Midterm Exam, Fall 2006, Solutions

ECSE-6968 – Physical Foundations of Solid-State Devices

Note: (***i***) Put your name on paper, show your work, underline results, and always show units.
(***ii***) Textbook, manuscript, excerpts, and calculators are allowed.

1. Assume that an electron has a kinetic energy $E = 0.025$ eV $= 0.025 \times 1.602 \times 10^{-19}$ CV and is propagating along the positive x direction in a constant potential given by $U(x) = U_0 = 0$.
   (a) Calculate the velocity of the electron (give numerical value).
   (b) Calculate the momentum of the electron (give numerical value).
   (c) Calculate the de Broglie wavelength of the electron (give numerical value).
   (d) Assume that the wave function of the electron is give by $\Psi(x, t) = \Psi_0 \exp(kx - \omega t)$. Calculate the wave number k of the wave function (give numerical value).
   (e) Calculate the temporal frequency (ω) of the wave function (give numerical value).

Solution:

(a) Kinetic energy is given by: $E = \dfrac{p^2}{2m} = \dfrac{mv^2}{2}$

$$\Rightarrow \quad v = \sqrt{\frac{2E}{m}} = \sqrt{\frac{2 \times 0.025\ \text{V} \times 1.602 \times 10^{-19}\ \text{C}}{9.1 \times 10^{-31}\ \text{kg}}} = 9.38 \times 10^4\ \frac{\text{m}}{\text{s}}$$

where we have used: J = CV = kg m^2 s^{-2} and eV = 1.6×10^{-19} CV

(b) The electron momentum is given by:

$$p = \sqrt{2mE} = \sqrt{2 \times 9.1 \times 10^{-31}\ \text{kg} \times 0.025 \times 1.602 \times 10^{-19}\ \text{CV}} = 8.54 \times 10^{-26}\ \frac{\text{kg m}}{\text{s}}$$

(c) Electron de Broglie wavelength:

$$\lambda = \frac{h}{p} = \frac{6.63 \times 10^{-34}\ \text{J s}}{8.54 \times 10^{-26}\ \text{kg m s}^{-1}} = 7.76 \times 10^{-9}\ \text{m} = 7.76\ \text{nm}$$

(d) Wave number: $k = \dfrac{2\pi}{\lambda} = \dfrac{2 \times 3.14}{7.76 \times 10^{-9}\ \text{m}} = 8.09 \times 10^8\ \text{m}^{-1}$

(e) Angular frequency: $E = \hbar\omega \quad \Rightarrow \quad \omega = \dfrac{E}{\hbar} = \dfrac{0.025\ \text{V} \times 1.6 \times 10^{-19}\ \text{C}}{1.05 \times 10^{-34}\ \text{J s}} = 3.80 \times 10^{13}\ \text{s}^{-1}$

where we have used: J = kg m^2 s^{-2} and J = CV

2. Assume that the dispersion relation of an electron in a semiconductor near the band minimum is given by $E = (9.04 \times 10^{-38}\ \text{kg m}^4\ \text{s}^{-2})\, k^2$.
   (a) Give the value of the curvature of the dispersion relation (give numerical value).
   (b) Calculate the value effective mass (in kg) of an electron obeying this dispersion relation (give numerical value).

Assume that the dispersion relation of a free electron is given by E = 100 meV = $\hbar^2 k^2 / (2m)$ where $m = 9.1 \times 10^{-31}$ kg.

(c) Calculate the particle velocity (give numerical value).

(d) Calculate the wave number k and the wavelength λ of the electron (give numerical value).

(e) Assume that the energy E in the equation $E = \hbar^2 k^2 / (2m)$ is purely kinetic, so that $E = \hbar\omega$. This is valid for free particles. Eliminate E from the last two equations and solve the resulting equation for ω. Calculate the group velocity of the electron with energy E = 100 meV using the equation $v_{gr} = \mathrm{d}\omega / \mathrm{d}k$ (give numerical value).

