DUE: THURSDAY FEBRUARY 17, 2000

SECOND MIDTERM ALERT: The second midterm exam will be given in class on Tuesday February 22, 2000 from 10–11:30 am in 283 Kerr Hall. This will be a closed book exam, although you will be allowed to consult two sheets of handwritten material of your choice. The exam will cover material primarily from chapters 5–7, 10 and 13 of Baierlein. However, the material from chapters 1–4 is still fair game.

All problems are taken from Baierlein unless otherwise indicated. *In order to earn total credit for a problem solution, you must show all work involved in obtaining the solution.* Late homework received before Tuesday February 22 will be graded at half credit. No homework sets accepted after solution sets are handed out.

1. The goal of this problem is to compute the contribution of the rotational degrees of freedom of a diatomic molecule to the specific heat of an ideal gas. Consider the quantum mechanical problem of a rigid rotator with moment of inertia $I \equiv \hbar^2/(2\varepsilon)$ [this defines the variable ε, which has units of energy]. One can show that the energy levels of this system are $\epsilon_\ell = \varepsilon\ell(\ell+1)$, where $\ell = 0, 1, 2\ldots$ can be any non-negative integer. The degeneracy of the ℓth energy level is equal to $2\ell+1$.

(a) Write down the partition function, $Z_R(T)$, for the rigid rotator, which is a function of the temperature T. (*NOTE:* the sum cannot be evaluated exactly.)

(b) Evaluate $Z_R(T)$ approximately for $kT \gg \varepsilon$ by converting the sum to an integral. [*HINT:* Change the integration variable to $x = \varepsilon\ell(\ell+1)/kT$. The resulting integral should then be simple to evaluate. If not, go back to part (a) and make sure you have not left something out!]

(c) Evaluate $Z_R(T)$ approximately for $kT \ll \varepsilon$ by taking the first two terms in the sum (and discarding the remaining terms).

(d) From the results of parts (b) and (c), evaluate the mean energy E and the specific heat C_V in the low-temperature and high-temperature limits. Does the high-temperature limit reproduce the expected value predicted by the equipartition theorem? Explain.

2. The Euler-MacLaurin summation formula states that:

$$\sum_{n=0}^{N} f(n) = \int_0^N f(x)\,dx + \tfrac{1}{2}\left[f(0) + f(N)\right] + \sum_{p=1}^{m} \frac{B_{2p}}{(2p)!}\left[f^{(2p-1)}(N) - f^{(2p-1)}(0)\right] + R_{m+1}(N)\,,$$

where the B_{2p} are Bernoulli numbers[1] and R_{m+1} is a remainder term which can be bounded. In the formula above, $f^{(r)}(0)$ denotes the rth derivative of the function f evaluated at 0. The Euler-MacLaurin summation formula is valid in the limit of $N \to \infty$ as long as all the derivatives above are finite and the remainder term does not diverge.[2] In many cases, this formula can be used to convert a sum to an integral and control the size of the correction terms.

(a) In problem 1 part (b), you evaluated Z_R in the limit of $kT \gg \varepsilon$ by converting a sum to an integral. Using the Euler-MacLaurin summation formula, show that a more accurate expression for Z_R in the limit of $kT \gg \varepsilon$ has the following form:

$$Z_R = \frac{kT}{\varepsilon} + a_1 + a_2\,\frac{\varepsilon}{kT} + \mathcal{O}\left(\varepsilon^2/(kT)^2\right)\,.$$

Explicitly evaluate the numbers a_1 and a_2.

(b) Using the result of part (a), compute the mean energy E and the specific heat C_V with the same level of accuracy. In particular, you should find that $C_V = 1 + A\varepsilon^2/(kT)^2$. What is the value of A?

(c) Using the expression for C_V in the low-temperature regime obtained in problem 1 part (d) and the improved result for C_V in the high-temperature regime obtained in part (b) above, sketch the graph of C_V as a function of T. Use your common sense to connect the small T and large T regimes while trying to be as accurate as you can.

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[1] Bernoulli numbers are defined via the Taylor series of the function $x/(e^x - 1)$. Specifically,

$$\frac{x}{e^x - 1} = \sum_{n=0}^{\infty} \frac{B_n x^n}{n!}\,.$$

For example, $B_0 = 1$, $B_1 = -1/2$, $B_2 = 1/6$, $B_3 = 0$, $B_4 = -1/30, \ldots$. In general, for positive integer n, $B_{2n+1} = 0$ and the B_{2n} are related to $\zeta(2n)$ as discussed in class.

[2] For a further discussion of this formula, see *e.g.*, *Mathematical Methods for Physicists*, 4th edition, by George B. Arfken and Hans J. Weber, pp. 337–342.

3. Chapter 13, problem 9 (p. 324).

4. Chapter 7, problem 1 (p. 162).

5. Chapter 7, problem 7 (p. 164).

6. Chapter 10, problem 5 (p. 242).

7. Chapter 10, problem 8 (p. 242).