Midterm Exam, Fall 2008

ECSE-6920 – Physical Foundations of Solid-State Devices, Prof. Schubert

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, which is in the ground state of an atom, is moving at a velocity of 1×10^6 m/s around the atom's core in a circular orbit.
   (a) Calculate the de Broglie wavelength of the electron.
   (b) Calculate the Bohr radius of this atom from the quantities calculated in (a).

   (a) Using de Broglie relation, $\lambda = h / p$ and $p = m_e v$, we can calculate the de Broglie wavelength of electron as,

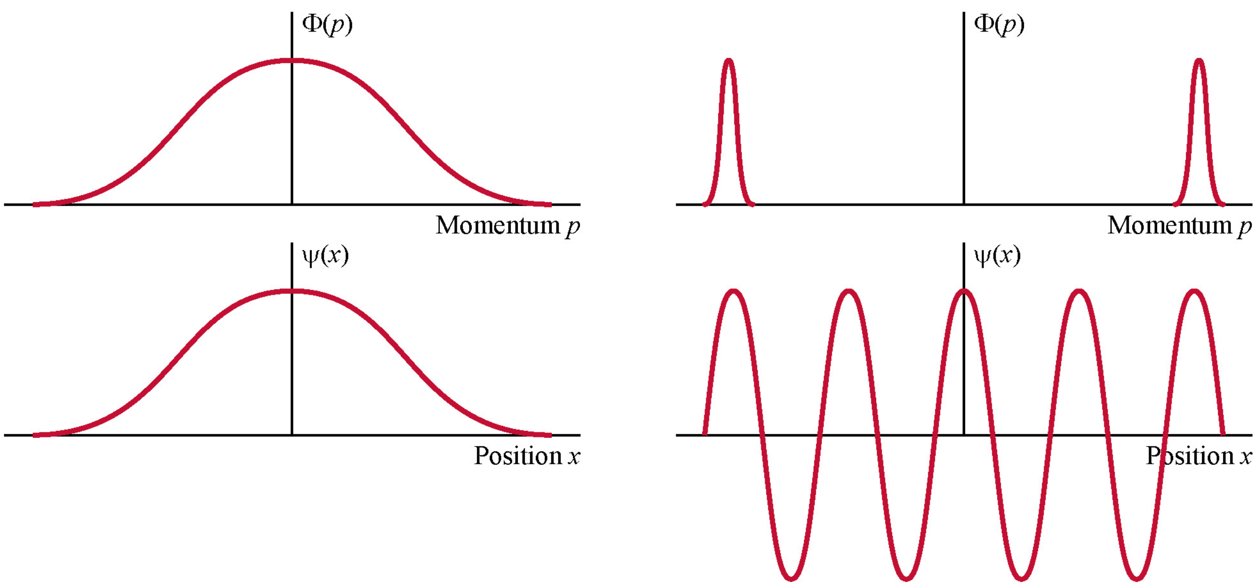
   $$\lambda_{electron} = h / p = h / m_e v = 6.63 \times 10^{-34} \text{ Js} / 9.1 \times 10^{-31} \text{ kg} \times 1 \times 10^6 \text{ m/s} = 7.28 \text{ Å}$$

   (b) From the Bohr-Sommerfeld quantization condition, $2\pi a_B = n \lambda$. For ground state, $n = 1$. Therefore, the Bohr radius of the electron in the ground state is given as,

   $$a_B = \lambda / 2\pi = 7.28 \text{ Å} / 2\pi = 1.16 \text{ Å}$$

2. Given is a momentum-space wave function, $\Phi(p)$, as shown in the figure below.
   (a) Sketch the corresponding real-space wave function $\psi(x)$.
   (b) Explain your choice of $\psi(x)$.

   (a) Corresponding real-space wave function $\psi(x)$.

