy eigenstate equation, in the subspace spanned by the seven states in *(a)* are

$$H|\psi\rangle = (T+V)|\psi\rangle = E|\psi\rangle$$

$$\frac{\hbar^2 b^2}{2m}\begin{pmatrix} 0 & & & & & & \\ & \frac{1}{4} & -t & & & & \\ & -t & \frac{1}{4} & & & & \\ & & & \frac{1}{2} & -t & -t & \\ & & & -t & \frac{1}{2} & & -t \\ & & & -t & & \frac{1}{2} & -t \\ & & & & -t & -t & \frac{1}{2} \end{pmatrix}|\psi\rangle = E|\psi\rangle$$

where

$$t = \frac{2mV_0}{\hbar^2 b^2}$$

The block-diagonal equation can be solved in subspaces independently. Let $E = \frac{\hbar^2 b^2}{2m} e$.

$\mathbf{k}_0$ subspace: $\quad e = 0$

$\mathbf{k}_1$ subspace: $\quad \left(\frac{1}{4} - e\right)^2 - t^2 = 0 \implies e = \frac{1}{4} \pm t$

$\mathbf{k}_2$ subspace: $\quad \left[\left(\frac{1}{2} - e\right)^2 - 4t^2\right]\left(\frac{1}{2} - e\right)^2 = 0 \implies e = \frac{1}{2} \text{ or } \frac{1}{2} \pm 2t$

So the energy eigenvalues are

$\mathbf{k}_0$ subspace: $\quad E = 0$

$\mathbf{k}_1$ subspace: $\quad E = \frac{1}{4}\frac{\hbar^2}{2m} \pm V_0$

$\mathbf{k}_2$ subspace: $\quad E = \frac{1}{2}\frac{\hbar^2}{2m} \text{ or } \frac{1}{2}\frac{\hbar^2 b^2}{2m} \pm 2V_0$

Problem 2.4 Tight binding for BCC and FCC lattices

Use

$$E = \langle 0| \hat{H} |\psi\rangle = \sum_n e^{i\mathbf{k}\cdot\mathbf{R}_n} \langle 0| \hat{H} |n\rangle$$

and take into account

(a) 8 nearest neighbours in BCC

$$E = \underbrace{\langle 0| \hat{H} |0\rangle}_{\epsilon_0} + \sum_{8 \text{ neighbours}} e^{i\mathbf{k}\cdot\mathbf{R}_n} \underbrace{\langle 0| \hat{H} |n\rangle}_{t}$$

$$E = \epsilon_0 + t \sum_{l,m,n=\pm 1} e^{\frac{i}{2}(lk_x a + mk_y a + nk_z a)}$$

$$E = \epsilon_0 + t \sum_{l=\pm 1} e^{\frac{i}{2}(lk_x a)} \sum_{m=\pm 1} e^{\frac{i}{2}(mk_y a)} \sum_{n=\pm 1} e^{\frac{i}{2}(nk_z a)}$$

$$E = \epsilon_0 + t\left(e^{iak_x/2} + e^{-iak_x/2}\right)\left(e^{iak_y/2} + e^{-iak_y/2}\right)\left(e^{iak_z/2} + e^{-iak_z/2}\right)$$

$$E = \epsilon_0 + 8t \cos\left(\frac{ak_x}{2}\right) \cos\left(\frac{ak_y}{2}\right) \cos\left(\frac{ak_z}{2}\right)$$

(b) 12 nearest neighbours in FCC

$$E = \epsilon_0 + t \sum_{l,m=\pm 1} e^{\frac{i}{2}(lk_x a + mk_y a)} + t \sum_{l,m=\pm 1} e^{\frac{i}{2}(lk_y a + mk_z a)} + t \sum_{l,m=\pm 1} e^{\frac{i}{2}(lk_z a + mk_x a)}$$

$$E = \epsilon_0 + 4t\left[\cos\left(\frac{ak_x}{2}\right)\cos\left(\frac{ak_y}{2}\right) + \cos\left(\frac{ak_y}{2}\right)\cos\left(\frac{ak_z}{2}\right) + \cos\left(\frac{ak_y}{2}\right)\cos\left(\frac{ak_x}{2}\right)\right]$$

Problem 2.5

Consider a two-dimensional band structure on a rectangular lattice

$$E(k) = 2t_1\cos(ak_x) + 2t_2\cos\big(bk_y\big)$$

(a)

