

## PHYS 813: Statistical Mechanics, Assignment 7

Due 4/30/09

1. Consider  $N$  noninteracting free particles in a box with periodic boundary conditions, in the momentum representation. The particles are in equilibrium with a heat bath and therefore are described by the canonical distribution. Denote the eigenfunctions of the one-particle Hamiltonian as

$$\phi_{\mathbf{k}}(\mathbf{r}) = \frac{1}{L^{3/2}} e^{i\mathbf{k}\cdot\mathbf{r}}.$$

Assume the many-particle wave function to be a product of one-particle functions.

- (a) Calculate the canonical partition function and compare your result with the classical one. Is your result physically acceptable? If not, what are the reasons for it?
  - (b) Calculate the canonical density matrix in the basis  $\phi_{\mathbf{k}}(\mathbf{r})$  and then transform it into the position representation (i.e., the matrix elements of  $\hat{\rho}$  should become functions of  $\mathbf{r}$  and  $\mathbf{r}'$ ).
2. Consider the trace of an operator  $\hat{O}$  defined as

$$\begin{aligned} \text{Tr}(\hat{O}) &= \sum'_{\mathbf{k}_1, \dots, \mathbf{k}_N} \langle \mathbf{k}_1, \dots, \mathbf{k}_N | \hat{O} | \mathbf{k}_1, \dots, \mathbf{k}_N \rangle \\ &= \sum_{\mathbf{k}_1, \dots, \mathbf{k}_N} C(\mathbf{k}_1, \dots, \mathbf{k}_N) \langle \mathbf{k}_1, \dots, \mathbf{k}_N | \hat{O} | \mathbf{k}_1, \dots, \mathbf{k}_N \rangle \end{aligned}$$

for  $N$  particles in a box with periodic boundary conditions, where  $\mathbf{k}_i$  is the wave vector of  $i$ th one-particle state. The prime in the first sum denotes restriction of the summation to such terms that a given state appears only once. In the second sum the summation is unrestricted but the numerical factor balances the repeated counting of the same state. Find an expression for  $C$  for the Maxwell-Boltzmann, Bose-Einstein, and Fermi-Dirac statistics. The factor may depend on  $N$  and the occupation numbers of one-particle wave functions.

3. Derive, for all three statistics, the relevant expressions for the quantity  $\langle n_\epsilon^2 \rangle - \langle n_\epsilon \rangle^2$ . Begin from finding the respective probabilities,  $p_\epsilon(n)$ , that there are exactly  $n$  particles in state  $\epsilon$ . Express your result in terms of the derivative of  $\langle n_\epsilon \rangle$  with respect to the chemical potential. Compare your result with the expression for the fluctuation of the number of particles for the classical grand canonical distribution.
4. Show that if the occupation number  $n_\epsilon$  of an energy level  $\epsilon$  is restricted to the values  $0, 1, 2, \dots, l$ , then the mean occupation number of that level is

$$\langle n_\epsilon \rangle = \frac{1}{z^{-1}e^{\beta\epsilon} - 1} - \frac{l+1}{(z^{-1}e^{\beta\epsilon})^{l+1} - 1}$$

Check next that  $l = 1$  gives the Fermi-Dirac result, whereas  $l \rightarrow \infty$  gives the Bose-Einstein result.

5. Show that for an ideal Bose gas both  $\gamma = C_p/C_V$  and  $C_p$  diverge at the critical temperature  $T_c$ , where  $C_p$  and  $C_V$  are heat capacities at constant pressure and volume, respectively.

(a) First, from the relation

$$pV/kT = \ln \mathcal{Z}(V, T, \mu) = - \sum \ln \left( 1 - e^{-(\epsilon_i - \mu)/kT} \right) = \frac{V}{\lambda^3} g_{5/2}(z),$$

where  $g_n(z) = \frac{1}{\Gamma(n)} \int_0^\infty \frac{x^{n-1} dx}{z^{-1}e^x - 1}$ , show that

$$\frac{1}{z} \left( \frac{\partial z}{\partial T} \right)_p = - \frac{5g_{5/2}(z)}{2Tg_{3/2}(z)}.$$

Similarly one can show (do not do this) that

$$\frac{1}{z} \left( \frac{\partial z}{\partial T} \right)_v = - \frac{3g_{3/2}(z)}{2Tg_{1/2}(z)}, \quad v = V/N.$$

(b) Show that at constant average number of particles  $N$ ,  $S$  depends only on  $z$ . You may use the formulas for the average energy and number of particles:  $U = (3/2)kT(V/\lambda^3)g_{5/2}(z)$  and  $N = (V/\lambda^3)g_{3/2}(z) + z/(1-z)$ .

(c) Now show that (show the first equality, as the second one is trivial)

$$\gamma = \frac{(\partial z / \partial T)_p}{(\partial z / \partial T)_v} = \frac{5g_{5/2}(z)g_{1/2}(z)}{3g_{3/2}(z)^2}$$

(d) Based on this equation, show the divergence of  $\gamma$  and  $C_p$ . *Hint:*  $z \rightarrow 1$  as  $T$  approaches  $T_c$  from above.

6. A gas of  $N$  spinless and noninteracting Bose particles of mass  $m$  is enclosed in a volume  $V$  at temperature  $T$ .

- (a) Find an expression for the density of single-particle states  $g(\epsilon)$  as a function of the single particle energy  $\epsilon$  using the classical expression. Sketch the result.
- (b) Write down an expression for the mean occupation number of a single-particle state  $\bar{n}_\epsilon \equiv \langle n_\epsilon \rangle$  as a function of  $\epsilon$ ,  $T$ , and the chemical potential  $\mu(T)$ . Draw this function on your sketch of part (a) for a moderately high temperature, i.e., the temperature above the Bose-Einstein transition. Indicate the place on the  $\epsilon$ -axis where  $\epsilon = \mu$ .
- (c) Write down an integral expression that implicitly determines  $\mu(T)$  (think of a quantity that remains unchanged as  $T$  decreases). On your sketch from point (a), mark the direction where  $\mu$  moves as  $T$  is lowered.
- (d) Find an expression for the Bose-Einstein transition temperature,  $T_c$ , below which one must have a macroscopic occupation of some single-particle states (consider a point where  $\mu(T)$  is already very close to its limit value but the number of particles in the ground state is still very small).
- (e) Describe  $\bar{n}_\epsilon(T)$  for  $T < T_c$ . Refer the results to the graph from point (a).
- (f) Find an exact expression for the total energy  $U(T, V)$  of the gas for  $T < T_c$ .