Température de Fusion

(1) $$P(x,p)\,dx\,dp = \frac{1}{Z} e^{-\frac{E}{kT}} dx\,dp$$

$$P(x)\,dx = \left(\int_{\substack{p\in\mathbb{R}\\ x \text{ fixé}}} P(x,p)\,dp\right) dx$$

$$= \frac{1}{Z}\left(\int e^{-\frac{p^2}{2mkT}} dp\right) e^{-\frac{\frac{1}{2}kx^2}{kT}} dx$$

$$\iint P(x,p)\,dx\,dp = 1 \iff Z = \iint e^{-\frac{E}{kT}} dx'\,dp'$$

$$= \left(\int e^{-\frac{p'^2}{2mkT}} dp'\right)\left(\int e^{-\frac{kx'^2}{2kT}} dx'\right)$$

donc

$$P(x)\,dx = \frac{e^{-\frac{k x^2}{2 k T}}\,dx}{\left(\int_{\mathbb{R}} e^{-\frac{k x'^2}{2 k T}}\,dx'\right)}$$

posons $\quad X^2 = \dfrac{k x'^2}{2 k T} \iff x' = \sqrt{\dfrac{2 k T}{k}}\, X$

$$\int e^{-\frac{k x'^2}{2 k T}}\,dx' = \left(\int e^{-X^2}\,dX\right)\sqrt{\frac{2 k T}{k}}$$

$$= \sqrt{\frac{2\pi k T}{k}}$$

$$\boxed{P(x)\,dx = \sqrt{\frac{k}{2\pi k T}}\, e^{-\frac{k x^2}{2 k T}}\,dx}$$

(2) $$\boxed{\langle x \rangle = \int x\, P(x)\, dx = 0}$$ car $x P(x)$ est une fonction impaire

$$\langle x^2 \rangle = \int x^2 P(x)\, dx = \int \left(\frac{2kT}{K}\right) X^2 e^{-X^2} dX \sqrt{\frac{2kT}{K}} \sqrt{\frac{K}{2\pi kT}}$$

avec $X^2 = \frac{K x^2}{2kT} \Longleftrightarrow x = \sqrt{\frac{2kT}{K}}\, X$

$$= \frac{2kT}{K\sqrt{\pi}} \cdot \frac{\sqrt{\pi}}{2} = \frac{kT}{K}, \quad \boxed{\langle x^2 \rangle = \frac{kT}{K}}$$

(3) on a $\Theta = \frac{\hbar\omega}{k} \Longleftrightarrow \left(\frac{K}{m}\right) = \omega^2 = \frac{\Theta^2 k^2}{\hbar^2}$

$$M = N_A\, m$$

$$K = m \frac{\Theta^2 k^2}{\hbar^2} = \frac{M\, \Theta^2 k^2}{N_A\, \hbar^2}$$

donc $x_0 = \langle x^2 \rangle^{1/2} = \left(\frac{kT}{K}\right)^{1/2} = \left(\frac{k T N_A \hbar^2}{M \Theta^2 k^2}\right)^{1/2}$

$$\boxed{x_0 = \frac{\hbar}{\Theta}\left(\frac{T N_A}{M k}\right)^{1/2} = \frac{\hbar N_A}{\Theta}\left(\frac{T}{MR}\right)^{1/2}}$$

(4) $\frac{x_0}{d}$ est presque constant, <u>en accord avec l'hypothèse de Lindemann.</u>

si on note $r = \frac{x_0}{d} = 4.10^{-2}$,

cela suggère la formule

$$r = \frac{x_0}{d} = \frac{\hbar N_A}{\Theta d}\left(\frac{T_F}{MR}\right)^{1/2}$$

$$\Longleftrightarrow \quad \boxed{\Theta = \frac{\hbar N_A}{r d}\left(\frac{T_F}{MR}\right)^{1/2}}$$