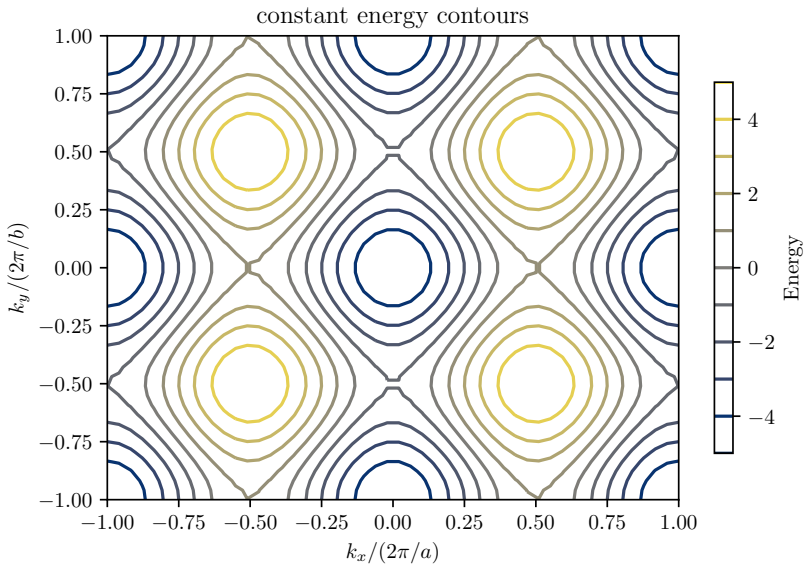
The energy is periodic over in k-space over $k_x \to k_x + \frac{2\pi}{a}$ and $k_y \to k_y + \frac{2\pi}{b}$ *independently*, so the reciprocal lattice is *rectangular* of dimensions $\frac{2\pi}{a}, \frac{2\pi}{b}$.

(b)

Correspondingly the real space lattice is also *rectangular* of dimensions a, b.

(c)

If $t_1 < t_2 < 0$ and $a < b$, we can plot some contours of constant energy.



From the graph, maxima are found at $(k_x, k_y) = (\pm\frac{\pi(2n+1)}{a}, \pm\frac{\pi(2m+1)}{b})$, for $n, m \in \mathbb{Z}$. Minima are found at $(k_x, k_y) = (\pm\frac{\pi 2n}{a}, \pm\frac{\pi 2m}{b})$. Saddle points are at $(k_x, k_y) = (\pm\frac{\pi 2n}{a}, \pm\frac{\pi(2m+1)}{b})$ or

$(k_x, k_y) = (\pm\frac{\pi(2n+1)}{a}, \pm\frac{\pi 2m}{b})$. Electron effective masses are given by

$$\begin{aligned}
\frac{\hbar^2}{m_{ij}} &= \partial_{k_i}\partial_{k_j}E(k) \\
\frac{\hbar^2}{m_{ij}} &= \partial^2_{k_i}E(k)\delta_{ij} \\
m^{*2} &= \det\big(m_{ij}\big) \\
m^* &= \begin{cases} \text{maxima} & -\frac{\hbar^2}{2ab\sqrt{t_1 t_2}} \\ \text{minima} & +\frac{\hbar^2}{2ab\sqrt{t_1 t_2}} \\ \text{saddle points} & \frac{\hbar^2}{2ab\sqrt{-t_1 t_2}} \implies \text{undefined} \end{cases}
\end{aligned}$$

(d)

Some contours with $-1 < E < 1$ are open. The energy of saddle points lie in this range.

(e)

The contours of constant energy

Near the extrema,

$$-|E - E_{ext}| \approx t_1 a^2 k_x^2 + t_2 b^2 k_y^2$$

We can parametrise the constant energy contours by

$$\begin{aligned}
k_x &= \sqrt{\frac{-|E - E_{ext}|}{t_1 a^2}}\cos(\alpha) \\
k_y &= \sqrt{\frac{-|E - E_{ext}|}{t_2 b^2}}\sin(\alpha)
\end{aligned}$$

In two dimensions, the density of states near the extrema can be found by integrating over the ellipse

$$\begin{aligned}
g(E) &= \int \frac{2\cdot\delta(E - E(\mathbf{k}))}{(2\pi)^2}\,\mathrm{d}\mathbf{k} \\
g(E) &= \int \frac{\mathrm{d}C}{2\pi^2}\frac{1}{\big|\nabla_\perp E(\mathbf{k})\big|} \\
g(E) &\approx \int_0^{2\pi}\frac{\mathrm{d}\alpha}{2\pi^2}\sqrt{\frac{k_y^2\frac{t_2 b^2}{t_1 a^2} + k_x^2\frac{t_1 a^2}{t_2 b^2}}{2t_1^2 a^4 k_x^2 + 2t_2^2 b^4 k_y^2}} \\
g(E) &\approx \frac{1}{\pi}\frac{1}{\sqrt{2t_1 a^2 t_2 b^2}} = \frac{\sqrt{2}}{\pi\hbar^2}|m^*|
\end{aligned}$$

Problem 2.6

(a)

Construct Bloch states

$$\left|\psi_p\right\rangle = \sum_n e^{i\mathbf{k}\cdot\mathbf{R}_n} \left|p_n\right\rangle$$

Consider 3 nearest neighbours

$$\begin{aligned}
\left|\psi_p\right\rangle &= \left|p_0\right\rangle + \left[e^{i\left(k_x a/2 + k_y a\sqrt{3}/2\right)} \left|p_1'\right\rangle + e^{i\left(-k_x a/2 + k_y a\sqrt{3}/2\right)} \left|p_2'\right\rangle + \left|p_3'\right\rangle\right] \\
\left|\psi_p\right\rangle &= \left|p_0\right\rangle + \left[e^{i\left(k_x a/2 + k_y a\sqrt{3}/2\right)} \left|p_1'\right\rangle + e^{i\left(-k_x a/2 + k_y a\sqrt{3}/2\right)} \left|p_2'\right\rangle + \left|p_3'\right\rangle\right] \\
\left|\psi_p'\right\rangle &= \left|p_0'\right\rangle + \left[e^{i\left(k_x a/2 - k_y a\sqrt{3}/2\right)} \left|p_1'\right\rangle + e^{i\left(-k_x a/2 - k_y a\sqrt{3}/2\right)} \left|p_2'\right\rangle + \left|p_3'\right\rangle\right]
\end{aligned}$$

