Physique des solides

Une introduction

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Dynamique du réseau 1

1. Problèmes du réseau gelé
2. Déplacements sous la condition BvK
3. Approche classique des vibrations harmoniques
    1. Séparation de Born-Oppenheimer
    2. Approximation harmonique
    3. Exemple : chaine mono-atomique
        1. Relation de dispersion
        2. Cas limites

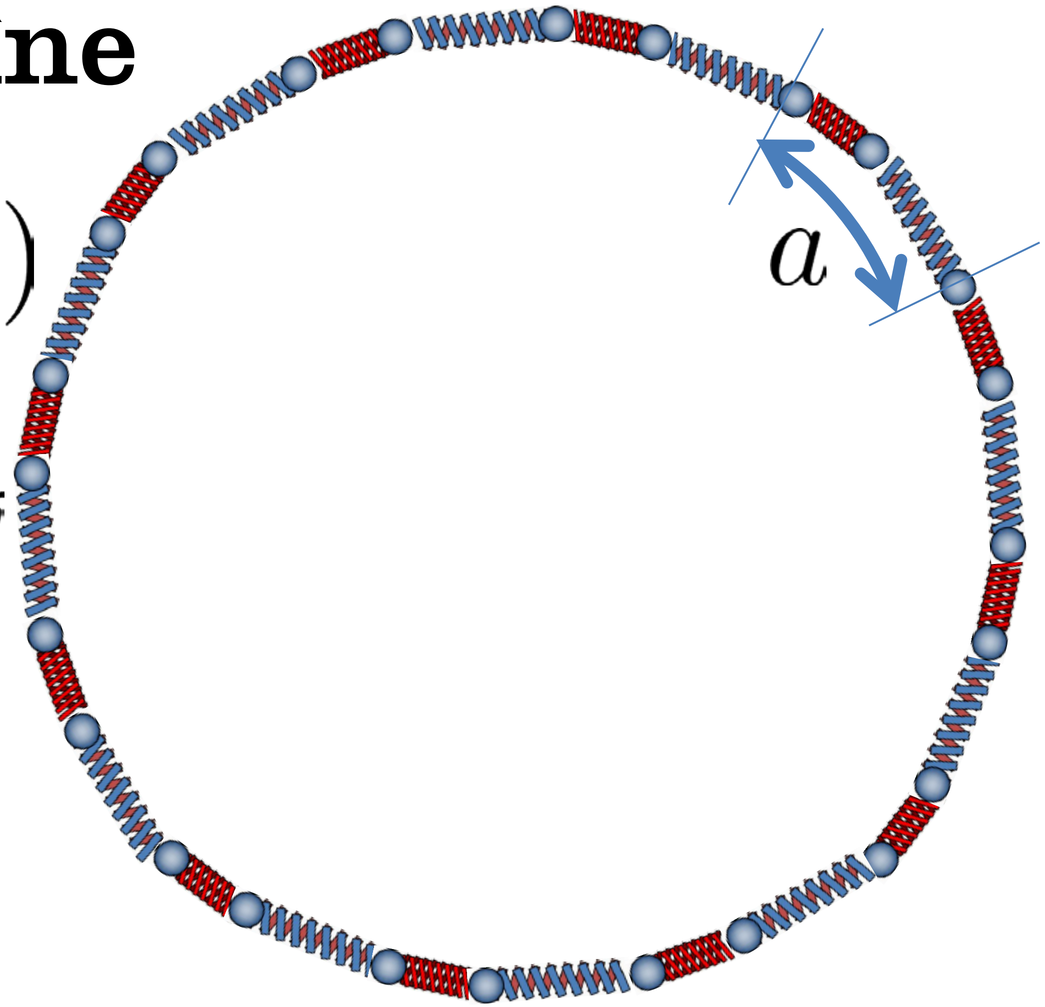
2. Déplacements sous BvK

Bouclage de la chaîne

$$\boldsymbol{u}_j(x,t) = \boldsymbol{u}_j(x+Na,t)$$

$$\boldsymbol{u}_j(x_j,t) = \sum_q A_{q,j} e^{iqx_j}$$

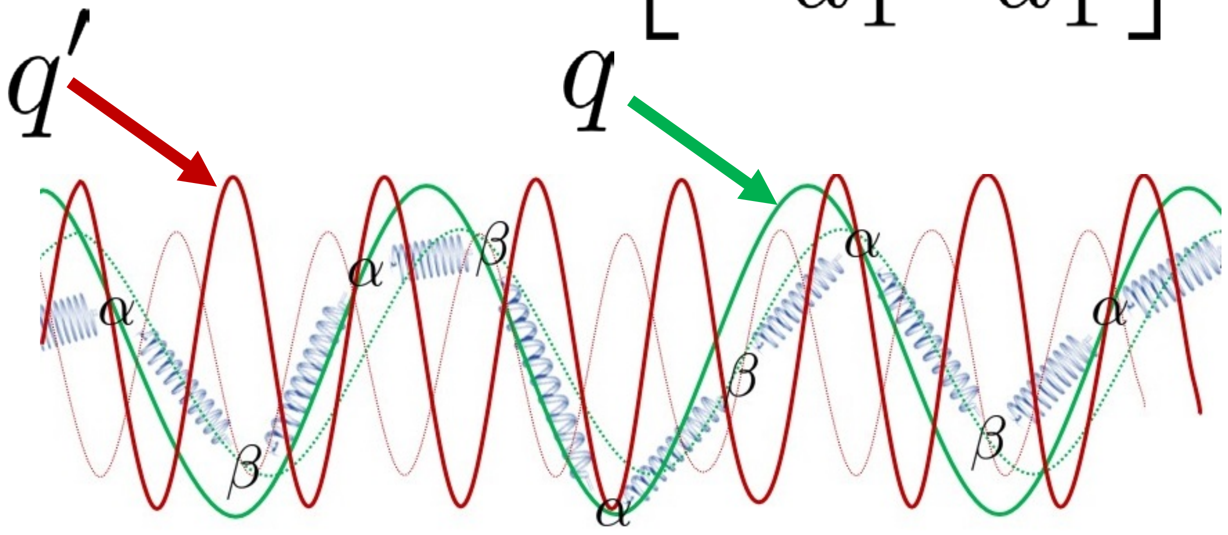
$$q = n\frac{2\pi}{L_1} = n\frac{2\pi}{N_1 a_1}$$



