PHYS4031 STATISTICAL MECHANICS   Problem Set 6   Due: 22 November 2016 (Tuesday)
"T+2" = 24 November 2016 (Thursday)

All problem sets should be handed in not later than 5pm on the due date. Drop your assignment in the PHYS4031 Box outside Rm.213. Work out the steps of the calculations in detail. While discussions with your classmates are encouraged, you should write up your answers independently.

6.0 *Reading Assignment*:

6.0 *Reading Assignment*: After the chapter on ferromagnetism and critical phenomena, we go back to develop the third ensemble theory (Part VI). The logic under our flow is as follows. In Chapter XI, we develop the grand canonical ensemble that deals with open systems (thus relaxing fixed N), and establish the Gibbs distribution, grand partition function, grand potential Ω, and the thermodynamics ($\langle E \rangle$, $\langle N \rangle$, S, F, etc.) systematically. The results are general and applicable to interacting and non-interacting systems. Chapter XII is a short chapter in which we apply the grand canonical ensemble theory to *non-interacting* fermions and bosons in general. We will re-derive the Fermi-Dirac and Bose-Einstein distributions and set up the equations for studying Ideal Fermi Gas and Ideal Bose Gas. The results in Ch.XII are still "general" in the sense that they are good for any spatial dimension and any energy dispersion relation. Good places to read include: Mandl (Sec.11.1-11.4,11.7), Bowley/Sanchez (Ch.9, Sec.10.1-2), Rosser (Ch.11,12), and Guenault (Ch.8,9).

After that, there are two remaining chapters. Chapter XIII on 3D ideal (non-relativistic) Fermi gas. It is covered in every undergraduate Statistical Mechanics textbook and usually the focus is on the $T = 0$ physics and low-temperature ($kT \ll E_F$) physics. These are important in solid state physics. We will also work out the correction to the ideal gas law due to the fermionic nature of the particles at high temperatures. The best way to learn is to explain to yourself the physics and to go through the derivations privately. Easier undergraduate textbooks skip the high-temperature discussion. Bowley/Sanchez (Ch.9, Sec.10.1-3), Mandl (Ch.11), and Guenault (Ch.8,9) are easy places to read. Greiner's *Thermodynamics and Statistical Mechanics* gives detailed derivations of almost all the results, including even the ultra-relativistic Fermi gas.

Chapter XIV discusses the physics of ideal Bose gas. In standard undergraduate courses, the focus is on the Bose-Einstein condensation, as discussed in a section in Bowley and Sanchez (Ch.10) and Mandl. For us, the notes also cover the equations that are valid at all temperatures and the correction to the ideal gas law due to the bosonic nature of the particles at high temperatures. The mathematical treatments of Fermi and Bose gases are very similar. BEC and cold-atom physics are hot topics in physics. For those who want to read more on BEC and Bose gases, relevant discussions are given in the two books (Statistical Mechanics and Introduction to Statistical Physics) by Kerson Huang. The author (K. Huang) contributed significantly to the physics of interacting bosons in the late 1950s, in his papers with T.D. Lee and C.N. Yang. The discussion in Pathria's *Statistical Mechanics* is also good. The techniques (laser cooling and trapping) that have led to the observation of BEC open up new possibilities in research. Ultra-cold atom/molecular gases and controllable optical lattices are currently hot topics in research. Interested students are directed to the books *Atomic Physics* by C.J. Foot and *Quantum Optics* by M. Fox for more information.

6.1 **Behavior of Heat Capacity within Mean Field Theory of the Ising model.**

In class (and class notes), we developed the mean field theory of the Ising model and obtained an expression for the partition function per spin and hence the Helmholtz free energy per spin $f(T)$. From $f(T)$, we could obtain the dependence of the magnetization m (per spin) and the susceptibility χ on $|T_c - T|$. In addition, we also explored how m and an applied field B are related near the critical point. These led to the critical exponents β, γ, and δ, respectively. The TA did the part on susceptibility in a sample question.

There is one more physical quantity to explore. **Evaluate** the mean energy (per spin) and hence **determine** how the heat capacity (per spin) behaves for $T < T_c$ and $T > T_c$. In particular, **comment** on the behavior, is it continuous or discontinuous across T_c?