where the subscripts label the 3 nearest neighbours. Do some algebra

$$\begin{aligned}
\left\langle p_0\right| \hat{H} \left|\psi_p\right\rangle &= E_p \\
\left\langle p_0'\right| \hat{H} \left|\psi_p\right\rangle &= \left[e^{i\left(k_x a/2 + k_y a\sqrt{3}/2\right)} + e^{i\left(-k_x a/2 + k_y a\sqrt{3}/2\right)} + 1\right] t \\
\left\langle p_0'\right| \hat{H} \left|\psi_p'\right\rangle &= E_p \\
\left\langle p_0\right| \hat{H} \left|\psi_p'\right\rangle &= \left[e^{i\left(k_x a/2 - k_y a\sqrt{3}/2\right)} + e^{i\left(-k_x a/2 - k_y a\sqrt{3}/2\right)} + 1\right] t^*
\end{aligned}$$

where

$$t = \left\langle p_0'\right| \hat{H} \left|p_i'\right\rangle = \left[\left\langle p_0\right| \hat{H} \left|p_i\right\rangle\right]^* = t^* \qquad \forall i \in 1, 2, 3$$

The eigenenergy satisfies determinant equation

$$\begin{vmatrix} E_p - E & tF(\mathbf{k}) \\ tF^*(\mathbf{k}) & E_p - E \end{vmatrix} = 0$$

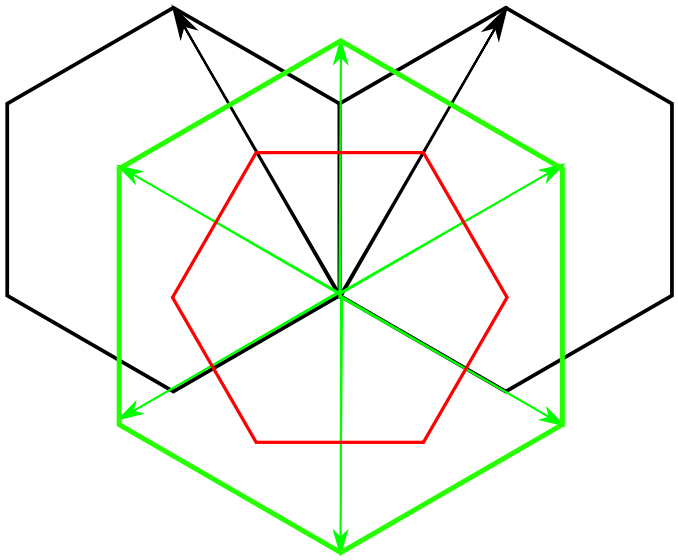
(b)

The reciprocal lattice vectors $\mathbf{b}_1$ and $\mathbf{b}_2$ are perpendicular to $\mathbf{t}_2$ and $\mathbf{t}_1$ respectively, and their inner products with t_1 and t_2 direction are 2π.

$$\begin{aligned}
\mathbf{b}_1 &= \frac{2\pi}{a\sqrt{3}} \begin{pmatrix} \sqrt{3} \\ 1 \end{pmatrix} \\
\mathbf{b}_2 &= \frac{2\pi}{a\sqrt{3}} \begin{pmatrix} -\sqrt{3} \\ 1 \end{pmatrix}
\end{aligned}$$

The lattice can be constructed from these two vectors. The first Brillouin zone is the enclosed by the perpendicular bisectors of the vectors from $\Gamma = (000)$ to the six nearest neighbours, a hexagon with one corner at

$$P = \frac{2\pi}{a\sqrt{3}}\frac{2}{\sqrt{3}}\hat{\mathbf{x}} = \frac{4\pi}{3a}\hat{\mathbf{x}}$$



(c)

$$\begin{vmatrix} E_p - E & tF(\mathbf{k}) \\ tF^*(\mathbf{k}) & E_p - E \end{vmatrix} = 0$$

$$E = E_p \pm t\left|F(\mathbf{k})\right|$$

Along zone corner and zone face directions,

$$F_P(\mathbf{k}) = 1 + 2\cos\left(\frac{ka}{2}\right)$$

$$F_Q(\mathbf{k}) = 1 + 2\cos\left(\frac{\sqrt{3}ka}{4}\right)\exp\left(-i\frac{\sqrt{3}ka}{4}\right)$$

(d)

A single layer of graphite will have a full lower band and an empty upper band which are touching, making it a semimetal.

(e)

Carbon nanotubes impose the periodic condition,

$$\mathbf{k} \cdot (m\mathbf{t}_1 + n\mathbf{t}_2) = 2\pi l$$

the allowed **k**s have constrained components perpendicular to the tube which must be integer multiples of $\frac{2\pi}{|m\mathbf{t}_1 + n\mathbf{t}_2|}$. Their components parallel to the tube are are constrained. Consequently, the loci of allowed **k** states are lines parallel to the tube.

