Applied Quantum Mechanics

Chapter 7 problems

LAST NAME FIRST NAME

Problem 7.1

(a) Write a computer program to calculate the chemical potential for n non-interacting electrons per unit volume at temperature, T.

(b) Calculate the value of the chemical potential for the case when electrons of effective mass $m^* = 0.07 \times m_0$ and carrier density $n = 1.5 \times 10^{18}\ \text{cm}^{-3}$ are at temperature $T = 300$ K

(c) Repeat (b), only now for the case when electrons have effective electron mass $m^* = 0.50 \times m_0$.

(d) Plot the Fermi-Dirac distribution function for the situations described by (b) and (c).

(e) Repeat (b), (c), and (d), only now for the case when temperature $T = 77$ K.

Your answer should include a print out of your computer program and plots.

Problem 7.2

(a) Show that $\dfrac{1}{e^{(E-\mu)/k_B T}+1} = 1 - \dfrac{1}{e^{(\mu-E)/k_B T}+1}$

(b) A semiconductor consists of a valance band with electron energy dispersion relation $E_{VB} = E(\mathbf{k})$ and a conduction band with electron energy dispersion relation such that $E_{CB} = E_0 - E(\mathbf{k})$, where E_0 is a constant such that the conduction band and valence band are separated by an energy band gap, E_g. Show that when particle number is conserved, the chemical potential is in the middle of the band gap with value $\mu = E_0/2$ and is independent of temperature.

Problem 7.3

(a) Calculate the average energy of electrons in a three-dimensional gas of electrons. Show that in the low temperature limit $\langle E_{3D}(T \to 0\ \text{K})\rangle = \dfrac{3}{5}E_F$ and in the high temperature limit $\langle E_{3D}(T \to \infty\ \text{K})\rangle = \dfrac{3}{2}k_B T$.

(b) Calculate the average energy of electrons in a two-dimensional gas of electrons. Show that in the low temperature limit $\langle E_{2D}(T \to 0\ \text{K})\rangle = \dfrac{1}{2}E_F$ and in the high temperature limit $\langle E_{2D}(T \to \infty\ \text{K})\rangle = k_B T$.

Problem 7.4

The anti-symmetric wave function that describes two identical indistinguishable non-interacting particles is given by the Slater determinant

$$\psi_a(x_1, x_2) = \frac{1}{\sqrt{2}}\begin{vmatrix} \psi_1(x_1) & \psi_1(x_2) \\ \psi_2(x_1) & \psi_2(x_2) \end{vmatrix}$$

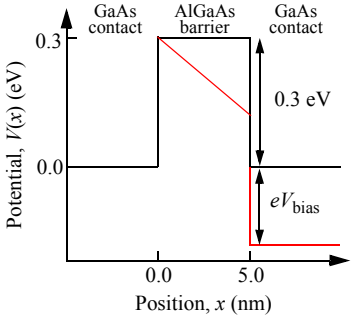
where rows label the single-particle state and columns label the particle. Position coordinate for particle 1 is x_1 and for particle 2 it is x_2.

(a) Plot $\psi_a(x_1, x_2)$ for the case when ψ_1 is the single-particle ground state of a one-dimensional rectangular potential well with infinite barrier energy and ψ_2 is the first excited state. Comment on the value of $|\psi_a(x_1, x_2)|^2$ when $x_1 = x_2$.

(b) Repeat the calculation in (a) but now for the case when ψ_1 is the single-particle first excited state and ψ_2 is the second excited state. Comment on your results.

(c) Repeat the calculations in (a) and (b) for symmetric wave functions $\psi_s(x_1, x_2)$. Comment on your results.

Problem 7.5



(a) Consider the conduction band minimum potential profile shown in the Fig. It consists of two GaAs contact layers and an AlGaAs potential energy barrier region. The contacts have the same *n*-type impurity concentration and the AlGaAs is intrinsic. The current due to a single electron in state $|\mathbf{k}\rangle$ with energy $E_\mathbf{k}$ is

$$J_e = e\frac{\hbar k_\perp}{m}T(E_\perp),$$

where $k_\perp = (\sqrt{2m(E_\perp - V(x))})/\hbar$ is the component of $\mathbf{k}$ perpendicular to the layer interface and $T(E_\perp)$ is the transmission coefficient. The total current flowing left-to-right involves all electron states in the left contact and so requires integrations over both $k_\perp$ and $k_\parallel$, where $k_\parallel = \sqrt{2mE_\parallel}/\hbar$ is the component of $\mathbf{k}$ parallel to the contact-barrier interface, and $E_k = E_\perp + E_\parallel$. If the probability of an electron mass m and charge e occupying state $|\mathbf{k}\rangle$ is given by the Fermi function $f(E_\mathbf{k}, \mu)$, the current due to the left contact is

$$J_L = e\int T(E_\perp)\frac{\hbar k_\perp}{m}\frac{dk_\perp}{2\pi}\int f(E_\mathbf{k}, \mu)\frac{d^2k_\parallel}{(2\pi)^2}$$

where μ is the chemical potential in the contact. Total current is the difference between the left contact and the right contact current. A positive bias voltage, V_{bias}, lowers the chemical potential energy of the right hand contact by eV_{bias}, and the total current is

$$J = e\int T(E_\perp)\frac{\hbar k_\perp}{m}\frac{dk_\perp}{2\pi}\int (f(E_\mathbf{k}, \mu) - f(E_\mathbf{k}, \mu - eV_{bias}))\frac{d^2k_\parallel}{(2\pi)^2}$$

