Theoretical Physics
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Chapter I Homework. Quantum Mechanics

HW-H1. 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 $\varepsilon_1 = -\varepsilon$. Then draw a solid horizontal line above your reference and label this line with energy $\varepsilon_2 = +\varepsilon$.

$\varepsilon_2 = +\varepsilon$ ____________________________

0 -

$\varepsilon_1 = -\varepsilon$ ____________________________

b) The Partition Function.

$$Z = \sum_i e^{-\frac{\varepsilon_i}{kT}} = e^{-\frac{\varepsilon_1}{kT}} + e^{-\frac{\varepsilon_2}{kT}} = e^{\frac{\varepsilon}{kT}} + e^{-\frac{\varepsilon}{kT}}$$

c) Occupation Numbers.

From the general formula $n_i = N \dfrac{e^{-\frac{\varepsilon_i}{kT}}}{Z}$ and $Z = e^{\frac{\varepsilon}{kT}} + e^{-\frac{\varepsilon}{kT}}$.

$$n_1 = N \frac{e^{\frac{\varepsilon}{kT}}}{Z} \qquad n_2 = N \frac{e^{-\frac{\varepsilon}{kT}}}{Z}$$

$$n_1 = N \frac{e^{\frac{\varepsilon}{kT}}}{e^{\frac{\varepsilon}{kT}} + e^{-\frac{\varepsilon}{kT}}} \qquad n_2 = N \frac{e^{-\frac{\varepsilon}{kT}}}{e^{\frac{\varepsilon}{kT}} + e^{-\frac{\varepsilon}{kT}}}.$$

d) Energy. $\overline{E} = \dfrac{n_1\varepsilon_1 + n_2\varepsilon_2}{n_1 + n_2} = \dfrac{n_1\varepsilon_1 + n_2\varepsilon_2}{N} = \dfrac{n_1}{N}\varepsilon_1 + \dfrac{n_2}{N}\varepsilon_2 = \dfrac{n_1}{N}(-\varepsilon) + \dfrac{n_2}{N}\varepsilon$

Use $\dfrac{n_1}{N} = \dfrac{e^{\frac{\varepsilon}{kT}}}{Z}$ and $\dfrac{n_2}{N} = \dfrac{e^{-\frac{\varepsilon}{kT}}}{Z}$ from Part (b) in $\overline{E} = \dfrac{n_1}{N}(-\varepsilon) + \dfrac{n_2}{N}\varepsilon$.

$$\overline{E} = \frac{e^{\frac{\varepsilon}{kT}}}{Z}(-\varepsilon) + \frac{e^{-\frac{\varepsilon}{kT}}}{Z}\varepsilon$$

$$\overline{E} = -\varepsilon\left[\frac{e^{\frac{\varepsilon}{kT}} - e^{-\frac{\varepsilon}{kT}}}{Z}\right] = -\varepsilon\left[\frac{e^{\frac{\varepsilon}{kT}} - e^{-\frac{\varepsilon}{kT}}}{e^{\frac{\varepsilon}{kT}} + e^{-\frac{\varepsilon}{kT}}}\right]$$

Hyperbolics: $\cosh x = \dfrac{e^x + e^{-x}}{2}$, $\sinh x = \dfrac{e^x - e^{-x}}{2}$, $\tanh x = \dfrac{\sinh x}{\cosh x}$

