Condensed Matter Physics : Answers to Examples 2

[1] 1D Case

Box length A: uniformly spaced k states in 1D separation $\frac{2\pi}{A}$ so

$$\frac{dN}{dk} = \frac{\delta N}{\delta k} \times 2 = \frac{1}{2\pi/A} \times 2 = \frac{A}{\pi}$$

(there are 2 spin states per k state) and:

$$g(\varepsilon) = \frac{dN}{d\varepsilon} = \frac{dN}{dk}\frac{dk}{d\varepsilon} = \frac{A}{\pi}\frac{1}{\hbar}\sqrt{\frac{2m}{\varepsilon}} \propto \varepsilon^{-1/2}$$

since:

$$\varepsilon = \frac{\hbar^2 k^2}{2m} \quad => \quad \frac{dk}{d\varepsilon} = \frac{1}{\hbar}\sqrt{\frac{2m}{\varepsilon}}$$

States will fill to $\pm k_F$ and the total number of particles in the system gives:

$$nA = 2k_F \times \frac{dN}{dK} = \frac{2k_F A}{\pi}$$

and:

$$k_F = \frac{n\pi}{2}$$

hence:

$$\varepsilon_F = \frac{\hbar^2 k_F^2}{2m} = \frac{(\hbar n\pi)^2}{8m}$$

2D Case

Take a square box of sides length A (remember Wigner showed the shape of the box does not matter – and a square is the easiest one algebraically): uniformly spaced k states in 2D separation $\frac{2\pi}{A}$ so:

$$\frac{dN}{dk} = \delta N.\frac{1}{\delta k} \times 2 = \frac{area\ between\ k\ and\ k + \delta k}{area\ per\ state}.\frac{1}{\delta k} \times 2 = \frac{2\pi k\delta k}{(2\pi/A)^2}.\frac{1}{\delta k} \times 2 = \frac{A^2 k}{\pi}$$

(there are 2 spin states per k state) and:

$$g(\varepsilon) = \frac{dN}{d\varepsilon} = \frac{dN}{dk}\frac{dk}{d\varepsilon} = \frac{A^2 k}{\pi}\frac{m}{\hbar^2 k} = \frac{A^2 m}{\hbar^2 \pi} \propto \varepsilon^0$$

since:

$$\varepsilon = \frac{\hbar^2 k^2}{2m} \quad => \quad \frac{d\varepsilon}{dk} = \frac{\hbar^2 k}{m}$$

States will fill a circle of radius to k_F and the total number of particles in the system gives

$$nA^2 = \frac{\pi k_F^2}{area\ per\ state} \times 2 = \frac{\pi k_F^2}{(2\pi/A)^2} \times 2$$

and:

$$k_F^2 = 2\pi n$$

hence:

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

[2]

$$p_F(\varepsilon_1) = \frac{1}{e^{\varepsilon_1 - \mu(T)/k_B T} + 1} = \frac{1}{e^{-\varepsilon_2 + \mu(T)/k_B T} + 1} = \frac{e^{\varepsilon_2 - \mu(T)/k_B T}}{1 + e^{\varepsilon_2 - \mu(T)/k_B T}} = 1 - \frac{1}{e^{\varepsilon_2 - \mu(T)/k_B T} + 1}$$
$$= 1 - p_F(\varepsilon_2)$$

Which means that if $g(\varepsilon)$ was constant around ε_F, then the chance of being unoccupied at a certain energy below the Fermi level would equal the chance of being occupied the same energy above the Fermi level and that you would not need to move the Fermi level in order to keep the same total number of electrons in the system – and remember the Fermi level is set at the point such that when you integrate $N = \int_0^\infty g(\varepsilon) p_F(\varepsilon) d(\varepsilon)$ you get the correct total number of electrons in the system.

