

Qual é a energia média,  $\langle E \rangle$ , de um oscilador harmônico clássico à temperatura absoluta T?

A energia total de um oscilador harmônico clássico, E, é dada por

$$E = T + U \Leftrightarrow E = \frac{1}{2}mv^2 + \frac{1}{2}Kr^2 \Leftrightarrow E = \frac{1}{2}m(v_x^2 + v_y^2 + v_z^2) + \frac{1}{2}K(x^2 + y^2 + z^2)$$

$$\langle E \rangle = \frac{\int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \left\{ \left[ \frac{1}{2}mv^2 + \frac{1}{2}Kr^2 \right] e^{-\frac{[\frac{1}{2}mv^2 + \frac{1}{2}Kr^2]}{K_B T}} \right\} dv_x dv_y dv_z dx dy dz}{\int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \left\{ e^{-\frac{[\frac{1}{2}mv^2 + \frac{1}{2}Kr^2]}{K_B T}} \right\} dv_x dv_y dv_z dx dy dz}$$

Ou rearranjando este integral de grau 6 de outra forma, temos que

$$\langle E \rangle = \frac{\overbrace{\int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \left\{ \left[ \frac{1}{2}mv^2 + \frac{1}{2}Kr^2 \right] e^{-\frac{[\frac{1}{2}mv^2 + \frac{1}{2}Kr^2]}{K_B T}} \right\} dx dy dz dv_x dv_y dv_z}^{I_1}}{\overbrace{\int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \left\{ e^{-\frac{[\frac{1}{2}mv^2 + \frac{1}{2}Kr^2]}{K_B T}} \right\} dx dy dz dv_x dv_y dv_z}^{I_2}}$$

Em primeiro lugar, vamos calcular os seguintes integrais triplos:

$$I_1 = \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \left\{ \left[ \frac{1}{2}mv^2 + \frac{1}{2}Kr^2 \right] e^{-\frac{[\frac{1}{2}mv^2 + \frac{1}{2}Kr^2]}{K_B T}} \right\} dx dy dz$$

$$I_2 = \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \left\{ e^{-\frac{[\frac{1}{2}mv^2 + \frac{1}{2}Kr^2]}{K_B T}} \right\} dx dy dz$$

Recorrendo às coordenadas esféricas, em que o elemento de volume  $dV$  é dado por

$$dV = dx \cdot dy \cdot dz = dr \cdot r d\theta \cdot r \sin \theta d\varphi = r^2 dr \cdot \sin \theta d\theta \cdot d\varphi$$

$$\begin{aligned} I_1 &= \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \left\{ \left[ \frac{1}{2}mv^2 + \frac{1}{2}Kr^2 \right] e^{-\frac{[\frac{1}{2}mv^2 + \frac{1}{2}Kr^2]}{K_B T}} \right\} dx dy dz = \\ &= \int_0^{2\pi} \int_0^\pi \int_0^\infty \left\{ \left[ \frac{1}{2}mv^2 + \frac{1}{2}Kr^2 \right] e^{-\frac{[\frac{1}{2}mv^2 + \frac{1}{2}Kr^2]}{K_B T}} \right\} r^2 dr \cdot \sin \theta d\theta \cdot d\varphi \end{aligned}$$

$$I_2 = \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \left\{ e^{-\frac{[\frac{1}{2}mv^2 + \frac{1}{2}Kr^2]}{K_B T}} \right\} dx dy dz = \int_0^{2\pi} \int_0^\pi \int_0^\infty \left\{ e^{-\frac{[\frac{1}{2}mv^2 + \frac{1}{2}Kr^2]}{K_B T}} \right\} r^2 dr \cdot \sin \theta d\theta \cdot d\varphi$$

Como  $e^{-\frac{[\frac{1}{2}mv^2]}{K_B T}}$  é independente com  $r$ ,  $\theta$  e  $\varphi$  (isto é,  $e^{-\frac{[\frac{1}{2}mv^2]}{K_B T}}$  não varia em função  $r$ ,  $\theta$  e  $\varphi$ ), então podemos passar o termo  $e^{-\frac{[\frac{1}{2}mv^2]}{K_B T}}$  para fora do integral triplo.

$$I_1 = e^{-\frac{[\frac{1}{2}mv^2]}{K_B T}} \int_0^{2\pi} \int_0^\pi \int_0^\infty \left\{ \left[ \frac{1}{2}mv^2 + \frac{1}{2}Kr^2 \right] e^{-\frac{[\frac{1}{2}Kr^2]}{K_B T}} \right\} r^2 dr \cdot \sin \theta d\theta \cdot d\varphi$$

$$I_2 = e^{-\frac{[\frac{1}{2}mv^2]}{K_B T}} \int_0^{2\pi} \int_0^\pi \int_0^\infty \left\{ e^{-\frac{[\frac{1}{2}Kr^2]}{K_B T}} \right\} r^2 dr \cdot \sin \theta d\theta \cdot d\varphi$$

$$\begin{aligned}
& \int_0^{2\pi} \int_0^{\pi} \int_0^{\infty} \left\{ \left[ \frac{1}{2}mv^2 + \frac{1}{2}Kr^2 \right] e^{-\frac{[\frac{1}{2}Kr^2]}{K_B T}} \right\} r^2 dr \cdot \sin \theta d\theta \cdot d\varphi = \\
&= \int_0^{2\pi} \int_0^{\pi} \int_0^{\infty} \left\{ \left[ \frac{1}{2}mv^2 r^2 + \frac{1}{2}Kr^4 \right] e^{-\frac{[\frac{1}{2}Kr^2]}{K_B T}} \right\} dr \cdot \sin \theta d\theta \cdot d\varphi \\
&= \int_0^{2\pi} d\varphi \int_0^{\pi} \sin \theta d\theta \int_0^{\infty} \left\{ \left[ \frac{1}{2}mv^2 r^2 + \frac{1}{2}Kr^4 \right] e^{-\frac{[\frac{1}{2}Kr^2]}{K_B T}} \right\} dr \\
&= [\varphi]_0^{2\pi} \cdot [-\cos \theta]_0^{\pi} \cdot \left\{ \frac{1}{2}mv^2 \int_0^{\infty} r^2 e^{-\frac{[\frac{1}{2}Kr^2]}{K_B T}} dr + \frac{1}{2}K \int_0^{\infty} r^4 e^{-\frac{[\frac{1}{2}Kr^2]}{K_B T}} dr \right\} = \\
&= 2\pi \cdot 2 \cdot \left\{ \frac{1}{2}mv^2 \cdot \left( \frac{2K_B T}{K} \right)^{\frac{3}{2}} \cdot \frac{\sqrt{\pi}}{4} + \frac{1}{2}K \cdot \left( \frac{2K_B T}{K} \right)^{\frac{5}{2}} \cdot \frac{3\sqrt{\pi}}{8} \right\} \\
&= \frac{mv^2}{2} \cdot \left( \frac{2\pi K_B T}{K} \right)^{\frac{3}{2}} + \left( \frac{2}{K} \right)^{\frac{3}{2}} \cdot (K_B T)^{\frac{5}{2}} \cdot \frac{3(\pi)^{\frac{3}{2}}}{2} \Rightarrow
\end{aligned}$$

