

PHYS 813: Statistical Mechanics, Assignment 10

Due 5/15/08

1. Consider an ideal quantum gas of N electrons in a cube of volume V at the temperature $T = 0$.
 - (a) Using the energy expression for a particle in the box, find to the leading order the number of states per energy interval.
 - (b) Calculate the total average energy \bar{E} in terms of the Fermi energy ϵ_F (the energy of the highest occupied state). Then find the relation between N and ϵ_F and eliminate ϵ_F from the expression for \bar{E} .
 - (c) Show that \bar{E} is an extensive quantity as a function of V and N (i.e., upon the increase of system size). Thus, \bar{E} is not proportional to N for a fixed volume, as one would expect for noninteracting particles. Explain the apparent paradox.
2. A white-dwarf star is thought to consist of helium nuclei which can be described classically and a degenerate electron gas. The gas can be considered degenerate despite the temperature of the star being about 10^7 K since the Fermi energy is much larger than kT due to high density.
 - (a) Because of the high densities, the relativistic effects should be important. Assuming that the density of a white-dwarf star is 10^7 g/cm³, find how the (nonrelativistic) Fermi energy compares to the electron rest energy.
 - (b) Calculate the pressure of the degenerate electron gas under these conditions, neglecting relativistic effects.
3. Despite its simplicity, the free-electron model of the electron conduction in metals predicts various properties quite successfully. Use this model to calculate the isothermal compressibility $\kappa = -(1/V)(\partial V/\partial p)_T$ of a metal as a function of the electron number density n and the Fermi energy ϵ_F at $T = 0$ K. You may use without proof the relation:

$$\frac{pV}{kT} = \ln \mathcal{Z}(V, T, \mu) = \frac{2V}{\lambda^3} f_{5/2}(z)$$

where $\mathcal{Z}(V, T, \mu) = \prod (1 + e^{-(\epsilon_i - \mu)/kT})$ is the grand canonical partition function expressed through single-particle energies ϵ_i and

$$f_n(z) = \frac{1}{\Gamma(n)} \int_0^\infty \frac{x^{n-1} dx}{z^{-1} e^x + 1},$$

with $\Gamma(n) = (n-1)(n-2)\dots\frac{1}{2}\sqrt{\pi}$ for half integer arguments and $z = e^{\mu/kT}$.

4. Consider the virial expansion

$$\frac{pv}{kT} = 1 - \sum_{j=1}^{\infty} \frac{j\beta_j}{j+1} \left(\frac{\lambda^3}{v}\right)^j$$

where v is the molar volume, β_j are functions of T called irreducible cluster integrals, and λ is the thermal length. Assume that only the terms with j equal to 1 and 2 are appreciable in the critical region. Determine the relationship between β_1 and β_2 at the critical point. Then find the ratio $kT_c/p_c v_c$, where the subscript c denotes the values at the critical point.

5. For a superconductor in a weak external magnetic field, the difference in the Gibbs free energy between the normal (G_n) and the superconducting (G_s) state can be expressed as $G_n - G_s = \mu_0 H_c(T)^2/2$ where μ_0 is the permeability of vacuum and $H_c(T)$ is the minimal magnetic field required to destroy superconductivity $H_c(T) = H_0 [1 - (T/\Upsilon)^2]$. The symbol Υ in the last expression denotes a constant and H_0 is clearly just the limit value of H_c at $T = 0$.

- (a) Find the entropy difference and the difference in specific heat between the normal and superconducting state.
- (b) Calculate the superconducting to normal transition temperature at zero field.
- (c) Is this a first-order (discontinuous entropy) or second-order (continuous entropy but discontinuous entropy derivative) phase transition?

Hint: This is a simple problem.

6. The detailed balance condition $\pi_{rs}/\pi_{sr} = e^{-\beta(E_s - E_r)}$ in Monte Carlo simulations, where π is the stochastic matrix and E is the energy, can be fulfilled in many ways. Also, one traditionally expresses the stochastic matrix as $\pi_{rs} = P_{rs}a_{rs}$, where P_{rs} is the probability that the system makes the *trial* move from configuration r to s and a_{rs} is the probability that this move is accepted.
- (a) In most simulation, one of the symmetric acceptance probabilities is assumed to be equal to one. For an arbitrary P_{rs} , specify the form of a_{rs} that maintains the detailed balance when $a_{sr} = 1$.
 - (b) Consider a system with energy levels $E_r = \hbar\omega(r + 1/2)$, $r = 0, 1, 2, \dots$. Assume the system can change its energy only by $\hbar\omega$, so that all probabilities P_{rs} depend on a single parameter, for example,

$$P_{rs} = \begin{cases} p & \text{if } s = r + 1 \\ 1 - p & \text{if } s = r - 1 \\ 0 & \text{otherwise} \end{cases}$$

Find the value of p that minimizes the probability that if the system is in state r , it will make *no* transition. Contrast this result with that of the Metropolis algorithm.