Statistical Mechanics / Quantum Mechanics

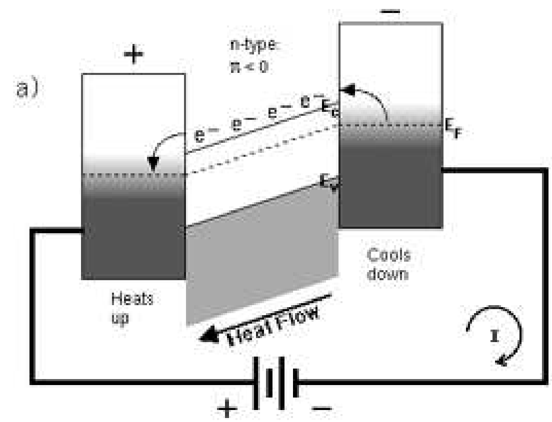
General Exam Questions for August 24, 2007

Instructions

Answer two questions from the Statistical Mechanics section and four questions from the Quantum Mechanics section, for a total of six problems. Put each of your solutions in a separate answer book. Make sure that you label and sign your name on the cover of each book.

I. Statistical Mechanics

1. A Peltier junction consists of two identical metallic electrodes separated by a semiconductor. The electrons in each of the electrodes behave like an ideal Fermi gas of Fermi level E_F in internal thermal equilibrium. The semiconductor acts like a wall separating the two gas containers that allows electrons of energy $E_C - E_F$ above the Fermi level to pass freely between the two electrodes, but provides an impenetrable barrier to electrons of lower energies.



   a) What is the average occupation probability for an individual electron state of energy $E_C - E_F$ above the Fermi level in one of the metal electrodes at temperature T? You may assume that $E_C - E_F \gg kT$. What physical parameter plays the role of the chemical potential μ?

   b) What potential difference V is required in order to keep the occupation probabilities of the two gases equal at E_C, in the case where the two electrodes are at different temperatures T_1 and T_2 and no current flows in the circuit?

   c) How much thermal energy ΔQ is removed from an electrode when an electron passes through the junction from that gas to the other side? *Hint: The overall neutrality of the metal ensures that the total number of electrons in each gas is stable; any net flow of electrons through the junction is compensated by electrons flowing in the external circuit loop (see figure) which enter and leave at energy E_F.*

   d) If thermal sources and sinks are attached to the two electrodes, this device can serve as a refrigerator. Show that the coefficient of performance $\epsilon = \Delta Q/\Delta W$ is the same as the Carnot refrigerator. You should assume that half of the electrical work dissipated in the junction is transferred to each of the two electrodes in the form of thermal energy.

2. At room temperature and pressure, hydrogen is stable as a gas of diatomic molecules. The two electrons in the molecular ground state share a common orbital that has zero angular momentum projection onto the bond axis passing through the two nuclei. At room temperature it is possible to ignore electronic excitations of the molecule and consider that all molecules in a gas in thermal

equilibrium at 300K are in the electronic ground state. The total nuclear spin I can be either 0 (parahydrogen) or 1 (orthohydrogen).

a) What rotational states are allowed? What are their energies and degeneracies?

b) What is the ratio of parahydrogen to orthohydrogen at room temperature T?

c) What is the ratio of parahydrogen to orthohydrogen at temperatures where kT is large compared to the lowest rotational level spacing but small compared to the ionization energy?

3. Consider a material with an equation of state

$$P = \frac{\alpha T}{V^2}$$

where α is a constant. The heat capacity of this material at constant volume is linear in temperature $C_V = A(V)T$.

a) Using Maxwell's relations or other equations, find the derivative of entropy $(\partial S/\partial V)_T$.

b) Prove that the coefficient $A(V)$ is independent of V.

c) Find $S(V, T)$ assuming that the value $S(T_0, V_0) = S_0$.

d) Find the heat capacity at constant pressure $C_P = T(\partial S/\partial T)_P$.

