Advanced Stat Mech - Assignment 1

Due date: January 18, 2019

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Note: Please submit the assignment to any one of TA's office on/before the due date. For the numerical parts, use your preferred programming language, plotting software, etc. and attach the print outs at the correct places of your solution. If you have any doubt regarding the assignment problems or the topics discussed in the class, feel free to discuss with the TA's or the instructor. Good luck!

Q1 $\boxed{\text{70 marks}}$

Probabilities and random walks

(a) *(Central limit theorem)* If X_i for $i = 1, 2, 3, .., N$ are independent, identically distributed random variables with zero mean and variance σ^2, then show that the random variable X (defined below) has Gaussian distribution function with zero mean and unit variance in the limit $N \to \infty$. $\boxed{15}$

$$X = \frac{X_1 + X_2 + ... + X_N}{\sigma\sqrt{N}}. \tag{1}$$

Now consider the individual random variables X_i to be Cauchy distributed. Does the above theorem hold? Repeat the same procedure as above for this case and find the distribution of X.

(b) *(Breaking stick)* Suppose you have a stick pf unit length. You break it into three pieces. What is the probability that you can make a triangle using these three pieces? (**Hint:** Triangle inequality.) $\boxed{5}$

(c) *(Random matrices)* Consider an ensemble of 2×2 real symmetric random matrices. Choose the entries from a uniform distribution of mean zero and unit variance. Create histograms for trace, individual eigenvalues and the spacing between the eigenvalues. Show the convergence with increasing size of the ensemble. Repeat the numerics by picking the entries from Gaussian distribution of zero mean and unit variance now. Show the convergence again. Do the results differ for these two choices? $\boxed{20}$

(d) *(Continuous time random walk on a 1d lattice)* A random walker moving on a one dimensional lattice can jump to the right with rate α and to the left with same rate. Derive the equation that describes the time evolution of the probability $P(i, t)$ to be at i'th site in time t. Next solve this equation to get $P(i, t)$ in terms of modified Bessel functions of first kind I_i. $\boxed{20}$

(e) *(Discrete time random walk on a 1d lattice)* Now consider a random walker moving in one dimensional lattice in discrete steps with probability $\frac{1}{2}$ to make a jump on either side. Derive the probability $P(r, N)$ for the walker to be at site r after N steps. Next consider N to be very large so that $P(r, N)$ can be approximated using Stirling's approximation. Show that $P(r, N)$ can now be written in the form $e^{-N\phi(\frac{r}{N})}$. Compute $\phi(x)$.($\phi(x)$ *is said to be the Large deviation function*). $\boxed{10}$

Q2 $\boxed{\text{30 marks}}$

Thermodynamics of fluid and magnetic systems

Please do the following questions parallelly for fluid systems $P, V, ...$ and magnetic systems $h, -M, ...$ Note that pressure P is replaced by the external magnetic field h and volume V by negative magnetization in magnetic systems. Take the number of particles N fixed in both cases.

(a) *(Thermodynamic potentials)* Consider the thermodynamic potentials – average energy U, enthalpy E, Gibbs potential G and Helmholtz potential A. Define them properly and write the corresponding differentials. Note the arguments of each potential. Write down the recipes to calculate entropy S, P (or h), V (or M) and temperature T from the thermodynamic potentials. Show that the knowledge of any one of the state functions is sufficient to calculate other state functions. $\boxed{15}$

(b) *(Response functions and convexity of potentials)* Define the basic response functions, namely the specific heat C_x with $x = P, V, h, M$ and compressiblity (magnetic susceptibility) κ_x (χ_x) with $x = T, S$ and write down the recipes to calculate these from the thermodynamic potentials. From that show that G is concave function of both temperature and pressure and A is concave function of temperature but convex function of volume (or magnetization). $\boxed{15}$