6.2 **Heat capacity within Landau Theory.**

This question is similar to 6.1. Starting from Landau's expression for the free energy as an expansion in the order parameter m, **discuss** the behavior of the heat capacity across T_c.

6.3 **Setting up mean field equations in the Random Field Ising Model.**

This is "harder". You are asked to develop a mean-field theory for the Ising model in the presence of a spatially dependent applied magnetic field.

Recall: In our discussion of the Ising model, there is a *uniform* applied magnetic field, and thus the parameter B in the Hamiltonian (energy expression $E(\{S_i\})$) does not depend on the location of the spin i. Then we could go through the following steps (conceptually): (i) Assume a yet-to-be-determined mean field $\langle S_i \rangle$ for the spin i and similarly for other spins j. (ii) Since one location is nothing special from another, the mean fields $\langle S_i \rangle = m_i = m$, are assumed to be independent of the location i. (iii) This makes life easier as the partition function and thus the free energy depends only on the mean field m (which remains an unknown). (iv) We can set up an equation to evaluate m (e.g. using the partition function or the free energy within mean field approximation). This gives a single equation for m that emphasizes self-consistency in the mean field formalism.

Consider the following variation of the Ising model. The Hamiltonian is given by

$$E(\{S_i\}) = -J \sum_{(ij)} S_i S_j - \sum_i B_i S_i \tag{1}$$

In particular, the applied magnetic field B_i could be different at different spin locations i.

Your task is to **set up mean field equations** for this **Random field Ising model**.

Hints: You may try to follow the formalism in the uniform field Ising model. That is to say, assume a mean field at each site i as $\langle S_i \rangle \equiv m_i$ and set up self-consistent equations for getting the m_i's. The key point is: **you cannot assume the yet-to-be-determined mean field m_i to be the same at each site**, instead you have the unknowns as m_i, one for each site i. At the end, you may check whether your equations could be reduced to the single equation when you make $B_i = B$ independent of locations.

How far to go? Your task is to get to the point that a set of equations (enough number of them) that can be solved for all the m_i's. You don't need to solve them – in fact you can't solve them unless you know the random fields B_i and do the calculations numerically.

Remarks: For students who want to explore further (no bonus of course), you may want to find out under what physical situations the random-field Ising model is useful. One could also try to play with random J_{ij} (random coupling), even to the extent that J_{ij} could be positive or negative values randomly assigned to the connections. This model is called a spin glass.

6.4 **Grand partition functions for non-interacting Fermions and Bosons with spin degeneracy factor.**

In Chapter XII, we derive the grand partition function for non-interacting fermions and bosons Q_F and Q_B, respectively. The answers are:

$$Q_F = \prod_{s.p.\ states\ i} \left[1 + e^{-\beta(\epsilon_i - \mu)}\right] \tag{2}$$

$$Q_B = \prod_{s.p.\ states\ i} \frac{1}{1 - e^{-\beta(\epsilon_i - \mu)}} = \left[1 - e^{-\beta(\epsilon_i - \mu)}\right]^{-1} \tag{3}$$

where the product is over all single-particle states i. Collectively, the two results can be written as

$$Q_{F,B} = \prod_{s.p.\ states\ i} \left[1 \pm e^{-\beta(\epsilon_i - \mu)}\right]^{\pm 1} \tag{4}$$

where the plus sign (minus sign) is for the fermionic (bosonic) case.

In some books, the authors could include a spin factor $(2s+1)$ into the result and write

$$Q_{F,B} = \prod_{s.p.\ states\ i} \left[1 \pm e^{-\beta(\epsilon_i - \mu)}\right]^{\pm(2s+1)} \tag{5}$$

where s is the spin of the particles. Recall that half-integer spins $s = 1/2, 3/2, \ldots$ are fermions and integer spins $s = 0, 1, 2, \ldots$ are bosons.

Tasks: **Explain** why it is OK to include the spin factor as shown in Eq. (5). From Eq. (5), one can calculate thermodynamic quantities by invoking the density of states $g(\epsilon)$.

Yet some authors do not use Eq. (5), but instead use Eq. (4). In doing so, the spin-degeneracy factor comes in when the density of states $g(\epsilon)$ is invoked in the calculations of thermodynamic quantities. **Explain** why both ways of handling the spin-degeneracy factor will give the same results and **point out the difference** in the densities of states when Eq. (4) and Eq. (5) are used.