2. Déplacements sous BvK

Bouclage de la chaîne

$$q \in \left[-\frac{\pi}{a_1}, \frac{\pi}{a_1} \right]$$



$$\boldsymbol{u}_j(x_j, t) = \sum_q A_{q,j} e^{iqx_j}$$

$$q = n\frac{2\pi}{L_1} = n\frac{2\pi}{N_1 a_1}$$

$$q' = (n + N_1)\frac{2\pi}{N_1 a_1} \equiv q$$

2. Déplacements sous BvK

Bouclage de la chaîne

$$q \in \left[-\frac{\pi}{a_1}, \frac{\pi}{a_1}\right]$$

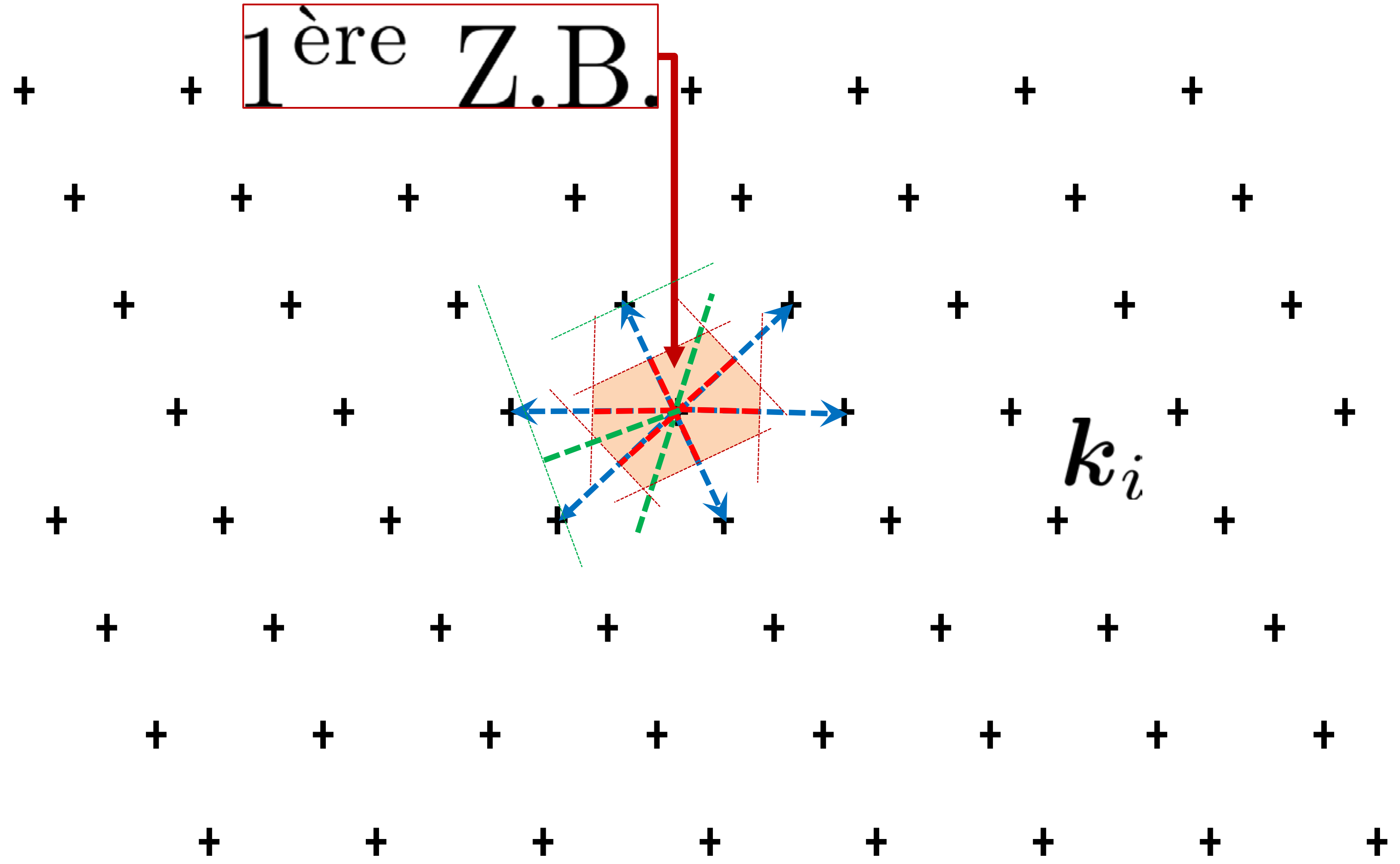
$$\boldsymbol{u}_j(x_j, t) = \sum_{k \in Z.B.} e^{ikx_j} \sum_{G \in R.R.} A_{k+G,j} e^{iGx_j}$$