The real situation is illustrated in this figure from the handout page 79:
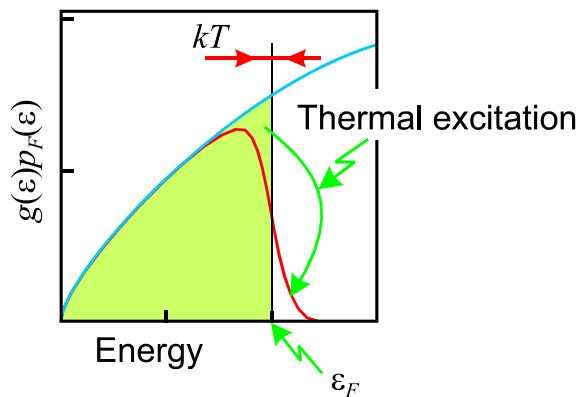
and so the question arises as by what fraction $g(\varepsilon)$ changes within kT of the Fermi level. Given $g(\varepsilon) \propto \varepsilon^{1/2}$ we have (where C is an appropriate constant):

$$g(\varepsilon) = C\varepsilon^{1/2}$$

$$\frac{dg(\varepsilon)}{d\varepsilon} = \frac{C}{2\varepsilon^{1/2}}$$

and the factional change in $g(\varepsilon)$ is for an energy change $\delta g(\varepsilon) = k_B T$:

$$\frac{\delta g(\varepsilon)}{g(\varepsilon)} = \frac{C}{2\varepsilon^{1/2}} \times \frac{1}{C\varepsilon^{1/2}} \times \delta\varepsilon = \frac{k_B T}{2\varepsilon} = \frac{1.38e-23 \times 300}{2 \times 5 \times 1.602e-19} = 0.0026$$

So at room temperature the fractional change in $g(\varepsilon)$ is only 0.0026 and so only the tiniest change in μ is needed to compenstate for this.

[3]   Heat capacity due to phonons is proportional to T³ at low temperatures

Heat capacity due to electrons is proportional to T[1]

So heat capacity is given by $C = \gamma T + \beta T^3$ (see handout page 82) where $\gamma = \frac{\pi^2}{2} N k_B \frac{1}{T_F}$ (handout page 75) where N is the number of electrons and $\frac{1}{T_F} = g(\varepsilon_F) \frac{2k_B}{3N}$ (handout page 80), and $\beta = N \frac{12\pi^4}{5} k_B \frac{1}{\theta_D^3}$ (see handout page 61) where N is the number of atoms (here equal to the number of electrons as each potatssium atom contributes 1 electron to the free electron gas).

So plotting C/T v T^2 gives a straight line intercept γ and gradient β.

From the graph, γ=2.1x10^{-3}Jmol^{-1}K^{-2} and β=(3.0x10^{-3}-2.0x10^{-3})/0.3 Jmol^{-1}K^{-4}

So:

$$\gamma = \frac{\pi^2}{3} k_B^2 g(\varepsilon_F)$$

Hence:

$$g(\varepsilon_F) = \frac{2.1e-3 * 3}{\pi^2 * (1.38e-23)^2} = 3.35e42 \text{ mol}^{-1}\text{J}^{-1}$$

But this is per mole of potassium – for easy comparison with the free electron model – which gives a value of 6.1e46 m^{-3}J^{-1} - i.e. a value per cubic meter we need to multiply by the number of moles per meter,

i.e. $g(\varepsilon_F) = 3.35e42 \text{ mol}^{-1}\text{J}^{-1} * \frac{860}{0.039} mol\ m^{-3} = 7.4e46 m^{-3}\text{J}^{-1}$

[4] The bulk of this question is covered on overheads 83 and 84, and then we need an expression for the Fermi energy of a free electron metal ($\varepsilon_F = \frac{\hbar^2}{2m}(3\pi^2 n)^{2/3}$ handout page 74). Each copper atom contributes 1 electron to the free electron gas so n for copper is 8900/0.0635*6.022e23=8.4e28m^{-3} giving:

$$B = \frac{2}{3} n\varepsilon_F = \frac{2}{3} n \frac{\hbar^2}{2m}(3\pi^2 n)^{2/3} = 63\text{GPa}$$

Which is (a) a significantly less than the actual bulk modulus (140 GPa). Unlike the alkali metals, transition metals have electrons in 'd' bands which have a relatively large size and so overlap in the solid – and compressing the solid increases this overlap, and hence the bulk modulus.

