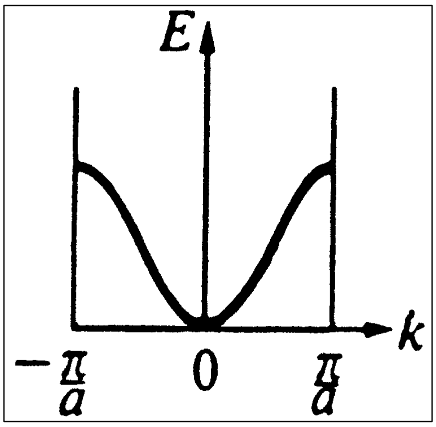
Condensed Matter Physics: Weekly Problem 5

These problems are to be formatively self-assessed by you, the student. Students taking part in the peer-marking pilot scheme will also be required to mark one of their peer's weekly problems. A mark scheme, out of 10, will be provided with each solution to aid your assessment before your timetabled weekly workshop. .

Summary: This problem will look at how the effective mass is related to the $E-(k)$ dispersion relationship (the energy bandstructure) for electrons in Bloch states (electrons moving a weak periodic potential).

In lectures, we saw that the interaction between the electrons and a periodic potential produced an $E(k)$ relationship with the general form as shown in the figure.



In this crystal, the energy bandstructure within the first Brillouin zone can be modelled by the *empirical* relationship:

$$E(k) = \alpha k^2 + \beta k^4$$

Where E is the electron energy, k is the wavevector and α, β are constants.

a. Use what you know about bandstructure to express α as a function of β. **[2 marks]**

b. Obtain an expression for the effective mass in terms of k and α. **[4 marks]**

c. Draw a qualitative sketch illustrating how the effective mass varies from $k = 0 \rightarrow \pi / a$.

What is the value of the effective mass at the point $k = \pi/(a\sqrt{3})$? What are the implications of this for the electron motion? **[4 marks]**

Condensed Matter Physics: Weekly Problem 5 - Solutions

When completing your assessment please enter the numerical marks for each question. Please also give information on any parts which you found difficult, as this will allow me to go over any common issues in the workshops. The workshops also provide the opportunity to individually talk to myself, and other staff members about any issues you faced when solving the problem. Information in the model solutions underlined/boxed in red is required for marks to awarded.

a. To determine the relationship between α and β we also need to recall that the electron velocity (group velocity) is zero at the Brillouin zone boundary:

$$\boxed{v_g\left(k = \pm\frac{\pi}{a}\right) = \frac{1}{\hbar}\left(\frac{dE}{dk}\right) = 0}$$ **[1 mark]**

At $k = \pi/a$, we get: $\boxed{2\alpha\left(\frac{\pi}{a}\right) + 4\beta\left(\frac{\pi}{a}\right)^3 = 0 \Rightarrow \alpha = -\beta\frac{2\pi^2}{a^2}}$ **[1 mark]**

b. We know that the effective mass is given by: $\boxed{m_{\text{eff}} = \hbar^2\left(\frac{d^2E}{dk^2}\right)^{-1}}$ **[1 mark]**

Thus, taking the derivatives we find:

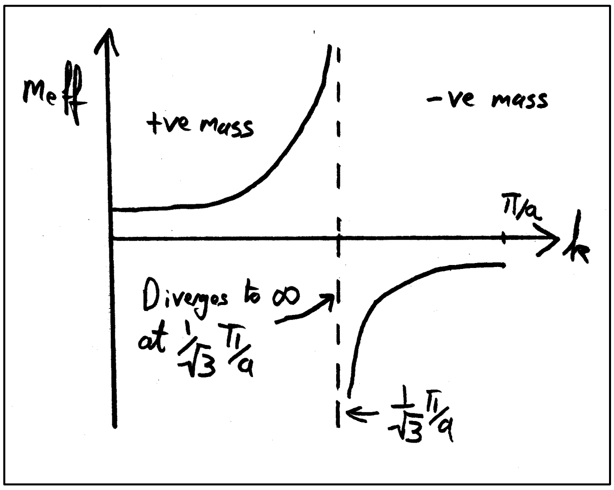
$$\boxed{\frac{dE}{dk} = 2\alpha k + 4\beta k^3 \Rightarrow \frac{d^2E}{dk^2} = 2\alpha + 12\beta k^2 \Rightarrow m_{\text{eff}} = \frac{\hbar^2}{2\alpha + 12\beta k^2}}$$ **[1 mark]**

Substituting in for β from above gives: $\boxed{m_{\text{eff}} = \frac{\hbar^2}{2\alpha\left[1 - 3\left(\frac{ak}{\pi}\right)^2\right]}}$ **[2 marks]**

c. The figure shows how the effective mass behaves across the Brillouin zone starting at a low positive value increasing until it diverges to infinity at the point $k = \pi/a\sqrt{3}$. **[1 mark]**

As k continues to increase the effective mass is negative returning to a low negative value at the Brillouin zone boundary.

An infinite effective mass means that the electron will not move in response to an external force (from an electric field for example). **[1 mark]**



[2 marks for diagram]