

## Problem 5

### I.

Consider an electron in a solid, for which the Schrödinger equation can be given by

$$i\hbar \frac{\partial}{\partial t} \Psi = H\Psi, \quad (\text{i})$$

where  $t$  is the time,  $\Psi$  is the wave function of the electron,  $H$  is the Hamiltonian for the electron,  $i$  is the imaginary unit, and  $\hbar$  is the reduced Planck constant (given by the Planck constant divided by  $2\pi$ ). Answer the following questions. Here,  $\omega = E/\hbar$ ,  $E$  is the energy of the electron, and  $k$  is the wavenumber of the electron (real number).

(1) Suppose  $H = -A \frac{\partial^2}{\partial x^2}$ , where  $A$  is a real positive constant, and  $x$  is the position. Assume that the wave function is given by  $\Psi = Ce^{i(kx - \omega t)}$ , where  $C$  is a constant.

(1-i) Derive the dispersion relationship between  $E$  and  $k$ .

(1-ii) An electron in this solid can be expressed as a free electron with an effective mass  $m$ . Derive  $m$ . Note that the momentum of an electron can be given by  $\hbar k$ .

(1-iii) Consider a one-dimensional solid with a length  $L$ . Find the possible values of  $k$  in this solid. Here, assume a periodic boundary condition with a period  $L$ .

(1-iv) Using the result of Question (1-iii), derive the density of states of an electron at an energy  $E$  in this one-dimensional solid.

(2) Suppose  $H = -A \left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right)$ , where  $A$  is a real positive constant, and  $x$ ,  $y$ , and  $z$  are positions.

Assume that the wave function is given by  $\Psi = Ce^{i(k_x x + k_y y + k_z z - \omega t)}$ , where  $C$  is a constant, and  $k_x$ ,  $k_y$ , and  $k_z$  are the wavenumber components in the  $x$ -,  $y$ -, and  $z$ -direction, respectively. Derive the density of states of an electron at an energy  $E$  in this three-dimensional solid.

(3) Suppose  $H = \begin{pmatrix} 0 & Bk \\ Bk & 0 \end{pmatrix}$ , where  $B$  is a positive real number. In this case, the Schrödinger equation for an electron can be given by

$$i\hbar \frac{\partial}{\partial t} |\Psi\rangle = H|\Psi\rangle, \quad (\text{ii})$$

where  $|\Psi\rangle$  is the state vector of the electron.

(3-i) Suppose  $|\Psi\rangle = \begin{pmatrix} \varphi_1 \\ \varphi_2 \end{pmatrix} e^{-i\omega t}$ , where  $\varphi_1$  and  $\varphi_2$  are time-independent values. Derive the dispersion relationship between  $E$  and  $k$ .

(3-ii) Derive the propagation speed of this electron given by  $dE/dk$ , and discuss the difference between this electron and a free electron.

II.

Consider a silicon (Si) p-n junction biased with a voltage  $V$  as shown in Fig. 1. An n-type Si and a p-type Si are uniformly doped with phosphorus (P) and boron (B), respectively. The doping concentrations of the n-type Si and the p-type Si are  $N_D$  and  $N_A$ , respectively. The activation rate of the dopants is 100%. Here,  $x$  is the position, and the interface between the n-type Si and the p-type Si is located at  $x = 0$ . The edges of the depletion layer are at  $x = -l_n$  and  $x = l_p$ . Here,  $k_B$  is the Boltzmann constant,  $q$  is the elementary charge,  $T$  is the temperature of the p-n junction,  $\epsilon_s$  is the permittivity of Si, and  $n_i$  is the intrinsic carrier density of Si. Answer the following questions, assuming that  $T$  is at room temperature.

- (1) Draw the band diagram of the p-n junction when  $V = 0$ . The Fermi level  $E_F$  and the intrinsic Fermi level  $E_i$  must be indicated in the band diagram.
- (2) Derive the built-in potential of the p-n junction  $V_{bi}$ . Here, the electron density at the thermal equilibrium condition can be given by  $n_i e^{(E_F - E_i)/k_B T}$ , and the hole density by  $n_i e^{(E_i - E_F)/k_B T}$ .
- (3) Derive and sketch the electro-static potential and electric field in the depletion layer using  $l_n$  and  $l_p$  when  $V = 0$ . Here, the electric field can be assumed to be zero in the n-type and p-type neutral regions.
- (4) Derive the depletion layer width  $W = l_n + l_p$  using  $V_{bi}$  when  $V = 0$ .
- (5) Draw the band diagram under a forward bias ( $V > 0$ ), and explain the reason why a current increases exponentially with respect to  $V$  using the energy distribution of electrons in the conduction band.
- (6) Under a reverse bias ( $V \ll 0$ ), there is a voltage range where a constant, non-zero current flows. Explain this reason using the distributions of minority carriers in the neutral regions.
- (7) Suppose crystal defects uniformly distribute in Si. Such crystal defects can be generation centers or recombination centers of electrons and holes. The effective recombination rate at the crystal defects per a unit volume is given by  $\frac{np - n_i^2}{n + p + 2n_i} \cdot \frac{1}{\tau}$ , where  $n$  is the electron density,  $p$  is the hole density, and  $\tau$  is the carrier lifetime. Derive the generation current density using the depletion layer width  $W$  under a reverse bias.

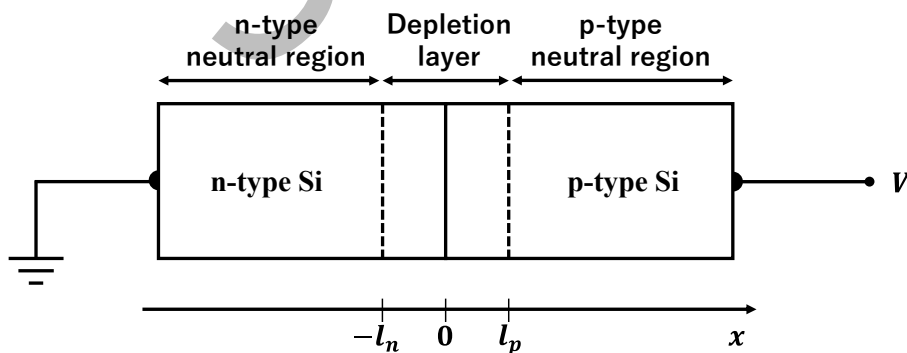


Fig. 1