Physics of Semiconductors (Problems for report)

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Choose two from the following eight problems and solve them.

I. Fundamentals in band theory

(i) Show that tight-binding approximation to the simple cubit lattice gives the dispersion as

$$E_n(\boldsymbol{k}) = E_n - \alpha_n - 2t \sum_{j=x,y,x} \cos k_j a. \tag{1}$$

Apply the same to the body-centered cubic and the face-centered cubit structures.

(ii) Wavefunctions at the top of valence band (Γ-point) in sp^3-bonding diamond structure semiconductors can be written to the second order of $k \cdot p$ approximation as

$$\text{Heavy hole band: } \left|\frac{3}{2}, \pm\frac{1}{2}\right\rangle = \frac{1}{\sqrt{6}}\left\{2|z\rangle\begin{pmatrix}\alpha\\ \beta\end{pmatrix} - (|x\rangle \pm i|y\rangle)\begin{pmatrix}\beta\\ \alpha\end{pmatrix}\right\}, \tag{2}$$

$$\text{Light hole band: } \left|\frac{3}{2} \pm \frac{3}{2}\right\rangle = \frac{1}{\sqrt{2}}(|x\rangle \pm i|y\rangle)\begin{pmatrix}\alpha\\ \beta\end{pmatrix}, \tag{3}$$

$$\text{Spin split-off band: } \left|\frac{1}{2}, \pm\frac{1}{2}\right\rangle = \frac{1}{\sqrt{3}}\left\{|z\rangle\begin{pmatrix}\alpha\\ \beta\end{pmatrix} + (|x\rangle + i|y\rangle)\begin{pmatrix}\beta\\ \alpha\end{pmatrix}\right\}. \tag{4}$$

where α and β are spin part of the wavefunction, and $|x\rangle$, $|y\rangle$, $|z\rangle$ are just showing the symmetry along the axes. The upper and lower rows for α and β correspond to the double sign $\pm$ or $\mp$.

Show that these functions diagonalize the spin-orbit interaction

$$H_{\text{so}} = \frac{C_{\text{so}}}{r^3}(\boldsymbol{l} \cdot \boldsymbol{\sigma}), \tag{5}$$

where $\boldsymbol{l}$ is the orbital angular momentum and $\boldsymbol{\sigma}$ is the vector of Pauli spin matrices.

II Si valley structure, carrier statistics, pn junction

(i) The conduction band bottom of Si consists of 6 equivalent valleys close to X-points (bit inside the first Brillouin zone). The effective transverse mass $m_t = 0.19m_0$, the effective longitudinal mass $m_l = 0.97m_0$, which were obtained from cyclotron resonance. The valence band top is at the Γ-point. It has degeneracy of heavy and light hole bands as well as strong non-parabolicity. Averaged effective mass for heavy hole is $m_{hh} = 0.49m_0$, and for light hole $m_{lh} = 0.16m_0$.

(1-a) Calculate the effective density of states N_c for the conduction band at temperature T.

(1-b) Also obtain the effective density of states N_v for the valence band.

(1-c) Calculate the np product (n_i^2) at 300K (the band gap at 300K is 1.1 eV).

(ii) Obtain 300K built-in potential of a Si pn diode, which is abruptly doped as $n = 1\times10^{17}\text{cm}^{-3}$, $p = 5 \times 10^{17}\text{cm}^{-3}$. Use the value of np product obtained in (1-c).

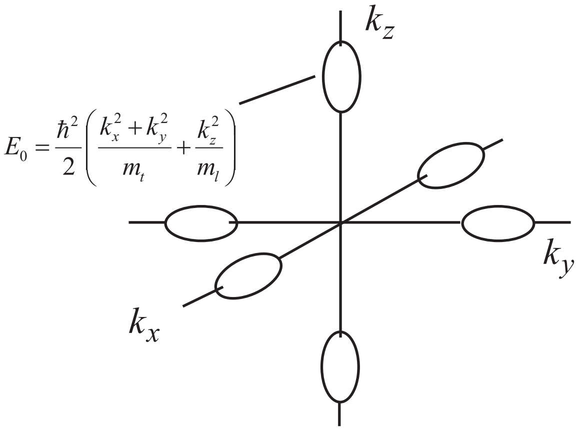


Figure 1: Schematic view of valley structure of Si conduction band. The six ellipsoidal bodies represent equi-energy surfaces for valleys close to X points.