Problem 2.7

(a)

$$\left|s(k)\right\rangle = \sum_n e^{ikR_n} \left|s^{(n)}\right\rangle$$
$$\left|d(k)\right\rangle = \sum_n e^{ikR_n} \left|n^{(d)}\right\rangle$$

(b)

Approximate $|s\rangle$ and $|d\rangle$ as an orthogonal basis, and consider only nearest neighbour interactions

$$H_{ss} = \sum_{n\in 0,\pm 1} e^{ikR_n} \left\langle s^{(0)}\right| \hat{H} \left|s^{(n)}\right\rangle$$
$$H_{ss} = \underbrace{\left\langle s^{(0)}\right| \hat{H} \left|s^{(0)}\right\rangle}_{E_{ss}} - \left(t_{s_0 s_1} e^{ika} + t_{s_0 s_{-1}} e^{-ika}\right)$$

where $t_{m_i n_j} = -\left\langle m^{(i)}\right| \hat{H} \left|n^{(j)}\right\rangle$. Exploiting the invariance of $\hat{H}$ under both parity and translation by a, $t_{s_0 s_1}$ and $t_{s_0 s_{-1}}$ can both be written as t_{ss}

$$H_{ss} = E_{ss} - 2t_{ss}\cos(ka)$$

Analogously,

$$H_{dd} = E_{dd} - 2t_{dd}\cos(ka)$$
$$H^*_{ds} = H_{sd} = \underbrace{\left\langle s^{(0)}\right| \hat{H} \left|d^{(0)}\right\rangle}_{\approx 0} - t_{sd}\left(e^{ika} + e^{-ika}\right)$$
$$H_{ds} = H_{sd} = -2t_{sd}\cos(ka)$$

where in the off-diagonal case we cannot use parity transform to equate two different matrix elements, but the local orbitals can always be chosen such that the matrix elements are real.

$$H\left|\psi\right\rangle = E(k)\left|\psi\right\rangle$$

$$\begin{vmatrix} E_s - 2t_{ss}\cos(ka) - E(k) & -2t_{sd}\cos(ka) \\ -2t_{sd}\cos(ka) & E_d - 2t_{dd}\cos(ka) - E(k) \end{vmatrix} = 0$$

(c)

t_{ss} is expected to be the strongest interaction because s orbitals are found more often than d orbitals where the Hamiltonian is strong..

(d)

When t_{ss} and t_{dd} are negligible and $|E_{dd} - E_{ss}| \ll 1$

$$E^2(k) - (E_{dd} + E_{ss})E(k) + E_{dd}E_{ss} - 4|t_{sd}|^2\cos^2(ka) = 0$$

$$E(k) = \frac{1}{2}(E_{dd} + E_{ss}) \pm \frac{1}{2}\sqrt{(E_{dd} - E_{ss})^2 + 16|t_{sd}|^2\cos^2(ka)}$$

$$E(k) = \frac{1}{2}(E_{dd} + E_{ss}) \pm 2|t_{sd}|\cos(ka)$$

(e)

The inclusion of small hopping terms creates band gaps at $k = 0$.

(f)

This model somewhat describes Cu.

Topic 3

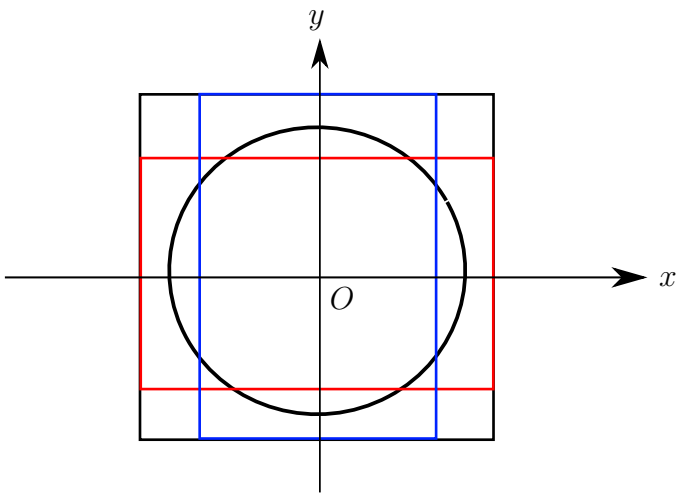
Problem 3.1

Read off $\frac{1}{\Delta(1/B)} = 1.8 \times 10^4$ T from the figure,

$$\Delta\left(\frac{1}{B}\right) = \frac{2\pi e}{\hbar A_k}$$
$$A_k = \frac{2\pi e}{\hbar}\frac{1}{\Delta(1/B)} = 1.72 \times 10^{20}\ \mathrm{m}^{-2}$$
$$k_F = \sqrt{\frac{A_k}{\pi}} = 7.40 \times 10^9\ \mathrm{m}^{-1}$$

Four electrons per Ru are distributed equally across the three bands, so the Fermi surface γ encloses $\frac{4}{3}$ electrons per lattice site.

$$\frac{4}{3} = \int_{\text{cylinder of radius } k_F} 2 \times \left(\frac{a}{2\pi}\right)^2 \mathrm{d}\mathbf{k} = 2\pi k_F^2 \left(\frac{a}{2\pi}\right)^2 \implies a = \sqrt{\frac{8\pi}{3}}\frac{1}{k_F} = 3.91 \times 10^{-10}\ \mathrm{m}$$



