PHYS 813: Statistical Mechanics, Assignment 9

Due 5/19/09

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 consistst 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/cm^3, 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. Use the free-electron model of the electrons in metals to calculate the isothermal compressibility $\kappa = -(1/V)(\partial V/\partial p)_{T,N}$ of a metal. First, do not assume low temperature and obtain an expression for κ in terms of the Fermi functions f_n defined below. Then show that for $T \to 0$ this expression simplifies to the one derived in a previous problem and depending on the Fermi energy ϵ_F. You may use without proof the relations:

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

where $\lambda = h/\sqrt{2\pi mkT}$, $\mathcal{Z}(V,T,\mu) = \Pi\left(1 + \mathrm{e}^{-(\epsilon_i-\mu)/kT}\right)$ is the grand canonical partition function expressed through single-particle energies ϵ_i, and

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

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

$$N = \frac{2V}{\lambda^3} f_{3/2}(z);$$

$$\frac{df_n(z)}{dz} = \frac{1}{z} f_{n-1}(z).$$

4. The density of (single-particle) states $g(\epsilon)$ is a different function of energy ϵ for different ideal Fermi gases (e.g., two-dimensional, three-dimensional, relativistic, etc.). However, at low temperature T, some properties of the systems depend on $g(\epsilon)$ in the same way. Show that, in particular, the chemical potential μ and heat capacity C_V are given by

$$\mu \approx \epsilon_{\mathrm{F}} \left[1 - \frac{\pi^2}{6} \left(\frac{\partial \ln g(\epsilon)}{\partial \ln \epsilon}\right)_{\epsilon=\epsilon_{\mathrm{F}}} \left(\frac{kT}{\epsilon_{\mathrm{F}}}\right)^2\right]$$

and

$$C_V \approx \frac{\pi^2}{3} k^2 T g(\epsilon_{\rm F})$$

where $\epsilon_{\rm F}$ is the Fermi energy. *Hint*: use the following asymptotic expansion of the integral

$$\int_0^\infty \frac{\phi(x)dx}{{\rm e}^{x-\xi}+1} = \int_0^\xi \phi(x)dx + \frac{\pi^2}{6}\left(\frac{d\phi}{dx}\right)_{x=\xi} + \cdots$$

valid for any well-behaving $\phi(x)$.

5. 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.

6. 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 premeability of vacuum and $H_c(T)$ is the minimal magnetic field required to destroy superconductivity $H_c(T) = H_0\left[1-(T/\Upsilon)^2\right]$. 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.

7. The detailed balance condition $\pi_{rs}/\pi_{sr} = {\rm e}^{-\beta(E_s-E_r)}$ in Monte Carlo simulations, where π is the stochastic matrix and E is the energy, can be fullfilled 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 $E_r = \hbar\omega(r + 1/2)$, $r = 0, 1, 2, \ldots$. Assume the system can change its energy only by $\hbar\omega$, so that all probabilities P_{rs} depend on a single parameter, for example,

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

   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.