$$\begin{aligned}
\Rightarrow I_1 &= \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \left\{ \left[ \frac{1}{2}mv^2 + \frac{1}{2}Kr^2 \right] e^{-\frac{[\frac{1}{2}mv^2 + \frac{1}{2}Kr^2]}{K_B T}} \right\} dx dy dz \\
&= e^{-\frac{[\frac{1}{2}mv^2]}{K_B T}} \cdot \left\{ \frac{mv^2}{2} \cdot \left( \frac{2\pi K_B T}{K} \right)^{\frac{3}{2}} + \left( \frac{2}{K} \right)^{\frac{3}{2}} \cdot (K_B T)^{\frac{5}{2}} \cdot \frac{3(\pi)^{\frac{3}{2}}}{2} \right\} \Rightarrow I_1 \\
&= \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \left\{ \left[ \frac{1}{2}mv^2 + \frac{1}{2}Kr^2 \right] e^{-\frac{[\frac{1}{2}mv^2 + \frac{1}{2}Kr^2]}{K_B T}} \right\} dx dy dz \\
&= \left( \frac{2\pi K_B T}{K} \right)^{\frac{3}{2}} \cdot e^{-\frac{[\frac{1}{2}mv^2]}{K_B T}} \cdot \left\{ \frac{mv^2}{2} + \frac{3K_B T}{2} \right\}
\end{aligned}$$

Agora precisamos de justificar alguns destes cálculos.

Substituição de variável:  $t^2 = \frac{Kr^2}{2K_B T} \Leftrightarrow t = r \cdot \sqrt{\frac{K}{2K_B T}} \Rightarrow dt = dr \cdot \sqrt{\frac{K}{2K_B T}} \Leftrightarrow dr = dt \cdot \sqrt{\frac{2K_B T}{K}}$

$$t^2 = \frac{Kr^2}{2K_B T} \Rightarrow r^4 = \frac{4 \cdot (K_B T)^2 \cdot t^4}{K^2}$$

$$\int_0^\infty r^2 e^{-\frac{[1/2Kr^2]}{K_B T}} dr = \int_0^\infty \frac{2 \cdot (K_B T) \cdot t^2}{K} e^{-t^2} \sqrt{\frac{2K_B T}{K}} dt = \left(\frac{2K_B T}{K}\right)^{\frac{3}{2}} \cdot \int_0^\infty t^2 e^{-t^2} dt$$

$$\int_0^\infty r^4 e^{-\frac{[1/2Kr^2]}{K_B T}} dr = \int_0^\infty \left(\frac{4 \cdot (K_B T)^2 \cdot t^4}{K^2}\right) e^{-t^2} \cdot \sqrt{\frac{2K_B T}{K}} dt = \left(\frac{2K_B T}{K}\right)^{\frac{5}{2}} \int_0^\infty t^4 e^{-t^2} dt$$

Agora precisamos calcular estes dois integrais recorrendo à técnica da integração por partes.

$$\int_0^\infty t^2 e^{-t^2} dt = \left[ \frac{-te^{-t^2}}{2} \right]_0^\infty - \left( \int_0^\infty \frac{-e^{-t^2}}{2} dt \right) = \underbrace{\left[ \frac{-te^{-t^2}}{2} \right]_0^\infty}_{0} + \frac{1}{2} \overbrace{\left( \int_0^\infty e^{-t^2} dt \right)}^{\frac{\sqrt{\pi}}{4}} = \frac{\sqrt{\pi}}{4}$$

$$\begin{aligned} \int_0^\infty t^4 e^{-t^2} dt &= \left[ \frac{-t^3 e^{-t^2}}{2} \right]_0^\infty - \left( \int_0^\infty \frac{-3t^2 e^{-t^2}}{2} dt \right) = \underbrace{\left[ \frac{-t^3 e^{-t^2}}{2} \right]_0^\infty}_0 - \left( \underbrace{\left[ \frac{3te^{-t^2}}{4} \right]_0^\infty}_0 - \left( \int_0^\infty \frac{3e^{-t^2}}{4} dt \right) \right) = \\ &= \underbrace{\left[ \frac{-t^3 e^{-t^2}}{2} \right]_0^\infty}_0 - \left( \underbrace{\left[ \frac{3te^{-t^2}}{4} \right]_0^\infty}_0 - \frac{3}{4} \overbrace{\left( \int_0^\infty e^{-t^2} dt \right)}^{\frac{3\sqrt{\pi}}{8}} \right) = \frac{3\sqrt{\pi}}{8} \end{aligned}$$

$$\int_{-\infty}^{+\infty} e^{-t^2} dt = 2 \cdot \int_0^\infty e^{-t^2} dt = \sqrt{\pi} \Leftrightarrow \int_0^\infty e^{-t^2} dt = \frac{\sqrt{\pi}}{2}$$

$$\int_0^\infty r^2 e^{-\frac{[\frac{1}{2}Kr^2]}{K_B T}} dr = \sqrt{\frac{2K_B T}{K}} \int_0^\infty t^2 e^{-t^2} dt = \left(\frac{2K_B T}{K}\right)^{\frac{3}{2}} \cdot \frac{\sqrt{\pi}}{4}$$

$$\int_0^\infty r^4 e^{-\frac{[\frac{1}{2}Kr^2]}{K_B T}} dr = \left(\frac{2K_B T}{K}\right)^{\frac{5}{2}} \int_0^\infty t^4 e^{-t^2} dt = \left(\frac{2K_B T}{K}\right)^{\frac{5}{2}} \cdot \frac{3\sqrt{\pi}}{8}$$

$$\frac{1}{2}mv^2 \int_0^\infty r^2 e^{-\frac{[\frac{1}{2}Kr^2]}{K_B T}} dr + \frac{1}{2}K \int_0^\infty r^4 e^{-\frac{[\frac{1}{2}Kr^2]}{K_B T}} dr = \frac{mv^2}{2} \cdot \left(\frac{2K_B T}{K}\right)^{\frac{3}{2}} \cdot \frac{\sqrt{\pi}}{4} + \sqrt{\frac{2}{K}} (K_B T)^{\frac{3}{2}} \cdot \frac{3\sqrt{\pi}}{8}$$

Agora, vamos calcularmo integral  $I_2$ .

