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Structure and Properties of Functional Materials

Exercise Set 6

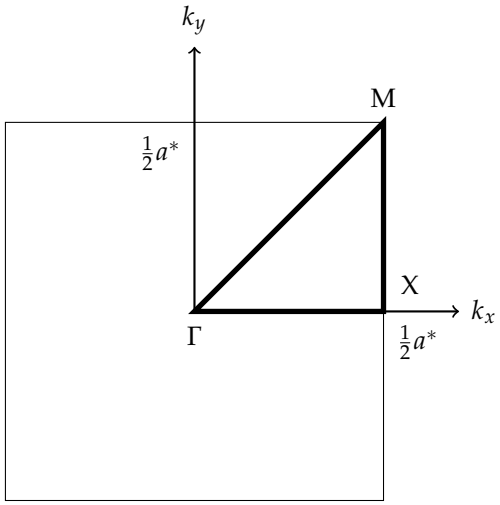
Friday, 1 March, 2013

1. Potassium metal has a body-centred cubic structure with cell parameter $a = 5.328\,\text{Å}$. Its electronic structure can be modelled as a free electron gas, with each atom contributing one electron to the gas.
   (a) Calculate the electron density n in this gas.
   (b) Calculate the Fermi wavevector k_F.
   (c) Calculate the Fermi level E_F.
   (d) Calculate the Fermi temperature T_F. Why is this so far above room temperature?
   (e) Why don't all electrons in a free electron gas contribute to its heat capacity? Which ones do, and why? Estimate the fraction of electrons that contribute to the heat capacity of this gas at $T = 300\,\text{K}$.

2. Suppose a triple axis spectrometer is used to measure the phonon dispersion of potassium, operating in constant-**Q** mode. Which modes (*i.e.*, what wavevector, and longitudinal or transverse) would you expect to see excited for each of the following values of **Q**? Explain your reasoning.
   (a) $\mathbf{Q} = (4.1, 0, 0)$
   (b) $\mathbf{Q} = (0.2, 2, 0)$
   (c) $\mathbf{Q} = (1.1, 0.9, 0)$
   (d) $\mathbf{Q} = (1.2, 0, 0)$

3. *For discussion and collaboration:*

Shown below is a plan of the Brillouin zone of a square (2D) lattice, with some high-symmetry points marked and a path through the Brillouin zone indicated with a thick line.



Consider first the section of the path from Γ to X; that is, from $\mathbf{k} = (0, 0)$ to $\mathbf{k} = (\frac{1}{2}a^*, 0)$. Sketch the dispersion curves (E against k) for the free-electron bands along this path up to $E \approx 10h^2/8ma^2$. Repeat (individually or as a class) for the path from X to M and M back to Γ.

Hint:

$$E = \frac{\hbar^2(\mathbf{k} - \mathbf{G})^2}{2m},$$

but since the reciprocal lattice vectors are $\mathbf{G} = a^*(i, j)$ where i, j are integers, the curves from Γ to X look like

$$E = \frac{\hbar^2(a^*)^2}{2m}\left((\delta - i)^2 + j^2\right)$$

where δ goes from 0 at Γ to $\frac{1}{2}$ at X. Sketch these for a few values of i and j.