Problem 5

I. The one-dimensional Schrödinger equation describing the behavior of an electron is expressed as

$$i\hbar\frac{\partial\psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi(x,t)}{\partial x^2} + V(x)\psi(x,t) \ .$$

Here, $\psi(x,t)$ is the electron wave function as a function of position x and time t, $V(x)$ is the potential as a function of x, m is the electron mass, $\hbar$ is Planck's constant h divided by 2π, and i is the imaginary unit. Answer the following questions.

(1) The wave function of energy eigenstates is expressed as

$$\psi(x,t) = \Phi(x)e^{-i\omega t},$$

where $\Phi(x)$ is a function of x and ω is the angular frequency. Using this equation, derive the time-independent Schrödinger equation.

(2) Consider the energy eigenstates of an electron confined by the potential $V(x)$ shown in Fig. 1, where $V(x) = 0$ for $0 \leqq x \leqq L$ and $V(x) = V_0$ for $x < 0$ and $L < x$. When the potential height V_0 is infinite, the solution for $\Phi(x)$ in the range $0 \leqq x \leqq L$ is given by

$$\Phi(x) = C_1 e^{ikx} + C_2 e^{-ikx} \ .$$

Here k is the wavenumber, which is a positive real number. C_1 and C_2 are constants. Note that $\Phi(x) = 0$ for $x < 0$ and $L < x$.

(2-i) Express the eigenenergy E as a function of k.

(2-ii) Find the value of k and the eigenenergy E.

(2-iii) Find the eigenfunction of the electron corresponding to each eigenenergy obtained above.

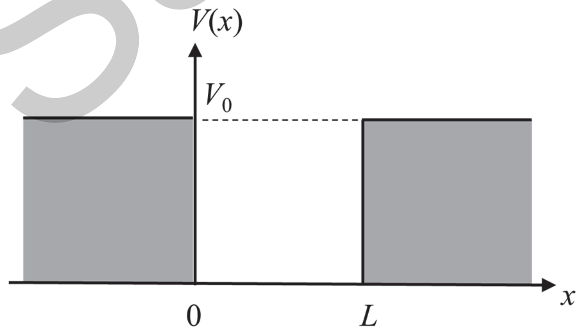

Fig. 1

(3) Consider the case where the potential height V_0 is finite in Fig. 1. When $V_0 > E$, the solution for the electron wavefunction $\Phi(x)$ confined by the potential barriers is given by

$$\Phi(x) = \begin{cases} B_1 \mathrm{e}^{k'x} & x < 0 \\ C_1 \mathrm{e}^{ikx} + C_2 \mathrm{e}^{-ikx} & 0 \leqq x \leqq L \\ B_2 \mathrm{e}^{-k'x} & L < x \end{cases}$$

where k' is a positive real number, and $k' = \frac{\sqrt{2m(V_0 - E)}}{\hbar}$. $B_1,\ B_2,\ C_1,$ and C_2 are constants.

(3-i) Using k', describe the penetration (penetration length) of the electron wavefunction into the potential barriers.

(3-ii) Give physical reasons why there is no penetration of the electron wavefunction into the potential barriers when V_0 is infinite.

(3-iii) What difference occurs in the eigenenergy value of the ground state when V_0 is infinite and when V_0 is finite? Also, how is the difference (between the eigenenergy values when V_0 is infinite and when V_0 is finite) in the excited states compared with the ground state? Here, it is not necessary to exactly calculate the electron wavefunctions and eigenenergy values when V_0 is finite.

(3-iv) In the electron system confined by the potential $V(x)$ as shown in Fig. 1, when electrons exist only in the ground state, light irradiation can induce a transition from the ground state to the excited states (In a semiconductor quantum well structure, this is called "inter-subband transition"). How do the photon energy and wavelength of the inter-subband transition change when V_0 is changed from infinite to finite? Here, it is not necessary to exactly calculate the electron wavefunctions and eigenenergy values when V_0 is finite.

II. Consider the conduction band and valence band of a three-dimensional intrinsic semiconductor crystal. The bottom energy of the conduction band is E_{C}, the top energy of the valence band is E_{V}, the Fermi level is E_{F}, the effective mass of electrons is m_{e}, the effective mass of holes is m_{h}, the band gap is E_{g}, the absolute temperature is T, Boltzmann's constant is k_{B}, Planck's constant is h, and $\hbar$ is h divided by 2π. In this semiconductor, the bandgap is about 1 eV, only one band each is considered for electrons and holes, respectively, carriers exist only near the Γ point (wavevector $\boldsymbol{k} = \mathbf{0}$), and the effective mass approximation can be applied. Answer the following questions.

(1) Express the kinetic energy E of the electron in the conduction band as a function of the wavevector $\boldsymbol{k}$.

(2) The density of states $g(E)$ of the electrons in the conduction band is expressed as

$$g(E) = \frac{1}{2\pi^2}\left(\frac{2m_{\mathrm{e}}}{\hbar^2}\right)^{\frac{3}{2}}(E - E_{\mathrm{C}})^{\frac{1}{2}}.$$

Derive this equation.

(3) Obtain the electron density n_0 in the conduction band of this semiconductor in thermal equilibrium near room temperature using E_{C}, E_{F}, m_{e}, T, k_{B}, and h. Assume that the Fermi-Dirac distribution can be approximated by the Boltzmann distribution. The following formula may be used in the derivation.

$$\int_0^{\infty} \sqrt{x}\ \exp\left(\frac{-x}{k_{\mathrm{B}}T}\right) dx = \frac{1}{2}\sqrt{\pi(k_{\mathrm{B}}T)^3}\ .$$

(4) Find the Fermi level E_{F} near room temperature.

(5) If this semiconductor is Si (silicon), what impurities should be doped to make it N-type or P-type, respectively? Indicate one element for each type, and describe the reason for your choice. Also, how does the Fermi level E_{F} change when the semiconductor is changed from intrinsic to N-type or P-type, respectively? Explain the above in about 5 lines. You may use diagrams if necessary.