(b) For an ideal gas of the same number density (n=N/V) we have:

$$P = \frac{N k_B T}{V} \qquad \left(\frac{\partial P}{\partial V}\right)_T = -\frac{N k_B T}{V^2} \qquad B = -V \left(\frac{\partial P}{\partial V}\right)_T = \frac{N k_B T}{V} = n k_B T = 0.35\text{GPa}$$

Which is very much smaller. The point here is that in a normal gas we are talking about particles where the number density is so low that we don't have to worry if they are Bosons

or Fermions – the number of particles per state is very small so the chance of multiple occupancy is very low. However, at the number densities we are talking about here, the simple ideal gas equation would imply more than one particle per k state – and as such breaks down for Fermions. For Fermions you would need to occupy states of higher energy because the lower ones are already full, so the total energy stored (as kinetic energy) is higher than would be suggested by the ideal gas, so the kinetic energy contribution to the bulk modulus is therefore much larger.

[5]

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

For He^3 m =0.003/6.022e23 =4.98e-27kg , n =81/m =1.63e28/m^3 and so ε_F=0.43meV. The main reason is that the mass of the He^3 atom is much smaller than that of the electron, but the number density is also low (compare with that for copper 8.4e28m^{-3} – see Q4 above).

In the He_2 dimer (held together by very weak van-der-Waals forces – binding energy about 0.95meV) the nuclear separation is 3.0Å, whereas if one had a close packed solid with the same number density as liquid He^3 the atomic separation would be 4.4 Å – i.e there is a fair bit of 'space' in liquid He^3 and so our calculation of the Fermi energy, whilst very approximate, has some meaning as a starting point in considering the properties of liquid He^3.

[6] The expression for thermal conductivity is:

$$\kappa = \frac{1}{3}C\langle c \rangle l$$

Where C is the heat capacity per unit volume, c is the speed of the objects carrying the heat and l is the mean free path of the heat carriers.
For a metal the electrons dominate the thermal conductivity on account of their high velocity, despite the low electronic heat capacity. For a metal the heat capacity is proportional to the temperature. The mean free path has contributions from geometric scattering (defects, grain boundaries) and scattering by phonons. For a reasonably pure metal at room temperature and above the phonon scattering dominates. Above the Debye temperature (about 340K for copper) the Dulong and Petit result holds for the heat capacity due to phonons (a constant $3k_B$ per atom) so the number of phonons increases linearly with temperature and so the scattering length decreases inversely with temperature cancelling out the linear rise in heat capacity with temperature. Stainless steel, by comparison, has a much lower thermal conductivity – due to the greatly reduced mean free path for the electrons. Since the number of phonons around in copper and stainless steel is not radically different – the increase in electron scattering must be due to more geometric scattering – Stainless steel is a non-homogeneous alloy with a complex microstructure giving many defects and grain boundaries for electron scattering. The mean free path for the electrons does not decrease therefore so strongly with temperature, and so the thermal conductivity rises as the temperature and the electronic contribution to the heat capacity increases.

[7] See Handout pages 98-105. Expressions for Eq and Eq-G on page 105 – the point of this part of the question is that you should work through this material for yourself to check you understand what is going on.

From page 105 of the handout we have (I use k not q etc to save having to re typeset everything with its associated mistakes):

$$\begin{pmatrix} E_{k,-1} & V_1/2 \\ V_1/2 & E_{k,0} \end{pmatrix} \begin{pmatrix} C_{k,-1} \\ C_{k,0} \end{pmatrix} = \varepsilon_k \begin{pmatrix} C_{k,-1} \\ C_{k,0} \end{pmatrix}$$

$$\Rightarrow \begin{pmatrix} E_{k,-1} - \varepsilon_k & V_1/2 \\ V_1/2 & E_{k,0} - \varepsilon_k \end{pmatrix} \begin{pmatrix} C_{k,-1} \\ C_{k,0} \end{pmatrix} = \mathbf{0}$$

$$\Rightarrow \left(E_{k,-1} - \varepsilon_k \right)\left(E_{k,0} - \varepsilon_k \right) - \left(\frac{V_1}{2} \right)^2 = 0$$