$$\begin{aligned} I_2 &= e^{-\frac{[\frac{1}{2}mv^2]}{K_B T}} \int_0^{2\pi} \int_0^\pi \int_0^\infty \left\{ e^{-\frac{[\frac{1}{2}Kr^2]}{K_B T}} \right\} r^2 dr \cdot \sin \theta d\theta \cdot d\varphi \\ &\int_0^{2\pi} \int_0^\pi \int_0^\infty \left\{ e^{-\frac{[\frac{1}{2}Kr^2]}{K_B T}} \right\} r^2 dr \cdot \sin \theta d\theta \cdot d\varphi = \int_0^{2\pi} d\varphi \int_0^\pi \sin \theta d\theta \int_0^\infty \left\{ r^2 e^{-\frac{[\frac{1}{2}Kr^2]}{K_B T}} \right\} dr \\ &= [\varphi]_0^{2\pi} \cdot [-\cos \theta]_0^\pi \cdot \int_0^\infty \left\{ r^2 e^{-\frac{[\frac{1}{2}Kr^2]}{K_B T}} \right\} dr = 2\pi \cdot 2 \cdot \int_0^\infty \left\{ r^2 e^{-\frac{[\frac{1}{2}Kr^2]}{K_B T}} \right\} dr \\ &= 4\pi \cdot \sqrt{\frac{2K_B T}{K}} \underbrace{\int_0^\infty t^2 e^{-t^2} dt}_{\frac{\sqrt{\pi}}{4}} = (\pi)^{\frac{3}{2}} \cdot \sqrt{\frac{2K_B T}{K}} \end{aligned}$$

$$\begin{aligned} I_2 &= e^{-\frac{[\frac{1}{2}mv^2]}{K_B T}} \int_0^{2\pi} \int_0^\pi \int_0^\infty \left\{ e^{-\frac{[\frac{1}{2}Kr^2]}{K_B T}} \right\} r^2 dr \cdot \sin \theta d\theta \cdot d\varphi = e^{-\frac{[\frac{1}{2}mv^2]}{K_B T}} \cdot \left(\frac{2\pi K_B T}{K}\right)^{\frac{3}{2}} \\ I_1 &= \left(\frac{2\pi K_B T}{K}\right)^{\frac{3}{2}} \cdot e^{-\frac{[\frac{1}{2}mv^2]}{K_B T}} \cdot \left\{ \frac{mv^2}{2} + \frac{3K_B T}{2} \right\} \end{aligned}$$

$$\begin{aligned}
\langle E \rangle &= \frac{\overbrace{\int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \left\{ \left[ \frac{1}{Z} m v^2 + \frac{1}{2} K r^2 \right] e^{-\frac{[\frac{1}{2} m v^2 + \frac{1}{2} K r^2]}{K_B T}} \right\} dx dy dz dv_x dv_y dv_z}^{I_1}}{\int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \left\{ e^{-\frac{[\frac{1}{2} m v^2 + \frac{1}{2} K r^2]}{K_B T}} \right\} dx dy dz dv_x dv_y dv_z} = \\
&= \frac{\int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \left( \left( \frac{2\pi K_B T}{K} \right)^{\frac{3}{2}} \cdot e^{-\frac{[\frac{1}{2} m v^2]}{K_B T}} \cdot \left\{ \frac{m v^2}{2} + \frac{3 K_B T}{2} \right\} \right) dv_x dv_y dv_z}{\int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \left( e^{-\frac{[\frac{1}{2} m v^2]}{K_B T}} \cdot \left( \frac{2\pi K_B T}{K} \right)^{\frac{3}{2}} \right) dv_x dv_y dv_z} \\
&= \frac{\left( \frac{2\pi K_B T}{K} \right)^{\frac{3}{2}} \cdot \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \left( e^{-\frac{[\frac{1}{2} m v^2]}{K_B T}} \cdot \left\{ \frac{m v^2}{2} + \frac{3 K_B T}{2} \right\} \right) dv_x dv_y dv_z}{\left( \frac{2\pi K_B T}{K} \right)^{\frac{3}{2}} \cdot \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \left( e^{-\frac{[\frac{1}{2} m v^2]}{K_B T}} \right) dv_x dv_y dv_z} \\
&= \frac{\int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \left( e^{-\frac{[\frac{1}{2} m v^2]}{K_B T}} \cdot \left\{ \frac{m v^2}{2} + \frac{3 K_B T}{2} \right\} \right) dv_x dv_y dv_z}{\int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \left( e^{-\frac{[\frac{1}{2} m v^2]}{K_B T}} \right) dv_x dv_y dv_z}
\end{aligned}$$

Então temos que

$$\begin{aligned} \langle E \rangle &= \frac{\int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \left( e^{-\frac{[\frac{1}{2}mv^2]}{K_B T}} \cdot \left\{ \frac{mv^2}{2} + \frac{3K_B T}{2} \right\} \right) d\nu_x d\nu_y d\nu_z}{\int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \left( e^{-\frac{[\frac{1}{2}mv^2]}{K_B T}} \right) d\nu_x d\nu_y d\nu_z} \\ &= \frac{\left\{ \int_{-\infty}^{+\infty} \left( e^{-\frac{[\frac{1}{2}mv_z^2]}{K_B T}} \right) \int_{-\infty}^{+\infty} \left( e^{-\frac{[\frac{1}{2}mv_y^2]}{K_B T}} \right) \int_{-\infty}^{+\infty} \left\{ \left( e^{-\frac{[\frac{1}{2}mv^2]}{K_B T}} \right) \cdot \left( \frac{m(v_x^2 + v_y^2 + v_z^2)}{2} + \frac{3K_B T}{2} \right) \right\} d\nu_x d\nu_y d\nu_z \right\}}{\int_{-\infty}^{+\infty} \left( e^{-\frac{[\frac{1}{2}mv_z^2]}{K_B T}} \right) d\nu_z \int_{-\infty}^{+\infty} \left( e^{-\frac{[\frac{1}{2}mv_y^2]}{K_B T}} \right) d\nu_y \int_{-\infty}^{+\infty} \left( e^{-\frac{[\frac{1}{2}mv^2]}{K_B T}} \right) d\nu_x} \end{aligned}$$

Agora, precisamos generalizar e em vez de calcular os integrais um a um, vamos fazer o seguinte:

Para i,j=x,y,z, temos  $\nu_i, \nu_j = \nu_x, \nu_y, \nu_z$  e o primeiro integral do numerador de  $\langle E \rangle$  em função de  $\nu_x$  fica

$$\begin{aligned} \int_{-\infty}^{+\infty} \left( e^{-\frac{[\frac{1}{2}mv_x^2]}{K_B T}} \cdot \left\{ \frac{mv_x^2 + (\sum_{j=y,z} mv_j^2)}{2} + 2K_B T \cdot \frac{3}{4} \right\} \right) d\nu_x &= \underbrace{\int_{-\infty}^{+\infty} \left( e^{-\frac{[\frac{1}{2}mv_x^2]}{K_B T}} \cdot \frac{mv_x^2}{2} d\nu_x + e^{-\frac{[\frac{1}{2}mv_x^2]}{K_B T}} \cdot \frac{(\sum_{j=y,z} mv_j^2)}{2} \right)}_{I_3} + \\ e^{-\frac{[\frac{1}{2}mv_x^2]}{K_B T}} \cdot 2K_B T \cdot \frac{3}{4} d\nu_x &= \underbrace{\int_{-\infty}^{+\infty} \left( e^{-\frac{[\frac{1}{2}mv_x^2]}{K_B T}} \cdot \frac{mv_x^2}{2} \right) d\nu_x}_{I_4} + \underbrace{\int_{-\infty}^{+\infty} \left( e^{-\frac{[\frac{1}{2}mv_x^2]}{K_B T}} \cdot \frac{(\sum_{j=y,z} mv_j^2)}{2} \right) d\nu_x}_{I_4} + \frac{3K_B T}{2} \cdot \\ \underbrace{\int_{-\infty}^{+\infty} \left( e^{-\frac{[\frac{1}{2}mv_x^2]}{K_B T}} \right) d\nu_x}_{I_5} \end{aligned}$$

$$I_3 = \int_{-\infty}^{+\infty} \left( e^{-\frac{[\frac{1}{2}mv_x^2]}{K_B T}} \cdot \frac{mv_x^2}{2} \right) d\nu_x \rightarrow \text{Substituição de variável} \left\{ \begin{array}{l} h^2 = \frac{mv_x^2}{2K_B T} \Leftrightarrow h = \sqrt{\frac{m}{2K_B T}} \nu_x \\ dh = \sqrt{\frac{m}{2K_B T}} d\nu_x \Leftrightarrow d\nu_x = \sqrt{\frac{2K_B T}{m}} dh \\ v_x^2 = \frac{2K_B T}{m} h^2 \Rightarrow \frac{mv_x^2}{2} = K_B T h^2 \end{array} \right.$$

