Thermal Physics

Energy of a particle in a 1D box

Consider a box of one dimension.

The kinetic energy is: $\mathrm{E} = \frac{\hbar^2}{2mL^2} n^2$, where n=1, 2, 3…

The average energy is: $\langle \mathrm{E} \rangle = \frac{\sum_{n=1}^{\infty} \frac{\hbar^2}{2mL^2} n^2 \exp\left(- \frac{\hbar^2}{2mL^2 k_B T} n^2 \right)}{\sum_{n=1}^{\infty} \exp\left(- \frac{\hbar^2}{2mL^2 k_B T} n^2 \right)}$

Approximating the summations with integrals:

$$\langle \mathrm{E} \rangle = k_B T \frac{\sum_{n=1}^{\infty} \frac{\hbar^2}{2mL^2 k_B T} n^2 \exp\left(- \frac{\hbar^2}{2mL^2 k_B T} n^2 \right)}{\sum_{n=1}^{\infty} \exp\left(- \frac{\hbar^2}{2mL^2 k_B T} n^2 \right)} \approx k_B T \frac{\int_0^{\infty} u^2 \exp\left(-u^2\right) du}{\int_0^{\infty} \exp\left(-u^2\right) du}$$

Both, the numerator and denominator are Gaussian integrals with values:

$\int_0^{\infty} \exp\left(-u^2\right) du = \frac{\sqrt{\pi}}{2}$ and $\int_0^{\infty} u^2 \exp\left(-u^2\right) du = \frac{\sqrt{\pi}}{4}$ then:

$$U = \langle \mathrm{E} \rangle \approx \frac{1}{2} k_B T$$