Midterm Exam, Fall 2007, Solutions

ECSE-6920 – 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 a one-dimensional wave function is given by

$$\psi = A\left(\frac{3}{16} - \frac{x^2}{L^2} + \frac{x^4}{L^4}\right) \qquad \text{for} \qquad -L/2 \le x \le L/2$$

$$\psi = 0 \qquad \text{for} \qquad x < -L/2 \ \text{ and } \ x > L/2$$

(a) Schematically sketch the wave function. Explain the purpose of the constant A.
(b) Are ψ and ψ' continuous?
(c) What is $\psi(x = 0)$?
(d) What is $\psi(x = L/2)$?
(e) For $A = 1 / (L^{1/2})$, is the wave function normalized? Give ***yes*** or ***no*** answer and explain.
(f) Calculate the position expectation value.
(g) Assume that the potential energy surrounding the wave function is given by

$$U = 0 \qquad \text{for} \qquad -L/2 \le x \le L/2$$

$$U = +U_0 \qquad \text{for} \qquad x < -L/2 \ \text{ and } \ x > L/2$$

What is the expectation value of the potential energy?
(h) Is the expectation value of the total energy zero or non-zero? (Explain)

Solution:

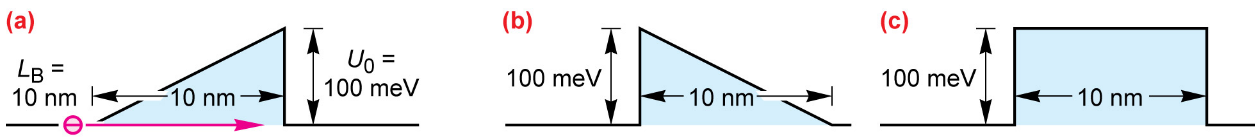
(a) A is the normalization constant. The value of constant A is chosen such that the wave function is normalized, i.e. the integral of (or the area under) the probability density function of the particle is 1.
(b) ψ is continuous. However, ψ' is not continuous.
(c) $\psi(x = 0) = \frac{3}{16}A$.
(d) $\psi(x = L/2) = 0$.
(e) For $A = 1 / (L^{1/2})$, the wave function is ***not*** normalized. The probability density function of the particle has its maxima at $x = 0$ where its value is $\left(\frac{3}{16}A\right)^2$. It is easily seen that the area under the probability function, which has to be equal to 1 for normalized wave function, is less than the area enclosed by rectangle with width = L and height = $\left(\frac{3}{16}A\right)^2$. For $A = 1 / (L^{1/2})$, the area of such a rectangle is $\frac{9}{256} \ll 1$.
(f) The position expectation value, $\langle x \rangle = \int_{-\infty}^{\infty} \psi^*(x)\ x\ \psi(x)\ \mathrm{d}x$.
The given wave function is an even function. Therefore, $\langle x \rangle = \int_{-\infty}^{\infty} even \times odd \times even\ \mathrm{d}x = \int_{-\infty}^{\infty} odd\ \mathrm{d}x = 0$.
(g) The expectation value of the potential energy $\langle U \rangle = \int_{-\infty}^{\infty} \psi^*(x)\ U(x)\ \psi(x)\ \mathrm{d}x$. For the potential energy, $\langle U \rangle = \int_{-\infty}^{-\frac{L}{2}} \psi^*(x)\ U(x)\ \psi(x)\ \mathrm{d}x + \int_{-L/2}^{+L/2} \psi^*(x)\ U(x)\ \psi(x)\ \mathrm{d}x + \int_{+L/2}^{\infty} \psi^*(x)\ U(x)\ \psi(x)\ \mathrm{d}x$. Therefore, $\langle U \rangle = 0$.

(h) The expectation value of the total energy, $\langle E\rangle = \langle E_{kin}\rangle + \langle E_{pot}\rangle = \langle E_{pot}\rangle$.

$$\langle E_{kin}\rangle = \int_{-\infty}^{\infty} \psi^*(x) \left(\frac{-\hbar^2}{2m}\frac{d^2}{dx^2}\right) \psi(x)\ \mathrm{d}x.$$

Second derivative of and even function is an even function. Therefore, $\langle E_{kin}\rangle = \int_{-\infty}^{\infty} even \times even\ \ \mathrm{d}x =$ non-zero. Therefore, the expectation value of total energy, $\langle E\rangle$, is non-zero.

2. An electron with effective mass $m^* = 0.5\ m_0$ tunnels through a barrier, shown in ***Figure*** (a) below that is triangular in shape with $U_0 = 100$ meV high and $L_B = 100$ Å = 10 nm wide.



(a) Give a formula for the tunneling barrier potential as a function of *x*.
(b) What is the tunneling probability of the electron calculated by using the WKB approximation?
(c) If a free electron with mass m_0 were to tunnel through the barrier, what would be its tunnel probability?
(d) Is the tunneling probability of the barrier shown in ***Figure*** (b) the same as the one shown in ***Figure*** (a)? If not, is it higher or lower?
(e) Is the tunneling probability of the barrier shown in ***Figure*** (c) the same as the one shown in ***Figure*** (a)? If not, is it higher or lower?