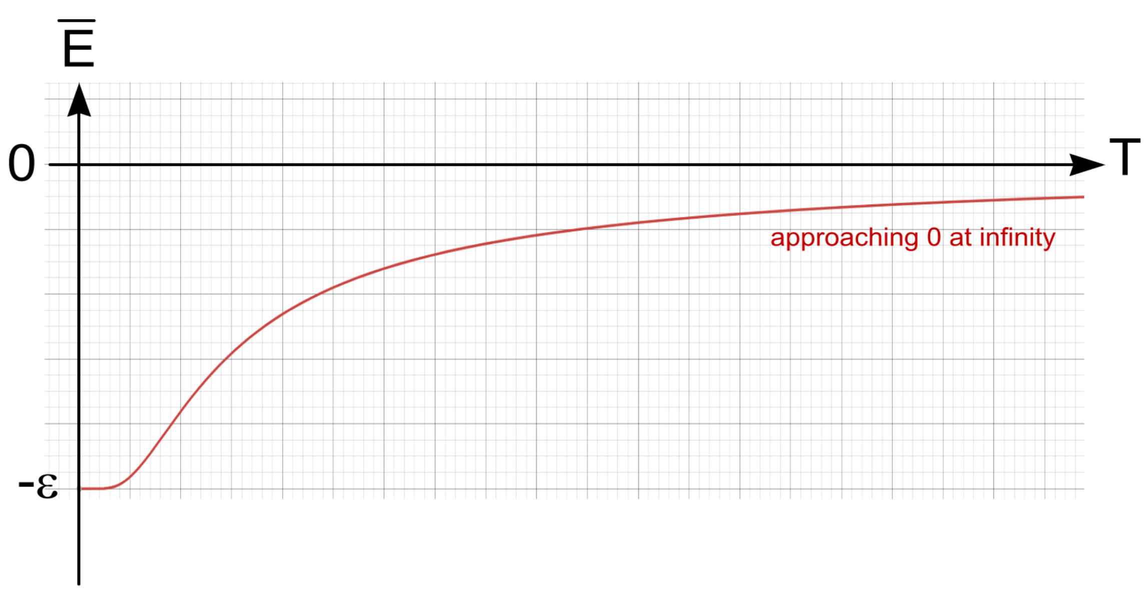
$$\overline{E} = -\varepsilon \tanh \frac{\varepsilon}{kT}$$

Sketch.

$$\lim_{T \to 0} \overline{E} = -\varepsilon \lim_{T \to 0} \tanh \frac{\varepsilon}{kT} = -\varepsilon \lim_{T \to 0}\left[\frac{e^{\frac{\varepsilon}{kT}} - e^{-\frac{\varepsilon}{kT}}}{e^{\frac{\varepsilon}{kT}} + e^{-\frac{\varepsilon}{kT}}}\right]$$

$$\lim_{T \to 0} \overline{E} = -\varepsilon \lim_{x \to \infty}\left[\frac{e^x - e^{-x}}{e^x + e^{-x}}\right] = -\varepsilon \lim_{x \to \infty}\left[\frac{e^x}{e^x}\right] = -\varepsilon$$

$$\lim_{T \to \infty} \overline{E} = -\varepsilon \lim_{T \to \infty}\left[\frac{e^{\frac{\varepsilon}{kT}} - e^{-\frac{\varepsilon}{kT}}}{e^{\frac{\varepsilon}{kT}} + e^{-\frac{\varepsilon}{kT}}}\right] = -\varepsilon \lim_{x \to 0}\left[\frac{e^x - e^{-x}}{e^x + e^{-x}}\right] = -\varepsilon\left[\frac{1-1}{1+1}\right] = 0$$



HW-H2. Two Quantum States Part II.

a) Limit $T \to 0$. As $T \to \text{small}$, then $\frac{\varepsilon}{kT} \to \text{large}$, $e^{\frac{\varepsilon}{kT}} \to \text{large}$, $e^{-\frac{\varepsilon}{kT}} \to \text{small}$.

$$n_1 = N \frac{e^{\frac{\varepsilon}{kT}}}{e^{\frac{\varepsilon}{kT}} + e^{-\frac{\varepsilon}{kT}}} \to N \frac{e^{\frac{\varepsilon}{kT}}}{e^{\frac{\varepsilon}{kT}}} = N \quad \text{and} \quad n_2 = N \frac{e^{-\frac{\varepsilon}{kT}}}{e^{\frac{\varepsilon}{kT}} + e^{-\frac{\varepsilon}{kT}}} \to 0$$

All particles are in the lowest energy state: $\overline{E} = -\varepsilon$. Note that the sum $n_1 + n_2 = N$, as always.

b) Limit $T \to \infty$. As $T \to \text{large}$, then $\frac{\varepsilon}{kT} \to \text{small}$, $e^{\frac{\varepsilon}{kT}} \to 1$, $e^{-\frac{\varepsilon}{kT}} \to 1$.

$$n_1 = N \frac{e^{\frac{\varepsilon}{kT}}}{e^{\frac{\varepsilon}{kT}} + e^{-\frac{\varepsilon}{kT}}} \to \frac{N}{2} \quad \text{and} \quad n_2 = N \frac{e^{-\frac{\varepsilon}{kT}}}{e^{\frac{\varepsilon}{kT}} + e^{-\frac{\varepsilon}{kT}}} \to \frac{N}{2}$$

Now $\overline{E} = 0$. The numbers check out again since $n_1 + n_2 = N$ as always.

c) Entropy. At T = 0, we have a most ordered state where all the particles are in the lowest energy level. There is only one way to have all the particles in the ground state. At T = infinity, we expect most disorder. Half the particles in each state provides for the most disorder, many ways to achieve this state. Just like there are many more ways to have a messy room.

