PHY 4523 Spring 2001 – Homework 4

Due at the start of class on Friday, March 2.

Answer all questions. To gain full credit you should explain your reasoning and show all working. Please write neatly and include your name on the front page of your answers.

1. *Canonical ensemble with continuous microstates.* (Based on Reif Problem 6.11.)

   Consider a pair of atoms which are constrained to move only along the x direction. Let x_j and p_j be the position and momentum of atom j ($j = 1, 2$). Assume that the total energy of the pair can be written

   $$E = \frac{p_1^2}{2m} + \frac{p_2^2}{2m} + U(x_1 - x_2) \tag{1}$$

   where m is the mass of each atom and $U(r)$ is the Lennard-Jones potential, which describes the atomic interaction in the group VIII elements He, Ne, Ar Kr, and Xe:

   $$U(r) = U_0 \left[\left(\frac{a}{r}\right)^{12} - 2\left(\frac{a}{r}\right)^{6} \right]. \tag{2}$$

   Here U_0 and a characterize the strength and range of the potential, respectively.

   Provided that the atoms are maintained in thermal contact with a heat reservoir, the expectation (mean) value of any quantity $y(x_1, p_1, x_2, p_2)$ can be written

   $$\langle y \rangle = \frac{\int dx_1 dp_1 dx_2 dp_2 \; y \, e^{-\beta E}}{\int dx_1 dp_1 dx_2 dp_2 \; e^{-\beta E}}. \tag{3}$$

   Using the preceding information,

   (a) calculate the mean separation between the atoms, $\bar{x}(T) = \langle |x_1 - x_2| \rangle$;

   (b) calculate the linear coefficient of thermal expansion, $\alpha = \dfrac{1}{\bar{x}} \dfrac{\partial \bar{x}}{\partial T}$.

   The following hints may simplify the problem:

   (i) Given the form of Eq. (1), it will prove advantageous to change integration variables in Eq. (3) from x_1 and x_2 to $x_1 + x_2$ and $x_1 - x_2$.

   (ii) You should be able to take advantage of the separability of Eq. (1) to greatly simplify Eq. (3) for the case $y = |x_1 - x_2|$.

   (iii) Expand the potential $U(r)$ about its minimum. You will need to figure out how many terms in the expansion you need to keep to obtain the leading term in α.

   (iv) When performing integrals of the form $\int_0^\infty dz \exp(-a_2 x^2 + a_3 x^3 + \ldots)$, it will be to your benefit to replace the exponential by $\exp(-a_2 x^2)(1 + a_3 x^3 + \ldots)$. Under what conditions is this approximation valid?

2. *Ideal gas in a gravitational field.*

   Do Reif Problem 7.2.

3. *Classical picture of electrical resistivity.*

   Do Reif Problem 7.8.