III CV characteristics of a GaAs pn diode

V_b (V)	C (pF)
0.0	408
-0.2	380
-0.4	350
-0.6	334
-0.8	313
-1.0	296
-1.2	283
-1.4	273

There is a GaAs (dielectric constant 13) $\mathrm{p}^+\mathrm{n}$ diode grown with molecular beam epitaxy. Doping is abrupt and uniform for both p and n layers. We have cut the grown film to a $1\mathrm{mm}^2$ area and measured the differential capacitance with applying the (negative) bias voltage V_b and obtained the results summarized in the table on the left.

Obtain the built-in potential in unit of V. The measured C contains some experimental errors.

Assume that the capacitance is dominated by the doping in the n layer and obtain the donor concentration in the n layer in the unit of cm^{-3}.

IV Various confinement potentials

Choose the material as GaAs (electron effective mass $m^* = 0.067m_0$) and calculate energy levels for various one-dimensional confinement (along z).

(i) Quantum well with infinite barrier height and width a = 10nm. Obtain energy levels for ground state, 1st and 2nd excited states.

(ii) The n-th eigen value of triangular potential

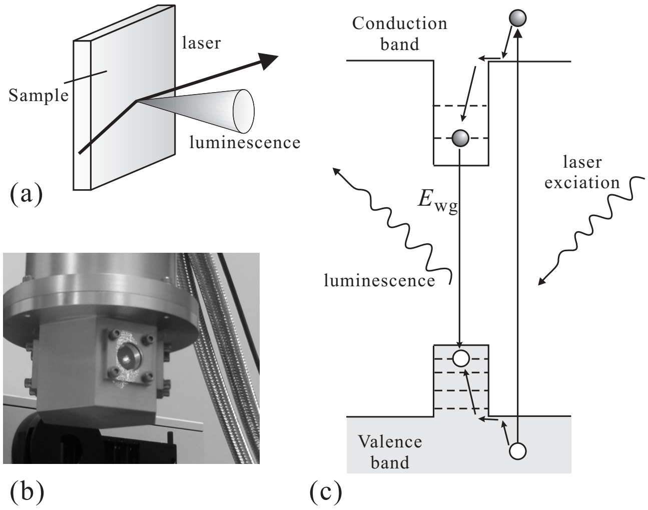
$$U(z) = \begin{cases} \infty & (z < 0) \\ e\mathcal{E}z & (z \geq 0). \end{cases} \tag{6}$$

Let $\mathcal{E}$ be 10^5 V/cm. And refer to appendix “Eigenstates of triangular potential”.

(iii) The n-th engenvalue of harmonic potential,

$$U(z) = \frac{m^*\omega^2}{2}z^2 \tag{7}$$

V Photoluminescence from quantum wells



The left figure illustrates a photoluminescence experiment. As shown in (a), the sample is illuminated with (in many cases laser) light with high energy, for electron-hole pairs to be created. The electron-hole pairs recombine to emit photons. (b) shows a photograph of a real apparatus (4K cryostat), which has three optical windows. Two of them are for inlet and outlet of the laser light and the middle one is to collect the luminescence from the sample.

As shown schematically in (c), such excited carriers migrate inside the sample, relax into the bound states in the quantum wells and recombine. Hence if such band to band emission dominates the luminescence, the energy of emitted photons is the energy difference between the ground states in the quantum well for electrons and holes.

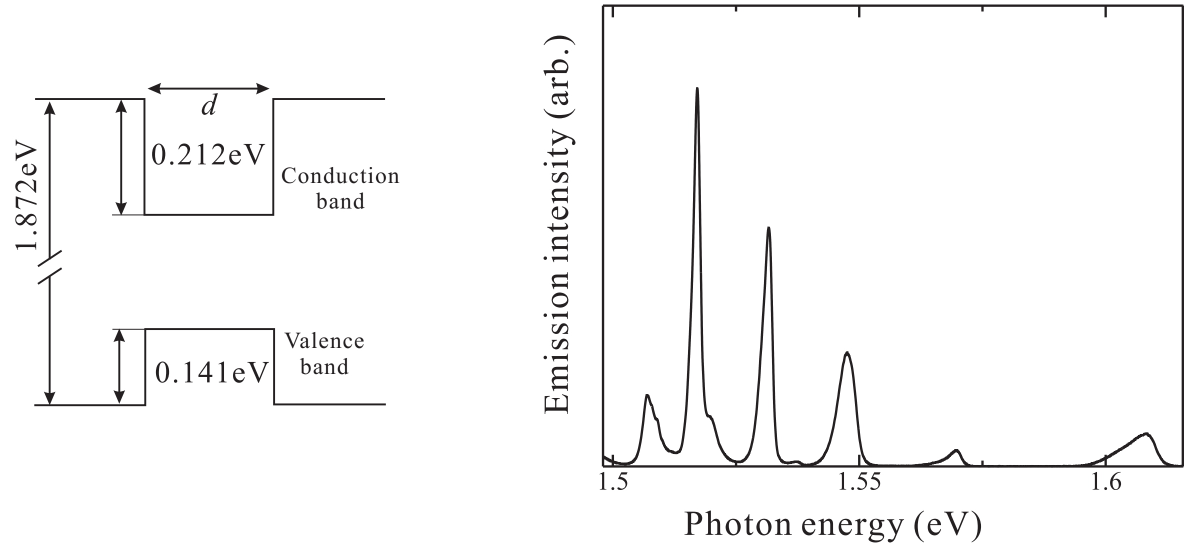
The quantum wells considered here consist of GaAs (well) and $\mathrm{Al_{0.3}Ga_{0.7}As}$ (barrier). At low temperatures the band diagram for such quantum wells can be drawn as in Fig.2(a). The effective electron mass in GaAs is $0.067m_0$ and that for heavy hole is $0.45m_0$. These values change in AlGaAs though the effect of the discontinuity is not very large and here we ignore it.