The Brillouin zone, and the three Fermi surfaces A, B, and γ all centered at the origin. The blue sheet is A which has dimensions $\frac{2}{3}\frac{2\pi}{a} \times \frac{2\pi}{a}$, while the red sheet B is the opposite. The circle is γ which has characteristic dimension k_F.

$$A_k^{(\alpha)} = \frac{2\pi e}{\hbar}\frac{1}{\Delta(1/B)} = 2.86 \times 10^{19}\ \mathrm{m}^{-2} \approx 0.11\left(\frac{2\pi}{a}\right)^2$$
$$A_k^{(\beta)} = \frac{2\pi e}{\hbar}\frac{1}{\Delta(1/B)} = 1.24 \times 10^{20}\ \mathrm{m}^{-2} \approx 0.48\left(\frac{2\pi}{a}\right)^2$$

The total area occupied by filled electron states in α and β would be equal to that in A and B, $2 \times \frac{2}{3}\left(\frac{2\pi}{a}\right)^2 \approx \left[0.48 + (1 - 0.11)\right]\left(\frac{2\pi}{a}\right)^2$, which implies α is an hole band and β a electron band.

Problem 3.2

$$N = 2\frac{1}{(2\pi/L)^3}\frac{4\pi}{3}k_F^3$$
$$k_F^3 = 3\pi^2\frac{N}{V} = 3\pi^2\frac{\rho N_A}{M}$$
$$A_k = \pi k_F^2 = \pi\left(3\pi^2\frac{\rho N_A}{M}\right)^{2/3}$$
$$\Delta\left(\frac{1}{B}\right) = \frac{2\pi e}{\hbar}\frac{1}{A_k} = 5.5 \times 10^{-5}\ \mathrm{T}^{-1}$$

for $B = 1$ T,

$$A_r = A_k\left(\frac{\hbar}{eB}\right)^2 = 7.46 \times 10^{-11}\ \mathrm{m}^2$$

Problem 3.3

$$E^{\pm} = \frac{1}{2}\frac{\hbar^2}{2m}\left[k^2 + \left(k - \frac{2\pi}{a}\right)^2\right] \pm \frac{1}{2}\sqrt{\left(\frac{\hbar^2}{2m}\right)^2\left[k^2 - \left(k - \frac{2\pi}{a}\right)^2\right]^2 + 4|U_0|^2}$$
$$E^{\pm} = \frac{1}{2}\frac{\hbar^2}{2m}\left[2k^2 - \frac{4\pi}{a}k + \frac{4\pi^2}{a^2}\right] \pm \frac{1}{2}\sqrt{\left(\frac{\hbar^2}{2m}\right)^2\left[\frac{4\pi}{a}k - \frac{4\pi^2}{a^2}\right]^2 + 4|U_0|^2}$$
$$\left.\frac{\mathrm{d}^2E^{\pm}}{\mathrm{d}k^2}\right|_{k=\frac{\pi}{a}} = \frac{\hbar^2}{m} \pm \left[4\left(\frac{\hbar^2}{m}\right)^2\left(\frac{\pi}{a}k - \frac{\pi^2}{a^2}\right)^2 + 4|U_0|^2\right]^{-\frac{1}{2}}\left(\frac{\hbar^2}{m}\right)^2\frac{2\pi^2}{a^2}$$
$$\left.\frac{\mathrm{d}^2E^{\pm}}{\mathrm{d}k^2}\right|_{k=\frac{\pi}{a}} = \frac{\hbar^2}{m} \pm \frac{1}{2|U_0|}\left(\frac{\hbar^2}{m}\right)^2\frac{2\pi^2}{a^2}$$
$$\frac{1}{m^*} = \frac{1}{m} + \frac{\hbar^2\pi^2}{m^2|U_0|a^2} \approx \frac{1}{m}\frac{4E_0}{E_{\mathrm{gap}}}$$
$$\frac{m^*}{m} \approx \frac{E_{\mathrm{gap}}}{4E_0} \implies m^* \sim E_{\mathrm{gap}}$$

From the given data

Crystal	$\frac{m^*}{E_{\text{gap}}} \sim$
InSb	6.5×10^{-2}
InAs	6.0×10^{-2}
InAs	5.1×10^{-2}

They are roughly the same orders of magnitude.

Problem 3.4

$$Z = 1 + \exp\bigl[-\beta(\epsilon - \mu)\bigr]$$
$$f_e(\epsilon) = \langle N_e \rangle = \frac{1}{\beta}\left(\frac{\partial \ln Z}{\partial \mu}\right)_{T,V} = \frac{1}{e^{\beta(\epsilon-\mu)} + 1}$$
$$f_h(\epsilon) = \langle N_h \rangle = \langle N_e + N_h \rangle - \langle N_e \rangle = \langle 1 \rangle - \langle N_e \rangle = 1 - f_e(\epsilon)$$
$$f_h(\epsilon) = \frac{e^{\beta(\epsilon-\mu)}}{e^{\beta(\epsilon-\mu)} + 1} = \frac{1}{e^{\beta(\mu-\epsilon)} + 1}$$

Problem 3.5

Drift velocity is the average velocity of charge carriers in the material which describes net movement and ignores individual thermal movements. *Electron mobility* $e\tau/m$ is a measure of relaxation time in the material. *Effective mass* is the mass which in vacuum would have lead to second derivative of dispersion curve equal to that of the *bare mass* in the external potential.