$$q = n\frac{2\pi}{L_1} = n\frac{2\pi}{N_1 a_1}$$

2. Déplacements sous BvK

Bouclage de la chaîne

$$q \in \left[-\frac{\pi}{a_1}, \frac{\pi}{a_1}\right]$$



2. Déplacements sous BvK

Bouclage de la chaîne

$$q \in \left[-\frac{\pi}{a_1}, \frac{\pi}{a_1}\right]$$

$$\boldsymbol{u}_j(x_j, t) = \sum_q A_{q,j} e^{iqx_j}$$

Volume d'un mode $\dfrac{(2\pi)^3}{V_{\mathrm{Xtal}}}$

$$q = n\frac{2\pi}{L_1} = n\frac{2\pi}{N_1 a_1}$$

$$v^* = \frac{(2\pi)^3}{v}$$ **modes**

2. Déplacements sous BvK

Bouclage de la chaîne

$$q \in \left[-\frac{\pi}{a_1}, \frac{\pi}{a_1}\right]$$

$$\boldsymbol{u}_j(x_j, t) = \sum_q A_{q,j} e^{iqx_j}$$

avec

EXO

$$q = n\frac{2\pi}{L_1} = n\frac{2\pi}{N_1 a_1}$$

$$\int_{-L/2}^{L/2} e^{iqx_j} e^{-iqx_j} dx_j = L\delta_{q,q'}$$

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3. Approche classique des vibrations harmoniques

Newton en couplage harmonique

$$W \approx \sum_{j,n} \sum_{\alpha=1}^{3} W_{j,n} + \sum_{j,n} \sum_{\alpha=1}^{3} \frac{\partial W}{\partial u_{\alpha,j}} u_{\alpha,j} + \sum_{j,n} \sum_{\alpha,\beta=1}^{3} \frac{1}{2} \frac{\partial^2 W}{\partial u_{\alpha,j} \partial u_{\beta,n}} u_{\alpha,j} u_{\beta,n}$$

cte | **cte=0** | **quadratique**

3. Approche classique des vibrations harmoniques

Newton en couplage harmonique

$$m\ddot{u}_{\alpha,j} = -2\sum_{n} V_{n,j}(u_{\alpha,j} - u_{\alpha,n})$$

$$-\omega_q^2 A_j(q) + \sum_{n} D_{n,j} A_n(q) = 0$$

$$\boldsymbol{u}_j(x_j, t) = \sum_{q} A_j(q) e^{i(qx_j - \omega_q t)}$$

en rassemblant tous les atomes

3. Approche classique des vibrations harmoniques

Newton en couplage harmonique

$$\widehat{H} = \sum_q \left(\widehat{a}_q^\dagger \widehat{a}_q + \frac{1}{2} \right) \hbar\omega_(q)$$

$$\ddot{\vec{A}}(q) - \widehat{D}\vec{A}(q) = 0$$

$$\widehat{D}\vec{A}(q) = \omega_q^2 \vec{A}(q)$$

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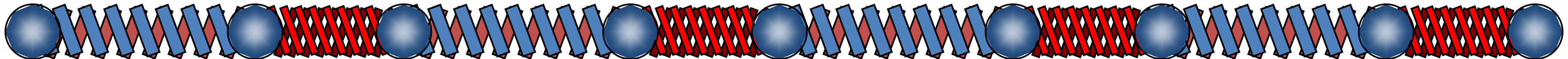
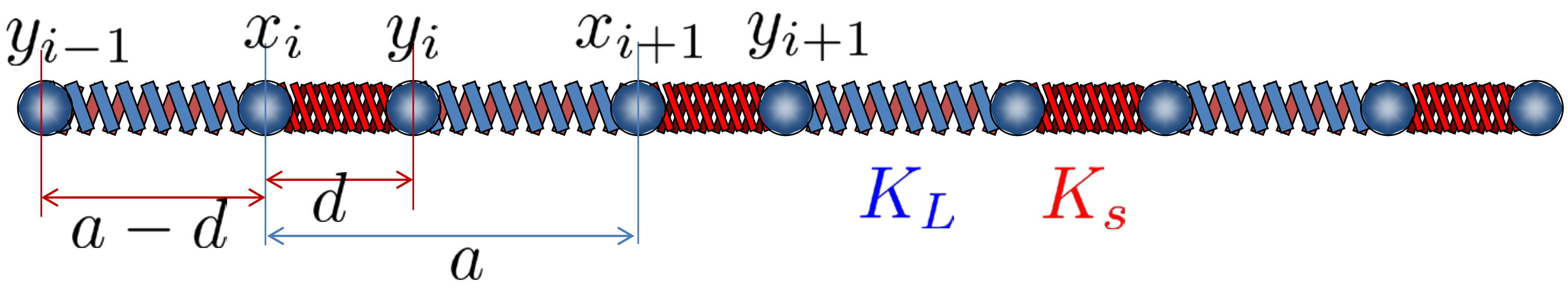


4. Chaîne mono-atomique asymetrique 1D

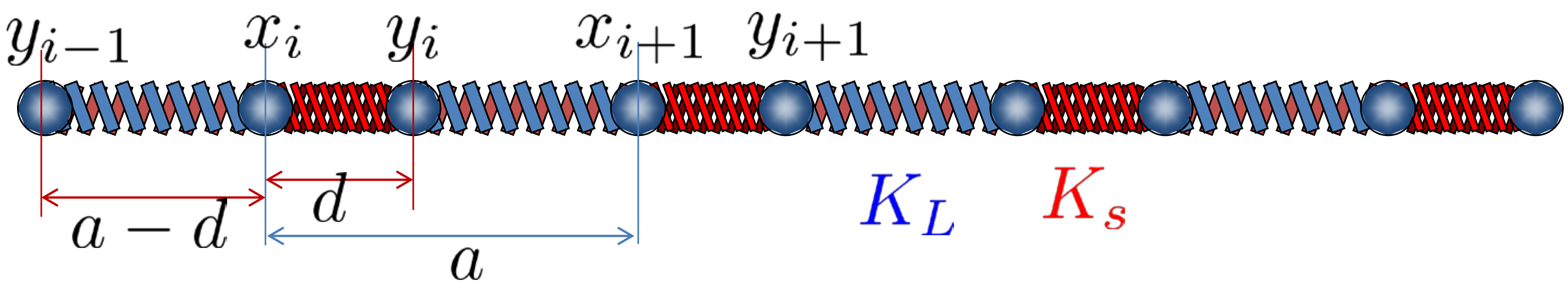


$$\begin{cases} m\ddot{x}_i = -K_s(x_i - y_i) - K_L(x_i - y_{i-1}) \\ m\ddot{y}_i = -K_s(y_i - x_i) - K_L(y_i - x_{i+1}) \end{cases}$$

