Qualifying Examination – Statistical Mechanics

Spring, 2015

1. (Fundamental concepts in statistical mechanics, 20 points)
   Please explain in brief the following terminologies in Statistical Mechanics.
   (a) Ergodic theorem and the postulate of equal *a priori* probability
   (b) Bose-Einstein condensation and its criterion
   (c) Correlation function
   (d) Critical phenomenon and order parameter
   (e) Fluctuation-dissipation theorem
   (f) (Classical) Liouville's theorem

2. (Canonical ensemble for classical gas, 20 points)
   (a) For an ideal classical gas consisting of N particles of mass m in a container of volume V and at temperature T, please
      (i) Write down its Partition function. (Note to include the factor $\frac{1}{N!}$ to prevent the Gibbs paradox.)
      (ii) Calculate its corresponding Helmholtz free energy, F. (Given the Gaussian integral $\int_{-\infty}^{\infty} e^{-x^2} dx = \sqrt{\pi}$.)
      (iii) Derive the familiar state equation, $PV=Nk_BT$, by $P = -\frac{\partial F}{\partial V}\Big|_{T,N}$.
      (iv) Calculate the entropy of this gas by $S = -\frac{\partial F}{\partial T}\Big|_{V,N}$. Take two such containers of different gas and open the partition to allow them to mix. What is the entropy change after the mixing?
   (b) To take into account that real particles (1) repel each other at close range, imagine each particle to be a hard sphere of volume v and (2) attract each other at long range, add a potential energy term[1] $-\alpha\left(\frac{N}{V}\right)^2 V$ to the free energy in (ii) of (a). Show that modifications (1) and (2) lead us to the Van der Waals equation: $\left[P + \alpha\left(\frac{N}{V}\right)^2\right](V - Nv) = Nk_BT$.

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[1] The parameter, α, describes the strength of pairwise attractive force between particles, while $\left(\frac{N}{V}\right)^2$ comes from the joint probability. Finally, the V factor comes from integrating the energy density $-\alpha\left(\frac{N}{V}\right)^2$ over the whole volume to obtain the potential energy.

3. (Random walk, 20 points)

(a) A drunkard is kicked out of the pub. Being fully intoxicated, he walks forward and backward with equal probability. According to the senior high-school math, the probability of finding him at position *n* after *N* steps is $P(n,N) = C^N_{N_\rightarrow}\left(\frac{1}{2}\right)^{N_\rightarrow}\left(\frac{1}{2}\right)^{N_\leftarrow}$ where $N_\rightarrow$ and $N_\leftarrow$ represent the number of steps forward and backward, respectively. Naturally,

$$N = N_\rightarrow + N_\rightarrow \text{ and } n = N_\rightarrow - N_\rightarrow. \qquad (1)$$

Assume $N \gg n \gg 1$ so that the Stirling formula can be used to approximate all large factorials: $\lim_{N\gg1} N! \approx N\ln N - N$. Show that $P(n,N)$ can be reduced to the Gaussian distribution: $P(n,N)\sim\frac{1}{\sqrt{N}}exp\left(-\frac{n^2}{4N}\right)$.

(b) Tom Witten of the University of Chicago has a simple theory[2] for the ridge-length distribution on a crumpled paper. He argues that any ridge of length ℓ must result from a consecutive (and thus hierarchical) decimation of the first and longest ridge, which equals roughly the length *L* of paper. So

$$\ell = L\frac{1}{3}\cdot\frac{2}{3}\cdot\frac{2}{3}\cdot\frac{1}{3}\cdot\frac{1}{3}\cdots \qquad (2)$$

where ℓ happens to fall in the shorter $\frac{1}{3}$ (or longer $\frac{2}{3}$) half of the previous ridge for $N_{\frac{1}{3}}$ (and $N_{\frac{2}{3}}$) number of times throughout a total of N=$N_{\frac{1}{3}} + N_{\frac{2}{3}}$ folds. Equation (2) can be re-expressed as $\ln\frac{R}{\ell} = N_{\frac{1}{3}}\ln\frac{3}{1} + N_{\frac{2}{3}}\ln\frac{3}{2}$ or

$$\ln\frac{R}{\ell} = \left(N_{\frac{1}{3}} + N_{\frac{2}{3}}\right)\frac{\ln\frac{9}{2}}{2} + \left(N_{\frac{1}{3}} - N_{\frac{2}{3}}\right)\frac{\ln 2}{2} \qquad (3)$$