$$\Rightarrow \varepsilon_k^2 - \left(E_{k,-1} + E_{k,0} \right)\varepsilon_k + E_{k,-1} E_{k,0} - \left(\frac{V_1}{2} \right)^2$$

$$\Rightarrow \varepsilon_k = \left(E_{k,-1} + E_{k,0} \right)/2 \pm \sqrt{ \left(E_{k,-1} + E_{k,0} \right)^2 /4 - E_{k,-1} E_{k,0} + \left(\frac{V_1}{2} \right)^2 }$$

$$\Rightarrow \varepsilon_k = \left(E_{k,-1} + E_{k,0} \right)/2 \pm \sqrt{ \left(E_{k,-1} - E_{k,0} \right)^2 /4 + \left(\frac{V_1}{2} \right)^2 }$$

Substituting back into the first line of

$$\begin{pmatrix} E_{k,-1} - \varepsilon_k & V_1/2 \\ V_1/2 & E_{k,0} - \varepsilon_k \end{pmatrix} \begin{pmatrix} C_{k,-1} \\ C_{k,0} \end{pmatrix} = \mathbf{0}$$

Gives:

$$\frac{C_{k,-1}}{C_{k,0}} = -\frac{V_1/2}{E_{k,-1} - \varepsilon_k} = \frac{V_1/2}{\left(E_{k,0} - E_{k,-1} \right)/2 \pm \sqrt{ \left(E_{k,-1} - E_{k,0} \right)^2 /4 + \left(\frac{V_1}{2} \right)^2 }}$$

Consider low values of k.

Now $E_{k,0} = \dfrac{\hbar^2 k^2}{2m}$ and $E_{k,-1} = \dfrac{\hbar^2 \left(k - G_0 \right)^2}{2m}$ so near $k=0$ $E_{k,0} \ll E_{k,-1}$

Setting $\Delta E = \left(E_{k,-1} - E_{k,0} \right)/2$ we have:

$$\frac{C_{k,-1}}{C_{k,0}} = \frac{V_1/2}{-\Delta E \pm \sqrt{ \left(\Delta E \right)^2 + \left(\frac{V_1}{2} \right)^2 }}$$

Taking the low energy solution (-) since $\Delta E \gg V_1/2$ (it's a weak potential) we have:

$$\frac{C_{k,-1}}{C_{k,0}} \approx \frac{V_1/2}{-2\Delta E}$$ and $C_{k,0} >> C_{k,-1}$ and the solution is essentially a plane wave of wavevector k (very little contribution from the other component wavevector k-G_0) and indeed energy

$$E_{k,0} = \frac{\hbar^2 k^2}{2m}.$$

Taking the high energy solution near k=0 (+ solution) we have:

$$\frac{C_{k,-1}}{C_{k,0}} = \frac{V_1/2}{-\Delta E + \sqrt{(\Delta E)^2 + \left(\frac{V_1}{2}\right)^2}} = \frac{V_1/2}{\Delta E} \cdot \frac{1}{-1+\sqrt{1+\left(\frac{V_1}{2\Delta E}\right)^2}}$$

$$\approx \frac{V_1/2}{\Delta E} \cdot \frac{1}{-1+\left(1+\frac{1}{2}\left(\frac{V_1}{2\Delta E}\right)^2\right)} = \frac{V_1/2}{\Delta E} \cdot 2\left(\frac{\Delta E}{V_1/2}\right)^2 = 2\left(\frac{\Delta E}{V_1/2}\right)$$

i.e. $C_{k,-1} >> C_{k,0}$ and the solution is essentially a plane wave of wavevector k-G_0 (very little contribution from the other component wavevector k) and energy $E_{k,-1} = \dfrac{\hbar^2(k-G_0)^2}{2m}$