Assuming that the donors and acceptors are fully ionised at 300 K, i.e. $k_B T \gg \Delta$. The intrinsic carrier density is small compared to the dopants density, so we are in the extrinsic regime

$$n = N_d - N_a = 2 \times 10^{22}\ \text{m}^{-3}$$

and the law of mass action gives

$$np = n_{in}^2 \implies p = \frac{n_{in}^2}{n} = 2.88 \times 10^{16}\ \text{m}^{-3}$$

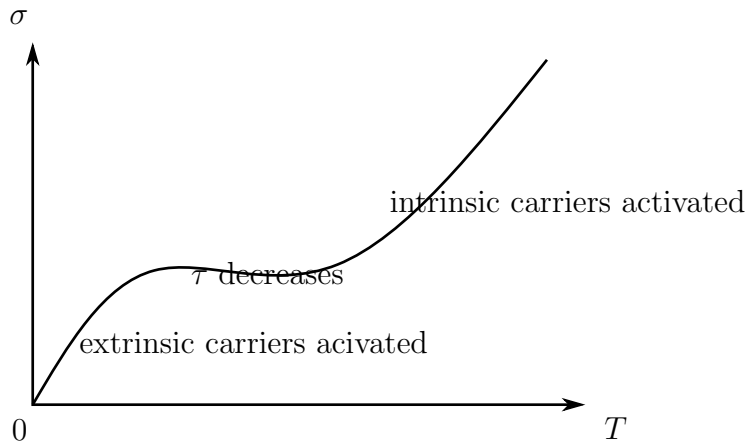
At low frequency

$$\sigma_0 = \frac{n_{\text{all carriers}} e^2 \tau}{m}$$

so we expect

- at low temperature, neither intrinsic nor extrinsic carriers are activated.

- at higher temperature in the extrinsic regime, the extrinsic carriers are activated and saturate to a level of n, while τ the relaxation time shortens with temperature rise.
- in the intrinsic regime more and more intrinsic carriers are activated.



Problem 3.6

Energy of hydrogenic donor orbit:

$$\frac{m_c^*}{m_e}\frac{1}{\epsilon^2} \times 13.6 \text{ eV} = 0.630 \text{ meV}$$

For donor orbits to overlap with each other significantly, their wavefunctions have to be closer in real space, that is when the "radius" of their orbit is similar to the inter-impurity distance

$$r_0 = \frac{4\pi\epsilon\epsilon_0\hbar^2}{m^* e^2} = \epsilon\frac{m_e}{m^*}a_{\text{Bohr}} = 6.35 \times 10^{-8} \text{ m} \gtrsim \left(\frac{1}{N_d}\right)^{\frac{1}{3}} \implies N_d \gtrsim 4 \times 10^{21} \text{ m}^{-3}.$$

Topic 4

Problem 4.1

At the edge of the depletion region $x = x_b$, $\phi = \phi_b$ and $\boldsymbol{\nabla}\phi_b = 0$.

$$\nabla^2\phi = -\frac{N_d e}{\epsilon\epsilon_0}$$
$$\phi = \phi_b - \frac{N_d e}{2\epsilon\epsilon_0}(x - x_b)^2$$

The depletion width is then given by

$$\sqrt{\frac{\phi_b}{\left(\frac{N_d e}{2\epsilon\epsilon_0}\right)}} = 2.58 \times 10^{-7}\ \text{m}$$

Problem 4.2

(a)

Assuming infinite potential well, the electron waves are bound in the z direction and free in the x and y directions

$$E_n(k) = \frac{\hbar^2}{2m}\left[\left(\frac{\pi n}{L}\right)^2 + k_x^2 + k_y^2\right] \qquad n \in \mathbb{Z}^+$$

(b)

The second lowest sub-band starts being filled at energy

$$E_2(0) = \frac{\hbar^2}{2m}\frac{\pi^2}{L^2}2^2 = E_1(k_{\max}^2) \implies k_{\max}^2 = \frac{\pi^2}{L^2}\left(2^2 - 1^2\right)$$

The number of states per area filled up to $k_{\max}$ is

$$\sigma = \int g_k \,\mathrm{d}k$$
$$\sigma = \frac{2}{(2\pi)^2}\pi k_{\max}^2$$
$$\sigma = \frac{3\pi}{2L^2}$$

(c)

For a well of finite depth, the energy of the highest bound state does not exceed V_0, if E_n for infinite well still holds (roughly)

$$\frac{\hbar^2}{2m}\frac{\pi^2}{L^2}N^2 \approx V_0$$
$$N \approx \frac{L}{\pi\hbar}\sqrt{2mV_0}$$

(d)

Bound solutions of finite potential well are either odd or even.

