Max Proft U5190335

1. Classical and Quantum Harmonic Oscillators.

$$H = \frac{p^2}{2m} + \underbrace{\frac{1}{2} m \omega^2 x^2} \qquad \omega = \frac{pK}{m}$$

Side Note: This does not make sense. The units of do not match which means that does not have units of Joules. Shouldn't it be $\omega = \sqrt{\frac{k}{m}}$?

For one oscillator we have:

$$Z_1 = \frac{1}{2\pi\hbar} \iint dx\, dp\; e^{-\beta H}$$

$$= \frac{1}{2\pi\hbar} \int_{-\frac{X}{2}}^{\frac{X}{2}} dx \int_{-\infty}^{\infty} dp\; e^{-\beta\left(\frac{1}{2m} + \frac{k^2 x^2}{m}\right)p^2}$$

Note: The oscillator can have momentum from $-\infty$ to ∞, but is forced to oscillate with $\frac{-X}{2} < x < \frac{X}{2}$.

Using Mathematica (Integral #1)

$$\cancel{= \frac{1}{\sqrt{2\pi\hbar^2}} \sqrt{\frac{m}{\beta+2}}}$$

$$= \int_{-\frac{X}{2}}^{\frac{X}{2}} \frac{\sqrt{m}}{\hbar\sqrt{2\pi\beta}} \frac{1}{\sqrt{1+2k^2x^2}}\, dx$$

Using Mathematica (Integral #2)

$$= \frac{\ln\left(1 + kX\left(kX + \sqrt{2 + k^2X^2}\right)\right)}{2k\hbar\sqrt{\frac{\beta\pi}{m}}}$$

For N identical oscillators we have

$$Z = \frac{1}{N!} Z_1^N$$

$$= \frac{1}{N!}\left(\frac{\ln\left(1 + kX\left(kX + \sqrt{2+k^2X^2}\right)\right)}{2k\hbar\sqrt{\frac{\beta\pi}{m}}}\right)^N$$

and $E = -\frac{\partial}{\partial\beta}\ln(Z)$

(Using Mathematica #3 Derivative)

$$\cancel{E \frac{1}{2\beta(N-1)!}\operatorname{Log}\left(\frac{\log\left(1+kx\left(kx+\sqrt{2+k^2x^2}\right)\right)}{2k\sqrt{\pi}\sqrt{\frac{\beta}{m}}\hbar}\right)^{n-1}}$$

$$= \frac{N}{2\beta},$$ which is independent of k, as required

Q2.

$$\varepsilon_n = \hbar\omega\left(n+\frac{1}{2}\right)$$
$$= \frac{\hbar p k}{m}\left(n+\frac{1}{2}\right)$$

For one Quantum harmonic oscillator we have:

$$Z_1 = \frac{1}{2\pi\hbar}\sum_{n=1}^{\infty} e^{-\beta\varepsilon_n}$$

(Mathematica, #4 Summation)

$$= \frac{1}{2\pi\hbar}\,\frac{1}{e^{kp\beta\hbar/m}-1}$$

For N identical oscillators we have:

$$Z = \frac{1}{N!}(Z_1)^N$$
$$= \left(\frac{1}{2\pi\hbar}\right)^N \frac{1}{N!}\left(e^{kp\beta\hbar/m}-1\right)^{-N}$$

The energy is given by:

$$E = -\frac{\partial}{\partial\beta}\ln(Z)$$

(Mathematica: #5 Derivative)

$$= \frac{kNp\hbar}{m}\left(1+\frac{1}{e^{kp\beta\hbar/m}-1}\right)$$, which is dependent on k.

Q3

T	β	Classical Z	Classical E	Quantum Z	Quantum E
$T \approx 0$	$\beta \to \infty$	$Z \to 0$	$E \to 0$	$Z \to 0$	$E = \frac{k N \rho \hbar}{m}$
$T \to \infty$	$\beta \approx 0$	$Z \to \infty$	$E \to \infty$	$Z \to \infty$	$E \to \infty$

#1 Integral

$$\text{Integrate}\left[\frac{1}{2\pi\hbar}\,\text{Exp}\left[-\beta\left(\frac{1}{2\,m}+\frac{k^2\,x^2}{m}\right)p^2\right],\ \{p,-\infty,\infty\}\right]$$

Out[4]= $$\text{ConditionalExpression}\left[\frac{1}{\sqrt{2\pi}\,\sqrt{\frac{\beta+2\,k^2\,x^2\,\beta}{m}}\,\hbar},\ \text{Re}\left[\frac{\beta+2\,k^2\,x^2\,\beta}{m}\right]>0\right]$$

#2 Integral

In[2]:= $$\text{Integrate}\left[\frac{1}{\sqrt{2\pi}\,\sqrt{\frac{\beta+2\,k^2\,x^2\,\beta}{m}}\,\hbar},\ \{x,-X/2,X/2\},\ \text{Assumptions}\to\{\beta\in\text{Reals},\ k\in\text{Reals},\ X\in\text{Reals}\}\right]$$

Out[2]= $$\text{ConditionalExpression}\left[\frac{\text{Log}\left[1+k\,X\left(k\,X+\sqrt{2+k^2\,X^2}\right)\right]}{2\,k\,\sqrt{\pi}\,\sqrt{\frac{\beta}{m}}\,\hbar},\ \beta\geq 0\ \&\&\ k\,\beta\geq 0\ \&\&\ X>0\right]$$

#3 Derivative

In[8]:= $$-D\left[\text{Log}\left[\frac{1}{n!}\left(\frac{\text{Log}\left[1+k\,X\left(k\,X+\sqrt{2+k^2\,X^2}\right)\right]}{2\,k\,\sqrt{\pi}\,\sqrt{\frac{\beta}{m}}\,\hbar}\right)^n\right],\ \beta\right]$$

Out[8]= $$\frac{n}{2\,\beta}$$

#4 Summation

In[9]:= $$\text{Sum}\left[\text{Exp}\left[-\frac{\beta\,\hbar\,p\,k}{m}\,(i+1)\right],\ \{i,0,\infty\}\right]$$

Out[9]= $$\frac{1}{-1+e^{\frac{k\,p\,\beta\,\hbar}{m}}}$$

#5 Derivative

In[13]:= $$\text{FullSimplify}\left[-D\left[\text{Log}\left[\left(\frac{1}{-1+e^{\frac{k\,p\,\beta\,\hbar}{m}}}\right)^n\right],\ \beta\right]\right]$$

Out[13]= $$\frac{\left(1+\frac{1}{-1+e^{\frac{k\,p\,\beta\,\hbar}{m}}}\right)k\,n\,p\,\hbar}{m}$$