PHYS4031 STATISTICAL MECHANICS

SAMPLE QUESTION FOR DISCUSSION IN WEEK 11 EXERCISE CLASSES (14, 16 November 2016)

You may want to think about them before attending exercise class.
SQ26: $f(m)$ of Ising model in the mean field approximation and Landau Theory
SQ27: Classical ideal gas by evaluating $Q(T,V,\mu)$ and the same physics comes out

SQ26 **Helmholtz free energy per spin f taken to be a function of m**

In class (and class notes), we evaluated the partition function and then the Helmholtz free energy per spin $f(T,B)$ from the mean field approximation of the Hamiltonian of the Ising model. The answer is

$$f = \overline{f} + \frac{Jzm^2}{2} - kT \ln \left[\cosh \left(\frac{Jzm}{kT} + \frac{B}{kT} \right) \right] \tag{1}$$

where $\overline{f} = -kT \ln 2$ is the entropy per spin at high temperature. It is just a constant term and therefore doesn't matter any more.

Physics Background: (a) Formally, we should take f as $f(T,B)$. From f, the mean field equation

$$m = \tanh \left(\frac{Jzm}{kT} + \frac{B}{kT} \right) \tag{2}$$

can be obtained in several ways, e.g. by the definition of $m = -(\partial f / \partial B)_T$. Solving Eq. (2) for m at $T > T_c$ only gives one solution $m = 0$. For $T < T_c$, Eq. (2) gives three real solutions (one positive, one negative, and $m = 0$). In this case, formally we should substitute the solutions into f and examine which solution gives the minimum f, as f should be a minimum at equilibrium. This is how Eq. (1) should be applied formally.

TA: With this idea, it implies that we should be able to get at the values of m by setting $(\partial f/\partial m)_{T,B} = 0$, which is a mathematical statement saying the value of m at equilibrium should be the one that extremizes f (so possibly including values that minimizes as well as maximizes f). Show that the condition also leads to the mean field equation Eq. (2).

Physics Background: (b) Although formally Eq. (2) can be solved to obtain $m(T,B)$ and then plugging $m(T,B)$ back into Eq. (1) really gives $f(T,B)$, it is suggestive that we could **look at Eq. (1) as a function of** $f(m,T)$.

TA: Let's consider $B = 0$. Construct $(f - \overline{f})/kT$ and write it in terms of m and T_c. Then plot $(f - \overline{f})/kT$ as a function of m for different values of T above, near, and below T_c. The plot should stress the different behavior as T varies across T_c.

TA: Starting from Eq. (1) with $B = 0$, expand the argument and show that the Helmholtz free energy per spin f can be written in the Landau form, namely

$$f = f_0 + a(T)\, m^2 + b\, m^4 \tag{3}$$

and identify the terms f_0, $a(T)$ and b.

Remarks: It happens that the behavior captured in Eq. (3) is the starting point of the Landau theory of continuous phase transition. Landau (1937) gave a phenomenological theory of continuous phase transition. He proposed a simple form of $f(m,B)$ (Eq. (3)) that captures the key features in the plot of Eq. (1), but emphasizes that these features need not come from the details of the physical problems under consideration, but more on the symmetry of the problem and that the phase below T_c breaks a symmetry in the Hamiltonian of the problem (realized by a changing sign in $a(T)$ as T goes across T_c). His theory had led to the idea of **spontaneous symmetry breaking**, which affected much of particle physics and condensed matter physics.

Knowing Lev D Landau: Landau is one of the greatest theoretical physicists of all time. He did ground breaking works across many fields, including magnetic properties of solids (Landau diamagnetism, Landau levels, ferromagnetism), continuous phase transitions, superfluidity and superconductivity, nuclear physics, neutron stars, QED, interacting electron systems (Fermi liquid theory), and neutrino spin. Any one of these works would have qualified him for a Nobel Prize. He finally was awarded the Prize in 1962 after he was hurt badly (and fatally) in a car accident. He established the whole of Soviet physics. He was a great teacher. His student Lifshitz helped him write a whole set of **Course of Theoretical Physics** covering all topics in physics. They are also called the "Landau and Lifshitz" series. There are 10 volumes, with 8 of them authored by Landau and Lifshitz (volumes 1 to 8), plus 2 by his students. The volumes cover Mechanics, Classical Theory of Fields, Quantum Mechanics, Quantum Electrodynamics, Statistical Physics, Fluid Mechanics, Theory of Elasticity, Electrodynamics of Continuous Media, Statistical Physics (Part 2), and Physical Kinetics. These books define the standard of an exam for students who wanted to become his students – called the *Theoretical Minimum*. That minimum is almost an unreachable maximum for many! But his high standard paid off later – those who passed his exam became leaders in Soviet/Russian physics and a few later won the Nobel Prize themselves. If you only read Feynman's Lectures and his other books, and Greiner's series (which are good for undergraduates), you ain't see nothing yet! Go to the library and enjoy *Landau and Lifshitz*.