Solution:

(a) The curvature of the dispersion relation is given by:

$$\frac{\mathrm{d}^2 E}{\mathrm{d}k^2} = 2 \times 9.04 \times 10^{-38} \text{ kg m}^4 \text{ s}^{-2} = 1.81 \times 10^{-37} \frac{\text{kg m}^4}{\text{s}^2}$$

(b) For an electron obeying this dispersion relation, the effective mass is given by:

$$m^* = \frac{\hbar^2}{\mathrm{d}^2 E / \mathrm{d}k^2} = \frac{(1.05 \times 10^{-34} \text{ kg m}^2 \text{ s}^{-1})^2}{1.81 \times 10^{-37} \text{ kg m}^4 \text{ s}^{-2}} = 6.09 \times 10^{-32} \text{kg}$$

(c) For a free electron, the velocity is given by:

$$v = \sqrt{\frac{2E}{m}} = \sqrt{\frac{2 \times 0.1 \text{ V} \times 1.60 \times 10^{-19} \text{ C}}{9.1 \times 10^{-31} \text{ kg}}} = 1.88 \times 10^5 \frac{\text{m}}{\text{s}}$$

(d) The wave number k is given by:

$$k = \frac{\sqrt{2mE}}{\hbar} = \frac{\sqrt{2 \times 9.11 \times 10^{-31} \text{ kg} \times 0.1 \text{ V} \times 1.6 \times 10^{-19} \text{ C}}}{1.05 \times 10^{-34} \text{ kg m}^2 \text{ s}^{-1}} = 1.63 \times 10^9 \text{ m}^{-1}$$

The wavelength of the electron $\lambda = \dfrac{2\pi}{k} = \dfrac{2 \times 3.14}{1.63 \times 10^9 \text{ m}^{-1}} = 3.85 \times 10^{-9} \text{ m}$

(e) $E = \dfrac{\hbar^2 k^2}{2m} = \hbar\omega$ ➔ $\omega = \dfrac{\hbar k^2}{2m}$ which is valid for a free electron. Thus the group velocity is given by

$$v_{gr} = \frac{\mathrm{d}\omega}{\mathrm{d}k} = \frac{\hbar k}{m} = \frac{\sqrt{2mE}}{m} = \sqrt{\frac{2E}{m}} = \sqrt{\frac{2 \times 0.1 \text{ V} \times 1.6 \times 10^{-19} \text{ C}}{9.11 \times 10^{-31} \text{ kg}}} = 1.87 \times 10^5 \frac{\text{m}}{\text{s}}$$

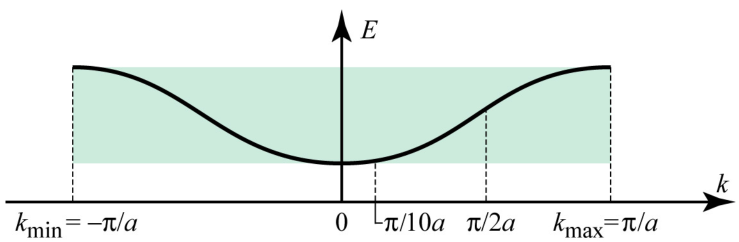
3. Consider an electron in a one-dimensional periodic structure along the x direction with lattice constant (period) a = 5 Å = 0.5 nm. Assume that there will be two allowed bands with a band width $2\Delta E_0$ and $2\Delta E_1$. Assume further that the dispersion relation of the lowest band is given by $E = E_0 - \Delta E_0 \cos ka$ where E_0 = 20 meV and ΔE_0 = 10 meV.

(a) Which of the following relations will be correct: (i) $\Delta E_0 > \Delta E_1$ (ii) $\Delta E_0 < \Delta E_1$ (iii) cannot be determined.
(b) What is the effective mass of the electron in the lowest band at the Brillouin center (give numerical value).
(c) Let us assume that the electron in the periodic lattice potential is accelerated by an electric field $\mathcal{E} = 1000$ V/cm along the positive x direction. After sufficiently long time, the mass of the electron becomes heavier. Give a reason for the fact that the electron mass increases.
(d) Give an estimate of the time it takes for the electron effective mass to become infinitely large.