Então temos que

$$\begin{aligned}
 I_3 &= \int_{-\infty}^{+\infty} \left( e^{\frac{-[\frac{1}{2}mv_x^2]}{K_B T}} \cdot \frac{mv_x^2}{2} \right) dv_x = \int_{-\infty}^{+\infty} (e^{-h^2} \cdot K_B T h^2) \cdot \sqrt{\frac{2K_B T}{m}} dh \Leftrightarrow I_3 = \sqrt{\frac{2K_B T}{m}} \cdot K_B T h^2 \cdot \underbrace{\int_{-\infty}^{+\infty} h^2 e^{-h^2} dh}_{\frac{\sqrt{\pi}}{2}} \\
 &\Leftrightarrow I_3 = \sqrt{\frac{2K_B T}{m}} \cdot K_B T \cdot \frac{\sqrt{\pi}}{2} = \sqrt{\frac{2\pi K_B T}{m}} \cdot \frac{K_B T}{2}
 \end{aligned}$$

Então temos que

$$I_3 = \sqrt{\frac{2\pi K_B T}{m}} \cdot \frac{K_B T}{2}$$

$$I_4 = \int_{-\infty}^{+\infty} \left( e^{\frac{-[\frac{1}{2}mv_x^2]}{K_B T}} \cdot \sum_{j \neq i} mv_j^2 \right) dv_x \rightarrow \text{Substituição de variável} \left\{
 \begin{array}{l}
 h^2 = \frac{mv_x^2}{2K_B T} \Leftrightarrow h = \sqrt{\frac{m}{2K_B T}} v_x \\
 dh = \sqrt{\frac{m}{2K_B T}} dv_x \Leftrightarrow dv_x = \sqrt{\frac{2K_B T}{m}} dh \\
 v_x^2 = \frac{2K_B T}{m} h^2
 \end{array}
 \right.$$

$$\begin{aligned}
 I_4 &= \int_{-\infty}^{+\infty} \left( e^{\frac{-[\frac{1}{2}mv_x^2]}{K_B T}} \cdot \left( \frac{\sum_{j=y,z} mv_j^2}{2} \right) \right) dv_x = \left( \frac{\sum_{j=y,z} mv_j^2}{2} \right) \cdot \int_{-\infty}^{+\infty} \left( e^{\frac{-[\frac{1}{2}mv_x^2]}{K_B T}} \right) dv_x \\
 &= \left( \frac{\sum_{j=y,z} mv_j^2}{2} \right) \cdot \int_{-\infty}^{+\infty} e^{-h^2} \sqrt{\frac{2K_B T}{m}} dh = \sqrt{\frac{2K_B T}{m}} \cdot \left( \frac{\sum_{j=y,z} mv_j^2}{2} \right) \cdot \underbrace{\left( \int_{-\infty}^{+\infty} e^{-h^2} dh \right)}_{\sqrt{\pi}} \\
 &= \sqrt{\frac{2K_B T}{m}} \cdot \left( \frac{\sum_{j=y,z} mv_j^2}{2} \right) \cdot \sqrt{\pi} = \sqrt{\frac{2\pi K_B T}{m}} \cdot \left( \frac{\sum_{j=y,z} mv_j^2}{2} \right)
 \end{aligned}$$

Então temos que

$$I_4 = \sqrt{\frac{2K_B T}{m}} \cdot \left( \frac{\sum_{j=y,z} m v_j^2}{2} \right) \cdot \sqrt{\pi} = \sqrt{\frac{2\pi K_B T}{m}} \cdot \left( \frac{\sum_{j=y,z} m v_j^2}{2} \right)$$

e como é óbvio

$$I_5 = \int_{-\infty}^{+\infty} \left( e^{-\frac{[\frac{1}{2}mv_x^2]}{K_B T}} \right) dv_x \rightarrow \text{Substituição de variável} \begin{cases} h^2 = \frac{mv_x^2}{2K_B T} \Leftrightarrow h = \sqrt{\frac{m}{2K_B T}} v_x \\ dh = \sqrt{\frac{m}{2K_B T}} dv_x \Leftrightarrow dv_x = \sqrt{\frac{2K_B T}{m}} dh \\ v_x^2 = \frac{2K_B T}{m} h^2 \end{cases}$$

$$I_5 = \int_{-\infty}^{+\infty} \left( e^{-\frac{[\frac{1}{2}mv_x^2]}{K_B T}} \right) dv_x = \sqrt{\frac{2K_B T}{m}} \underbrace{\int_{-\infty}^{+\infty} e^{-h^2} dh}_{\sqrt{\pi}} = \sqrt{\frac{2K_B T}{m}} \cdot \sqrt{\pi} = \sqrt{\frac{2\pi K_B T}{m}}$$

De seguida, temos que:

$$\begin{aligned}
& \int_{-\infty}^{+\infty} \left( e^{\frac{-[\frac{1}{2}mv_x^2]}{K_B T}} \cdot \left\{ \frac{mv_x^2}{2} + \left( \frac{\sum_{j=y,z} mv_j^2}{2} \right) + 2K_B T \cdot \frac{3}{4} \right\} \right) dv_x \\
&= \int_{-\infty}^{+\infty} \left( e^{\frac{-[\frac{1}{2}mv_x^2]}{K_B T}} \cdot \frac{mv_x^2}{2} + e^{\frac{-[\frac{1}{2}mv_x^2]}{K_B T}} \cdot \left( \frac{\sum_{j=y,z} mv_j^2}{2} \right) + e^{\frac{-[\frac{1}{2}mv_x^2]}{K_B T}} \cdot \frac{3K_B T}{2} \right) dv_x \\
&= \underbrace{\int_{-\infty}^{+\infty} \left( e^{\frac{-[\frac{1}{2}mv_x^2]}{K_B T}} \cdot \frac{mv_x^2}{2} \right) dv_x}_{I_3} + \underbrace{\int_{-\infty}^{+\infty} \left( e^{\frac{-[\frac{1}{2}mv_x^2]}{K_B T}} \cdot \left( \frac{\sum_{j=y,z} mv_j^2}{2} \right) \right) dv_x}_{I_4} + \frac{3K_B T}{2} \\
&\cdot \underbrace{\int_{-\infty}^{+\infty} \left( e^{\frac{-[\frac{1}{2}mv_x^2]}{K_B T}} \right) dv_x}_{I_5} = \sqrt{\frac{2\pi K_B T}{m}} \cdot \frac{K_B T}{2} + \sqrt{\frac{2\pi K_B T}{m}} \cdot \left( \frac{\sum_{j=y,z} mv_j^2}{2} \right) + \frac{3K_B T}{2} \cdot \sqrt{\frac{2\pi K_B T}{m}} = \\
&= \sqrt{\frac{2\pi K_B T}{m}} \left\{ 2K_B T + \left( \frac{\sum_{j=y,z} mv_j^2}{2} \right) \right\}
\end{aligned}$$