$$x_i = Xe^{iqna}e^{i\omega_q t}$$

$$y_i = Ye^{iq(na+d)}e^{i\omega_q t}$$

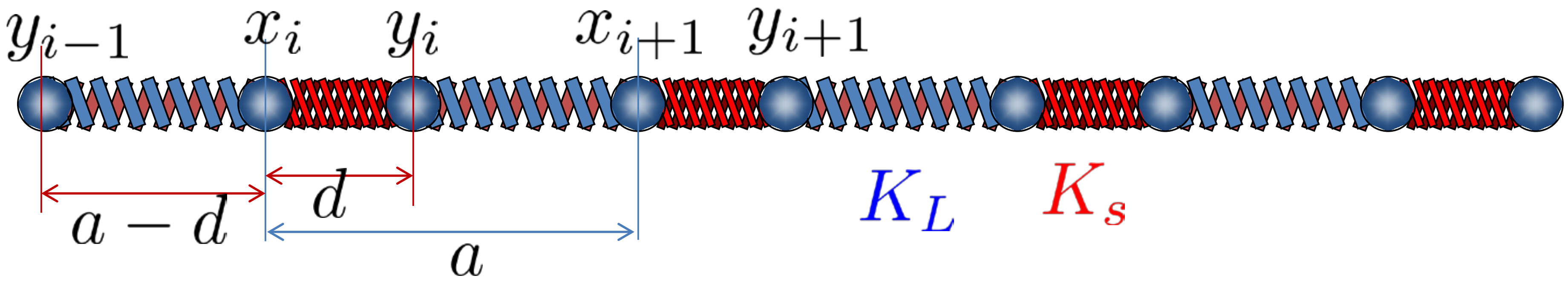
4. Chaîne mono-atomique asymetrique 1D



$$\begin{cases} -\omega_q^2 X = -\Omega_s^2 (X - Ye^{iqd}) - -\Omega_L^2 (X - Ye^{iq(-a+d)}) \\ -\omega_q^2 Ye^{iqd} = -\Omega_s^2 (Ye^{iqd} - X) - -\Omega_L^2 (Ye^{iqd} - Xe^{iqa}) \end{cases}$$

$$x_i = Xe^{iqna} e^{i\omega_q t}$$
$$y_i = Ye^{iq(na+d)} e^{i\omega_q t}$$

4. Chaîne mono-atomique asymetrique 1D

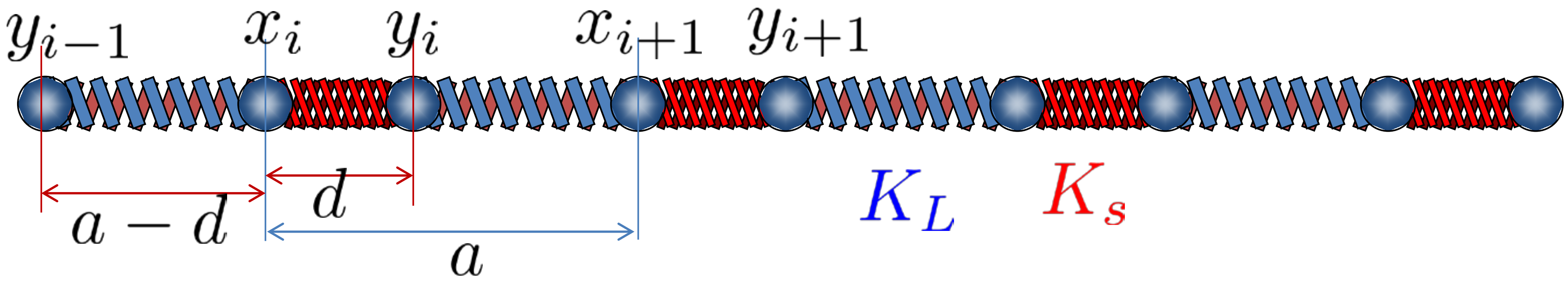


$$\begin{cases} (\Omega_s^2+\Omega_L^2-\omega_q^2)X-(\Omega_s^2+\Omega_L^2 e^{-iqa})Ye^{iqd}=0 \\ -(\Omega_s^2+\Omega_L^2 e^{iqa})Xe^{-iqd}+(\Omega_s^2+\Omega_L^2-\omega_q^2)Y=0 \end{cases}$$

