Statistical Physics Spring 2019: Tutorial Sheet 1 (Instructor: K. Damle)

Due April 10 2019 in class

1. Consider a simple harmonic oscillator with oscillation frequency ω and mass m in 1-dimension.

   - Characterize the surface of constant energy E in phase space: What does it look like in geometric terms?
   - Find the 'volume' in phase-space occupied by states with energy $\leq E$ in classical mechanics. What are the dimensions of this 'volume'?
   - Find the number of states with energy $\leq E$ in the corresponding quantum problem
   - When E is large, show that the two answers are proportional to each other. What is the proportionality constant?

2. As we have discussed, the entropy of an equilibrium system considered as a function of energy, *i.e.* $S(E)$, can be calculated by taking the logarithm of the number of states that 'have total energy E' for a macroscopic system [question: why is 'have total energy E' in quotes above?]. Apply this to a system of N independent oscillators (distinguishable) having total energy

   $$E = \frac{1}{2}\hbar\omega N + M\hbar\omega$$

   where M is a large integer, and do the following

   - Calculate the entropy $S(E)$
   - Determine the temperature T, or rather, find E as a function of T.
   - Now, find the probability that a given oscillator out of these N (say the first oscillator) is in a particular quantum state n. To do this, assume that all states of total energy E are equally likely.

3. Consider an insulating ionic solid in which each ion carries a net magnetic moment $g\mu_B m_J$ in the $\hat{z}$ direction, where the quantum number m_J is of course allowed to take values $-J, -J+1 \ldots + J$ appropriate for a ground state ionic multiplet of total angular momentum J. An external field $B\hat{z}$ couples to these moments to give the magnetic contribution E_M to the energy of the solid

$$E_M = -\sum_{i=1}^{N} g\mu_B m_J(i) B$$

where i indexes the lattice sites on which the ions live.

   - Assuming that weak dipolar interactions between the ions are enough to equilibriate the system but not strong enough to affect the thermodynamics, calculate the linear magnetic susceptibility (*i.e.* for weak fields B).
   - Take the high temperature limit of the formula you derive. Is the resulting expression familiar?

4. The measured heat capacity per mole $c = \frac{1}{N}\frac{dE}{dT}$ of a system has been fit to an empirical formula

$$c(T) = \frac{T}{\Delta} \exp\left(-(T - T_f)^2/\Delta^2\right)$$

Assuming that the entropy per mole $s(T)$ obeys the third law of thermodynamics, calculate the $T \to \infty$ limit of $s(T)$ under the assumption that T_f/Δ is very very large.

5. Let P_m be the probability that a system is in eigenstate with energy E_m. If we define the entropy by $S = -\sum_m P_m \log(P_m)$, and demand that S be as large as it can be subject to the constraint that the mean energy $\langle E \rangle$ (with mean $\langle ... \rangle$ taken with respect to the probabilities P_m) be some fixed value $\bar{E}$, then what choice of P_m satisfies this demand?

6. The density matrix of a free particle is given as

$$\hat{w} = \exp(-\hat{H}/T)$$

with $\hat{H} = \hat{p}^2/2m$. Assume that the particle is in a box of linear dimension L with periodic boundary conditions. In the $L \to \infty$ limit, what is the coordinate space representation of $\hat{w}$?

7. Assuming a classical canonical distribution

    - calculate the classical partition function of an ideal gas of N indistinguishable particles of mass m enclosed in an infinitely tall cylinder of cross-sectional area A placed in a uniform gravitational field.
    - Also calculate the mean energy and heat capacity
    - Now calculate the Helmholtz free energy F.
    - Compare your result for the heat capacity with that of an ideal gas without an external gravitational field. Explain the difference.

8. A substrate has N_0 trapping sites at which a gas molecule can be trapped on its surface. Only one gas molecule can be trapped in a given trapping site at a time. However, the trapped molecule can be in one of three different trapped states with three different energies ϵ_1, ϵ_2, and ϵ_3.