Fazendo Para i=x,y,z, temos  $v_i = v_x, v_y, v_z$  e

$$\int_{-\infty}^{+\infty} \left( e^{\frac{-[\frac{1}{2}mv_i^2]}{K_B T}} \right) dv_i = \int_{-\infty}^{+\infty} e^{-h^2} \cdot \sqrt{\frac{2K_B T}{m}} dh = \sqrt{\frac{2K_B T}{m}} \cdot \underbrace{\int_{-\infty}^{+\infty} e^{-h^2} dh}_{\sqrt{\pi}} = \sqrt{\frac{2\pi K_B T}{m}}$$

Conclusão:

$$\int_{-\infty}^{+\infty} \left( e^{\frac{-[\frac{1}{2}mv_i^2]}{K_B T}} \right) dv_i = \int_{-\infty}^{+\infty} \left( e^{\frac{-[\frac{1}{2}mv_x^2]}{K_B T}} \right) dv_x = \int_{-\infty}^{+\infty} \left( e^{\frac{-[\frac{1}{2}mv_y^2]}{K_B T}} \right) dv_y = \int_{-\infty}^{+\infty} \left( e^{\frac{-[\frac{1}{2}mv_z^2]}{K_B T}} \right) dv_z = \sqrt{\frac{2\pi K_B T}{m}}$$

E o denominador de  $\langle E \rangle$  fica igual a

$$\int_{-\infty}^{+\infty} \left( e^{\frac{-[\frac{1}{2}mv_z^2]}{K_B T}} \right) dv_z \int_{-\infty}^{+\infty} \left( e^{\frac{-[\frac{1}{2}mv_y^2]}{K_B T}} \right) dv_y \int_{-\infty}^{+\infty} \left( e^{\frac{-[\frac{1}{2}mv_x^2]}{K_B T}} \right) dv_x = \left[ \int_{-\infty}^{+\infty} \left( e^{\frac{-[\frac{1}{2}mv_i^2]}{K_B T}} \right) dv_i \right]^3 = \left[ \sqrt{\frac{2\pi K_B T}{m}} \right]^3 = \left( \frac{2\pi K_B T}{m} \right)^{\frac{3}{2}}$$

$$\begin{aligned}
\langle E \rangle &= \frac{\int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \left( e^{-\frac{[\frac{1}{2}mv^2]}{K_B T}} \cdot \left\{ \frac{mv^2}{2} + \frac{3K_B T}{2} \right\} \right) d\nu_x d\nu_y d\nu_z}{\int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \left( e^{-\frac{[\frac{1}{2}mv^2]}{K_B T}} \right) d\nu_x d\nu_y d\nu_z} \\
&= \frac{\left\{ \int_{-\infty}^{+\infty} \left( e^{-\frac{[\frac{1}{2}mv_z^2]}{K_B T}} \right) \int_{-\infty}^{+\infty} \left( e^{-\frac{[\frac{1}{2}mv_y^2]}{K_B T}} \right) \int_{-\infty}^{+\infty} \left\{ \left( e^{-\frac{[\frac{1}{2}mv_x^2]}{K_B T}} \right) \cdot \left( m(v_x^2 + v_y^2 + v_z^2) + 2K_B T \cdot \frac{3}{4} \right) \right\} d\nu_x d\nu_y d\nu_z \right\}}{\int_{-\infty}^{+\infty} \left( e^{-\frac{[\frac{1}{2}mv_z^2]}{K_B T}} \right) d\nu_z \int_{-\infty}^{+\infty} \left( e^{-\frac{[\frac{1}{2}mv_y^2]}{K_B T}} \right) d\nu_y \int_{-\infty}^{+\infty} \left( e^{-\frac{[\frac{1}{2}mv^2]}{K_B T}} \right) d\nu_x}
\end{aligned}$$

$$\int_{-\infty}^{+\infty} \left( e^{-\frac{[\frac{1}{2}mv_z^2]}{K_B T}} \right) d\nu_z \int_{-\infty}^{+\infty} \left( e^{-\frac{[\frac{1}{2}mv_y^2]}{K_B T}} \right) d\nu_y \int_{-\infty}^{+\infty} \left( e^{-\frac{[\frac{1}{2}mv^2]}{K_B T}} \right) d\nu_x = \left( \frac{2\pi K_B T}{m} \right)^{\frac{3}{2}}$$

$$\begin{aligned}
& \int_{-\infty}^{+\infty} \left( e^{-\frac{[\frac{1}{2}mv_y^2]}{K_B T}} \right) \int_{-\infty}^{+\infty} \left\{ \left( e^{-\frac{[\frac{1}{2}mv_x^2]}{K_B T}} \right) \cdot \left( \frac{m(v_x^2 + v_y^2 + v_z^2)}{2} + \frac{3K_B T}{2} \right) \right\} dv_x dv_y = \\
&= \int_{-\infty}^{+\infty} \left( e^{-\frac{[\frac{1}{2}mv_y^2]}{K_B T}} \right) \left\{ \sqrt{\frac{2\pi K_B T}{m}} \left\{ 2K_B T + \left( \frac{\sum_{j=y,z} mv_j^2}{2} \right) \right\} \right\} dv_y \\
&= \int_{-\infty}^{+\infty} \left\{ 2K_B T \cdot \sqrt{\frac{2\pi K_B T}{m}} \cdot \left( e^{-\frac{[\frac{1}{2}mv_y^2]}{K_B T}} \right) + \sqrt{\frac{2\pi K_B T}{m}} \cdot mv_y^2 \cdot \left( e^{-\frac{[\frac{1}{2}mv_y^2]}{K_B T}} \right) + \sqrt{\frac{2\pi K_B T}{m}} \cdot mv_z^2 \right. \\
&\quad \left. \cdot \left( e^{-\frac{[\frac{1}{2}mv_y^2]}{K_B T}} \right) \right\} dv_y = \int_{-\infty}^{+\infty} 2K_B T \cdot \sqrt{\frac{2\pi K_B T}{m}} \cdot \left( e^{-\frac{[\frac{1}{2}mv_y^2]}{K_B T}} \right) dv_y \\
&\quad + \int_{-\infty}^{+\infty} \sqrt{\frac{2\pi K_B T}{m}} \cdot \frac{mv_y^2}{2} \cdot \left( e^{-\frac{[\frac{1}{2}mv_y^2]}{K_B T}} \right) dv_y + \int_{-\infty}^{+\infty} \sqrt{\frac{2\pi K_B T}{m}} \cdot \frac{mv_z^2}{2} \cdot \left( e^{-\frac{[\frac{1}{2}mv_y^2]}{K_B T}} \right) dv_y \\
&= 2K_B T \cdot \sqrt{\frac{2\pi K_B T}{m}} \cdot \int_{-\infty}^{+\infty} \left( e^{-\frac{[\frac{1}{2}mv_y^2]}{K_B T}} \right) dv_y + \sqrt{\frac{2\pi K_B T}{m}} \cdot \int_{-\infty}^{+\infty} \frac{mv_y^2}{2} \cdot \left( e^{-\frac{[\frac{1}{2}mv_y^2]}{K_B T}} \right) dv_y + \sqrt{\frac{2\pi K_B T}{m}} \\
&\quad \cdot \frac{mv_z^2}{2} \cdot \int_{-\infty}^{+\infty} \left( e^{-\frac{[\frac{1}{2}mv_y^2]}{K_B T}} \right) dv_y
\end{aligned}$$

