

Chapter 6 problems

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**Problem 6.1**

(a) Numerically calculate the chemical potential for  $n_0$  non-interacting electrons per unit volume at temperature,  $T$ .

(b) Calculate the value of the chemical potential for electrons of effective mass  $m_e^* = 0.07 \times m_0$  and carrier density  $n_0 = 1.5 \times 10^{18} \text{ cm}^{-3}$  at temperature  $T = 300 \text{ K}$ .

(c) Repeat (b) for electrons with effective electron mass  $m_e^* = 0.50 \times m_0$ .

(d) Plot the Fermi-Dirac distribution function for case (b) and (c).

(e) Repeat (b), (c), and (d) for the case when temperature  $T = 77 \text{ K}$ .

**Problem 6.2**

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

(b) A semiconductor has valance band electron energy dispersion relation  $E_{\text{VB}} = E(\mathbf{k})$  and conduction band electron energy dispersion relation  $E_{\text{CB}} = E_0 - E(\mathbf{k})$ , where  $E_0$  is a constant such that the conduction band and valance 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 6.3**

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

that  $\langle E_{3\text{D}}(T \rightarrow \infty \text{ K}) \rangle = \frac{3}{2} k_B T$  in the high temperature limit.

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

**Problem 6.4**

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

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

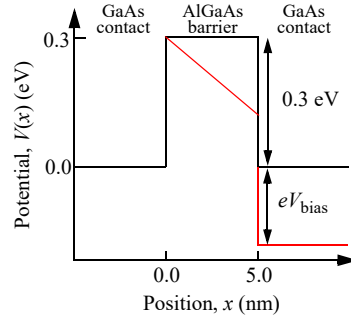
where rows label the single-particle state and columns label the particle. Position coordinate for particle 1 is  $x_1$  and for particle 2 it is  $x_2$ .

(a) Plot  $\Psi_a(x_1, x_2)$  for the case when  $\psi_1$  is the single-particle ground state of a one-dimensional rectangular potential well with infinite barrier energy and  $\psi_2$  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  $\psi_1$  is the single-particle first excited state and  $\psi_2$  is the second excited state. Comment on the results.

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

### Problem 6.5



(a) Consider the conduction band minimum potential profile shown in the figure. 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

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

where  $k_{\perp}$  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

$k_{\parallel} = \sqrt{2m_e^*E_{\parallel}}/\hbar$  is the component of  $\mathbf{k}$  parallel to the contact-barrier interface, and  $E_{\mathbf{k}} = E_{\perp} + E_{\parallel}$ . If the probability of an electron mass  $m_e^*$  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

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

where  $\mu$  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,  $V_{\text{bias}}$ , lowers the chemical potential energy of the right hand contact by  $eV_{\text{bias}}$ , and the total current is

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

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

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

(b) Calculate current density through the potential barrier using an effective electron mass  $m_e^* = 0.07 \times m_0$  and a voltage bias range of  $0 < V_{\text{bias}} < 0.3 \text{ V}$ . As in the figure, assume that the potential change due to  $V_{\text{bias}}$  is linear 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  $n_0 = 10^{18} \text{ cm}^{-3}$  and  $n_0 = 10^{16} \text{ cm}^{-3}$  and when temperature has value  $T = 300 \text{ K}$  and  $T = 4.2 \text{ K}$ . Explain what is observed when the voltage bias range is extended to  $0 < V_{\text{bias}} < 2.3 \text{ V}$ .

### Problem 6.6

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

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

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

where  $m_0$  is the electron mass.

(b) Find the expression for  $\mu_{\text{min}}^{2D}(T)$  of a two-dimensional electron gas.

(c) Find  $\mu_{\text{min}}^{1D}(T)$  for a one-dimensional electron gas.

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

### Problem 6.7

Three identical indistinguishable non-interacting 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  $E_{\text{total}} = 13.5 \times \hbar\omega$ , and (c) when total energy is  $E_{\text{total}} = 48.5 \times \hbar\omega$ . (d) Repeat (a) - (c) for the case when there are five particles. Comment on anything learned.

### Problem 6.8

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

$$\hat{H} = -t_{\text{hop},1} \sum_{\langle i,j \rangle, \sigma_s} (\hat{c}_{2,\sigma_s}^\dagger \hat{c}_{1,\sigma_s} + \hat{c}_{1,\sigma_s}^\dagger \hat{c}_{2,\sigma_s}) + U \sum_i \hat{n}_{i,\uparrow} \hat{n}_{i,\downarrow}$$

where  $t_{\text{hop},1}$  is the nearest neighbor hopping matrix element,  $U$  is the additional energy associated with two electrons of opposite spin occupying the same lattice site, the elec-

tron 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  $t_{\text{hop},1}$  by finding the eigenvalues for the matrix. Plot the eigenenergies as a function of the ratio  $U/t_{\text{hop},1}$ .

(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 is learned.

### Problem 6.9

Explain why the statement “The wave function  $\psi(\mathbf{r})$  is a function of three-dimensional real-space” is incorrect.

### Problem 6.10

An electron gas obeys Fermi-Dirac statistics at temperature  $T$  and is constrained to motion in the  $x$ -direction. A potential barrier of infinite energy is placed at position  $x = 0$  such that potential  $V(x > 0) = \infty$  and  $V(x \leq 0) = 0$ .

(a) By considering a region that confines electrons of effective electron mass  $m_e^*$  from  $x = 0$  to  $x = L < 0$ , find the normalized electron energy eigenstates and explain how taking the limit  $L \rightarrow -\infty$  creates a continuum of states.

(b) At sufficiently high temperatures the Fermi-Dirac distribution may be approximated by a Maxwell-Boltzmann distribution. Find an analytic expression for the electron density  $n = n(x, T)$  in terms of a characteristic length scale,  $\lambda_e = \hbar / \sqrt{2m_e^*k_B T}$ . Explain why  $n$  has a smaller value near  $x = 0$  than when  $x \ll -\lambda$ . Plot the density  $n = n(x, T)$  at temperatures  $T = 300$  K,  $T = 100$  K, and  $T = 10$  K for electrons with effective electron mass  $m_e^* = 0.07 \times m_0$ .

(c) When temperature  $T < E_F/k_B$  the Fermi-Dirac distribution may not be approximated by a Maxwell-Boltzmann distribution. Find and explain the spatial dependence of carrier concentration  $n = n(x, T)$  for temperatures  $T = 300$  K,  $T = 100$  K,  $T = 10$  K, and  $T = 0$  K.

$$\text{Note } \int_0^\infty e^{-a\xi^2} d\xi = \frac{1}{2} \sqrt{\frac{\pi}{a}} \text{ and } \int_{\xi=0}^{\xi=\infty} e^{-a\xi^2} \cos(b\xi) d\xi = \sqrt{\frac{\pi}{4a}} e^{\frac{-b^2}{4a}} \text{ for } \text{Re } a > 0.$$

### Problem 6.11

A fermion system has chemical potential  $\mu(T = 3 \text{ K}) = 52.1 \text{ meV}$  and  $\mu(T = 300 \text{ K}) = 38.9 \text{ meV}$ . Plot the Fermi-Dirac distribution  $f(E)$  and the Bose distribution  $g(E)$  as a function of energy  $0 < E < 200 \text{ meV}$ . Explain the difference in the curves obtained. What is expected to happen to the distribution functions in the high-temperature limit?