$$x_i = Xe^{iqna}e^{i\omega_q t}$$

$$y_i = Ye^{iq(na+d)}e^{i\omega_q t}$$

4. Chaîne mono-atomique asymetrique 1D

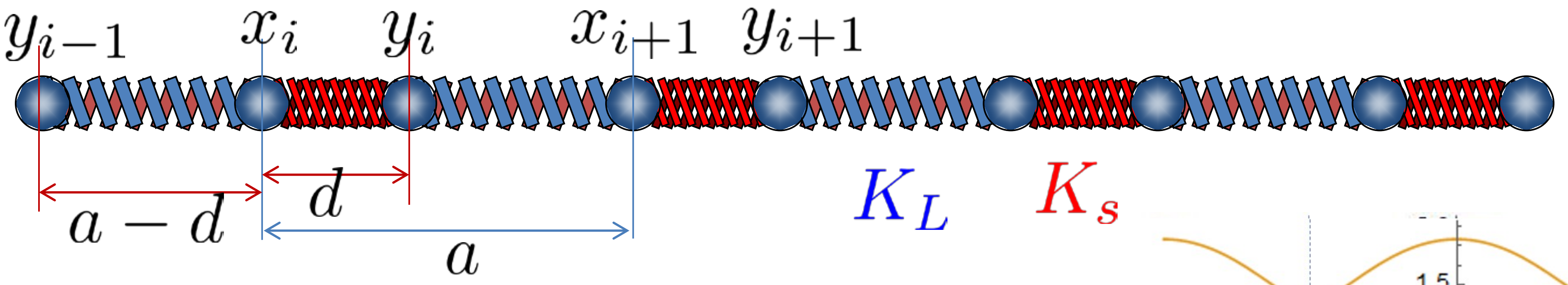


$$\begin{pmatrix} \Omega_s^2 + \Omega_L^2 & -(\Omega_s^2 + \Omega_L^2 e^{-iqa})e^{iqd} \\ -(\Omega_s^2 + \Omega_L^2 e^{iqa})e^{-iqd} & \Omega_s^2 + \Omega_L^2 \end{pmatrix} \begin{pmatrix} X \\ Y \end{pmatrix} = \omega_q^2 \begin{pmatrix} X \\ Y \end{pmatrix}$$

$$\omega_q^2 = (\Omega_s^2 + \Omega_L^2) \pm \sqrt{\Omega_s^4 + \Omega_L^4 + 2\Omega_s^2\Omega_L^2 \cos qa}$$

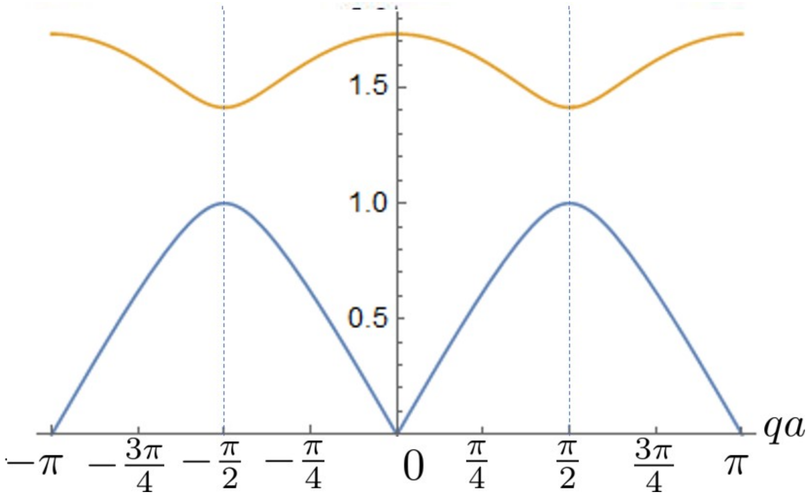
Période $\frac{2\pi}{a}$ **2 atomes/maille** ➡ **2 branches**

4. Chaîne mono-atomique asymetrique 1D



K_L K_s

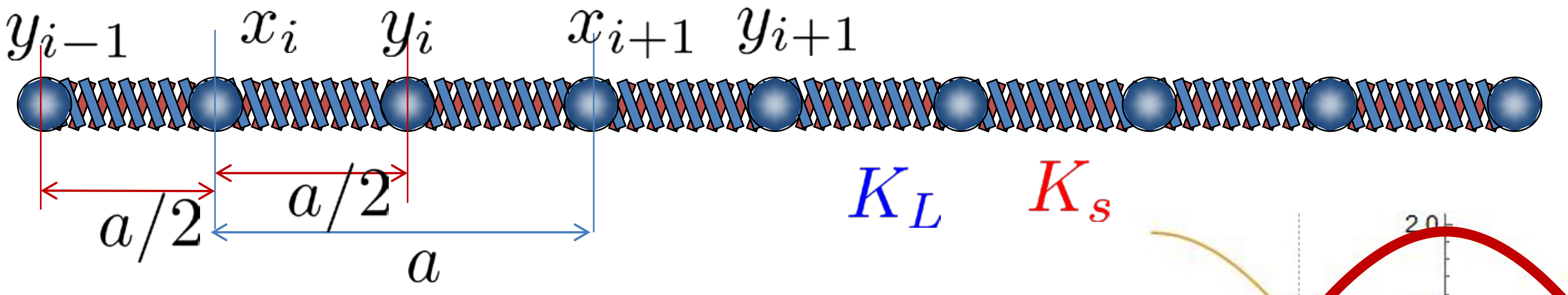
K_L ➡ K_s



$$\omega_q^2 = (\Omega_s^2 + \Omega_L^2) \pm \sqrt{\Omega_s^4 + \Omega_L^4 + 2\Omega_s^2\Omega_L^2 \cos qa}$$

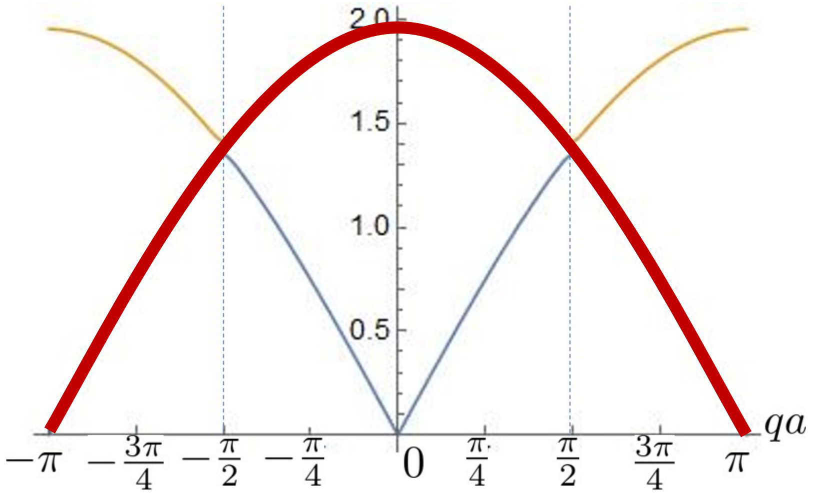
Période $\frac{2\pi}{a}$ **2 atomes/maille ➡ 2 branches**