$$\int_{-\infty}^{+\infty} \frac{mv_y^2}{2} \cdot \left( e^{-\frac{[\frac{1}{2}mv_y^2]}{K_B T}} \right) dv_y \rightarrow \text{Substituição: } \begin{cases} h^2 = \frac{mv_y^2}{2K_B T} \Leftrightarrow h = \sqrt{\frac{m}{2K_B T}} v_y \\ dh = \sqrt{\frac{m}{2K_B T}} dv_y \Leftrightarrow dv_y = \sqrt{\frac{2K_B T}{m}} dh \\ v_y^2 = \frac{2K_B T}{m} h^2 \Rightarrow K_B T h^2 = \frac{mv_y^2}{2} \end{cases}$$

$$\int_{-\infty}^{+\infty} \frac{mv_y^2}{2} \cdot \left( e^{-\frac{[\frac{1}{2}mv_y^2]}{K_B T}} \right) dv_y = K_B T \cdot \int_{-\infty}^{+\infty} h^2 \cdot (e^{-h^2}) \cdot \sqrt{\frac{2K_B T}{m}} dh = K_B T \cdot \sqrt{\frac{2K_B T}{m}} \cdot \underbrace{\int_{-\infty}^{+\infty} h^2 e^{-h^2} dh}_{\frac{\sqrt{\pi}}{2}} = K_B T \cdot \sqrt{\frac{2K_B T}{m}}.$$

$$\frac{\sqrt{\pi}}{2} \Rightarrow \int_{-\infty}^{+\infty} \frac{mv_y^2}{2} \cdot \left( e^{-\frac{[\frac{1}{2}mv_y^2]}{K_B T}} \right) dv_y = \frac{K_B T}{2} \cdot \sqrt{\frac{2\pi K_B T}{m}}$$

$$\sqrt{\frac{2\pi K_B T}{m}} \cdot \int_{-\infty}^{+\infty} \frac{mv_y^2}{2} \cdot \left( e^{-\frac{[\frac{1}{2}mv_y^2]}{K_B T}} \right) dv_y = \sqrt{\frac{2\pi K_B T}{m}} \cdot \frac{K_B T}{2} \cdot \sqrt{\frac{2\pi K_B T}{m}} = \frac{K_B T}{2} \cdot \left( \frac{2\pi K_B T}{m} \right)$$

$$\int_{-\infty}^{+\infty} \left( e^{-\frac{[\frac{1}{2}mv_y^2]}{K_B T}} \right) dv_y = \int_{-\infty}^{+\infty} e^{-h^2} \cdot \sqrt{\frac{2K_B T}{m}} dh = \sqrt{\frac{2K_B T}{m}} \cdot \underbrace{\int_{-\infty}^{+\infty} e^{-h^2} dh}_{\sqrt{\pi}} = \sqrt{\frac{2\pi K_B T}{m}}$$

$$\sqrt{\frac{\pi}{m}} \cdot (2K_B T)^{\frac{3}{2}} \cdot \int_{-\infty}^{+\infty} \left( e^{-\frac{[\frac{1}{2}mv_y^2]}{K_B T}} \right) dv_y = \sqrt{\frac{\pi}{m}} \cdot (2K_B T)^{\frac{3}{2}} \cdot \sqrt{\frac{2\pi K_B T}{m}} = 2K_B T \cdot \left( \frac{2\pi K_B T}{m} \right)$$

$$\sqrt{\frac{2\pi K_B T}{m}} \cdot \frac{mv_z^2}{2} \cdot \int_{-\infty}^{+\infty} \left( e^{-\frac{[\frac{1}{2}mv_y^2]}{K_B T}} \right) dv_y = \sqrt{\frac{2\pi K_B T}{m}} \cdot \frac{mv_z^2}{2} \cdot \sqrt{\frac{2\pi K_B T}{m}} = \frac{2\pi K_B T}{m} \cdot \left( \frac{mv_z^2}{2} \right)$$