Real experimental photoluminescence spectrum for quantum wells $d =$ 5nm, 7.5nm, 10nm, 15nm at 4K is shown in Fig.2(a) (actually these quantum well are grown in a single film).

(i) Obtain the binding energies for the ground states of electrons and holes for the diagram in Fig.2(a), with $d =$ 5 nm, 7.5 nm, 10 nm, 15 nm.

(ii) From the above results calculate the energies of photon emission for band to band transitions.

(iii) The very left two peaks in Fig.2(b) are from bulk (GaAs substrate). The remaining four peak positions should also have some shifts from the above calculations. The shifts are due to binding energies of **excitions**. Namely, though it is not mentioned in the present lectures, the dominant luminescence is not due to the direct



(a) (b)

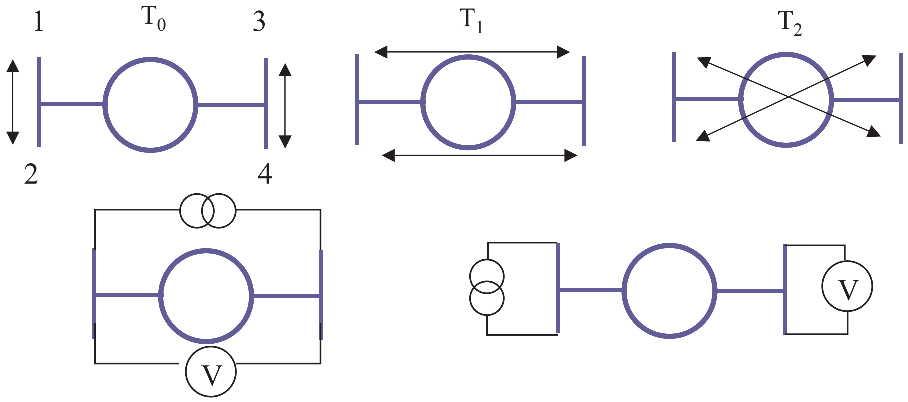
Figure 2: (a) Energy diagram for $\mathrm{GaAs/Al_{0.3}Ga_{0.7}As}$ quantum well. (b) Photoluminescence spectrum obtained at 4K in the experiment described here.

transition between the bound states but from recombination in bound states (excitons) of an electron and a hole.

Estimate the exciton binding energy for each quantum well from the above result of experiment and calculation. Does the binding energy increase or decrease with decreasing well width? C

VI Coherent transport I

(i) Derive Landauer formula for a four terminal quantum wire with transmission coefficient T by using Landauer-Buettiker formalism.
(ii) Treat an AB ring as a four terminal conductor with transmission coefficients shown in the upper row in the following figure.



Upper left: transmission coefficient between terminals 1-2 and 3-4 are T_0. Similarly, middle and right mean the coefficients are T_1 for 1-3 and 2-4, T_2 for 1-4 and 2-3. Lower left: circuit configuration for ordinary four terminal resistance R_c. The symbol of overlapping two shifted open circles is a constant current source. The encircled V is a voltmeter. Lower right is for "non-local" four terminal resistance R_{nl}.

Under the approximation $T_0 \gg T_1, T_2$, obtain the expression for ordinary four terminal resistance R_c, the measurement setup for which is shown in lower left in the above figure and that for so called non-local resistance R_{nl}

VII Coherent transport II

(i) Let MT be a transfer matrix of a potential barrier with a complex transmission coefficient t and a complex reflection coefficient r. Show that MT can be expressed as follows.