$$\psi_{\text{odd}}(x) = \begin{cases} \sin\left(\frac{\sqrt{2mE}}{\hbar}x\right) & |x| < \frac{L}{2} \\ \sin\left(\frac{\sqrt{2mE}}{\hbar}\frac{L}{2}\right)\exp\left(-\frac{\sqrt{2m(V_0-E)}}{\hbar}\left(|x|-\frac{L}{2}\right)\right) & |x| > \frac{L}{2} \end{cases}$$
$$\psi_{\text{even}}(x) = \begin{cases} \cos\left(\frac{\sqrt{2mE}}{\hbar}x\right) & |x| < \frac{L}{2} \\ \cos\left(\frac{\sqrt{2mE}}{\hbar}\frac{L}{2}\right)\exp\left(-\frac{\sqrt{2m(V_0-E)}}{\hbar}\left(|x|-\frac{L}{2}\right)\right) & |x| > \frac{L}{2} \end{cases}$$

Matching the wavefunction and its first derivative at $|x| = \frac{L}{2}$, we get two forms which the solutions might take

$$\tan\left(\frac{\sqrt{2mE}}{\hbar}\frac{L}{2}\right) = \begin{cases} \sqrt{\frac{V_0-E}{E}} \\ -\sqrt{\frac{E}{V_0-E}} \end{cases}$$

For real solutions of $0 < E < V_0$, $\sqrt{\frac{V_0-E}{E}}$ ranges from $+\infty$ to 0, intersecting the tangent above the x-axis between $n\pi + \left[0, \frac{\pi}{2}\right]$. That is exactly

$$\text{ceil}\left[\frac{\sqrt{2mV_0}}{\hbar}\frac{L}{2}\Big/\pi\right]$$

times. $-\sqrt{\frac{E}{V_0-E}}$ ranges from 0 to $-\infty$, intersecting the tangent below the x-axis (ignore $E = 0$ solution). The curves meet somewhere in $n\pi + \left[\frac{\pi}{2}, \pi\right]$

$$\text{ceil}\left[\left(\frac{\sqrt{2mV_0}}{\hbar}\frac{L}{2} - \frac{\pi}{2}\right)\Big/\pi\right]$$

Add both up, the number of bound solutions is

$$\text{ceil}\left[\frac{\sqrt{2mV_0}}{\hbar\pi}\frac{L}{2}\right] + \text{ceil}\left[\frac{\sqrt{2mV_0}}{\hbar\pi}\frac{L}{2} - \frac{1}{2}\right] = 1 + \text{floor}\left[\frac{\sqrt{2mV_0}}{\hbar}\frac{L}{\pi}\right]$$

Problem 4.3

Sorry I did not finish brief notes questions on time.

Problem 4.4

Use the NFE model,

$$H = \begin{pmatrix} E_0(1+2\kappa) & U \\ U & E_0(1-2\kappa) \end{pmatrix}$$

$$\big[E_0(1+\kappa^2) - E\big]^2 - E_0 4\kappa^2 = U^2 E = E_0 \left[1 \pm \sqrt{\frac{U^2}{E_0^2} + 4\kappa^2}\right]$$

The 1D density of states in κ is

$$g_\kappa = \frac{2}{2\pi/L}\frac{\mathrm{d}k}{\mathrm{d}\kappa} = \frac{2}{2\pi/L}\frac{\pi}{a} = \frac{L}{a} = N$$

The change in electronic energy is

$$E_{\text{elec}} = \frac{1}{N}\int_1^0 \mathrm{d}\kappa\, g_\kappa \left(\sqrt{U^2 + 4\kappa^2 E_0^2} - 2\kappa E_0\right)$$

$$E_{\text{elec}} = |U| \int_0^1 \mathrm{d}\kappa \left(\frac{2\kappa E_0}{|U|} - \sqrt{1 + \left(\frac{2\kappa E_0}{U}\right)^2}\right)$$

$$E_{\text{elec}} = |U| \int_0^1 \mathrm{d}x \left(\frac{x}{\alpha} - \sqrt{1 + \left(\frac{x}{\alpha}\right)^2}\right)$$

where $x = \kappa$, $\alpha = \frac{|U|}{2E_0}$. In the limit $\alpha \ll 1$, $\sinh^{-1}(1/\alpha) = \ln\big(2/\alpha\big)$

$$\begin{aligned} E_{\text{elec}} &= |U| \int_0^1 \mathrm{d}x \left(\frac{x}{\alpha} - \sqrt{1 + \left(\frac{x}{\alpha}\right)^2}\right) \\ &= |U| \left[\frac{1}{2\alpha} - \alpha \int_0^{\sinh^{-1}(1/\alpha)} \cosh^2 u \,\mathrm{d}u\right] \\ &= |U| \left[\frac{1}{2\alpha} - \frac{\alpha}{4}\int_0^{\ln\left(2/\alpha\right)} e^{2u} + e^{-2u} + 2\,\mathrm{d}u\right] \end{aligned}$$

$$= \frac{1}{2}|U|\alpha \ln \alpha$$
$$= \frac{\hbar^2\pi^2}{2ma^2}\alpha^2 \ln \alpha$$

Problem 4.5

Singlet(triplet) state:

$$|\psi\rangle = \frac{1}{\sqrt{2}}\big(|ab\rangle \pm |ba\rangle\big)$$
$$\rho(r) = \Big|\langle\psi|\left(|r\rangle \otimes I\right)\Big|^2 + \Big|\langle\psi|\left(I \otimes |r\rangle\right)\Big|^2$$
$$\rho(r) = \frac{1}{2}\big|\psi_a(r)\,|b\rangle \pm \psi_b(r)\,|a\rangle\big|^2 + \frac{1}{2}\big||a\rangle\,\psi_b(r) \pm |b\rangle\,\psi_a(r)\big|^2$$
$$\rho(r) = \psi_a^2(r) + \psi_b^2(r) \pm 2\psi_a(r)\psi_b(r)\,\langle a|b\rangle$$

However $|\psi\rangle$ is not normalised. If it were, the singlet state would have lower charge density in the middle.