SQ27 **Classical ideal gas - revisited using the calculation scheme of the Grand Partition Function.**

The third ensemble theory (grand canonical ensemble theory) deals with a system having variables (T, V, μ). A model set up is one with the system embedded in a bath. The wall allows exchanges of energy *and* particles between the system and the bath. The bath is huge and set the temperature T and chemical potential μ of the system.

We worked out in class the probability of finding a system to have exactly N particles and in a state of energy $E_i(N)$ has the form

$$P(E_i(N), N) \propto e^{-E_i(N)/kT+\mu N/kT} \tag{4}$$

Normalizing the probability gives the Gibbs distribution

$$P(E_i(N), N) = \frac{1}{Q} e^{-E_i(N)/kT+\mu N/kT} \tag{5}$$

where $Q(T, V, \mu)$ is the grand partition function given by

$$Q(T, V, \mu) = \sum_{N=0}^{\infty} \sum_{N\text{-particle states } i} e^{-E_i(N)/kT+\mu N/kT} \tag{6}$$

Then the grand potential $\Omega(T, V, \mu) = -kT \ln Q(T, V, \mu)$ and everything follows. This is the grand ensemble theory. Done!

One observation is that Eq. (6) can be written as

$$\begin{aligned} Q(T, V, \mu) &= \sum_{N=0}^{\infty} \sum_{N\text{-particle states } i} e^{-E_i(N)/kT+\mu N/kT} \\ &= \sum_{N=0}^{\infty} e^{\mu N/kT} \sum_{N\text{-particle states } i} e^{-E_i(N)/kT} \\ &= \sum_{N=0}^{\infty} \xi^N Z(T, V, N) \end{aligned} \tag{7}$$

where

$$\xi \equiv e^{\mu/kT} \tag{8}$$

and $Z(T, V, N)$ is the partition function of the system when it has N particles.

Let's see how it works! Here, we do something unpractical, but yet educational. We want to construct $Q(T, V, \mu)$ for a **classical ideal gas**. Of course, we need not do that for the physics. We have done it in microcanonical and canonical ensemble theories. But it will be nice to see how things works out fine.

Eq. (7) suggests that if we know $Z(T, V, N)$ for all values of N, then one can construct $Q(T, V, \mu)$. It doesn't sound clever – if we know $Z(T, V, N)$ then we can get the physics! Nonetheless, let's try it and see how things work.

Here, TA will demonstrate how to obtain the Grand Partition Function $Q(T, V, \mu)$ of a classical ideal gas and the same old physics.

(a) The single-particle partition function z for a non-relativistic free particle was evaluated by several methods to be $z = V/\lambda_{th}^3$, where λ_{th} is the thermal de Broglie wavelength. Using z to construct the partition function Z and then use Z to construct the grand partition function $Q(T, V, \mu)$ for a classical ideal gas.

(b) Using $Q(T, V, \mu)$, find $\Omega(T, V, \mu)$. This Ω is the one you worked out in the mid-term exam. It is given by $\Omega = E - TS - \mu N$.

Hence, calculate thermodynamic quantities from Ω (or from Q) and recover the physics of a classical ideal gas.

(c) In a mid-term exam question, you showed that $\Omega = -pV$. Hence, a short cut to the equation of state of a system is

$$pV = kT \ln Q \ . \tag{9}$$

Apply this relation and check that the well-known result of a classical ideal gas results.

Important remarks: This completes our discussion on the classical ideal gas in statistical mechanics, namely using all the three ensemble theories. And this simple example illustrates the deeper mathematical relationships among microcanonical, canonical, and grand canonical ensemble theories.

(d) As a by-product, obtain an expression for μ/kT and show that it is in agreement with the result

$$\frac{\mu}{kT} = -\ln\left[\frac{V}{N}\frac{1}{\lambda_{th}^3}\right] \tag{10}$$

previously obtained by the microcanonical and canonical ensembles. Hence, point out that ξ (defined in Eq. (8)) is small (dimensionless number) in classical ideal gas.

[Remark: Note one more time the form of μ and it is **negative for a classical ideal gas**. As a quantum gas would become a classical gas at high temperatures [recall the de Broglie wavelength shrinks as temperature rises], we expect the chemical potential μ to shift to smaller (and eventually negative) values as temperature increases.]