Q3 $\boxed{\text{30 marks}}$

Ensembles and classical ideal gas

(a) *(Entropy maximization)* In any statistical population the most probable configuration is given by the maximization of the Gibbs entropy defined as $S_{\text{Gibbs}} = -\Sigma_\alpha p_\alpha \log p_\alpha$ where p_α is the probability of αth microstate which satisfies $\Sigma_\alpha p_\alpha = 1$. Show that the maximum entropy is given by the microcanonical ensemble for which all microstates are equally likely. Next consider that in addition to the constraint $\Sigma_\alpha p_\alpha = 1$, we also have the average energy $\langle E\rangle = \Sigma_\alpha p_\alpha E_\alpha$ fixed. Show that the entropy will be maximized by the canonical ensemble. Now add one more constraint of the fixed average number of particles $\langle N\rangle = \Sigma N_\alpha p_\alpha$. Show that the maximization of entropy corresponds to the Grand canonical ensemble. Comment on the equivalence of all these ensembles in the thermodynamic limit, $\boxed{20}$

(b) *(Classical ideal gas in grand canonical ensemble)* Consider the classical ideal gas at temperature T and fugacity z in the grand canonical ensemble. Show that the probability distribution for finding the number of particle N in the system is Poisson distribution given as, $\boxed{10}$

$$P(N) = \frac{\langle N\rangle^N e^{-\langle N\rangle}}{N!}. \tag{2}$$

Q4 $\boxed{\text{50 marks}}$

Ideal Fermi and Bose gas

Consider an ideal Fermi gas at temperature T enclosed in a box of volume V. We can derive the expressions of N, E and P to be the following:

$$N = \frac{V}{\lambda^3} f^-_{3/2}(z), \quad E = \frac{3VK_BT}{2\lambda^3} f^-_{5/2}(z), \quad P = \frac{2E}{3V}, \tag{3}$$

where $f^-_\nu(z) = \frac{1}{\Gamma[\nu]}\int_0^\infty dx \frac{x^{\nu-1}}{z^{-1}e^x+1}$.

(a) Show that as $T \to 0$ $\boxed{5}$

$$f^-_\nu(z) = \sum_0^\infty \frac{(\beta\mu)^{\nu-m}}{\Gamma[|\nu-m|+1]} I_m, \text{with} \tag{4}$$

$$I_m = \frac{1}{\Gamma[m+1]}\int_{-\infty}^{\infty} dt\, t^m \frac{d}{dt}\left(\frac{-1}{e^t+1}\right) = \begin{cases} 0, \text{for } m = odd \\ 2f_m^-(1), \text{for } m > 0 \\ 1, \text{for m=0} \end{cases} \tag{5}$$

(b) Using this expansion in the expression of N and E, find the leading order correction for non zero temperature. Compute the specific heat in $T \to 0$ limit. Plot C_v as a function of T qualitatively over full range. $\boxed{15}$

(c) A metal can be modelled as a collection of free electrons and vibrating ions. The ions can be shown to contribute T^3 to the specific heat. Given this information and the results obtained above, discuss a technique that can be used to distinguish metals and non-metals. $\boxed{5}$

(d) *(Free Bose gas and first look at a phase transition)* Discuss Bose-Einstein condensation. For a free Bose gas in 3d calculate the condensation temperature T_c. Calculate C_V and discuss about its behavior around T_c. If you find a cusp singularity in C_v at T_c discuss about its existence only at thermodynamic limit and convince yourself about the crucial role played by the thermodynamic limit in the theory of phase transitions. Is there a transition in lower dimensions? Discuss mathematically. $\boxed{25}$

Q5 $\boxed{\text{30 marks}}$

Interacting gas and virial coefficients

(a) *(Second virial coefficient)* Evaluate explicitly the second virial coefficient $B_2(T)$ for the following interaction potentials : $\boxed{15}$

$$(i)\ u(\vec{r}) = \begin{cases} \infty & \text{if } |\vec{r}| < a \\ 0 & \text{if } |\vec{r}| \geq a \end{cases}, \qquad (ii)\ u(\vec{r}) = \begin{cases} \infty & \text{if } |\vec{r}| < a \\ -\epsilon & \text{if } a < |\vec{r}| < R \\ 0 & \text{if } |\vec{r}| \geq R \end{cases}$$

For case (ii) interpret the behaviour of $B_2(T)$ in $T \to \infty$ and $T \to 0$, both for $\epsilon > 0$ and $\epsilon < 0$.