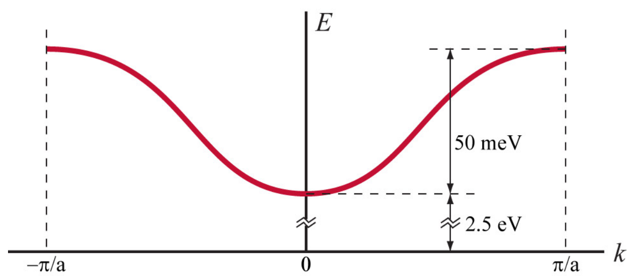


   (b) The choice of the real-space wave functions is based on the following knowledge: The momentum-space representation is obtained by taking the Fourier transform of the real-space wave function and vice-versa. For the first case, the inverse Fourier transform of a

Gaussian function results in another Gaussian function. For the second case, the presence of momentum of same magnitude but opposite sign represents two waves propagating in positive and negative direction and thus a standing wave. The two-maxima get increasingly pronounced with increasing number of nodes of the wave function. We know that the momentum-space representation has maxima at $(n + 1)\, h / (2L)$ where L is the width of an infinite potential well.

3. Assume that the dispersion relation of the conduction band of a semiconductor within the first Brillouin zone is cosine-function shaped with (i) a minimum at $k = 0$, (ii) an amplitude of 25 meV, and (iii) a full-period width of $2\pi / a = 2\pi / 5$ Å $= 2\pi / 0.5$ nm. Assume further that the semiconductor has an energy gap of $E_g = 2.5$ eV.
   (a) Sketch the dispersion relation of the conduction band within the first Brillouin zone.
   (b) Calculate the effective mass of electrons near the minimum at $k = 0$.
   (c) Calculate the photon momentum of light emitted by the semiconductor.
   (d) Assume that an electron-hole recombination event occurs with the electron having a momentum equal to the photon momentum and a hole having a momentum of $p = 0$. Under these conditions, is momentum conservation satisfied?
   (e) Express the electron momentum as a percentage of the momentum the electron would have at the Brillouin zone edge.
   (f) What meaningful conclusion can be drawn from the results of this exercise?

(a) Dispersion relation within first Brillouin zone.



(b) From the given information we can write, $E = 25 \times 10^{-3} \times\ (1 - \cos(ak)) + 2.5$ eV
The effective mass is given as,

$$m^* = \hbar^2 / (\mathrm{d}^2E / \mathrm{d}k^2) = \hbar^2 / (a^2 \times 25 \times 10^{-3} \times \cos(ak))$$

Therefore, effective mass at $k = 0$ is,

$$m^*_{(k=0)} = \hbar^2 / (a^2 \times 25 \times 10^{-3} \times 1) = 1.11 \times 10^{-29}\ \text{kg} = 12.2\ m_e$$

(c) Wavelength of the photo emitted by the semiconductor can be calculated as,

$$\lambda_{photon} = hc / E = 6.63 \times 10^{-34}\ \text{Js} \times 3 \times 10^8\ (\text{m/s}) / (2.5 \times 1.6 \times 10^{-19}\ \text{J}) = 497\ \text{nm}.$$

We can calculate the photon momentum from the photon wavelength as below,

$$p_{photon} = h / \lambda_{photon} = 6.63 \times 10^{-34}\ \text{Js} / 497 \times 10^{-9}\ \text{m} = 1.33 \times 10^{-27}\ \text{kg m/s}$$

(d) Yes.

(e) Electron momentum at the zone boundary is given as,

$p_{max} = \hbar\pi / a = 6.6 \times 10^{-25}$ kg m/s

The momentum of electron participating in the recombination event can be expressed as a percentage of electron momentum at the zone boundary as below,

$p_{photon} / p_{electron,\ max} = 0.2\ \%$

(f) This exercise reveals that the momentum difference between electron and holes taking part in radiative recombination event must be much smaller than the maximum momentum at the zone boundary. Therefore, optical transitions are "vertical" in k-space. Carriers taking part in radiative recombination are usually located near the center of the first Brillouin zone, *i.e.* near $k = 0$. The exercise also shows that radiative recombination cannot occur in indirect-gap semiconductors, which have substantial difference between the location of conduction-band minima and valence-band maxima.