4. Chaîne mono-atomique asymetrique 1D



K_L K_s

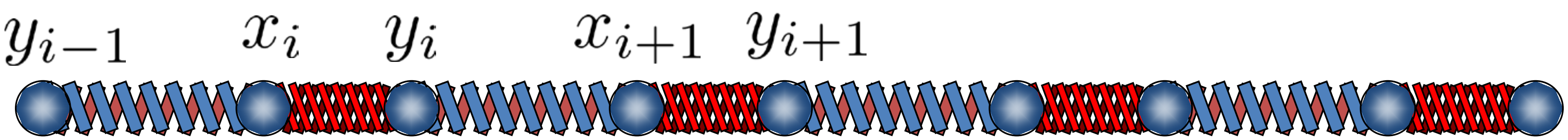
K_L → K_s



$$\omega_q^2 = 2\Omega^2 \left(1 \pm |\cos(qa/2)|\right)$$

Période $\frac{4\pi}{a}$ **1 atome/maille** → **1 branche**

4. Chaîne mono-atomique asymetrique 1D

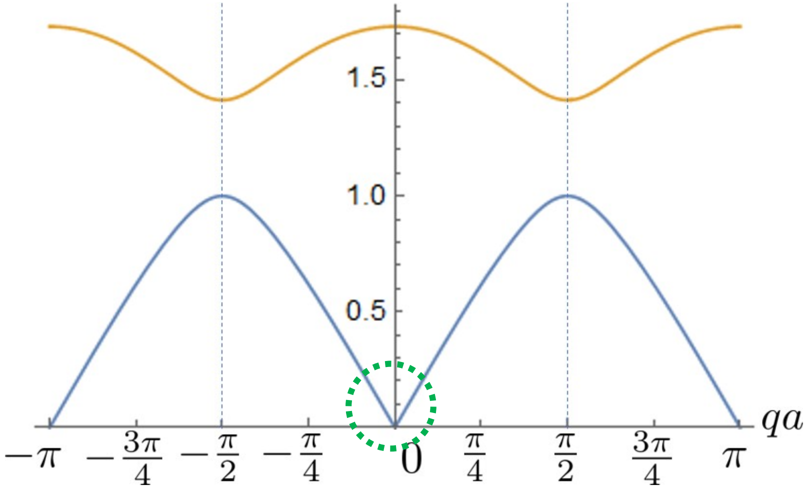


EXO

$$q \longrightarrow 0$$

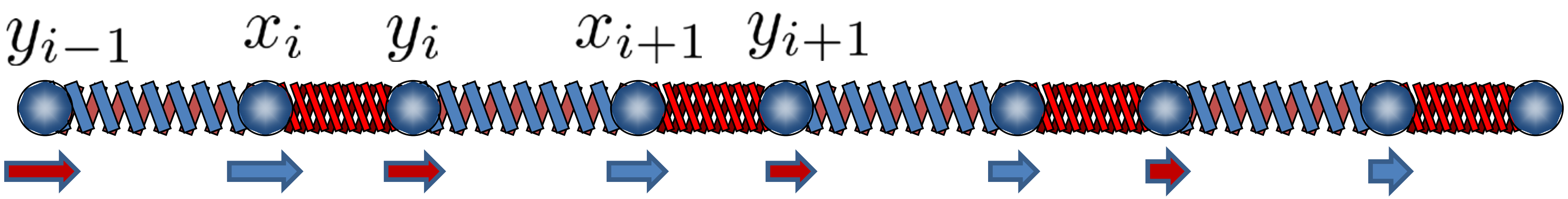
$$\omega_q \longrightarrow \left[\frac{1}{2m}\frac{K_s K_L}{K_s + K_L} a^2\right]^{1/2} q$$

$$c = \frac{\partial \omega_q}{\partial q} \longrightarrow \left[\frac{Ka}{2m/a}\right]^{1/2}$$



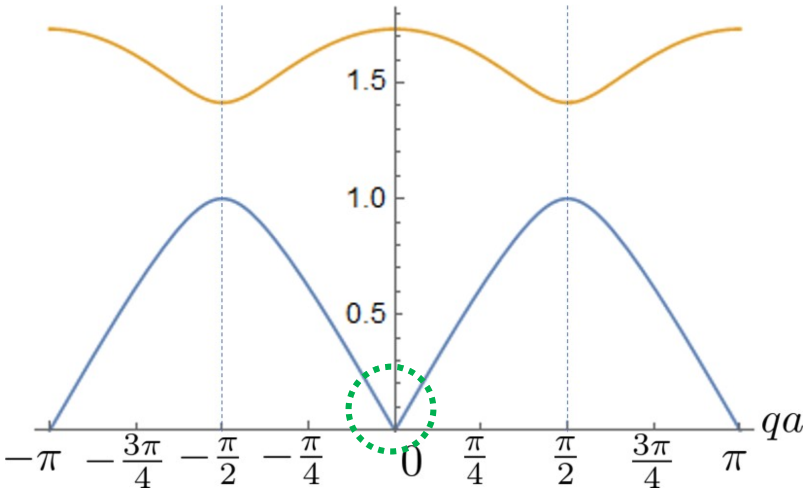
$$\omega_q^2 = (\Omega_s^2 + \Omega_L^2) \pm \sqrt{\Omega_s^4 + \Omega_L^4 + 2\Omega_s^2\Omega_L^2 \cos qa}$$

