PHYS 328 HOMEWORK #10-- SOLUTIONS

1. Consider the nth energy level in a hydrogen atom. An electron in this level can have n - 1 values of angular momentum, and for each value of angular momentum, can have 2 L + 1 values of the azimuthal quantum number. Thus, the total number of equivalent energy states available to this electron can be expressed as :

$$\sum_{L=0}^{L=n-1} (2L+1) = 2\sum_{L=0}^{n-1} L + \sum_{L=0}^{n-1} 1$$

Let's find the value of the last sum; we are simply adding the number one n times (remember, there are n values from 0 to n - 1), so the last sum contributes a value n to the total number of states.

How can we find the value of the first summation; in other words, how do we sum L from 0 to n - 1? You may know that it is well known that the sum of the first k integers is k (k + 1)/2, but let me try to motivate that. Suppose you have integers 1 through k. You can sum them by grouping them in pairs : (1 + k) + (2 + (k - 1)) + (3 + (k - 2)) + ... you can see that the sum of each group is k + 1, and that there are k/2 such pairings, so that the sum of all the integers is $(k + 1)\times k/2$, or k (k + 1)/2. (If there are an odd number of integers, the analysis varies a bit but you get the same result).

Thus the value of the first sum is 2(n-1) n/2 = n(n-1); when we add this to n we get:

total number of energy levels $= n^2 - n + n = n^2$

You may remember from chemistry that the total number of electrons in an energy level is $2n^2$; this takes into account that two electrons of different spin orientations may have the same n, l, m quantum numbers.

2. Given that :

$$\int \frac{\mathrm{dx}}{\mathrm{x}^2 + \mathrm{a}^2} = \frac{1}{\mathrm{a}} \arctan \left| \frac{\mathrm{x}}{\mathrm{a}} \right|$$

we can easily show the definite integral :

$$\int_0^\infty \frac{\mathrm{dx}}{\mathrm{x}^2 + \mathrm{a}^2} = \frac{\pi}{2\,\mathrm{a}}$$

Now, if we differentiate both sides with respect to a we get :

$$\frac{\mathrm{d}}{\mathrm{da}} \int_0^\infty \frac{\mathrm{dx}}{\mathrm{x}^2 + \mathrm{a}^2} = \frac{\mathrm{d}}{\mathrm{da}} \left(\frac{\pi}{2\,\mathrm{a}}\right)$$

The derivative on the right easily yields :

$$\frac{-\pi}{2 a^2}$$

On the left, we get :

$$\frac{d}{da} \int_0^\infty \frac{dx}{x^2 + a^2} = \int_0^\infty \frac{d}{da} \left(\frac{dx}{x^2 + a^2} \right) = \int_0^\infty \frac{-2 a dx}{\left(x^2 + a^2 \right)^2}$$

These two expressions must be equal, so :

$$\int_0^\infty \frac{-2 \, \mathrm{a} \, \mathrm{dx}}{\left(x^2 + \mathrm{a}^2\right)^2} = \frac{-\pi}{2 \, \mathrm{a}^2} \Rightarrow \int_0^\infty \frac{\mathrm{dx}}{\left(x^2 + \mathrm{a}^2\right)^2} = \frac{\pi}{4 \, \mathrm{a}^3}$$

Repeating the process we get :

$$\frac{d}{da} \int_0^\infty \frac{dx}{(x^2 + a^2)^2} = \frac{d}{da} \left(\frac{\pi}{4 a^3}\right) = -\frac{3\pi}{4 a^4}$$

The derivative on the left becomes :

$$\frac{d}{da} \int_0^\infty \frac{dx}{(x^2 + a^2)^2} = \int_0^\infty \frac{d}{da} \left(\frac{dx}{(x^2 + a^2)^2} \right) = \int_0^\infty -\frac{2 \cdot 2 a}{(x^2 + a^2)^3} dx$$

Equating the two expressions :

$$\int_0^\infty -\frac{2\cdot 2a}{\left(x^2+a^2\right)^3} \, dx = -\frac{3\pi}{4a^4} \Rightarrow \int_0^\infty \frac{dx}{\left(x^2+a^2\right)^3} = \frac{3\pi}{16a^5}$$

What does Mathematica - bot think?

 $\label{eq:linear} Integrate[1 \ / \ (x^2 + a^2)^3, \ \{x, \ 0, \ \infty\}, \ \mbox{Assumptions} \rightarrow \mbox{Re}[a] > 0]$

3 π

16 a⁵

Efficient, sure, but lacking in the panache of our solution.

3. In the high temperature limit, the equipartition theorem tells us that the average energy of N oscillators is f/2 N k T. For an Einstein oscillator, f = 2 so that the average energy of the ensemble is N k T. Therefore, the heat capacity is

$$C = \frac{dE}{dT} = N k$$

and using the result in the text for the standard deviation of the energy :

$$\sigma_{\rm E} = k \, \mathrm{T} \, \sqrt{\mathrm{C}/\mathrm{k}} = k \, \mathrm{T} \, \sqrt{\mathrm{N}\,\mathrm{k}/\mathrm{k}} = k \, \mathrm{T} \, \sqrt{\mathrm{N}}$$

The fractional fluctuation in energy is found by dividing the standard deviation by the energy :

$$\frac{\sigma_{\rm E}}{\bar{\rm E}} = \frac{\rm k\,T\,\sqrt{N}}{\rm N\,k\,T} = \frac{1}{\sqrt{\rm N}}$$

We have seen previously in the class how $1/\sqrt{N}$ is a good measure of relative fluctuation around the mean. For large systems, i.e., Avogadro sized, $1/\sqrt{N}$ is a tiny number, indicating that any fluctuations around the mean are so small as to be unmeasurable.