The singlet state has more charge density in the middle where Coulomb interaction is strong.

Problem 4.6

$$M = -\frac{1}{V}\frac{\partial F}{\partial H}$$
$$Z = \sum_{J_z=-J}^{J} \exp(-\beta g_L \mu_B H J_z)$$
$$F = -\frac{1}{\beta}\ln Z$$

$$\frac{\partial Z}{\partial H} = -\beta g_L \mu_B \sum_{J_z=-J}^{J} J_z \exp(-\beta g_L \mu_B H J_z)$$
$$\frac{\partial^2 Z}{\partial H^2} = (\beta g_L \mu_B)^2 \sum_{J_z=-J}^{J} J_z^2 \exp(-\beta g_L \mu_B H J_z)$$
$$M = \frac{1}{VZ\beta}\frac{\partial Z}{\partial H}$$

$$\chi = \frac{\partial M}{\partial H} = \frac{1}{VZ\beta}\left[-\frac{1}{Z}\left(\frac{\partial Z}{\partial H}\right)^2 + \frac{\partial^2 Z}{\partial H^2}\right]$$

At zero field $|\beta g_L \mu_B H J| \ll 1$,

$$Z = \sum_{J_z=-J}^{J} 1 = 2J+1$$
$$\frac{\partial Z}{\partial H} = -\beta g_L \mu_B \sum_{J_z=-J}^{J} J_z = 0$$
$$\frac{\partial^2 Z}{\partial H^2} = (\beta g_L \mu_B)^2 \frac{1}{3} J(J+1)(2J+1)$$
$$\chi = \frac{(\beta g_L \mu_B)^2}{3V\beta} J(J+1)$$

Problem 4.7

I understood these concepts really poorly.

Problem 4.8 Band magnets

(a) Stoner's expression

$$\chi = \mu_0 \frac{\mu_B^2 g(E_F)}{1 - \frac{Ug(E_F)}{2}} = \chi_{\text{Pauli}}\left(1 - \frac{Ug(E_F)}{2}\right)^{-1}$$
$$U = \frac{2}{g(E_F)}\left(1 - \frac{\chi_P}{\chi}\right)$$

We have reason to speculate the enhancements are due to Coulomb repulsion of these metals.

(b)

Stoner-Hubbard model expects the Coulomb repulsions to be:

metal	U
Ca	0.864 eV
Sc	0.668 eV
Pd	0.648 eV

(c)

In Stoner-Hubbard model ferromagnetic metals are marked by

$$\frac{Ug(E_F)}{2} \geq 1 \implies g(E_F) \geq \frac{2}{U}$$

Sommerfeld coefficient is the electron heat capacity divided by temperature

$$\begin{aligned} C_{el} &= \frac{\pi^2}{3} g(E_f) k_B^2 T \\ \gamma &= \frac{\pi^2}{3} g(E_f) k_B^2 \\ \gamma &\leq \frac{\pi^2}{3} \frac{2}{U} k_B^2 = 9.43 \times 10^{-3}\ \mathrm{J\,K^{-2}\,mol^{-1}} \end{aligned}$$

Problem 4.9

(a)

H is the magnetic field, M_i are magnetisations of the sublattices, and a, b, λ are phenomenological coefficients.

We had Curie law from earlier

$$\chi \propto \frac{1}{k_B T}$$

so the temperature dependence of a_is are

$$a_i = \frac{1}{\chi_i} - \lambda_{\text{self exchange}} = \frac{T - T_c}{C_i}$$

(b) decoupled equations

Near the ordering temperature T_N, $M_i^3 \sim 0$,

$$M_1 \approx \frac{\lambda_1}{a_1} M_2; \qquad M_2 \approx \frac{\lambda_2}{a_2} M_1$$

The decoupled equations are (below T_N where $M \neq 0$)

$$(\lambda_1 \lambda_2 - a_1 a_2) = a_2 b_1 M_1^2 = a_1 b_2 M_2^2$$

(c) critical behaviour

$$a_1(T_N)a_2(T_N) = \lambda_1\lambda_2$$

Close to T_N,

$$M_2 = \sqrt{\frac{\lambda_1\lambda_2 - a_1a_2}{a_1b_2}}$$

$$M_2 \approx \sqrt{\frac{a_1'a_2 + a_2'a_1}{a_1b_2}(T_N - T)}$$

$$M_1 = \sqrt{\frac{\lambda_1\lambda_2 - a_1a_2}{a_2b_1}}$$

$$M_1 \approx \sqrt{\frac{a_1'a_2 + a_2'a_1}{a_2b_1}(T_N - T)}$$