4. Chaîne mono-atomique asymetrique 1D



$$q \longrightarrow 0$$

Limite acoustique

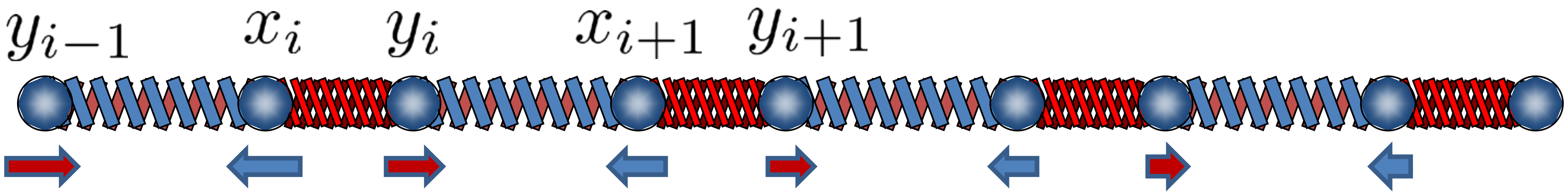


$$c = \frac{\partial \omega_q}{\partial q} \longrightarrow \left[\frac{Ka}{2m/a}\right]^{1/2}$$

$$\omega_q^2 \approx 0$$

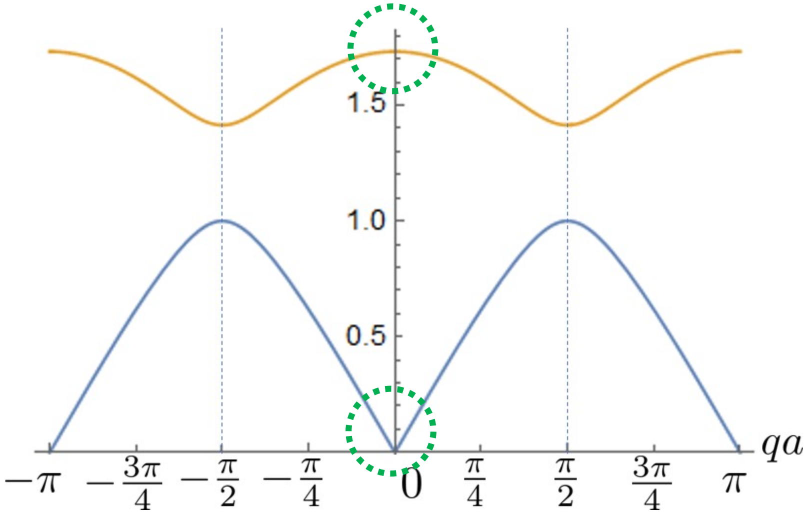
$$(\Omega_s^2 + \Omega_L^2)X - (\Omega_s^2 + \Omega_L^2)Y = 0$$

4. Chaîne mono-atomique asymetrique 1D



$$q \longrightarrow 0$$

EXO



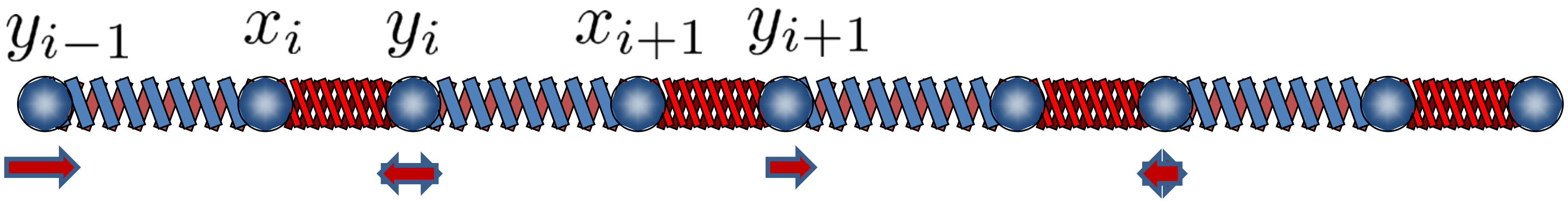
$$\omega_q \longrightarrow \sqrt{2(\Omega_s^2 + \Omega_L^2)}$$

$$c = \frac{\partial \omega_q}{\partial q} \longrightarrow 0$$

$$\omega_q^2 = (\Omega_s^2 + \Omega_L^2) \pm \sqrt{\Omega_s^4 + \Omega_L^4 + 2\Omega_s^2\Omega_L^2 \cos qa}$$

$$(\Omega_s^2 + \Omega_L^2 - \omega_q^2)X - (\Omega_s^2 + \Omega_L^2 e^{-iqa})Ye^{iqd} = 0$$

4. Chaîne mono-atomique asymetrique 1D



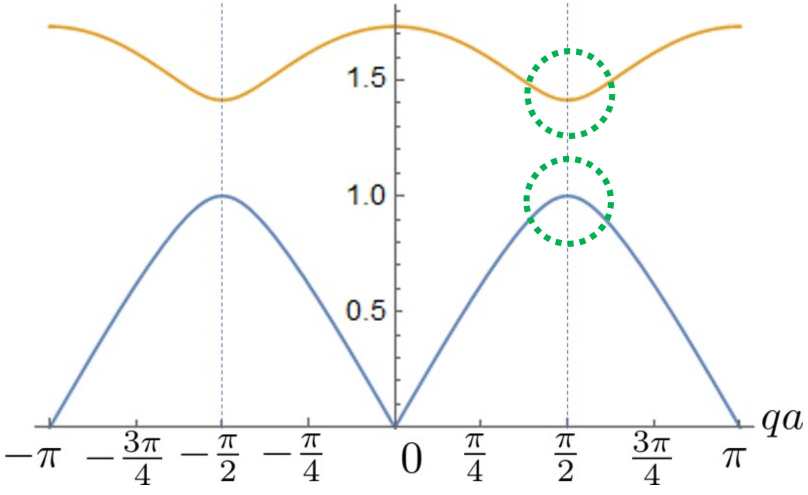
$$q \longrightarrow \frac{\pi}{a}$$

EXO

$$\omega_q \longrightarrow \sqrt{(\Omega_s^2 + \Omega_L^2) \pm |\Omega_s^2 - \Omega_L^2|}$$

