Condensed Matter Physics: Workshop 6 (12-16 March 2018)

Summary: In the nearly-free electron model the interaction between the periodic potential and the electron wavefunctions modifies the behaviour of the electrons.

This problem aims to show how energy band structure and the shape of the $E(k)$ relationship (the energy-wavevector dispersion relation) can be used to determine the behaviour of electrons in a solid with a weak periodic potential – electrons in Bloch states. We start with an energy-wavevector $E(k)$ relationship for an electron in a one-dimensional system, with a lattice constant of a:

$$E(k) = y(k^2 + zk^4)$$

E is the energy, k the wavevector and y and z are constants. In the model, the first Brillouin zone extends from $-\pi/a \rightarrow \pi/a$ (as is the case for a cubic lattice).

a. In small groups discuss:

- **i.** What are the key features of the nearly-free electron model?
- **ii.** What is the Bloch theorem, and what does it tell us about electrons in a periodic potential?

b. Write down expressions for the following:

- **i.** The first derivative of the dispersion relation $dE \, / \, dk$.
- **ii.** The electron group velocity.
- **iii.** The second derivative $d^2E \, / \, dk^2$.
- **iv.** The electron effective mass.

c. We will now look at the motion of the Bloch electrons in this system (as determined from the $E(k)$ dispersion relation):

- **i.** Write down the value of the wavevector k at which the electron wave is a standing wave.
- **ii.** What is the significance of this k value?
- **iii.** What is the group velocity of the standing wave?
- **iv.** Using the result from (c) determine an expression for z.
- **v.** Sketch the general shape of this $E(k)$ curve.
- **vi.** What is the ratio of the effective masses evaluated at the centre of the first Brillouin zone and the first Brillouin zone boundary?
- **vii.** What is the significance of positive and negative effective masses?
- **viii.** Assume that $m_{\text{eff}} = m_e$ at the centre of the Brillouin zone. From this determine the value of the energy E at the Brillouin zone boundary.
- **ix.** Show that for small k the electron has an effective mass almost equal to that of a free electron mass.