Due June 6, Thursday

Problem 1 (20 points) *BEC transition and finite scaling.*

We have seen that Eq. 14.25 leads to two distinct regimes, Eqs. 14.28 and 14.29, separated by the phase boundary $n\lambda^3 = g_{3/2}(1)$. However, it is of importance to realize that this occurs only in the thermodynamic limit $N \to \infty$, with $n = N/V$ remaining finite. In this problem, we shall see how this transition occurs using numerical analysis. For this, our strategy is to **solve Eq. 14.25**, and it alone, and see how the results contained in Eqs. 14.28 and 14.29 will just follow.

(a) Eq. 14.25 contains three variables, $y = 1/(n\lambda^3)$, z, and N. Solving for z, we get the function $z(y,N)$. Then, **the BEC condensate fraction**

$$f(y,N) = \frac{n(0)}{N} = \frac{1}{N}\cdot\frac{1}{z^{-1}-1}$$

can be obtained. Fix the value of N at about 1000, and plot the function $f(y,N=1000)$ as a function of y. You must include $y_c = 1/\zeta(1.5)$ in the y range of the plot, since that is the most interesting point. Repeat this for several values of N, increasing about 10 fold each time, up to say, $N = 10^9$. Plot all $f(y,N)$ functions for $N = 10^3, 10^4, ..., 10^9$ in one plot and compare them. Discuss the behavior of $f(y,N)$ at $y = y_c$ and explain how the discontinuous behavior emerges at that point as N becomes large. [Hint: $f(y,N) = 1$ at $y = 0$, and it starts out from that point as a line with a negative slope $= -\zeta(1.5)$. As the line approaches the point $(y,f) = (y_c, 0)$, it bends, slowing down as the slope approaches zero, and smoothly connects to the zero function for $y \gg y_c$. Note that $f(y,N)$ is an analytic function of y for any finite N, but its "transition zone" defined by the y range $[y_c - \Delta y, y_c + \Delta y]$, in which the crossover regime from the negative sloped line to the zero function occurs, decreases to zero width ($\Delta y \to 0$) as $N \to \infty$. *This non-analyticity* in the thermodynamic limit is the hall-mark of a phase transition.]

(b) To infer the existence of a phase transition, or the value of the transition temperature, from a numerical work is a highly non-trivial task, since a numerical work cannot be done on an infinite system. An important technique in this regard is **the finite size scaling analysis**. The central conjecture of the finite scaling analysis is the following scaling hypothesis: any finite size thermodynamic function, say ϕ, near the phase transition is given by

$$\phi_L(T,V) = L^\lambda\, \psi\left(\frac{L}{\xi}\right), \qquad T \approx T_c$$

where ξ is the correlation length (lecture 17), and L is the linear size of the system ($N \propto L^3$). The exponent λ is determined by critical exponents (like those discussed in lectures 16, 17) of the problem, and the scaling function ψ depends on the system under consideration and the quantity ϕ being calculated. For the BEC condensate fraction considered above, $\lambda = 1$. Then, the value of T_c can be deduced from the numerical analysis, if one plots

$$\frac{\phi_L(T,V)}{L^\lambda} \propto \frac{f(y,N)}{N^{\lambda/3}}$$

for different values of N and then identifies the common intersection point of all curves. If the scaling hypothesis is correct, then such an intersection point must be well-defined for large enough N values, since at a phase transition $\xi \to \infty$ (lecture 17) and, thus, $\psi\left(\frac{L}{\xi}\right) \to \psi(0) = L$ independent as $T \to T_c$. Use this technique to verify that, indeed, the BEC transition occurs at $y = y_c$ from the curves that you have created in part (a).

Problem 2 (20 points) *BEC transition.*

A verbatim copy of a recent qualifier exam problem

Consider a two dimensional ideal gas model of (1) bosons with the dispersion relation $\varepsilon_{\vec{k}} = \hbar^2 k^2/2m$, and (2) "relativistic" bosons with the dispersion relation $\varepsilon_{\vec{k}} = \hbar v k$, where v is a positive constant (not necessarily equal to the speed of light). An elementary criterion for the existence of the Bose-Einstein condensation at a critical temperature T_B is $N_T \equiv \sum_{\varepsilon_{\vec{k}} \neq 0} n(\varepsilon_{\vec{k}}, \mu = 0, T = T_B) = N$, where n is the usual Bose-Einstein function. Show that this criterion leads to the conclusion that the system does not undergo a Bose-Einstein condensation at any finite temperature in the case of (1), while it does undergo a Bose-Einstein condensattion at a finite temperture in the case of (2). In the latter case, determine T_B in terms of other quantities (N/A, v, ...). The spin of the boson can be set to 0, and the thermodynamic limit ($N \to \infty$, $A \to \infty$, $N/A \to$ constant; A is the area) should be considered. Useful integral: $\int_0^\infty dx\, x/(e^x - 1) \approx 1.645$.