4. A classical gas of non-interacting atoms is in thermal equilibrium at temperature T in a container of volume V and surface area A. The potential energy of the atoms in the bulk is zero. Atoms adsorbed on the surface have a potential energy $V = -E_0$ and behave as an ideal two-dimensional gas. The two gases are in thermal equilibrium with each other, with density $n = N_{\text{bulk}}/V$ in the bulk and areal density $\sigma(n, T) = N_{\text{surface}}/A$ on the surface.

a) What are the chemical potentials of the two gases in terms of n, σ, E_0 and T?

b) Find an analytical expression for $\sigma(n, T)$.

Useful integral:

$$\int_{-\infty}^{\infty} e^{-x^2/2} dx = \sqrt{2\pi}$$

II. Quantum Mechanics

1. The water molecule consists of two hydrogen atoms bonded to an oxygen atom. The angle between the hydrogen bonds is approximately 105°. At excitation energies too small to excite vibrational levels or electronic transitions, the free molecule behaves as a quantum mechanical asymmetric top with angular coordinates given by the Euler angles ϕ, θ, ψ. The Hamiltonian for this problem is given by

$$H_{\text{rot}} = \frac{1}{2I_1}J_1^2 + \frac{1}{2I_2}J_2^2 + \frac{1}{2I_3}J_3^2.$$

It is convenient to order the molecular body axes such that $I_1 > I_2$ and the third axis is aligned with the molecular electric dipole moment. The three operators obey the standard commutation relations

$$[J_i, J_j] = i\epsilon_{ijk}J_k.$$

The eigenfunctions of this Hamiltonian may be expanded in terms of the D-functions $D^j_{m,\kappa}(\phi, \theta, \psi)$ which have the following behavior under the J_i operators.

$$\begin{aligned} J^2 D^j_{m,\kappa} &= \hbar^2 j(j+1) D^j_{m,\kappa} \\ J_3 D^j_{m,\kappa} &= \hbar\kappa D^j_{m,\kappa} \\ J_\pm D^j_{m,\kappa} &= \hbar\sqrt{j(j+1) - \kappa(\kappa \pm 1)}\, D^j_{m,\kappa\pm 1} \end{aligned}$$

The quantum number κ represents the projection of the angular momentum onto the principal molecular axis corresponding to I_3. It is restricted to the range $[-j, j]$. The other magnetic quantum number m is restricted to the same range and indicates the orientation of the system within the fixed laboratory frame. Other than contributing an additional degeneracy factor $2j + 1$ to each level in the spectrum, it does not play an explicit role in the eigenvalue problem.

a) Sketch the molecule, labeling the three molecular axes in your figure. What restriction on the allowed values of κ is implied by the symmetry of the molecule?

b) Rewrite H_{rot} in terms of the quantum operators J^2, J_3^2, and $J_\pm = J_1 \pm iJ_2$.

c) What are the energy eigenvalues of the four lowest-lying states? What are the corresponding eigenstates, expanded in the basis $|j, m, \kappa\rangle$?

2. A nanomachine contains a pendulum that consists of an approximately massless arm of length ℓ that swings freely about a fixed point on one end. To the other end of the arm is attached a bob of mass m. The pendulum is constrained to swing in a vertical plane, in which it can move freely through the full 360° subject to uniform gravitational acceleration g.

   a) Write down the Hamiltonian for this system in terms of the angle θ that the arm makes with the vertical, and its conjugate momentum.

   b) Consider the gravitational constant g to be a small parameter. In the limit of zero g, what are the energy eigenvalues and corresponding wavefunctions for this pendulum?

   c) Compute the ground-state wavefunction to the lowest non-vanishing order in g.

   d) Compute the ground-state energy to the lowest non-vanishing order in g.

