Problems:

1. Last week we calculated the high and low T behavior of the quantum oscillator from a microcanonical (fixed NVE) perspective, where we count states with specific energy. This week, we tackle the same question, but from the perspective of the canonical partition function (fixed NVT), where we take advantage of the partition function machinery.

   Recall that the energy of a quantum oscillator is given by

   $$E_n = \left(n + \frac{1}{2}\right)\epsilon_0$$

   where $\epsilon_0/2$ is the ground state energy, and n is an integer from zero to infinity describing the occupied energy level.

   (a) Calculate the partition function Z for the quantum oscillator. You will find it helpful to remember the expression for an infinite geometric sum.

   Solution 1a. We begin with three useful equations: first, the equations dictating the energetic steps of a quantum oscillator; second, the infinite geometric sum identity; and third, the partition function definition.

   $$E_{oscillator} = \epsilon_0(n \ + \ \frac{1}{2}) \tag{1}$$

   $$\sum_{i=0}^{\inf} a \cdot r^i = \frac{a}{1-r} \tag{2}$$

   $$Z = \sum_{states} e^{-\beta E_{state}} = \sum_{states} e^{-\frac{E_{state}}{kT}} \tag{3}$$

   Substituting (1) into (3), we find:

   $$Z = \sum_{states} e^{-\beta E_{state}} = \sum_{states} e^{-\frac{E_{state}}{kT}} \tag{4}$$

   (b) From the partition function, evaluate the mean energy U.

   (c) Evaluate the $T \to 0$ and $T \to \infty$ limits of the energy. Check that your results are consistent with the previous week. Isn't this approach much nicer?

2. Schroeder 6.22, parts (a) and (b) only. Be sure that you understand the simple paramagnet described on p. 232-3.

3. In the "Zipper" model for the formation of double-standed DNA from two single strands, the cooperativity of bonding requires that strands zip (or unzip) only from one end, so that the n^{th} link between strands only forms if bonds $(1, 2, \ldots, n-1)$ are all intact, mimicking a zipper. For each intact bond, $E = -\epsilon$, while each open bond has $E = 0$.

(a) For DNA of length N bases, show that the partition function is given by

$$Z = \frac{e^{(N+1)\beta\epsilon} - 1}{e^{\beta\epsilon} - 1}.$$

The finite geometric series you proved in Schroeder 6.22 is helpful.

(b) Determine the average number of bonded links $\langle n \rangle$. To calculate this, take advantage of the fact that the average number of links $\langle n \rangle = -U/\epsilon$.

(c) For $T = 0$, all links must be intact. For $kT \ll \epsilon$ (*i.e.* low T, but not zero), determine the average number of bonded links to first order in $e^{-\beta\epsilon}$. To do so, you will want to take advantage of that $e^{-\beta\epsilon} \ll 1$ at low temperature.

4. Schroeder 6.26. Including rotations is a step toward extending the ideal gas description to simple molecular systems, like H_2 or N_2. Be sure you understand Schroeder's discussion from p. 234-236.

5. Schroeder 6.51.