Solution:
(a) $\Delta E_0 < \Delta E_1$
(b) From the textbook, the effective mass of the electron can be calculated by using Eq. (8.48):

$$m_0^* = \frac{\hbar^2}{\Delta E_0 \, a^2} = \frac{(1.05\times10^{-34}\text{ J s})^2}{10\times10^{-3}\text{ C}\times1.6\times10^{-19}\text{ V}\times(0.5\times10^{-9}\text{ m})^2} = 2.76\times10^{-29}\text{ kg} = 30\, m_0$$

(c) The dispersion relation has the following basic form:



The energy is a function of wave vector, as shown in the figure above. The effective mass for $k > 0$ can be expressed by

$$m^* = m_0^* \left(1 + \frac{E - (E_0 - \Delta E_0)}{\Delta E_0}\right),$$

where m_0^* is the effective mass at the bottom of the band as given in Eq. (8.48). The bottom of the band occurs at the energy $E_0 - \Delta E_0$. The bandwidth of the band is $2\Delta E_0$. Hence Eq. (8.49) indicates that the effective mass increases over m_0^* for higher energies.

An alternative explanation is based on the equation:

$$m^* = \frac{\hbar^2}{\mathrm{d}^2 E / \mathrm{d}k^2}$$

The equation states that the effective mass is inversely proportional to the curvature of the E-versus-k function. Because the curvature of the $E(k)$ function (shown in the above figure) decreases as the energy increases, the effective mass increases.

(d) At $k = 0$, the effective mass of the electron is at the minimum point and it will increases with the increase of k. At $k = \pi/(2a)$, the effective mass is infinitely large.

$$\frac{\mathrm{d}k}{\mathrm{d}t} = -\frac{1}{\hbar} e\,\mathcal{E} \;\;\Rightarrow\;\; \Delta k = -\frac{1}{\hbar} e\,\mathcal{E}\,\Delta t\,.$$

$$\text{Thus } \Delta t = -\frac{\hbar}{e\,\mathcal{E}}\Delta k = \frac{1.05\times 10^{-34}\,\mathrm{J\,s}}{1.6\times 10^{-19}\,\mathrm{C}\times 100\,000\ \mathrm{V\,m^{-1}}}\,\frac{\pi}{0.5\times 2\times 10^{-9}\,\mathrm{m}} = 2.1\times 10^{-11}\,\mathrm{s}\,.$$

4. An electron with effective mass $m^* = 0.067\ m_0$ tunnels through a barrier that is 100 meV high and 100 Å = 10 nm wide.
   (a) Give a formula that allows one to calculate the tunneling probability of the electron.
   (b) Calculate the tunneling probability of the electron (give numerical value).
   (c) Consider that the effective mass of the electron doubles. Does the tunneling probability (i) increase or (ii) decrease?
   (d) Calculate the tunneling probability of the twice-as-heavy electron (give numerical value).

Solution:

(a) Eq. (9.21) can be used to calculate the tunneling probability:

$$T = \exp\left(-\int_{x=0}^{L_\mathrm{B}} 2\hbar^{-1}\sqrt{2m^*[U(x)-E]}\ \mathrm{d}x \right)$$

For $U(x)$ = constant = U, we obtain

$$T = \exp\left(-2\hbar^{-1}\sqrt{2m^*(U-E)}\ L_\mathrm{B} \right)$$

(b) The tunneling probability of the electron is given by:

$$T = \exp\left(-2\hbar^{-1}\sqrt{2m^*[U(x)-E]}L_\mathrm{B} \right)$$

$$= \exp\left(-2\,\frac{\sqrt{2\times 0.067\times 9.11\times 10^{-31}\ \mathrm{kg}\times(0.1\,\mathrm{V}\times 1.6\times 10^{-19}\,\mathrm{C})}}{1.05\times 10^{-34}\,\mathrm{J\,s}} \times 10\times 10^{-9}\ \mathrm{m} \right) = 2.21\times 10^{-4}$$

(c) The tunneling probability decreases as the electron mass increases.

(d) By using the same equation, we obtain

$$T = \exp\left(-2\hbar^{-1}\sqrt{2m^{*}[U(x)-E]}L_{\mathrm{B}}\right)$$

$$= \exp\left(-2\frac{\sqrt{4\times 0.067\times 0.911\times 10^{-30}\ \mathrm{kg}\times(0.1\,\mathrm{V}\times 1.6\times 10^{-19}\,\mathrm{C})}}{1.05\times 10^{-34}\,\mathrm{J\,s}}\times 10\times 10^{-9}\ \mathrm{m}\right) = 6.75\times 10^{-6}$$