PHYS4031 STATISTICAL MECHANICS

SAMPLE QUESTIONS FOR DISCUSSION in WEEK 4 EXERCISE CLASSES
(26,28 September 2016)

You may want to think about them before attending exercise class.
SQ8 - Volume of a D-dimensional sphere of radius R
SQ9 - Learning physics by inspecting the classical ideal gas result - what if it is D-dim?
SQ10 - Interstitial or Frenkel Defects (Microcanonical ensemble approach)

SQ8 **Mathematical Skills VI - Volume of a D-dimensional "sphere".** (You do not need to memorize the final result Eq. (7) for exam purposes.)

You know that πR^2 is the area of a circle (2D "sphere) and $\frac{4}{3}\pi R^3$ is the volume of a 3D sphere. How about higher dimensions? We used the answer in carrying out the microcanonical ensembe calculations for a classical ideal gas.

The **volume** of a hyper-sphere of radius R in D dimensions is formally given by

$$V_D(R) = \int \cdots \int_{0 \leq x_1^2 + \cdots x_D^2 \leq R^2} dx_1 \cdots dx_D. \tag{1}$$

(TA: Why is it?) We want to carry out this integral. This problem makes use of the Gaussian integral and the Gamma function, as introduced in Problem Set 1.

To proceed, by dimensional analysis, the **surface area** of a hyper-sphere of radius r can be written as:

$$A_D(r) = S_D \, r^{D-1} \tag{2}$$

where S_D is a constant to be determined. If we can find S_D, then $V_D(R)$ follows immediately since

$$V_D(R) = \int_0^R S_D \, r^{D-1} dr = \frac{S_D}{D} R^D. \tag{3}$$

Eq. (3) amounts to adding up shells to form a sphere as in an onion. Thus the whole problem becomes that of determining S_D in Eq. (2).

To get S_D, we consider the following integral:

$$I_D \equiv \int_{-\infty}^{\infty} dx_1 \int_{-\infty}^{\infty} dx_2 \cdots \int_{-\infty}^{\infty} dx_D \; e^{-(x_1^2 + x_2^2 + \cdots + x_D^2)} \tag{4}$$

where the integrals are over all space in D dimensions.

(a) Noting that I_D is a product of Gaussian integrals, show that

$$I_D = \pi^{D/2}. \tag{5}$$

(b) The integrand in I_D is "spherically symmetrical" (just like the spherically symmetrical potentials you encountered in atomic problems or in central force problems) and this allows us to treat Eq. (4) in a different way. Treating the integral over all D-dimensional space by adding up "spherical shells" of different radii, show that

$$I_D = \frac{S_D}{2} \, \Gamma(\frac{D}{2}) \tag{6}$$

where Γ is the Gamma Function (see Problem Set 1 about the Gamma functions).

(c) Hence, show that the volume of a D-dimensional hypersphere is given by

$$\boxed{V_D(R) = \frac{\pi^{D/2}}{\Gamma(\frac{D}{2}+1)} \; R^D.} \tag{7}$$

Remarks: This formula is needed for studying classical ideal gas within microcanonical ensemble (if we do not want to invoke any particle-in-a-big-box QM) in getting $W^{<}(E, V, N)$. It can also be used to study a collection of classical oscillators (Problem 2.6). To see that it is right, write down the explicit results for $D = 1, 2, 3, 4$. I think one can also do a mathematical induction proof. I hope that you are happy as you have just learnt something that goes beyond high school mathematics!

SQ9 **Learning physics by inspecting a result - Classical ideal gas.**

After a laborious calculation, the entropy of a 3D classical ideal gas was shown to be

$$S(E,V,N) = k \ln \left[\left(\frac{V}{N} \right)^{N} \left(\frac{4\pi m E}{3h^2 N} \right)^{3N/2} \right] + \frac{5}{2} Nk \tag{8}$$

This is (one form of) the Sackur-Tetrode Equation. This is exact, but looks a bit complicated. After taking derivatives, we have $E = \frac{3}{2}NkT$ and $pV = NkT$, results that you know in high school!

Natural extensions of the problem could be: How about classical ideal gas in 1D, 2D, 4D, etc.? Life is short and we don't want to waste our time doing these calculations one by one. Could we get at the results based on inspecting Eq. (8)?

TA: Lead the students through the following line of thought. We see that there is $\frac{3}{2}$ in $E = \frac{3}{2}NkT$. This 3/2 must come from the 3/2 in the power in Eq. (8). So the question is **where does the "3" come from and where does the "2" come from?** You may lead the students back to an expression of $W^{<}(E,V,N)$ or $W(E,V,N;\Delta E)$ and see how "3" and "2" enter into the expression.

Hence, predict how E goes in various dimension? You may add in discussions on other situations.

SQ10 **Interstitial Defects Problem - Microcanonical Ensemble Approach, again!** See Ch.IV appendix.

In Ch.IV Appendix A, we discussed the Schottky defect problem using microcanonical ensemble approach. Defects are extremely important to materials properties, as a perfect crystal is something too ideal. In fact, one can even make use of defects to control materials properties (e.g., in making swords). The example in Ch.IV is the simplest case in which n atoms are taken out (or excited from) of a regular array of N atoms and these atoms migrate (move) to the surface sites - forming Schottky defects. In the example, we don't care about how to put the n atoms onto the surface.

Interstitial or Frenkel defects: Here is an alternative scenario to the atoms after they are excited out of their positions in a regular array of N atoms. In a crystal, there are places **in between** where the atoms usually sit. When atoms get excited and go into these sites, they form **interstitial defects** or **Frenkel defects**. Let's say there are N' possible interstitial places that the excited atoms can get into (no double occupancy (too crowded) please). The energy required to create one such defect is ϵ. Consider a state of energy $E = n\epsilon$, i.e., n Frenkel defects are created. Thus, (E, N, N') or (n, N, N') defines a macrostate. Typically, $n \ll N, N'$, but these numbers are much bigger than unity.

TA: Follow the standard microcanonical ensemble approach - Count W, find S, derive $1/T$ in terms of E, N, N' and find $n(T)$. This shows the number of thermally created defects at a temperature T. Also, obtain the heat capacity and sketch how it depends on temperature T.

[**Important remarks**: In reality, excited atoms inside a crystal can do a lot of things – some go to the surface sites (Schottky defects) and some go to the interstitial positions (interstitial or Frenkel defects). Different excitations may require different energies, e.g., ϵ' for an excitation to surface states and ϵ for interstitial defects. Experiments usually cannot control one process to happen and one doesn't. Experimental data are a combination of all effects! Only in theoretical treatments can we separate them and consider them one by one. One should appreciate the complex reality that experimentalists face everyday! For a discussion on defects, see the chapters on "Point Defects" and "Dislocations" in *Introduction to Solid State Physics* by C. Kittel.]