Problem 3 (20 points) *Bose gas and a metal surface.*

One of the last year's exam problems

Equilibrium between a metal surface and a BEC volume gas. Consider a He gas with pressure P and in equilibrium with a metal surface. The energy of a He atom on the metal surface with no kinetic energy is $-\phi$. He atoms can freely move around on the metal surface, forming a two dimensional gas system. Let us call this phase the "surface gas" phase as opposed to the "volume gas" phase outside of the metal surface. We do not consider interactions between He atoms. Find the number of He atoms per unit area for the surface gas, as a function of P, T, ϕ and fundamental constants

(a) for T near room temperature, and

(b) for T below the Bose-Einstein condensate transition temperature for the volume gas.

In both cases, assume that P is near atmospheric pressure.

[Notes: For full credit, you need to show the derivation for key quantities such as μ, for part (a), using the classical ideal gas model. For part (b), the known value of μ can be used without derivation. Helpful formula: $\int_{-\infty}^{\infty} dx\, e^{-x^2} = \sqrt{\pi}$.]

Problem 4 (20 points) *Lattice gas theory.* Within the lattice gas theory (Section 15.2.2), we assign an energy value ε_0, when a molecule occupies a small volume element, the size of which is on the order of the excluded volume $\Omega/2$. Thus, the Hamiltonian is given by

$$\mathcal{H} = \varepsilon_0 \sum_i n_i - \varepsilon \sum_{\langle i,j \rangle} n_i n_j$$

where n_i is the occupancy of each volume element, with $n_i = 0, 1$ is sufficient to consider by assumption of a very small volume. Here, ε is the attraction (if $\varepsilon > 0$) energy scale for nearest neighbor pairs of molecules ($\langle i, j \rangle \equiv$ nearest neighbor pair of lattice indices). As ε_0 is the energy reference, we can set it to zero (in other words, it can be absorbed into the chemical potential μ), and we can write

$$Q = \sum_{\{n_i = 0,1\}} \exp\left[\beta\mu \sum_i n_i + \beta\varepsilon \sum_{\langle i,j \rangle} n_i n_j\right].$$

(a) Consider the case when $\varepsilon = 0$. You might worry that we assumed no such thing as "the kinetic energy" in the above Hamiltonian. This is *not* the case, as we will show now. Prove that this model correctly predicts the classical limit of the grand potential, $\Phi = -Nk_BT$ (Eq. 8.13), thus giving the classical ideal gas equation of motion, $PV = Nk_BT$ (and everything else) in the limit of the small fugacity $z \equiv e^{\beta\mu} \to 0$. This result shows that we must have introduced the kinetic energy in the above setup. Where did we do so?

(b) Now, consider the more general case $\varepsilon \neq 0$. Finish the program presented in page 8: i.e., upon the transformation $\sigma_i = 2n_i - 1$, what are the *effective field* H and the *effective exchange constant* J such that this problem maps to the Ising problem (Eqs. 15.16 and 15.14)? You can find $\varepsilon = \varepsilon(H, J)$ and $\mu = \mu(H, J)$ or, equivalently, $H = H(\varepsilon, \mu)$ and $J = J(\varepsilon, \mu)$.

Problem 5 (30 points) *Van der Waals theory and phase transition.* Consider the van der Waals equation of state (at the time of this writing, we have yet to derive this equation in class, we will do so, soon; in the mean time, you can read page 310 of the textbook).

$$(P + an^2)(V - bN) = Nk_BT$$

We can re-write this equation in a dimensionless form as

$$P_r = \frac{8T_r}{3v_r - 1} - \frac{3}{v_r^2}$$

where $P_r = P/P_c, T_r = T/T_c, v_r = v/v_c$ (where $v = 1/n$) are reduced dimensionless thermodynamic variables and

$$P_c = \frac{a}{27b^2}, \quad v_c = 3b, \quad T_c = \frac{8a}{27bk_B}$$

are the critical pressure, the critical molecular volume, and the critical temperature, respectively, within this theory. In this problem, we are *not* interested in the derivation of the above dimensionless form of the van der Waals equation from the first form. This is doable by anyone with patience. We will simply take this dimensionless form of the equation and explore it.

(a) Verify explicitly that $P_r(T_r, V_r)$ satisfies

$$\begin{aligned} P_r(T_r = 1, v_r = 1) &= 1, \\ \left.\frac{\partial P_r}{\partial v_r}\right|_{v_r=1,\, T_r=1} &= 0, \\ \left.\frac{\partial^2 P_r}{\partial v_r^2}\right|_{v_r=1,\, T_r=1} &= 0. \end{aligned}$$

(b) Find the equation of state for $T_r = 1$ and small $P_r - 1$ and small $v_r - 1$. You must verify the exponent δ, discussed in Section 16.4.

(c) Using a computer program, plot three isotherms $P_r(T_r = \text{fixed}, v_r)$ for three values of T_r: one just above T_c, one at T_c, and the third just below T_c. Choose the last one so that P_r does not become unphysical. Keep in mind that $v_r > 1/3$. Your plot should demonstrate clearly the behaviors summarized in Fig. T12.3.

