Capacité thermique : modèle quantique d'oscillateurs couplés
Debye 1912

① la distance entre les atomes p et p+1 est

$$r_p = u_{p+1} + a - u_p$$

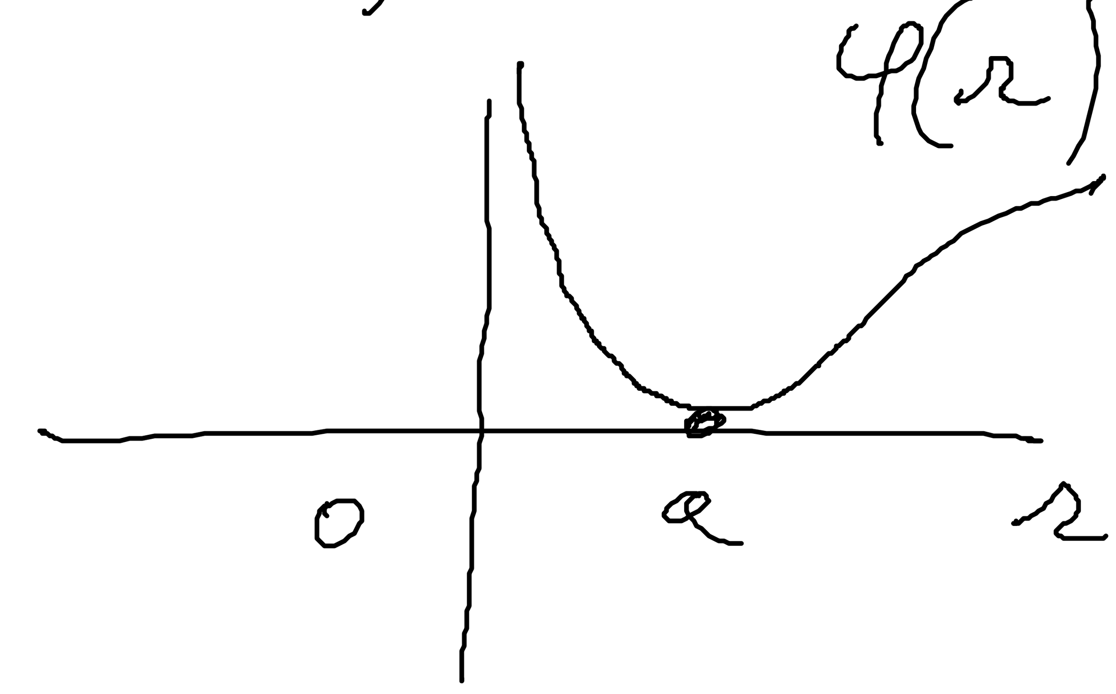
donc
$$E = \sum_{p=0}^{N-1} \varphi(r_p) = \sum_{p=0}^{N-1} \varphi(u_{p+1} + a - u_p)$$

si $|u_{p+1} - u_p| \ll a$,

$$\varphi(a + u_{p+1} - u_p) = \varphi(a) + \varphi'(a)\cdot(u_{p+1} - u_p) + \frac{1}{2}\varphi''(a)(u_{p+1} - u_p)^2 + \cdots$$

or

$\varphi'(a) = 0$ car minimum de φ



donc
$$E = N\varphi(a) + \sum_{p=0}^{N-1} \frac{1}{2}\varphi''(a)(u_{p+1} - u_p)^2$$

$$E = E_0 + \frac{m}{2}\omega_0^2 \sum_{p=0}^{N-1} (u_{p+1} - u_p)^2$$

avec $E_0 = N\,\varphi(a)$

$$\frac{m}{2}\omega_0^2 = \frac{1}{2}\varphi''(a) \Leftrightarrow \omega_0 = \left(\frac{\varphi''(a)}{m}\right)^{1/2}$$

(2) Loi de Newton pour l'atome $p \in \{0, \dots, N-1\}$

$$m\frac{d^2u_p}{dt^2} = \text{Force} = -\frac{dE}{du_p}$$

$$= -m\omega_0^2\left((u_p - u_{p-1}) - (u_{p+1} - u_p)\right)$$

$$= m\omega_0^2\left(u_{p+1} - 2u_p + u_{p-1}\right)$$

$$\Leftrightarrow \frac{d^2u_p}{dt^2} = \omega_0^2\left(u_{p+1} - 2u_p + u_{p-1}\right) \quad (*)$$

(3) Si $u_p = u_0 e^{i(kpa - \omega t)}$

alors $(*) \Leftrightarrow -\omega^2 u_p = \omega_0^2\left(e^{ika} - 2 + e^{-ika}\right)u_p$

$$\Leftrightarrow \omega^2 = \omega_0^2\left(2 - 2\cos(ka)\right)$$

$$= 4\omega_0^2\sin^2\left(\frac{ka}{2}\right)$$ car $\cos 2x = 1 - 2\sin^2 x$

$$\iff \quad \omega = 2\omega_0 \left|\sin\left(\frac{ka}{2}\right)\right|$$

k : fréq