When I first learned about this problem years ago, I had expected incorrectly that all the particles would be in the higher energy state at super high temperatures. However, if all the particles where up in the higher state, that would mean a very ordered state, as there is only one way to do that. So at high temperatures we get a “chaotic messy” state with half of the particles in each energy level.

HW-I3. Infinite Quantum States. Max Planck's discrete energy levels are $E_n = nhf$.
(a) Give the partition function as a summation from zero to infinity for these states.

$$Z = \sum_n e^{-\frac{E_n}{kT}} = e^{-\frac{nhf}{kT}} = 1 + e^{-\frac{hf}{kT}} + e^{-\frac{2hf}{kT}} + e^{-\frac{3hf}{kT}} +$$

Let $r = e^{-\frac{hf}{kT}}$. Then $Z = 1 + r + r^2 + r^3 + \ldots = \frac{1}{1-r} = \frac{1}{1-e^{-\frac{hf}{kT}}}$.

(b) Average Energy.

$$\overline{E} = \frac{\sum_n E_n e^{-\frac{E_n}{kT}}}{Z} = \frac{\sum_n (nhf) e^{-\frac{nhf}{kT}}}{Z}$$

$$\overline{E} = \frac{\sum_n E_n e^{-\frac{E_n}{kT}}}{Z} = \frac{\sum_n (nhf) e^{-\frac{nhf}{kT}}}{Z}$$

Let $x = \frac{hf}{kT}$. Then $\overline{E} = \frac{hf \sum_n n e^{-nx}}{Z}$.

Using

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

$$\sum_n n e^{-nx} = -\frac{d}{dx}(1-e^{-x})^{-1} = -(-1)(1-e^{-x})^{-2}(-e^{-x})(-1)$$

$$\sum_n n e^{-nx} = \frac{e^{-x}}{(1-e^{-x})^2} = \frac{e^{-\frac{hf}{kT}}}{(1-e^{-\frac{hf}{kT}})^2}$$

$$\overline{E} = \frac{hf \sum_n n e^{-nx}}{Z} = \frac{hf}{Z} \frac{e^{-\frac{hf}{kT}}}{(1-e^{-\frac{hf}{kT}})^2}$$

$$\overline{E} = \frac{hf\sum_n ne^{-nx}}{Z} = \frac{hf}{\left[\dfrac{1}{1-e^{-\frac{hf}{kT}}}\right]}\frac{e^{-\frac{hf}{kT}}}{(1-e^{-\frac{hf}{kT}})^2}$$

$$\overline{E} = \frac{hf\sum_n ne^{-nx}}{Z} = hf\,\frac{e^{-\frac{hf}{kT}}}{1-e^{-\frac{hf}{kT}}}$$

$$\overline{E} = \frac{hf\sum_n ne^{-nx}}{Z} = hf\,\frac{e^{-\frac{hf}{kT}}}{1-e^{-\frac{hf}{kT}}}\frac{e^{\frac{hf}{kT}}}{e^{\frac{hf}{kT}}} = hf\,\frac{1}{e^{\frac{hf}{kT}}-1}$$

$$\overline{E} = \frac{hf}{e^{\frac{hf}{kT}}-1}.$$

(c) Classical Result. We want the result when the Planck constant is very small. For small z, $e^z \approx 1+z$. Therefore,

$$\overline{E} \approx \frac{hf}{1+\dfrac{hf}{kT}-1} = \frac{hf}{(hf)/(kT)} = kT$$

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:

$$S_n = a + ar + ar^2 + \ldots + ar^{n-1} = a\left[\frac{1-r^n}{1-r}\right].$$

Derivation Below.

$$S_n = a + ar + ar^2 + \ldots + ar^{n-1}$$

$$rS_n = ar + ar^2 + ar^3 ... + ar^n$$

$$rS_n - S_n = ar^n - a$$

$$S_n(r-1) = a(r^n - 1)$$

$$S_n = \frac{a(r^n - 1)}{r - 1} \text{ and } S_n = \frac{a(1 - r^n)}{1 - r}$$

Note that if r < 1 and n goes to infinity: $S_\infty = \frac{a(1-0)}{1-r} = \frac{a}{1-r}$.

If $a = 1$, then $Z = 1 + r + r^2 + r^3 + ... = \frac{1}{1-r}$, as we know from before.