(b) *(One dimensional hard-rod gas)* Consider a one-dimensional gas of indistinguishable hard particles of mass m confined inside a finite region of length ('volume') L. The particles are interacting via the potential $\boxed{15}$

$$u(x - x') = \begin{cases} \infty & \text{if } |x - x'| < a \\ 0 & \text{if } |x - x'| \geq a \end{cases}$$

The hard sphere nature of the particles means that no particle can get within a distance $a/2$ of the ends $x = 0$ and $x = L$. This means there is a one-body potential acting as well, where

$$v(x) = \begin{cases} \infty & \text{if } x < a/2 \\ 0 & \text{if } a/2 \leq x \geq L - a/2 \\ \infty & \text{if } x > L - a/2. \end{cases}$$

So the Hamiltonian of the system can be written as

$$H_N = \sum_{i=1}^{N} \frac{p_i^2}{2m} + \sum_{i=1}^{N-1} u(x_i - x_{i-1}) + v(x_1) + v(x_N).$$

1. Show that the partition function $Z_N = \frac{1}{N!}\left(\prod_{i=1}^{N}\int\int \frac{dp_i dx_i}{h}\right)\exp(-\beta H_N)$ is explicitly given

by:

$$Z_N = \frac{1}{\lambda^N N!}(L - Na)^N, \quad \text{where,} \quad \lambda = \frac{h}{\sqrt{2\pi m K_B T}}.$$

2. Also show that the equation of state is given by

$$p = \frac{nK_BT}{1 - na}, \quad \text{where,} \quad n = N/L.$$

Q6 $\boxed{\text{20 marks}}$

Kinetic theory

(a) *(BBGKY hierarchy of equations)* Using the Liouville's equation and defining the s-particle density f_s, etc. derive the BBGKY hierarchy of equations, $\boxed{10}$

$$\left[\frac{\partial}{\partial t} + \sum_{n=1}^{s} \frac{\vec{p}_n}{m} \cdot \frac{\partial U}{\partial \vec{q}_n} - \sum_{n=1}^{s} \left(\frac{\partial U}{\partial \vec{q}_n} + \sum_{l} \frac{\partial V(\vec{q}_n - \vec{q}_l)}{\partial \vec{q}_n}\right) \cdot \frac{\partial}{\partial \vec{p}_n}\right] f_s$$
$$= \sum_{n=1}^{s} \int dV_{s+1} \frac{\partial V(\vec{q}_n - \vec{q}_l)}{\partial \vec{q}_n} \cdot \frac{\partial f_{s+1}}{\partial \vec{p}_n}. \quad (6)$$

The Hamiltonian has the usual form $H(\mathbf{p}, \mathbf{p}) = \sum_{i=1}^{N} \left[\vec{p}_i^2/2m + U(\vec{q}_i)\right] + \frac{1}{2}\sum_{i,j} V(\vec{q}_i - \vec{q}_j)$.

(b) *(Vlasov equation)* In the limit of high particle density $n = N/V$, or large interparticle interaction range λ, such that $n\lambda^3 >> 1$, the collision terms are dropped from the left-hand side of the equations in the BBGKY hierarchy. Assume that the N-body density is a product of one-particle densities, that is, $\rho = \prod_{i=1}^{N} \rho_1(\mathbf{x}_i, t)$ where $\mathbf{x}_i \equiv (\vec{p}_i, \vec{q}_i)$. Calculate the densities f_s, and their normalizations. Hence show that once the collision terms are eliminated, all the equations in the BBGKY hierarchy are equivalent to the single equation $\boxed{10}$

$$\left[\frac{\partial}{\partial t} + \frac{\vec{p}}{m} \cdot \frac{\partial}{\partial \vec{q}} - \frac{\partial U_{eff}}{\partial \vec{q}} \cdot \frac{\partial}{\partial \vec{p}}\right] f_1(\vec{p}, \vec{q}, t) = 0 \quad (7)$$

where $U_{eff}(\vec{q}, t) = U(\vec{q}) + \int d\vec{x}' V(\vec{q} - \vec{q}') f_1(\vec{\mathbf{x}}', t)$.