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Physics 603 **HOMEWORK ASSIGNMENT #6** Spring 2014

Due date for problems on Tuesday, April 1 [deadline on April 3].

1. (10) Read carefully PB sections 5.3 A, B, C, which were not covered in class. Use 5.3C to do this problem from Kardar; you may cite equations in PB in your answer rather than working everything out explicitly. (Note that traces of products are invariant under cyclic permutation of the multiplied matrices.

Quantum harmonic oscillator: consider a single harmonic oscillator with the Hamiltonian

$$\mathcal{H} = \frac{p^2}{2m} + \frac{m\omega^2 q^2}{2}, \quad \text{with} \quad p = \frac{\hbar}{\mathrm{i}}\frac{\mathrm{d}}{\mathrm{d}q}.$$

(a) Find the partition function Z, at a temperature T, and calculate the energy $\langle \mathcal{H} \rangle$.

(b) Write down the formal expression for the canonical density matrix ρ in terms of the eigenstates ($\{|n\rangle\}$), and energy levels ($\{\epsilon_n\}$) of $\mathcal{H}$.

(c) Show that for a general operator $A(x)$,

$$\frac{\partial}{\partial x}\exp[A(x)] \neq \frac{\partial A}{\partial x}\exp[A(x)], \qquad \text{unless} \qquad \left[A, \frac{\partial A}{\partial x}\right] = 0,$$

while in all cases

$$\frac{\partial}{\partial x}\operatorname{tr}\{\exp[A(x)]\} = \operatorname{tr}\left\{\frac{\partial A}{\partial x}\exp[A(x)]\right\}.$$

(d) Note that the partition function calculated in part (a) does not depend on the mass m, that is, $\partial Z/\partial m = 0$. Use this information, along with the result in part (c), to show that

$$\left\langle \frac{p^2}{2m} \right\rangle = \left\langle \frac{m\omega^2 q^2}{2} \right\rangle.$$

(e) Using the results in parts (d) and (a), or otherwise, calculate $\langle q^2 \rangle$.

2. (15) Statistics of deuterium (which has spin 1):

a) Discuss the wave functions needed to describe molecules of ortho-deuterium (o-D_2) and para-deuterium (p-D_2).

b) Write down the partition functions for a system of N molecules of i) o-D_2, ii) p-D_2, iii) equilibrium D_2. Note that it is not straightforward to write the partition function for normal D_2, You may assume that $Z_{vib} = 1$ and $Z_{electr} = 1$. (In each of these two approximations, indicate which characteristic energy is much greater than k_BT.)

c) Find expressions for the equilibrium ratios of o-D_2 to p-D_2 at i) very high *T* and ii) low *T*.

3. (10) PB 6.1 and the following part of 6.2:

For BE and FD statistics show that $\langle n_\varepsilon^2\rangle - \langle n_\varepsilon\rangle^2 = \langle n_\varepsilon\rangle \pm \langle n_\varepsilon\rangle^2$, respectively. Show then that in both cases the right-hand side is $k_B T\left(\frac{\partial\langle n\rangle}{\partial\mu}\right)_T$.

4. (5) PB 6.10. Part a) should be familiar and is mostly to help you do part b. In part b, relate d *T*/*T* to d*p*/*p* for adiabatic systems and then use your result in part a).