    Assuming that there are negligible interactions between trapped molecules, assuming that the surrounding volume of gas is big enough that the number of trapped molecules is a negligible fraction of the total, and assuming that the process of trapping and release happens fast enough that the entire system can reach equilibrium, calculate the chemical potential μ of the molecules in terms of the mean number $\bar{N}$ of trapped molecules, the temperature T, and the energy levels $\epsilon_{1/2/3}$

9. A polymer chain is made of N monomer units. Each monomer unit can be in one of two conformational states γ and δ. Corresponding energies are ϵ_γ and ϵ_δ, and the linear extent that each monomer unit occupies when in this conformational state is correspondingly l_γ, l_δ. So each configuration of the polymer chain can be described in terms of the conformational states of the individual monomer units that make up the polymer chain (*e.g.* $\gamma\delta\gamma\gamma\delta$...). Assume that the polymer experiences a constant tension T_n, that the polymer is in contact with

the surrounding medium at temperature T long enough to equilibriate, and that individual monomers can change their conformational state fast enough to be in equilibrium with respect to their conformational states as well.

Under these assumptions, calculate the mean length $\langle L \rangle = \langle \sum_{i=1}^{N} l_i \rangle$ as a function of T and T_n in equilibrium.

10. If two systems I and II are in equilibrium with each other at temperature T, show that

$$\langle (E_I - \langle E_I \rangle)^2 \rangle = \langle (E_{II} - \langle E_{II} \rangle)^2 \rangle = T^2/(C_I^{-1} + C_{II}^{-1})$$

where C_I and C_{II} are the heat capacities of the two systems.

What does this formula reduce to when one of the systems is very large compared to the other?

11. For a gas of N non-interacting particles occupying total volume V (*i.e.* with mean density $\rho \equiv N/V$), show that the number n of particles in a macroscopic sub-volume Ω is given by the Poisson distribution

$$P(n) = \frac{(\rho\Omega)^n}{n!} \exp(-\rho\Omega)$$

12. Consider an ionic insulating solid where each ion has total angular momentum quantum number $J = 1/2$. In a small external field $B\hat{z}$ along the $\hat{z}$ direction, the energy of the system is $E = -B \sum_{i=1}^{N} m_J(i)$ where each $m_J(i)$ can take values $\pm 1/2$.

- When the energy is fixed at $E = kB - BN/2$ (where $0 \le k \le N$ is an integer), how many different states can the system have at this energy?
- From the above, calculate the entropy as a function of energy $S(E)$.
- From this, calculate the temperature T as a function of energy.
- Invert this to work out $E(T)$.
- Using the above expressions for S and E for large N, calculate $\log Z_G$, where Z_G is the partition function in the Gibbs ensemble at temperature T

- Now calculate $\log(Z_G)$ directly from its definition in terms of the Gibbs distribution at temperature T. Does this agree with your earlier result obtained from expression for S and E?

13. Consider a system of fermionic atoms F (confined to a container with rigid walls) that can be of two types which we label as ↑ and ↓ (you may think of these as two possible polarizations of an internal 'spin' degree of freedom, although in real life examples it is a bit more complicated).

    An ↑ fermion $F_\uparrow$ can form a bosonic 'molecule' (bound state) B by combining with a ↓ fermion $F_\downarrow$. Conversely, a B molecule can dissociate into a $F_\uparrow$ and $F_\downarrow$. That is, we have

    $$F_\uparrow + F_\downarrow \rightleftharpoons B$$

    This 'reaction' (in both directions) is assumed to proceed slowly enough that we may think of the B molecules as being a stable bosonic species in its own right in addition to viewing the $F_\uparrow$ and $F_\downarrow$ as being stable fermionic atoms. However, this reaction does happen quickly enough (in both directions) to ensure that the fermionic and bosonic systems reach a common thermal equilibrium characterized by a single temperature T and a single chemical potential μ in the grand-canonical description (as the number of fermionic atoms N_F is not separately conserved, nor is the number of bosonic molecules N_B).