(d) Study Fig. T12.2 and the accompanying text. Below T_c, the physical isotherm is different from the isotherm plotted in solid line in Fig. T12.2, since between v_3 and v_1, the isotherm is replaced by the dotted *horizontal* line connecting 3, 2, and 1. This horizontal line corresponds to the mixed phase of gas and liquid. Imagine that this system of gas+liquid is contained in a cylinder, with a piston whose position defines the total volume of the system. The system is kept at a constant temperature below T_c, while you slide piston in or out to change the total volume. Let us suppose that the initial total volume is very large (pure gas phase). The cylinder wall is transparent so that you can see what is going on. Describe what you will see as you press on the lid so as to decrease the volume all the way to the pure liquid phase (reaching point 3 from the right, and then following a steeply rising liquid phase isotherm on the left side). Describe what happens to the *total* Gibbs free energy, as you do so. Plot it as a function of pressure.

(e) Now, consider two isotherms at T and $T + dT$, both below T_c. We are interested in the phase coexistence regime 1-2-3 only. By considering the Gibbs free energy change between these two coexistence regimes, show that

$$\left.\frac{dP}{dT}\right|_{coexistence} = \frac{\Delta S}{\Delta V}$$

where $\Delta V = V_1 - V_3$ and $\Delta S = S_1 - S_3 = L/T$, where L is the latent heat. This is the Clausius-Clapeyron equation for the vapor pressure curve.

Problem 6 (20 points) *Landau theory.* For the given Landau free energy of Eq. 16.34, calculate the magnetization per spin, the magnetic susceptibility, and the specific heat, below and above T_c, in terms of a, b_0, and c. Assuming that $a(T)$ and $c(T)$ are smooth and finite at T_c. Also, note the conditions stated in Eqs. 16.32, 16.33.

This problem is basically reproducing Lecture 16, but only using the Landau free energy. This means that the physical quantities are calculated in terms of abstract parameters a, b_0 and c, and they are calculated only for T near T_c. The calculated results must be verified to reproduce the results of Lecture 16 (Eqs. 16.18, 16.23, 16.24, 16.30), by appropriately identifying a, b_0 and c for the Ising model case.

Problem 7 (20 points) *Landau theory.*

A verbatim copy of a recent qualifier exam problem

Consider the Landau theory of phase transition, and for simplicity consider a scalar (Ising) order parameter m. Write the free energy as

$$F(m,h) = -hm + \frac{a(T)}{2}m^2 + \frac{u}{4}m^4 + \frac{v}{6}m^6\,,$$

where h is a magnetic field, u and v are assumed independent of T, and

$$a(T) = \alpha(T - T_c)\,.$$

1. For the case of $h = 0$ show graphically that the transition is first order (i.e. discontinuous) if $u < 0$ and second order (i.e. continuous) if $u > 0$.

2. From now on assume $u > 0$ and neglect v. Above the transition temperature T_c show that Landau theory predicts that the magnetic susceptibility χ, defined by
$$\chi = \left.\frac{\partial m}{\partial h}\right|_{h\to 0^+} ,$$
diverges as
$$\chi = \frac{C_+}{t^\gamma} \quad (T > T_c) ,$$
where $t \equiv (T - T_c)/T_c$ is the reduced temperature, the (universal) critical exponent, γ, is equal 1, and C_+ is the called a critical amplitude. Note that C_+ is *not* universal since it depends on the parameters in the Landau free energy.

3. However, we can define the corresponding amplitude below T_c in an analogous manner, i.e.
$$\chi = \frac{C_-}{|t|^\gamma} \quad (T < T_c) .$$
(You should note that, in contrast to the situation above T_c, m itself is *not* zero in the $h \to 0^+$ limit.) Show that the ratio C_+/C_- *is* universal according to Landau theory and find its universal value.
Note: Such critical amplitude ratios, like exponents, are believed to be universal also in an exact theory, though the universal values of amplitude ratios and exponents will, in general, be different from those predicted by Landau theory.

Problem 8 (40 points) Construct a Metropolis Monte Carlo code for a two dimensional Ising magnet with the periodic boundary condition. (A partial python code example is provided on the homework page of the course web site: it should be enough for part (a), and should be easily extensible for parts (b,c).) In the following, assume a ferromagnetic model, except in (b).

(a) Pick at least three temperatures, including one well above T_c, one near T_c, and one well below T_c. Start from the initial configuration where the system is magnetized up on the left half and down on the right half. Run the same number of runs (suggestion: ~ 2000 for 40×40 lattice). Compare the final configurations for different temperatures and discuss the results.

(b) Do the same for the anti-ferromagnetic model ($J < 0$). Discuss the results.

(c) Measure the magnetization and the spin correlation function
$$\Gamma_{ij} \;\equiv\; \overline{\langle \sigma_i \sigma_j \rangle} - \overline{\langle \sigma_i \rangle}\,\overline{\langle \sigma_j \rangle}$$
Examine these quantities at least for three temperatures. Try to demonstrate the existence of long range correlations near the critical point, and the spontaneous symmetry breaking below T_c.