

Theoretical Physics
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Chapter I Homework. Quantum Mechanics

HW-I1. Maxwell-Boltzmann Velocity Distribution (Classical). We know the following integral from earlier in our course.

$$\int_{-\infty}^{\infty} e^{-\alpha x^2} dx = \sqrt{\frac{\pi}{\alpha}}. \text{ Therefore, } \int_0^{\infty} e^{-\alpha x^2} dx = \frac{1}{2} \sqrt{\frac{\pi}{\alpha}}.$$

Also note that

$$\int_0^{\infty} x^2 e^{-\alpha x^2} dx = -\frac{d}{d\alpha} \left[\frac{1}{2} \sqrt{\frac{\pi}{\alpha}} \right] = \frac{1}{4\alpha} \sqrt{\frac{\pi}{\alpha}}.$$

You can simply just use the above integrals when needed below since we have derived the results in our course and above. The velocity probability distribution for particles in a gas moving only in one dimension can be written as

$$f(v_x) = A e^{-\beta E_x}, \text{ where } \beta = \frac{1}{kT} \text{ from class and } E_x = \frac{1}{2} m v_x^2.$$

(a) Find the normalization constant A from $\int_{-\infty}^{+\infty} f(v_x) dv_x = 1$.

(b) In 3D, $f(v_x)dv_x f(v_y)dv_y f(v_z)dv_z = A e^{-\beta E_x} A e^{-\beta E_y} A e^{-\beta E_z} dv_x dv_y dv_z$.

Confirm by integration in spherical velocity coordinates (v, θ, ϕ) that you get 1.

Hint: $dv_x dv_y dv_z$ gets replaced by $v^2 \sin \theta dv d\theta d\phi$ where the v integration goes from 0 to ∞ , the θ integration goes from 0 to π , and the ϕ integration goes from 0 to 2π .

(c) What is $f(v)$ in terms of v and the simplest constants such that $\int_0^{\infty} f(v) dv = 1$

Now you have found what this function specifically is, the function $f(v)$ we encountered in the abstract in "deriving" the ideal gas law. Hint: Look at your work for Part (b). What is left after you integrate over the angles but have not yet integrated over v ? All that stuff in the integrand is $f(v)$. But be sure to express the constant A^3 in terms of k , T , π , etc.

HW-12. Two Quantum States.

a) The Sketch. Sketch a dotted horizontal line to represent a zero reference energy point. Then draw a solid horizontal line below this reference and label this line with energy $\mathcal{E}_1 = -\mathcal{E}$. Then draw a solid horizontal line above your reference and label this line with energy $\mathcal{E}_2 = +\mathcal{E}$.

b) The Partition Function. At temperature T give the partition function for this system. Hint: Recall from notes for Class H that the partition function Z is the sum of exponentials where each exponent has a minus energy for the i^{th} energy level divided by kT .

c) Occupation Numbers. Then give the most probable occupation numbers n_1 and n_2 for each of these states if the total number of particles is some large value $N = n_1 + n_2$. Hint: The occupation numbers are your n_i that can be found in Chapter H or the Class Notes H.

d) Energy. Show that the average energy $\overline{E} = \frac{n_1\mathcal{E}_1 + n_2\mathcal{E}_2}{n_1 + n_2} = -\mathcal{E} \tanh \frac{\mathcal{E}}{kT}$.

e) What are the occupation numbers n_1 and n_2 and average energy \overline{E} in the limit as the temperature approaches absolute zero, i.e., $T \rightarrow 0$.

f) What are the occupation numbers n_1 and n_2 and average energy \overline{E} in the limit as the temperature approaches infinity, i.e., $T \rightarrow \infty$.

g) Compare your results for (e) and (f) in terms of entropy, i.e., the disorder of the system, using words. Why do you expect your answers for (e) and (f) to come out the way they do in terms of entropy?

The point values for this problem are not equally distributed among the parts. Most weight is assigned to the energy formula, sketch, and entropy discussion of the two limiting cases.

HW-13. Infinite Quantum States. Max Planck's discrete energy levels are $E_n = nhf$.

(a) Partition Function. Show that the partition function can be worked out and expressed

as $Z = \frac{1}{1 - e^{-\frac{hf}{kT}}}$. Set up the partition function (Class Notes H) according to the

definition of the partition function. Then, you will need and may use the following

mathematical formula $Z = 1 + r + r^2 + r^3 + \dots = \frac{1}{1 - r}$, where $r = e^{-\frac{hf}{kT}} < 1$.

By the way, here is the derivation of this math formula, but you need not include the derivation in your homework.

$$Z = 1 + r + r^2 + r^3 + \dots \quad \text{and} \quad rZ = r + r^2 + r^3 + \dots \quad \text{where } r < 1.$$

Each series has an infinite number of terms, each getting smaller and smaller since $r < 1$. Subtracting your two infinite sums,

$$Z - rZ = 1, \quad Z(1 - r) = 1, \quad \text{and} \quad Z = \frac{1}{1 - r}, \quad \text{the desired result.}$$

(b) Average Energy. Calculate the average energy. Let the oscillator occupation number

for each energy level n be N_n and the total number of oscillators be

$N = \sum_n N_n = N_0 + N_1 + N_2 + \dots$. Energy level $E_n = nhf$ as noted above

in part a. With this notation, the average energy is then

$$\bar{E} = \frac{\sum_n N_n E_n}{N} = \frac{\sum_n N_n nhf}{N}.$$

From Class H notes, $N_n = N \frac{e^{-\beta E_n}}{Z}$, where Z is your partition function and

$\beta = \frac{1}{kT}$. When you calculate the average energy you will need this derivative trick:

$$\sum_n n e^{-nx} = -\frac{d}{dx} \sum_n e^{-nx} = -\frac{d}{dx} \left[\frac{1}{1 - e^{-x}} \right].$$

Your answer will be the prize:
$$\bar{E} = \frac{hf}{e^{\frac{hf}{kT}} - 1}.$$

(c) You get the classical result by making "h" small, just as you get the classical formulas from relativity by making "c" large. What average energy when h is very small.

You should use the Taylor's expansion $e^z \approx 1 + z$? The equipartition theorem in classical thermodynamics says you get $kT/2$ for each degree of freedom, i.e., each way the system can absorb energy. Remember the ideal gas with $3kT/2$? Here, an oscillator has one degree for kinetic energy along the direction of the "spring" and one degree for its potential energy. So you should get kT for your classical average energy.

You are finished. However, it is highly recommended that sometime, as an exercise on your own, you derive the result for a finite sum of n terms:

$$S_n = a + ar + ar^2 + \dots + ar^{n-1} = a \frac{(1 - r^n)}{1 - r}.$$