$$\begin{aligned}
& \int_{-\infty}^{+\infty} \left( e^{-\frac{[\frac{1}{2}mv_y^2]}{K_B T}} \right) \left\{ \int_{-\infty}^{+\infty} \left\{ \left( e^{-\frac{[\frac{1}{2}mv_x^2]}{K_B T}} \right) \cdot \left( \frac{m(v_x^2 + v_y^2 + v_z^2)}{2} + 2K_B T \cdot \frac{3}{4} \right) \right\} dv_x \right\} dv_y = \\
&= \int_{-\infty}^{+\infty} \left( e^{-\frac{[\frac{1}{2}mv_y^2]}{K_B T}} \right) \left\{ \sqrt{\frac{2\pi K_B T}{m}} \left\{ 2K_B T + \frac{(\sum_{j=y,z} mv_j^2)}{2} \right\} \right\} dv_y \\
&= \int_{-\infty}^{+\infty} \left\{ \sqrt{\frac{\pi}{m}} \cdot (2K_B T)^{\frac{3}{2}} \cdot \left( e^{-\frac{[\frac{1}{2}mv_y^2]}{K_B T}} \right) + \sqrt{\frac{2\pi K_B T}{m}} \cdot \frac{mv_y^2}{2} \cdot \left( e^{-\frac{[\frac{1}{2}mv_y^2]}{K_B T}} \right) + \sqrt{\frac{2\pi K_B T}{m}} \cdot \frac{mv_z^2}{2} \right. \\
&\quad \left. \cdot \left( e^{-\frac{[\frac{1}{2}mv_y^2]}{K_B T}} \right) \right\} dv_y = \int_{-\infty}^{+\infty} \sqrt{\frac{\pi}{m}} \cdot (2K_B T)^{\frac{3}{2}} \cdot \left( e^{-\frac{[\frac{1}{2}mv_y^2]}{K_B T}} \right) dv_y \\
&+ \int_{-\infty}^{+\infty} \sqrt{\frac{2\pi K_B T}{m}} \cdot \frac{mv_y^2}{2} \cdot \left( e^{-\frac{[\frac{1}{2}mv_y^2]}{K_B T}} \right) dv_y + \int_{-\infty}^{+\infty} \sqrt{\frac{2\pi K_B T}{m}} \cdot \frac{mv_z^2}{2} \cdot \left( e^{-\frac{[\frac{1}{2}mv_y^2]}{K_B T}} \right) dv_y \\
&= \sqrt{\frac{\pi}{m}} \cdot (2K_B T)^{\frac{3}{2}} \cdot \int_{-\infty}^{+\infty} \left( e^{-\frac{[\frac{1}{2}mv_y^2]}{K_B T}} \right) dv_y + \sqrt{\frac{2\pi K_B T}{m}} \cdot \int_{-\infty}^{+\infty} \frac{mv_y^2}{2} \cdot \left( e^{-\frac{[\frac{1}{2}mv_y^2]}{K_B T}} \right) dv_y + \sqrt{\frac{2\pi K_B T}{m}} \\
&\cdot \frac{mv_z^2}{2} \cdot \int_{-\infty}^{+\infty} \left( e^{-\frac{[\frac{1}{2}mv_y^2]}{K_B T}} \right) dv_y = 2K_B T \cdot \left( \frac{2\pi K_B T}{m} \right) + \frac{K_B T}{2} \cdot \left( \frac{2\pi K_B T}{m} \right) + \frac{2\pi K_B T}{m} \cdot \left( \frac{mv_z^2}{2} \right) \Rightarrow \\
&\Rightarrow \int_{-\infty}^{+\infty} \left( e^{-\frac{[\frac{1}{2}mv_y^2]}{K_B T}} \right) \left\{ \int_{-\infty}^{+\infty} \left\{ \left( e^{-\frac{[\frac{1}{2}mv_x^2]}{K_B T}} \right) \cdot \left( \frac{m(v_x^2 + v_y^2 + v_z^2)}{2} + 2K_B T \cdot \frac{3}{4} \right) \right\} dv_x \right\} dv_y = \\
&= \frac{5K_B T}{2} \cdot \left( \frac{2\pi K_B T}{m} \right) + \frac{2\pi K_B T}{m} \cdot \left( \frac{mv_z^2}{2} \right) \\
&\Rightarrow \int_{-\infty}^{+\infty} \left( e^{-\frac{[\frac{1}{2}mv_y^2]}{K_B T}} \right) \left\{ \int_{-\infty}^{+\infty} \left\{ \left( e^{-\frac{[\frac{1}{2}mv_x^2]}{K_B T}} \right) \cdot \left( \frac{m(v_x^2 + v_y^2 + v_z^2)}{2} + \frac{3K_B T}{2} \right) \right\} dv_x \right\} dv_y \\
&= \frac{5K_B T}{2} \cdot \left( \frac{2\pi K_B T}{m} \right) + \frac{2\pi K_B T}{m} \cdot \left( \frac{mv_z^2}{2} \right)
\end{aligned}$$

$$\begin{aligned} & \Rightarrow \int_{-\infty}^{+\infty} \left( e^{-\frac{[\frac{1}{2}mv_y^2]}{K_B T}} \right) \left\{ \int_{-\infty}^{+\infty} \left\{ \left( e^{-\frac{[\frac{1}{2}mv_x^2]}{K_B T}} \right) \cdot \left( \frac{m(v_x^2 + v_y^2 + v_z^2)}{2} + \frac{3K_B T}{2} \right) \right\} dv_x \right\} dv_y \\ & = \left( \frac{2\pi K_B T}{m} \right) \cdot \left( \frac{5K_B T}{2} + \left( \frac{mv_z^2}{2} \right) \right) \end{aligned}$$

$$\begin{aligned} & \left\{ \int_{-\infty}^{+\infty} \left( e^{-\frac{[\frac{1}{2}mv_z^2]}{K_B T}} \right) \int_{-\infty}^{+\infty} \left( e^{-\frac{[\frac{1}{2}mv_y^2]}{K_B T}} \right) \left\{ \int_{-\infty}^{+\infty} \left\{ \left( e^{-\frac{[\frac{1}{2}mv_x^2]}{K_B T}} \right) \cdot \left( \frac{m(v_x^2 + v_y^2 + v_z^2)}{2} + \frac{3K_B T}{2} \right) \right\} dv_x \right\} dv_y \right\} dv_z \\ & = \int_{-\infty}^{+\infty} \left( e^{-\frac{[\frac{1}{2}mv_z^2]}{K_B T}} \right) \cdot \left( \frac{2\pi K_B T}{m} \right) \cdot \left( \frac{5K_B T}{2} + \left( \frac{mv_z^2}{2} \right) \right) dv_z \\ & = \left( \frac{2\pi K_B T}{m} \right) \cdot \int_{-\infty}^{+\infty} \left( e^{-\frac{[\frac{1}{2}mv_z^2]}{K_B T}} \right) \cdot \left( \frac{5K_B T}{2} + \left( \frac{mv_z^2}{2} \right) \right) dv_z \\ & = \frac{5K_B T}{2} \cdot \left( \frac{2\pi K_B T}{m} \right) \cdot \int_{-\infty}^{+\infty} \left( e^{-\frac{[\frac{1}{2}mv_z^2]}{K_B T}} \right) dv_z + \left( \frac{2\pi K_B T}{m} \right) \cdot \int_{-\infty}^{+\infty} \left( \frac{mv_z^2}{2} \right) \left( e^{-\frac{[\frac{1}{2}mv_z^2]}{K_B T}} \right) dv_z \end{aligned}$$

$$\int_{-\infty}^{+\infty} \left( \frac{mv_z^2}{2} \right) \left( e^{-\frac{[\frac{1}{2}mv_z^2]}{K_B T}} \right) dv_z \rightarrow \text{Substituiçāo: } \begin{cases} h^2 = \frac{mv_z^2}{2K_B T} \Leftrightarrow h = \sqrt{\frac{m}{2K_B T}} v_z \\ dh = \sqrt{\frac{m}{2K_B T}} dv_z \Leftrightarrow dv_z = \sqrt{\frac{2K_B T}{m}} dh \\ v_z^2 = \frac{2K_B T}{m} h^2 \Rightarrow K_B T h^2 = \frac{mv_z^2}{2} \end{cases}$$

$$\int_{-\infty}^{+\infty} \left( \frac{mv_z^2}{2} \right) \left( e^{-\frac{[\frac{1}{2}mv_z^2]}{K_B T}} \right) dv_z = \int_{-\infty}^{+\infty} (K_B T h^2) (e^{-h^2}) \sqrt{\frac{2K_B T}{m}} dh = K_B T \cdot \sqrt{\frac{2K_B T}{m}} \cdot \underbrace{\int_{-\infty}^{+\infty} h^2 e^{-h^2} dh}_{\frac{\sqrt{\pi}}{2}} = K_B T \cdot \sqrt{\frac{2K_B T}{m}} \cdot \frac{\sqrt{\pi}}{2} \Rightarrow$$