Solution:

(a) The formula for the tunneling barrier potential as a function of *x*.

i. $U_0 = 10\left(\frac{\text{meV}}{\text{nm}}\right)x$ for $0\ \le x \le 10\ \text{nm}$

ii. $U_0 = 0$ for $x < 0\ \text{ and }\ x > 10\ \text{nm}$

(b) The tunneling probability of the electron calculated by using the WKB approximation is

$$T_{m^*} = \mathrm{e}^{-\int_{x=0}^{L_B} 2\hbar^{-1}\sqrt{2m^*[U(x)-E]}.dx} = \mathrm{e}^{-15.33} = 2.2 \times 10^{-7}$$

(c) The tunnel probability a free electron with mass m_0 is

$$T_{m_0} = e^{-21.68} = 3.8 \times 10^{-10}$$

(d) The tunneling probability of the barrier shown in ***Figure*** (b) is the ***same*** as the one shown in ***Figure*** (a).

(e) The tunneling probability of the barrier shown in ***Figure*** (c) is ***lower*** than the one shown in ***Figure*** (a).

3. Given are the dispersion relations (energy band structures) of (a) gallium arsenide and (b) silicon.
   (a) Identify a direct and an indirect band-gap semiconductor material. (Explain)
   (b) Which material has a smaller conduction-band electron effective mass, Si or GaAs?
   (c) Can an effective mass become negative? (Explain)
   (d) If so, show one region in the *E*-versus-*k* diagram, in which the electron effective mass is negative? (Mark location in figure)
   (e) Highlight the range of *k* values in the figure for which the materials have an electron effective mass and hole effective mass that can be assumed to be a constant.
   (f) A dispersion relation is given by $E = \alpha k^2$, where $\alpha = 5 \times 10^{-39}$ J m^2. Calculate the numerical value of the effective mass.
   (g) For E = 100 meV, calculate the particle velocity.
   (h) For E = 100 meV, calculate wave number k.
   (i) For E = 100 meV, calculate the wavelength λ.
   (j) If the above E is purely kinetic, calculate the group velocity.

Solution:

(a) GaAs is direct band-gap and Si is indirect band-gap material. The conduction-band minimum of GaAs occurs directly above the valence-band maximum, i.e. along the same direction in *k*-space, allowing a direct transition of electron from conduction-band to valence-band, without any change in momentum. Such a transition is not possible in Si as the conduction-band minimum and the valence-band maximum occur in different direction in *k*-space.

(b) GaAs has smaller conduction-band electron effective mass.

(c) Yes. Effective mass is proportional to the curvature of the band structure. Therefore, the effective mass takes a negative value where the slope of the band structure decreases with increasing value of $|k|$.

(d) See figure. The red ellipses indicate the region in the E-versus-k diagram, in which the electron effective mass is negative.

(e) See figure. The yellow highlights indicate the range of k values in the figure for which the materials have an electron effective mass and hole effective mass that can be assumed to be a constant, because the dispersion relation in these regions can be approximated with a parabola.

(f) Effective mass $m^* = 1.11 \times 10^{-30}$ kg.

(g) The particle velocity is given by,

$$v = \sqrt{\frac{2E}{m^*}} = \sqrt{\frac{2 \times 100 \times 10^{-3}\text{eV} \times 1.602 \times 10^{-19}\,\text{C}}{1.11 \times 10^{-30}\,\text{kg}}} = 1.7 \times 10^5\ \frac{\text{m}}{\text{s}}$$

(h) The wavenumber k is given by,

$$k = \frac{\sqrt{2m^*E}}{\hbar} = \frac{\sqrt{2 \times 1.11 \times 10^{-30}\,\text{kg} \times 100 \times 10^{-3}\,\text{eV} \times 1.602 \times 10^{-19}\,\text{C}}}{1.05 \times 10^{-34}\,\text{kg.m}^2\text{.s}^{-1}}$$
$$= 1.8 \times 10^9\ \text{m}^{-1}$$

(i) The wavelength of the particle $\lambda = \frac{2\pi}{k} = \frac{2\times 3.14}{1.8\times 10^9\ \text{m}^{-1}} = 3.5 \times 10^{-9}$ m.

(j) The group velocity $v_{gr} = \frac{\text{d}\omega}{\text{d}k}$. For the given particle, $E = \frac{\hbar^2 k^2}{2m^*} = \hbar\omega$. Therefore, $\omega = \frac{\hbar k^2}{2m^*}$.

Thus, $v_{gr} = \frac{d}{dk}\left(\frac{\hbar k^2}{2m^*}\right) = \frac{\hbar k}{m^*} = \frac{1.05\times10^{-34}\ \mathrm{kg\,m^2\ s^{-1}} \times 1.8\times10^{9}\ \mathrm{m^{-1}}}{1.11\times10^{-30}\ \mathrm{kg}} = 1.7 \times 10^5\ \frac{\mathrm{m}}{\mathrm{s}}$