Starting from this expression, use the one and two-dimensional densities of states to convert the integrals to energy and evaluate the integration over $k_\parallel$ to show that

$$J = \frac{emk_B T}{\pi^2 \hbar^3} \int_0^\infty T(E_\perp) \ln\left(\frac{1 + e^{(\mu - E_\perp)/k_B T}}{1 + e^{(\mu - E_\perp - eV_{bias})/k_B T}} \right) dE_\perp$$

(b) Use MATLAB to calculate current density through the potential barrier. Use an effective electron mass $m = 0.07 \times m_0$ and an initial voltage bias range of $0 < V_{bias} < 0.3$ V. The code developed for Problem 4.3 may be used to calculate the transmission probability, $T(E_\perp)$. As in the Fig., assume that the potential change due to V_{bias} appears linearly with position across the barrier. Plot the calculated current density using both linear and log scales. Explain the dependence of current density on voltage bias that you observe when impurity concentration has value $n = 10^{18}$ cm^{-3} and $n = 10^{16}$ cm^{-3} and when temperature has value $T = 300$ K and $T = 4.2$ K. Explain what you observe when you extend the voltage bias range to $0 < V_{bias} < 2.3$ V.

Problem 7.6

The minimum value of chemical potential μ_{min} at finite absolute temperature T may be found by assuming a particle distribution function that is obtained in the $T \to \infty$ limit.

(a) Show that in this case a three-dimensional electron gas of fixed density n_{3D} has minimum chemical potential

$$\mu_{min}(T) = k_B T \ln\left(\frac{n_{3D}}{2} \left(\frac{2\pi\hbar^2}{m_0 k_B T} \right)^{\frac{3}{2}} \right)$$

where m_0 is the electron mass.

(b) Find the expression for $\mu_{min}(T)$ of a two-dimensional electron gas.

(c) Find the expression for $\mu_{min}(T)$ of a one-dimensional electron gas.

(d) Plot the exact μ and minimum μ_{min} from part (a), (b), and (c), for normalized chemical potential μ / E_F as a function of normalized thermal energy $k_B T / E_F$, where E_F is the Fermi energy. Explain the differences you observe.

Problem 7.7

Three particles in a one-dimensional harmonic oscillator potential obey the Pauli exclusion principle. Assuming that any two microscopically distinguishable arrangements of the system with the same total energy are equally likely (the ergodic theorem), plot the probability of occupation as a function of energy for (a) the lowest energy state of the system, (b) when the total energy is $E_{total} = 13.5 \times \hbar\omega$, and (c) when total energy is $E_{total} = 48.5 \times \hbar\omega$. (d) Repeat (a) - (c) for the case when there are five particles. Comment on anything you learn.

Problem 7.8

The Hubbard model is used to describe systems in terms of interacting particles on a lattice. For a one-dimensional (1D) lattice with only two sites, the Hamiltonian for electrons of spin $\sigma = \uparrow$ or $\downarrow$ is

$$\hat{H} = -t \sum_{\langle i,j\rangle,\sigma} (\hat{c}^{\dagger}_{2,\sigma}\hat{c}_{1,\sigma} + \hat{c}^{\dagger}_{1,\sigma}\hat{c}_{2,\sigma}) + U\sum_{i}\hat{n}_{i,\uparrow}\hat{n}_{i,\downarrow}$$

where t is the nearest neighbor hopping matrix element, U is the additional energy associated with two electrons of opposite spin occupying the same lattice site, i, the electron creation and annihilation operators are $\hat{c}^{\dagger}$ and $\hat{c}$ respectively, and $\hat{n}$ is the electron number operator.

(a) If there are a total of two electrons in the system ($N = 2$), write down all possible states in the Fock particle number basis.

(b) Using the Fock basis and $\hat{H}$, calculate all matrix elements and derive expression for the eigenenergies in terms of the coupling strengths U and t by finding the eigenvalues for the matrix. Plot the eigenenergies as a function of the ratio U/t.

(c) Repeat (a) and (b) for the same one-dimensional lattice with two sites, but now for the cases when $N = 1, 3, 4$ and comment on what you learn.