While $\left(N_{\frac{1}{3}} - N_{\frac{2}{3}}\right)$ mimics $N_\rightarrow - N_\rightarrow$ of Eq.(1), the first term of Eq.(3) can be thought of as describing the presence of wind. You see, a wind is going to sway and carry the drunkard along its direction. Therefore, the eventual position *n* (which role is now played by $\ln\frac{R}{\ell}$) of the drunkard depends on the wind speed, $\frac{\ln\frac{9}{2}}{2}$, and the "time", $N = N_{\frac{1}{3}} + N_{\frac{2}{3}}$, he stays out in the wind. Please use the above information to modify the result of (a) to predict the distribution function for ridge length ℓ on a crumpled sheet.

[2] T. A. Witten, Rev. Mod. Phys. **79**, 643 (2007).

4. (One-dimensional Ising model, 20 points)

The Hamiltonian of one-dimensional Ising model is

$$H = -J\sum_{i=1}^{N-1} S_i S_{i+1} - B\sum_{i=1}^{N} S_i$$

where $S_i = \pm 1$ and B is the external magnetic field. When the coupling constant J is positive/negative, the Hamiltonian favors parallel/antiparallel alignments for the spins.

(a) Please show that the magnetization, $M = \sum_{i=1}^{N} \langle S_i \rangle$ where $\langle\ \rangle$ denotes the statistical average, is always zero in the absence of B. In other words, there is no phase transition into a magnetic state at any temperature T.

(b) Find the magnetic susceptibility, $\chi \equiv \frac{dM}{dB}$, when B is much less than both J and $k_B T$.

5. (Debye and Einstein models, 20 points)

The Dulong-Petit law states that the specific heat C_V of a crystal is a constant (of temperature T), which equals $\frac{k_B}{2}$ multiplied by its degrees of freedom. So it came as a huge blow and challenge when experiments showed that C_V in fact varies with T. This puzzle helped to bring about the advent of QM. Among the various theories that attempted to amend this discrepancy, the model proposed by the great Einstein turned out to be a blunder….

(a) Einstein assumed that the phonon frequency ω is a constant. Please derive his prediction for the temperature dependence of C_V.

(b) In contrast, Debye allowed the frequency to vary as $\omega = vk$ where v is the sound velocity in the solid and k the wave momentum. Please again derive $C_V(T)$ based on the Debye model and compare with that of Einstein's at extremely low and high temperatures. (Note that the largest value of k is not zero, but equals $\frac{\pi}{a}$ where a denotes the lattice constant of the solid.)

6. (Fitting of real experimental data, 加分題, 10 points)

Cutting a long rod of length L by half, one gets two rods of length $L/2$. Further cut renders four rods of length $L/4$. Repeating this procedure by $n \gg 1$ times gives 2^n number of length-$L/2^n$ rods. Plot the number $N(\ell)$ as a function of rod length ℓ <u>in a histogram</u>（長條圖）for ALL rods that ever exist. What kind of distribution function do you obtain? Note that the answer is not $N(\ell) = L/\ell$. (註：長條圖的做法是先針對 x-軸參數選取一個固定間隔，並且把在每一間隔的棍子數目加起來當成新的 y 軸參數；由於棍子的長度越差越小，數據點在橫軸的分佈是 x 越小、點越密，因此小 x 的長條圖間隔會分到比較多的數據點，因此可以預期最後長條圖給出的 $N(\ell) \propto \frac{1}{\ell^{\alpha}}$分佈，對應的冪次方$\alpha$應該會大於 1）