Thermal Physics - PH441 **John Waczak**
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Simple harmonic oscillator(s)

Recall the that the energy of a single, simple harmonic oscillator is given by $E_n = (n + \frac{1}{2})\hbar\omega$. Typically to solve for this kind of thing we look for normal modes in a differential equation with specified boundary conditions. Normal modes are nice because we can view them as non-interacting.

First, let's find our partition function:

$$
\begin{aligned}
Z &= \sum_{n=0}^{\infty} e^{-\beta(n+1/2)\hbar\omega} \\
&= e^{-\beta\hbar\omega/2} \sum_{n=0}^{\infty} e^{-\beta\hbar\omega n} \\
\text{let } \xi &= e^{-\beta\hbar\omega} \\
\text{let } \Xi &= \sum_{n=0}^{\infty} e^{-\beta\hbar\omega n} \\
\Xi &= \sum_{n=0}^{\infty} \xi^n \\
&\text{Note: this is the geometric series} \\
\Xi &= \frac{1}{1-\xi} \\
\Rightarrow Z &= \frac{e^{-\beta\hbar\omega/2}}{1-e^{-\beta\hbar\omega}}
\end{aligned}
$$

Now that we have our partition function Z the next logical thing is to calculate the Helmholtz free energy.

$$
\begin{aligned}
F &= -kT\ln Z \\
&= -kT\ln\left(\frac{e^{-\beta\hbar\omega/2}}{1-e^{-\beta\hbar\omega}}\right) \\
&= \frac{kT\beta\hbar\omega}{2} + kT\ln(1-e^{-\beta\hbar\omega}) \\
&= \frac{\hbar\omega}{2} + kT\ln(1-e^{-\beta\hbar\omega})
\end{aligned}
$$

Now that we have F we can find the entropy as usual.

$$
\begin{aligned}
S &= -\left(\frac{\partial F}{\partial T}\right)_V \\
&= -k\ln(1-e^{-\beta\hbar\omega}) - \frac{kT(-e^{-\beta\hbar\omega})}{1-e^{-\beta\hbar\omega}}\left(\frac{-\hbar\omega}{kT}\right) \\
&= \frac{\hbar\omega}{T}\frac{e^{-\beta\hbar\omega}}{1-e^{-\beta\hbar\omega}} - k\ln(1-e^{-\beta\hbar\omega})
\end{aligned}
$$

Now recall that $U = \langle E \rangle = \langle (n + 1/2)\hbar\omega \rangle = (\langle n \rangle + \frac{1}{2})\hbar\omega$. Considering this, solve for U.

$$\begin{aligned}
U &= F + TS \\
&= \frac{\hbar\omega}{2} + kT\ln(1 - e^{-\beta\hbar\omega}) + \hbar\omega\frac{e^{-\beta\hbar\omega}}{1 - e^{-\beta\hbar\omega}} - kT\ln(1 - e^{-\beta\hbar\omega}) \\
&= \frac{\hbar\omega}{2} + \hbar\omega\frac{e^{-\beta\hbar\omega}}{1 - e^{-\beta\hbar\omega}} \\
\text{Furthermore: } \langle n \rangle &= \frac{e^{-\beta\hbar\omega}}{1 - e^{-\beta\hbar\omega}} = \frac{1}{e^{\beta\hbar\omega} - 1}
\end{aligned}$$

Now let's consider the high and low temperature limits of this

$$\begin{aligned}
\text{High temp} &\Rightarrow \beta\hbar\omega << 1 \\
\langle n \rangle &= (e^{\beta\hbar\omega} - 1)^{-1} \\
&= \frac{1}{1 + \beta\hbar\omega + ... - 1} \\
&= \frac{kT}{\hbar\omega} \quad \text{"Equipartition result"} \\
\text{Low temp} &\Rightarrow \beta\hbar\omega >> 1 \\
\langle n \rangle &= \frac{e^{-\beta\hbar\omega}}{1 - e^{-\beta\hbar\omega}} \\
&\approx e^{-\beta\hbar\omega}(1 + e^{-\beta\hbar\omega}) \quad \text{using } (1+z)^p \\
&= e^{-\beta\hbar\omega} + e^{-2\beta\hbar\omega}
\end{aligned}$$