3. The Schrodinger equation for an electron of mass m in a spherically symmetric potential $V(r)$ is conveniently written as

$$\left[-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial r^2}+\frac{2}{r}\frac{\partial}{\partial r}\right)+\frac{1}{2mr^2}L^2+V(r)\right]\psi(\vec{r})=E\psi(\vec{r})$$

where $\vec{L}$ is the angular momentum operator.

   a) Consider the hydrogen atom with the potential

$$V(r)=-\frac{e^2}{r}$$

   Assume that the electron is in the s-wave ground state of the hydrogen atom

$$\psi_0(\vec{r})=NR(r)$$

   where $R(r)$ is of the form $e^{-\beta r}$. Find the energy eigenvalue E and β in terms of $\hbar$, m, and e.

   b) An electron is in the ground state of tritium which has a nucleus with one proton and two neutrons. A nuclear reaction instantaneously changes the nucleus to ^{3}He which has two protons and one neutron. Calculate the probability that the electron is in the ground state of ^{3}He after the transition, assuming that the nuclear beta decay occurs with negligible nuclear recoil.

Useful integral:

$$\int_0^\infty r^2 e^{-\gamma r} dr = \frac{2}{\gamma^3}$$

4. Consider a variational estimate of the ground state energy for a particle of mass m in the one-dimensional potential

$$V(x) = \begin{cases} \infty, & x < 0 \\ 0, & 0 < x < a \\ V_0, & x > a \end{cases}$$

The Hamiltonian is given by the following expression.

$$H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)$$

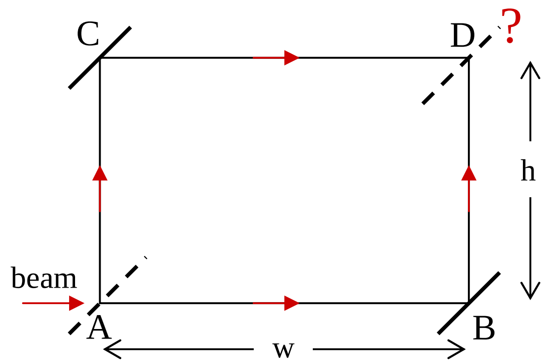
a) As a variational ansatz use $\psi(x) = \sin(\pi x/L)$ for $0 \le x \le L$, and $\psi(x) = 0$ otherwise, where the variational parameter L is slightly greater than the width a of the potential well. Here you may assume that $V_0 \gg \hbar^2/(ma^2)$, that is, the height of the potential is much larger than the ground state energy. Calculate an approximate value for

$$\Delta \equiv L - a \ll a$$

by minimizing the expectation value of the Hamiltonian in the state ψ.

b) Compute the ground state energy to leading order in Δ/a.

5. Consider a beam of mono-energetic neutrons split into two beams at point A using a Bragg mirror, as shown in the figure, such that the intensities of the two beams are equal. The two beams undergo further reflections at points B and C and are combined again using a second Bragg mirror at point D. The sides of the rectangle ABCD are at right angles and lie in a plane. For the purpose of this problem, the Bragg mirrors may be treated as ideal planar interfaces of negligible thickness.



   a) Show quantitatively and describe in words what happens when a wave packet is split at A. What are the amplitudes and phase shifts induced by the mirror in the transmitted and reflected waves? Answer the same questions for what happens when the two packets come together again at D.

   b) The closed loop formed by the paths ABD and ACD is rotated by an angle δ about segment AC. Again, show quantitatively and describe in words what happens when a wave packet in each beam is brought together at D.

   c) Imagine that the incident neutron beam contains r particles per second. What is the rate of neutrons emerging from point D as a function of δ? Does this apparatus create or destroy neutrons?

6. Consider an isotropic harmonic oscillator in two dimensions. The Hamiltonian is given by the following form.

$$H = \frac{p_x^2}{2m} + \frac{p_y^2}{2m} + \frac{m\omega^2}{2}\left(x^2 + y^2\right).$$

Its eigenfunctions can be represented by the eigenkets $|n_x n_y\rangle$ where n_x is the eigenvalue of the operator $a_x^+ a_x^-$ with $a_x^\pm = (m\omega x \mp i p_x)/\sqrt{2m\hbar\omega}$. Similar expressions also apply to the y degrees of freedom.

   a) What are the energies of the three lowest lying states? Is there any degeneracy?

   b) If a perturbation, $V = \delta m\omega^2 xy$ with $\delta \ll 1$ is applied, find the first order energy eigenket in terms of the unperturbed eigenkets $|n_x n_y\rangle$ and the corresponding first order energy shift for each of the three states found above.