PHYS-552: Final Exam

Due 25th of May, 5PM sharp!!!

May 23, 2012

1 Density matrix

- Derive the equation governing the time-development of the density matrix. What is the classical analog of this equation?
- For a classical system the microcanonical ensemble requires the *equal a priori probabilities* postulate. Can one construct the microcanonical ensemble for a quantum system based on the postulate of equal a priori probabilities alone? Why or why not?
- The density matrix for a harmonic oscillator is given by

$$\langle q|\exp(-\beta\hat{H})|q'\rangle = \left[\frac{m\omega}{2\pi\hbar\sinh(\beta\hbar\omega)}\right]^{\frac{1}{2}} \times \exp\left[-\frac{m\omega}{4\hbar}\left\{(q+q')^2\tanh\left(\frac{\beta\hbar\omega}{2}\right)+(q-q')^2\tanh\left(\frac{\beta\hbar\omega}{2}\right)\right\}\right], \tag{1}$$

  with the Hamiltonian given by

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial q^2}+\frac{m\omega^2}{2}q^2. \tag{2}$$

  Calculate the spread in momentum ($\langle p^2\rangle - \langle p\rangle^2$).

2 Chemical equilibrium

Consider the reaction

$$H_2 + D_2 \Longleftrightarrow 2HD, \tag{3}$$

taking place at finite but low temperature.

- Given that the nuclear spin of a hydrogen atom is $I = \frac{1}{2}$ and of that of a deuterium atom is $I = 1$, identify which constituent molecules are fermions which are bosons.
- Within the Born-Oppenheimer approximation calculate the relations between the rotational constants and the vibrational frequencies of the three molecular species.
- Calculate the equilibrium constant of the reaction, assuming that the constituent molecules are non-interacting quantum gases. Assume also that only the ground electronic state of each molecule is populated.

- It has been speculated that under certain conditions H_2/D_2 molecules can form a superfluid states. If this was true, how many superfluid components would a system of H_2 molecules have? Of the two isotopes which one would have a lower superfluid temperature, H_2 or D_2?

3 1D Ising model

The Hamiltonian of the one-dimensional ferromagnetic Ising model is given by

$$H = -J \sum_{i=1}^{N} \sigma_i \sigma_{i+1} \tag{4}$$

- Calculate the relation between the energy and the entropy in the micro-canonical ensemble.
- The dimer-dimer correlation function of the Ising model is defined as

$$D_{ijkl} = \langle \sigma_i \sigma_j \sigma_k \sigma_l \rangle - \langle \sigma_i \sigma_j \rangle \langle \sigma_k \sigma_l \rangle, \tag{5}$$

  where $i.j$ and k, l are nearest neighbor pairs. Calculate this function for the one-dimensional ferromagnetic Ising model.

4 Landau theory of phase transitions

- Define the term order parameter ($\eta(Y,T)$), assuming it depends on two variables, one of which is temperature T, the other being a generalized force Y. Sketch the typical behavior of the order parameter as a function of temperature for a first order and a second order phase transition, indicating what happens at the critical temperature T_c.

Assuming the free energy to be of the form

$$G(Y.T) = A_0(Y,T) + A_1(Y,T)\eta + A_2(Y,T)\eta^2 + A_3(Y,T)\eta^3 + A_4(Y,T)\eta^4. \tag{6}$$

- Argue that in the absence of an external field coupled to the order parameter $A_1(Y,T) = 0$.
- Argue that $A_4(Y,T)$ is positive.
- Setting $A_3(Y,T) = 0$ show that a second order phase transition results when $A_2(Y,T)$ is varied. Assuming $A_2(Y,T) = a(T - T_c)$, calculate the free energy as a function of temperature, and indicate what happens at the phase transition.
- Discuss under what circumstances does a first-order phase transition occur. Sketch the free energies as a function of the order parameter below, at, and above the phase transition temperature.
- The effect of *hysteresis* refers to the persistence of a phase below or above the phase transition temperature. For example, suppose the system is at high temperature, and it is in a disordered state. Cooling below the

phase transition temperature does not immediately result in the system becoming ordered. Conversely, the ordered state persists if one approaches the phase transition temperature from below. Which type of transition (first or second) would you expect to display hysteresis and why? Explain in terms of the behavior of the free energy in Landau theory.

5 Ideal gases of bosons and fermions

- Pathria & Beale (3rd Edition!!!) 7.34.
- Calculate the specific heat for a three and two-dimensional system of ideal fermions.
- For a three-dimensional system of ideal fermions with Fermi wave vector k_F calculate the quantity

$$\langle FS|\hat{n}(\mathbf{r})\hat{n}(\mathbf{r}')|FS\rangle, \tag{7}$$

where $|FS\rangle$ indicates the ground state of the system. (Hint: one way to do this is by expressing the product of second quantized density operators in reciprocal space.)

6 Renormalization group theory

One is given a system characterized by a Hamiltonian $H(\vec{K}, \vec{\sigma})$, where $\vec{K}$ indicates the vector of parameters (can be coupling constants, external fields, temperature, etc. or combinations thereof) and $\vec{\sigma}$ denotes the state space of the system (for instance spins in the Ising model).

- In renormalization group theory one defines a blocking transformation of the spins. In such a transformation a group of spins are "blocked" together, and a new spin associated with each block is defined,

$$\sigma'_I = A(\sigma_i; i \in I). \tag{8}$$

Subsequently a new Hamiltonian is sought, which describes the behaviour of the "blocked" spins. The new Hamiltonian ($H(\vec{K}', \vec{\sigma}')$) in general will have a different set of parameters $\vec{K}'$. Write the equation which fixes the parameters of the new Hamiltonian.

- Determining the new Hamiltonian can be viewed as a transformation of the parameters

$$\vec{K}' = \vec{R}(\vec{K}). \tag{9}$$

Such transformations can have fixed points, i.e. points for which

$$\vec{K}^* = \vec{R}(\vec{K}^*). \tag{10}$$

Give examples of different types of fixed points and explain their mathematical significance.

- For the ferromagnetic Ising model in two dimensions on a triangular lattice apply a blocking transformation and try to find the fixed points. Possible blocking transformations are: form a new spin out of three spins in the corner of triangles, and define the block spin to be the spin of one particular corner of the triangle, or use the majority rule.