4. We are asked to find an expression for the average energy of a system where the energy is linearly dependent on some coordinate, i.e.,

E = c |q|

where c is some constant. Following the procedure outlined in class, we begin by computing the partition function :

$$Z = \sum_{q}^{\Box} e^{-\beta c |q|} = \frac{1}{\Delta q} \Sigma e^{-\beta c |q|} \Delta q$$

Allowing Δq to approach zero, we can turn the sum into an integral; making use of the symmetry of |q| we can write :

$$Z = \frac{1}{\Delta q} \int_{-\infty}^{\infty} e^{-\beta c |q|} dq = \frac{1}{\Delta q} \cdot 2 \int_{0}^{\infty} e^{-\beta c q} dq = \frac{2}{\Delta q} \left(\frac{-1}{\beta c}\right) (0-1) = \frac{2}{\beta c \Delta q}$$

Having an analytical expression for Z, we can find the average energy from :

$$\overline{E} = \frac{-1}{Z} \frac{\partial Z}{\partial \beta} = -\frac{\beta c \Delta q}{2} \left(\frac{2}{c \Delta q}\right) \left(\frac{-1}{\beta^2}\right) = \frac{1}{\beta} = k T$$

5. We grind and find using :

$$v_{rms} = \sqrt{3 \text{ k T} / \text{m}}$$
$$v_{max} = \sqrt{2 \text{ k T} / \text{m}}$$
$$\overline{v} = \sqrt{8 \text{ k T} / (\pi \text{ m})}$$

Substituting values, we have :

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Clear[k, temp, mass]
k = 1.38 × 10<sup>^</sup>-23; temp = 300; mass = 32 × 1.67 × 10<sup>^</sup>-27;
factor = Sqrt[k temp / mass];
Print["The rms speed = ", Sqrt[3] factor, " m/s"]
Print["The most probable speed = ", Sqrt[2] factor, " m/s"]
Print["The average speed = ", Sqrt[8 / π] factor, " m/s"]
The rms speed = 482.089 m/s
The most probable speed = 393.624 m/s
The average speed = 444.158 m/s
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6. Following the treatment in the text, we find the most probable velocity of a nitrogen molecule at this temperature :

$$v_{max} = \sqrt{2 \text{ k T / m}} = \sqrt{2 \cdot 1.38^{-23} \text{ J / K} \cdot 1000 \text{ K} / (28 \cdot 1.67 \times 10^{-27} \text{ kg})} = 768 \text{ m / s}$$

The required speed for escape, 11, 000 m/s is 14.3 times this, so we can use text eq. 6.55 with $x_{min} = 14.3$ to compute:

$$P(v > v_{exc}) = \frac{4}{\sqrt{\pi}} \int_{14.3}^{\infty} x^2 e^{-x^2} dx$$

Integrating numerically gives :

 $(4 / \text{Sqrt}[\pi])$ NIntegrate $[x^2 \text{Exp}[-x^2], \{x, 14.3, \infty\}]$

 2.51172×10^{-88}

Which is really small. Realizing that the lifetime of the Earth is approx. 4.5 billion years (or 10^{17} secs), it is highly unlikely that the Earth will lose much nitrogen over geological history. However, for hydrogen and helium, the masses are much smaller and:

$$v_{max}(H_2) = 2874 \text{ m/s}$$

so that $x_{\min} = 11,000/2874 = 3.83$ and:

$$P(v > v_{esc}) = \frac{4}{\sqrt{\pi}} \int_{3.83}^{\infty} x^2 e^{-x^2} dx$$

Print["The probability of H_2 escape = ", (4 / Sqrt[π]) NIntegrate[x^2 Exp[-x^2], {x, 3.83, ∞ }]]

The probability of H_2 escape = 1.9017×10^{-6}

While a small number, we should not be surprised that over the lifetime of the Earth, hydrogen molecules have essentially all escaped, so that there is no free H left in the Earth's atmosphere. A similar result will follow for Helium which is only twice as massive as hydrogen molecules (where x_{\min} will be $\sqrt{2}$ times larger for He than H_2

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Print["The probability of He escape = ",
 (4 / Sqrt[\pi]) NIntegrate[x^2 Exp[-x^2], {x, Sqrt[2] 3.83, \omega\]]
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The probability of He escape = 1.12757×10^{-12}

Since the moon and Earth are roughly the same distance from the sun, we should expect the same temperatures in the planet's exospheres. However, on the moon the escape velocity is much lower (2400 m/s), so the value of x_{min} for nitrogen on the moon is 2400/768 = 3.12, leading to a probability of exceeding the escape velocity of:

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(4 / \text{Sqrt}[\pi]) NIntegrate [x^2 \text{Exp}[-x^2], \{x, 3.12, \infty\}]
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0.000218681

or $2.2 \cdot 10^{-4}$, suggesting a high probability of escape, consistent with the observation that the moon has no atmosphere today.