4. Assume a perturbation hamiltonian operator has the following function: $H' = A_0 \exp(i\, \omega_0\, t)$.

(a) ***First***, we assume that A_0 is a constant that does ***not*** depend on x, i.e. A_0 = constant. Assume further that this perturbation acts on an occupied quantum mechanical state j, possessing even-function symmetry. Next we consider the possibility of a quantum mechanical transition between this state j and another state m. Can such a transition occur?

(b) Justify your answer given under (a).

(c) ***Second***, we assume that $A_0(x)$ has the following spatial dependence: $A_0(x) = x \exp(-x^2)$. Is $A_0(x)$ an even-symmetry or an odd-symmetry function?

(d) Could this perturbation excite an electron from the valence band to the conduction band of a semiconductor? (Justify your answer)

(a) No.

(b) Transition matrix element of two wave functions $\psi_m{}^0$ and $\psi_j{}^0$ is given as,

$$H'_{mj} = \left\langle \psi_m^0 \middle| H' \middle| \psi_j^0 \right\rangle = \int_{-\infty}^{\infty} \psi_m^{0\,*}(x) H'(x)\, \psi_j^0(x) \mathrm{d}x\ .$$

Since A_0 is constant H' is also constant and independent of x, and therefore can be taken out of the integral. Then, due to orthogonality of eigenfunctions for any choice of $\psi_m{}^0$, $\left\langle \psi_m^0 \middle| \psi_j^0 \right\rangle = 0$; forcing the transition matrix element to be zero, thus the disallowing transition.

(c) $A^0(x) = -A^0(-x)$. Therefore, $A_0(x)$ is an odd-symmetry function.

(d) Yes.

ψ_0 = Valence band wave function = odd symmetry function

ψ_0 = Conduction band wave function = even symmetry function

H' = Perturbation Hamiltonian = odd symmetry function

$\int_{-\infty}^{\infty} even \times odd \times odd\ \mathrm{d}x \neq 0\ .$

5. Consider a infinite quantum well having its left-hand-side wall at $x = -$ (1/2) L_{QW} and its right-hand-side wall at $x = +$ (1/2) L_{QW}.

(a) Make a careful qualitative plot the wave functions $\psi_0(x)$, $\psi_1(x)$, $\psi_2(x)$, and $\psi_3(x)$.

(b) Make a careful qualitative plot of the product $\psi_0(x)\ \psi_1(x)$.

(c) Is the area under the curve, i.e. $\int_{-0.5 L_{\mathrm{QW}}}^{0.5 L_{\mathrm{QW}}} \psi_0(x)\ \psi_1(x)\, \mathrm{d}x$, zero, or non-zero?

(d) Make a careful qualitative plot of the product $\psi_0(x)\ \psi_2(x)$.

(e) Is the area under the curve, i.e. $\int_{-0.5 L_{\mathrm{QW}}}^{0.5 L_{\mathrm{QW}}} \psi_0(x)\ \psi_2(x)\, \mathrm{d}x$, zero, or non-zero?

(f) Make a careful qualitative plot of the product $\psi_1(x)\ \psi_3(x)$.

(g) Is the area under the curve, i.e. $\int_{-0.5 L_{\mathrm{QW}}}^{0.5 L_{\mathrm{QW}}} \psi_1(x)\ \psi_3(x)\, \mathrm{d}x$, zero, or non-zero?

(h) Make a careful qualitative plot of the product $\psi_3(x)\ \psi_3(x)$.

(i) Is the area under the curve, i.e. $\int_{-0.5 L_{\mathrm{QW}}}^{0.5 L_{\mathrm{QW}}} \psi_3(x)\ \psi_3(x)\, \mathrm{d}x$, zero, or non-zero?

(a) and (b) See figure below.

(c) Zero (orthogonality of wave functions or eigenvalues).

(d) See figure below.

(e) Zero (orthogonality of wave functions or eigenvalues).

(f) See figure below.

(g) Zero (orthogonality of wave functions or eigenvalues).

(h) See figure below.

(i) Non-zero.