Considering now $k \approx \dfrac{G_0}{2} = \dfrac{\pi}{a}$ - now ΔE is smaller than $V_1/2$ and we have:
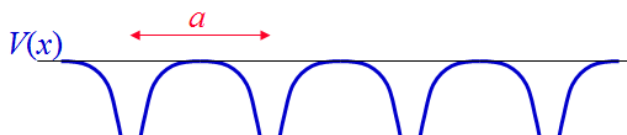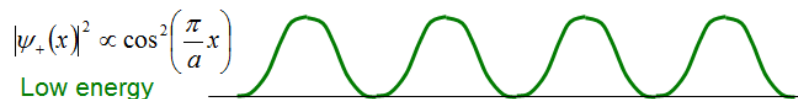
$$\frac{C_{k,-1}}{C_{k,0}} = \frac{V_1/2}{-\Delta E \pm \sqrt{(\Delta E)^2 + \left(\frac{V_1}{2}\right)^2}} = \frac{1}{-\left(\frac{\Delta E}{V_1/2}\right) \pm \sqrt{1+\left(\frac{\Delta E}{V_1/2}\right)^2}}$$

$$\approx \frac{1}{-\left(\frac{\Delta E}{V_1/2}\right) \pm \left(1+\frac{1}{2}\left(\frac{\Delta E}{V_1/2}\right)^2\right)} = \frac{1}{\pm 1 - \frac{1}{2}\left(\frac{\Delta E}{V_1/2}\right)} = \frac{1}{\pm 1 - \frac{\Delta E}{V_1}} \approx \pm 1 + \frac{\Delta E}{V_1}$$

i.e. the coefficients are of comparable sizes the combination giving the cos^2 and sin^2 solutions of overhead 104:
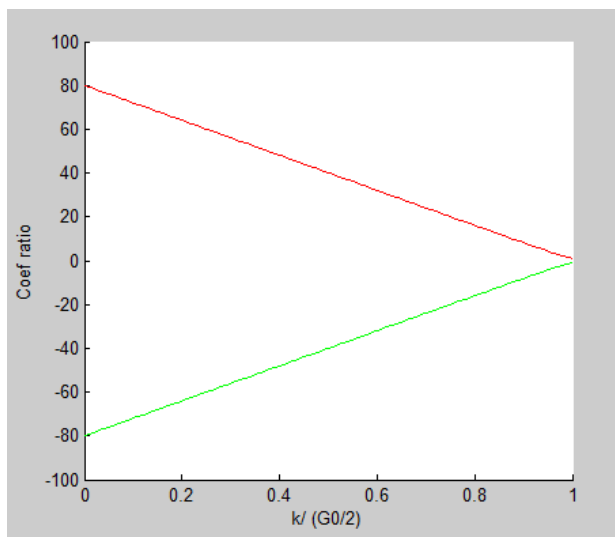
$$\psi_+(x) = \frac{1}{2}\left(|\varphi_{G_1/2}\rangle + |\varphi_{G_1/2}\rangle\right) \propto \cos\left(\frac{\pi}{a}x\right)$$

$$\psi_-(x) = \frac{1}{2}\left(|\varphi_{G_1/2}\rangle - |\varphi_{G_1/2}\rangle\right) \propto \sin\left(\frac{\pi}{a}x\right)$$

Note the way the figure is drawn there is a potential minimum at x=0 i.e. if we replace the atom like wells of V(x) with a simple cosine potential, (as we have in this maths) then V_1 is negative.

$|\psi_+(x)|^2 \propto \cos^2\left(\frac{\pi}{a}x\right)$
Low energy

$|\psi_-(x)|^2 \propto \sin^2\left(\frac{\pi}{a}x\right)$
High energy

$V(x)$

When you sketch the coefficient ratio – its not frightfully illuminating:

The red line is $\dfrac{C_{k,-1}}{C_{k,0}}$ for the high energy mode (+) and the green curve is $\left. 1 \middle/ \dfrac{C_{k,-1}}{C_{k,0}} \right.$ for the low energy mode (-)
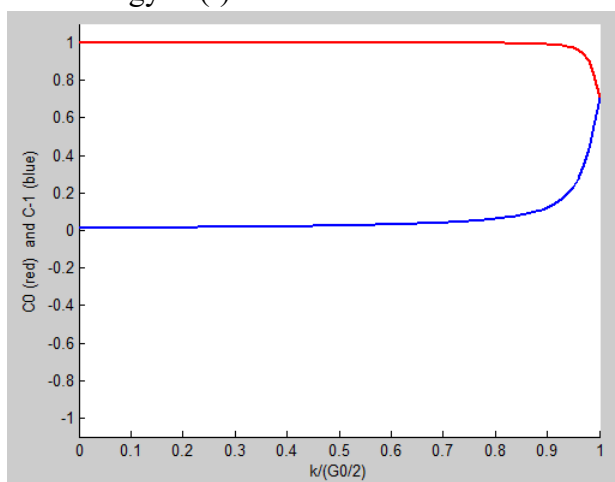
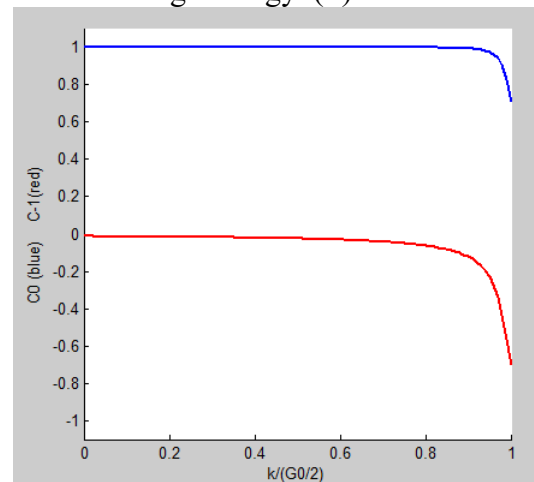Zooming in shows the expected behaviour as you approach the zone boundary:
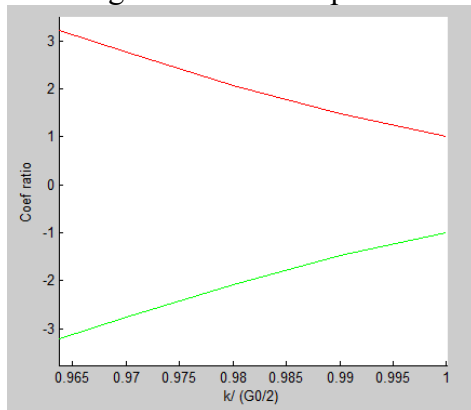
Really the purpose of considering the ratio is to enable one to see what happens to $C_{k,0}$ and $C_{k,-1}$.

So the mode coefficients look like:

Low energy   (-)

high energy (+)

[8] See discussion on overheads 107 and 108. For the material to be an insulator the energy of the lower band at its highest point – i.e. in the corner of the unit cell - i.e. at $(\pi/a, \pi/a)$ must be lower than that of the second band at its lowest point – i.e. at the middle of the side: $(\pi/a, 0)$.

[9] See overheads 112 - 121. The key point is that for a nearly full band, whilst all the electrons in the band contribute to the energy, momentum and current carried by the band it is easier to consider the motion of fictitious, notional 'absences' of an electron with energy and momentum given by the dispersion relation of the 'hole band'.

Balancing the Lorentz force to the centripetal acceration for a charged particle moving with velocity v perpendicular to the field gives: $F = |e\mathbf{v} \times \mathbf{B}| = m^*.2\pi f.v$ hence $v = \dfrac{eB}{2\pi m^*}$

Then read of the peak frequencies and use the equation to get m* for each.

In 3D there are many bands and the carriers in each will have characteristic masses.

[10] Donors contribute electrons to the conduction band. A donated electron at rest a long way from the donor will be in a k state at the bottom of the conduction band. If this electron approaches the donor its energy will drop by the binding energy of the bound state that results when it 'feels' the electrostatic attraction of the donor ion.

The formulae for this question are given on overhead 122.

If the donor hydrogen like wavefunctions do not overlap – the electrons in the donor states are stuck in the orbitals around the donor. If the wavefunctions do overlap then the electrons can tunnel from donor to donor – making a 'donor band' so they will conduct even at low temperatures where the donor states are not ionised. These ideas are expanded in the appendix on the tight binding approach, but this is not examinable.)

[11] All 'bookwork' from overheads 127-139, the idea of this question is for you to try and formulate this in your own words and discuss this topic with your supervisor once you have done so.