    The single particle eigenstates available to the fermions are thus labeled by a momentum $\mathbf{p}$ and a 'spin' $\sigma = \pm 1/2$, where $\sigma = +1/2$ corresponds to $F_\uparrow$ and $\sigma = -1/2$ corresponds to $F_\downarrow$. The energy $\epsilon^F_\sigma(\mathbf{p}) = p^2/2m$ independently of σ, while the single particle eigenstates available to the molecules have energy dispersion $\epsilon^B(\mathbf{p}) = -E_B + p^2/4m$, where $E_B \geq 0$ is the binding energy and the $4m$ in the denominator is because the mass of the bosonic molecule is twice the fermionic atom mass m.

    To analyze the equilibrium state of this mixture, we further assume that there are no interparticle interactions we need to include in our description and proceed as follows

    - Write down an expression in terms of $n^F_\sigma(\mathbf{p})$ and $n^B(\mathbf{p})$ for the conserved total number N_{tot} to which the chemical potential μ

couples in our grand canonical description. Here $n^F_\sigma(\mathbf{p})$ and $n^B(\mathbf{p})$ are respectively the number of F particles in state $|\mathbf{p}\sigma\rangle$ and B particles in state $|\mathbf{p}\rangle$, and $\mathbf{p}$ takes on values $2\pi\hbar\vec{n}/L$, with $\vec{n} \equiv (n_x, n_y, n_z)$ integers ranging from $-\infty$ to $+\infty$ as is appropriate for a system confined with periodic boundary conditions to a box of volume L^3.

- Write down an expression for the total energy in terms of $n^F_\sigma(\mathbf{p})$, $n^B(\mathbf{p})$ and $\epsilon^F_\sigma(\mathbf{p})$ and $\epsilon^B(\mathbf{p})$.
- Using the above, calculate $Z_{\text{grand}} = Tr\exp(-\beta(H_{\text{tot}} - \mu N_{\text{tot}}))$ to obtain an answer in the form of an infinite product.
- From this, calculate the expectation value of N_{tot} by differentiating $\log(Z_{\text{grand}})$ with respect to $\beta\mu$.
- From this, take the naive thermodynamic limit and express the total density $\rho_{\text{tot}} = N_{\text{tot}}/L^3$ as a sum of two integrals.

  $$\rho_{\text{tot}} = I_F + I_B$$

  where I_F is the contribution of the fermions and I_B the contribution of the bosons.
- We now need to use this expression to solve for μ in terms of ρ_{tot} and T. To do this, first argue that since the total density is finite, $\mu \leq -E_B$.

For the rest of the problem, consider the simpler case of a marginally bound molecule with $E_B = 0$.

- Now, argue that for low enough temperature $I_F + I_B$ is bounded above by a small number that will be less than any non-zero ρ_{tot} for the allowed range of μ, thus leading to an inconsistency.
- Thus, argue that at low enough temperature, we need to carefully include a condensate density contribution $2n^B_0$ in addition to the two integrals, and thereby modify the naive thermodynamic limit expression for ρ_{tot}. Thus

  $$\rho_{\text{tot}} = I_F + I_B + 2n^B_0$$

- Calculate in the $T \to 0$ limit, the value of μ
- Calculate in the same limit the value of the condensate density n_0^B.
- Obtain the expectation value of the number of fermionic atoms in the same limit
- Obtain the expectation value of the total number of bosonic molecules (including condensate) in the same limit
- Show that the value of μ remains unchanged as the system is heated to slightly above absolute zero.
- Using the above, calculate the temperature dependence of the condensate density as the temperature is raised slightly above zero. Write your answer in the form $A - BT^p$ and identify the constants A and B and the power p.
- The transition temperature at which the condensate disappears on heating is the temperature at which this formula predicts that the condensate density is zero. Use this to calculate T_c in terms of total density ρ_{tot} and other system parameters.

Endnote: If you find this interesting look up 'Resonantly paired fermionic superfluids' by V. Gurarie and L. Radzihowsky in Annals of Physics, **322**, *2-119 (2007) available in our library*