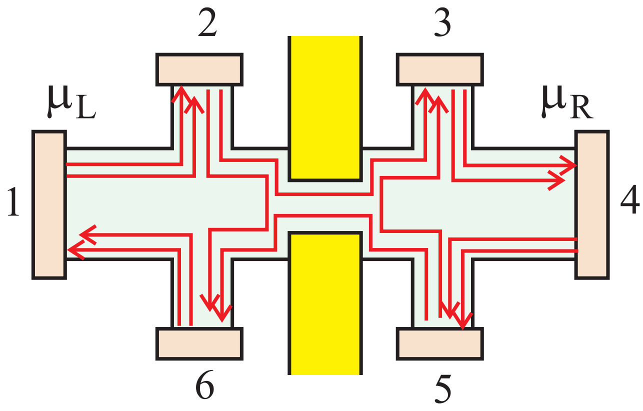
$$M_T = \begin{pmatrix} 1/t^* & -r^*/t^* \\ -r/t & 1/t \end{pmatrix}. \tag{8}$$

(ii) If an AB ring is a double slit system, the probability amplitude of outgoing wavefunction is written as

$$|\psi|^2 = |\psi_1|^2 + |\psi_2|^2 + 2|\psi_1||\psi_2| \cos\theta \tag{9}$$

which gives if we put $|\psi_1| = |\psi_2|$ and $\theta = -\pi$, zero. The result is apparently against the requirement of unitarity. Also in $\theta = e\Phi/\hbar + \theta_0$, if $\theta \neq 0$, Onsager reciprocity is also broken (Φ is magnetic flux piercing through the ring). Discuss what is wrong in the above "double slit model".

VIII Electric transport through edge modes



Let us consider a sample in the shape called “Hall bar”, which is illustrated in the left figure. The main difference between the present sample and ordinary Hall bar samples is a quantum point contact (QPC) placed in the center of the sample. Now a perpendicular magnetic field is applied and the sample is in the integer quantum Hall effect with the filling factor ν. Let the QPC be a state through which χ channels of the edge modes pass and the rests are reflected. A current source is connected to terminals 1 and 4. The chemical potentials of other terminals can be measured with ideal potentiometers.

Obtain the following quantities with Landauer-Büttiker formula.

(i) The longitudinal resistance R_{L} determined from the voltage between 2 and 3 (or 5 and 6).

(ii) The longitudinal resistance R_{H} determined from the voltage between 2 and 6 (or 3 and 5).

Appendix: Eigenstates in a triangular potential

Let us consider one dimensional triangular potential on x-axis. The time independent Schrödinger equation is written as

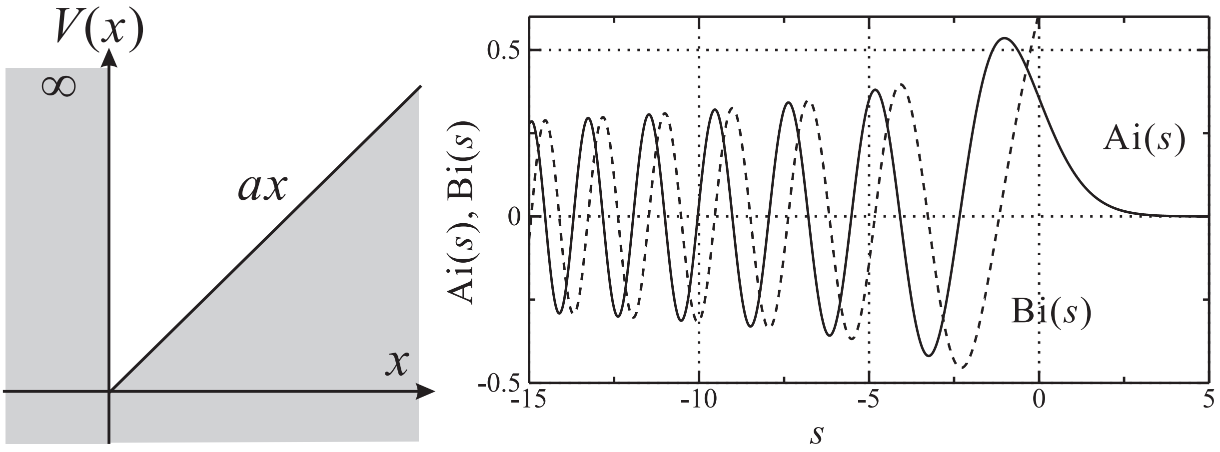
$$\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+V(x)\right)\psi=E\psi,\qquad V(x)=\begin{cases}ax & (x>0,\quad a>0)\\ \infty & (x\le 0)\end{cases}. \tag{10}$$