$$\int_{-\infty}^{+\infty} \left( \frac{mv_z^2}{2} \right) \left( e^{-\frac{[\frac{1}{2}mv_z^2]}{K_B T}} \right) dv_z = \frac{K_B T}{2} \cdot \sqrt{\frac{2\pi K_B T}{m}} \Rightarrow \left( \frac{2\pi K_B T}{m} \right) \cdot \int_{-\infty}^{+\infty} \left( \frac{mv_z^2}{2} \right) \left( e^{-\frac{[\frac{1}{2}mv_z^2]}{K_B T}} \right) dv_z = \frac{K_B T}{2} \cdot \left( \frac{2\pi K_B T}{m} \right)^{\frac{3}{2}}$$

$$\int_{-\infty}^{+\infty} \left( e^{-\frac{[\frac{1}{2}mv_z^2]}{K_B T}} \right) dv_z \rightarrow Substituição: \begin{cases} h^2 = \frac{mv_z^2}{2K_B T} \Leftrightarrow h = \sqrt{\frac{m}{2K_B T}} v_z \\ dh = \sqrt{\frac{m}{2K_B T}} dv_z \Leftrightarrow dv_z = \sqrt{\frac{2K_B T}{m}} dh \\ v_z^2 = \frac{2K_B T}{m} h^2 \Rightarrow K_B T h^2 = \frac{mv_z^2}{2} \end{cases}$$

$$\int_{-\infty}^{+\infty} \left( e^{-\frac{[\frac{1}{2}mv_z^2]}{K_B T}} \right) dv_z = \int_{-\infty}^{+\infty} e^{-h^2} \sqrt{\frac{2K_B T}{m}} dh = \sqrt{\frac{2K_B T}{m}} \cdot \underbrace{\int_{-\infty}^{+\infty} e^{-h^2} dh}_{\frac{\sqrt{\pi}}{2}} = \sqrt{\frac{2\pi K_B T}{m}} \Leftrightarrow$$

$$\Leftrightarrow \int_{-\infty}^{+\infty} \left( e^{-\frac{[\frac{1}{2}mv_z^2]}{K_B T}} \right) dv_z = \sqrt{\frac{2\pi K_B T}{m}} \Leftrightarrow$$

$$\Leftrightarrow \frac{5K_B T}{2} \cdot \left( \frac{2\pi K_B T}{m} \right) \cdot \int_{-\infty}^{+\infty} \left( e^{-\frac{[\frac{1}{2}mv_z^2]}{K_B T}} \right) dv_z = \frac{5K_B T}{2} \cdot \left( \frac{2\pi K_B T}{m} \right) \cdot \sqrt{\frac{2\pi K_B T}{m}} \Leftrightarrow$$

$$\Leftrightarrow \frac{5K_B T}{2} \cdot \left( \frac{2\pi K_B T}{m} \right) \cdot \int_{-\infty}^{+\infty} \left( e^{-\frac{[\frac{1}{2}mv_z^2]}{K_B T}} \right) dv_z = \frac{5K_B T}{2} \cdot \left( \frac{2\pi K_B T}{m} \right)^{\frac{3}{2}}$$

Então temos que

$$\left\{ \int_{-\infty}^{+\infty} \left( e^{-\frac{[\frac{1}{2}mv_z^2]}{K_B T}} \right) \int_{-\infty}^{+\infty} \left( e^{-\frac{[\frac{1}{2}mv_y^2]}{K_B T}} \right) \left\{ \int_{-\infty}^{+\infty} \left( e^{-\frac{[\frac{1}{2}mv_x^2]}{K_B T}} \right) \cdot \left( \frac{m(v_x^2 + v_y^2 + v_z^2)}{2} + \frac{3K_B T}{2} \right) dv_x \right\} dv_y \right\} dv_z =$$

$$= \int_{-\infty}^{+\infty} \left( e^{-\frac{[\frac{1}{2}mv_z^2]}{K_B T}} \right) \cdot \left( \frac{2\pi K_B T}{m} \right) \cdot \left( \frac{5K_B T}{2} + \left( \frac{mv_z^2}{2} \right) \right) dv_z =$$

$$\begin{aligned}
&= \left( \frac{2\pi K_B T}{m} \right) \cdot \int_{-\infty}^{+\infty} \left( e^{-\frac{[\frac{1}{2}mv_z^2]}{K_B T}} \right) \cdot \left( \frac{5K_B T}{2} + \left( \frac{mv_z^2}{2} \right) \right) dv_z = \\
&= \frac{5K_B T}{2} \cdot \left( \frac{2\pi K_B T}{m} \right)^{\frac{3}{2}} + \frac{K_B T}{2} \cdot \left( \frac{2\pi K_B T}{m} \right)^{\frac{3}{2}} = \\
&= \frac{6K_B T}{2} \cdot \left( \frac{2\pi K_B T}{m} \right)^{\frac{3}{2}}
\end{aligned}$$

Então que o numerador de  $\langle E \rangle$  é dado por

$$\int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \left\{ \left[ \frac{1}{2}mv^2 + \frac{1}{2}Kr^2 \right] e^{-\frac{[\frac{1}{2}mv^2 + \frac{1}{2}Kr^2]}{K_B T}} \right\} dv_x dv_y dv_z dx dy dz = \frac{6K_B T}{2} \cdot \left( \frac{2\pi K_B T}{m} \right)^{\frac{3}{2}}$$

e como é óvio de calcular

$$\int_{-\infty}^{+\infty} \left( e^{-\frac{[\frac{1}{2}mv_z^2]}{K_B T}} \right) dv_z \int_{-\infty}^{+\infty} \left( e^{-\frac{[\frac{1}{2}mv_y^2]}{K_B T}} \right) dv_y \int_{-\infty}^{+\infty} \left( e^{-\frac{[\frac{1}{2}mv^2]}{K_B T}} \right) dv_x = \left( \frac{2\pi K_B T}{m} \right)^{\frac{3}{2}}$$

Então temos que

$$\begin{aligned}
\langle E \rangle &= \frac{\int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \left\{ \left[ \frac{1}{2}mv^2 + \frac{1}{2}Kr^2 \right] e^{-\frac{[\frac{1}{2}mv^2 + \frac{1}{2}Kr^2]}{K_B T}} \right\} dv_x dv_y dv_z dx dy dz}{\int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \left\{ e^{-\frac{[\frac{1}{2}mv^2 + \frac{1}{2}Kr^2]}{K_B T}} \right\} dv_x dv_y dv_z dx dy dz} \Leftrightarrow \\
&\Leftrightarrow \langle E \rangle = \frac{\frac{6K_B T}{2} \cdot \left( \frac{2\pi K_B T}{m} \right)^{\frac{3}{2}}}{\left( \frac{2\pi K_B T}{m} \right)^{\frac{3}{2}}} \Leftrightarrow \langle E \rangle = \frac{6K_B T}{2} \Leftrightarrow \langle E \rangle = 3K_B T \\
U = N_A \cdot \langle E \rangle &\Leftrightarrow U = N_A \cdot 3K_B T \Leftrightarrow U = 3 \overbrace{N_A K_B}^{R=N_A K_B} T / mole \Leftrightarrow U = 3RT / mole
\end{aligned}$$

Calor específico a volume constante:  $C_v = \frac{dU}{dT} \Leftrightarrow C_v = \frac{d}{dT}(3RT/mole) \Leftrightarrow C_v = 3R/mole$

$C_v = 3R/mole \Rightarrow$  Lei de Dulong e Petit