With adopting the transformation of the variable

$$s=\left(\frac{2ma}{\hbar^2}\right)^{1/3}\left(x-\frac{E}{a}\right), \tag{11}$$

the Schrödinger equation is transformed into

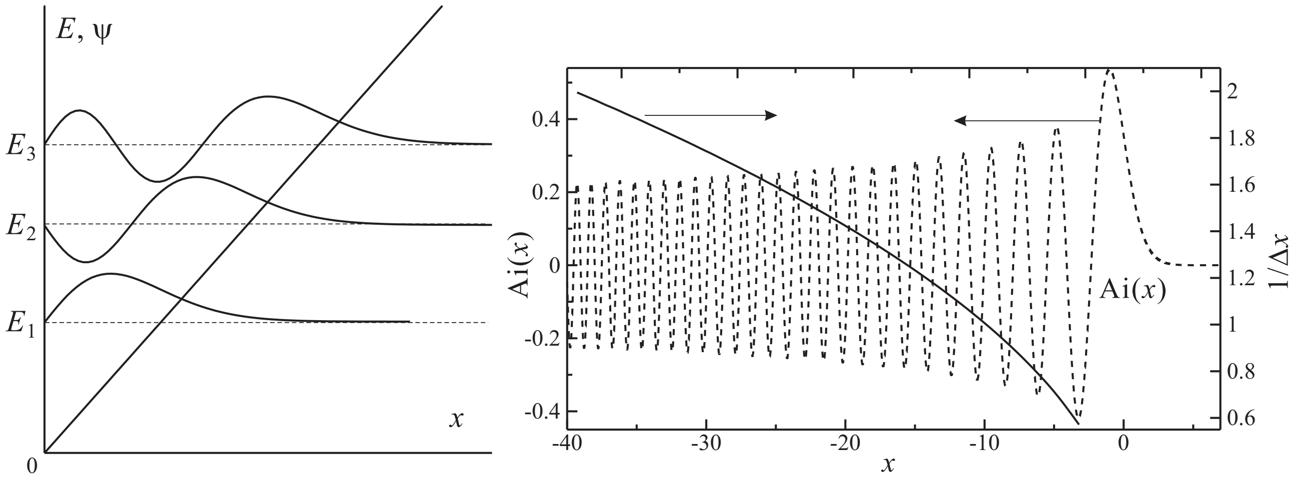
$$\frac{d^2\psi}{ds^2}=s\psi. \tag{12}$$



(a)

(b)

Figure 3: (a) illustrates a triangular potential. (b) illustrates Airy functions.



(a) (b)

Figure 4: (a) illustrates eigenenergies and eigenfunctions in a triangular potential for $n = 1, 2, 3$ from the ground state. (b) Let $\mathit{\Delta} x$ be the intervals of zero points in Airy function. In this figure $1/\mathit{\Delta} x$ is plotted against the midpoints between the zero points. The broken line is Airy function.

The equation is now in the form of differential equation called Airy's (or Stokes') differential equation.

The solutions to (12) are called **Airy functions** and classified with the asymptotic behavior in $s \to \infty$ into Ai for $\psi \to 0$ and Bi for $\psi \to \infty$. Some representatives of them are plotted in Fig.3(b).

As basis for the bound state wavefuntions, we should adopt Ai, which are zero at infinity. The asymptotic form for $s \to \pm\infty$ is given as

$$\mathrm{Ai}(s) \sim \frac{1}{2\sqrt{\pi}s^{1/4}} \exp\left(-\frac{2}{3}s^{3/2}\right) \quad (s \to \infty) \tag{13}$$

$$\sim \frac{1}{\sqrt{\pi}|s|^{1/4}} \cos\left(\frac{2}{3}|s|^{3/2} - \frac{\pi}{4}\right) \quad (s \to -\infty). \tag{14}$$

In $x < 0$, $V = \infty$ and $\psi = 0$, the boundary condition at $x = 0$ is thus $\psi(+0) = 0$. Ai(s) has many zeros and the boundary condition requires that one of which must fit to $x = 0$. Let us write such zero points as $s_1, s_2, \cdots s_n, \cdots$ in the order of the absolute value of s, then the energy eigenvalue E_n is obtained from (11) as

$$E_n = -\left(\frac{\hbar^2 a^2}{2m}\right)^{1/3} s_n. \tag{15}$$

From the asymptotic form (14),

$$s_n \sim -\left(\frac{3\pi(4n-1)}{8}\right)^{2/3} \tag{16}$$

is the asymptotic solution of s_n for $n \to \infty$.