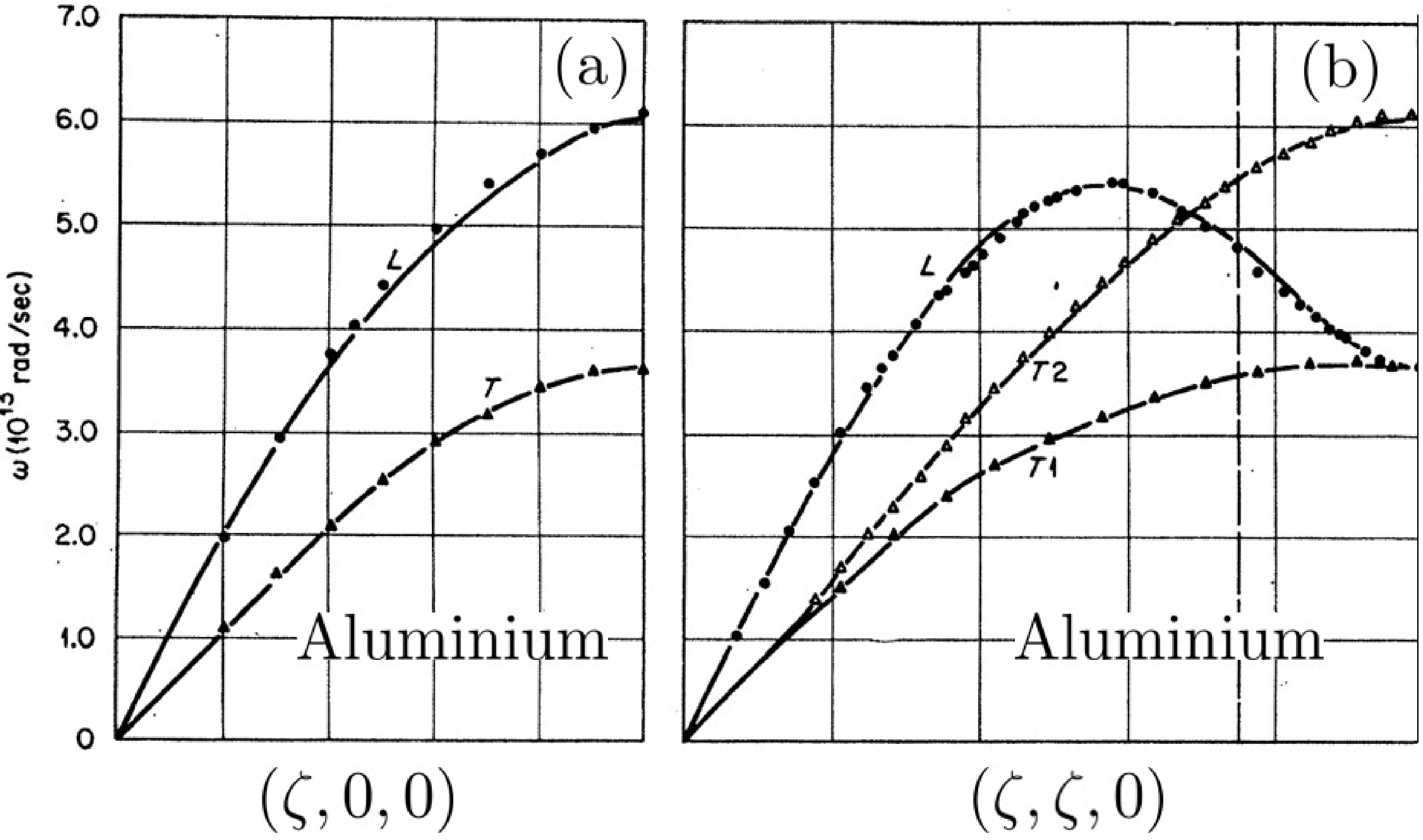
$$c = \frac{\partial \omega_q}{\partial q} \longrightarrow 0$$

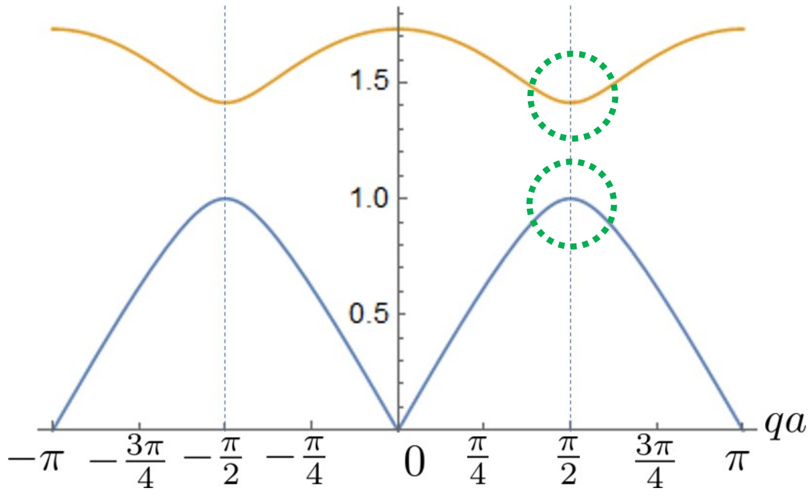
Diffraction onde mécanique !



$$\omega_q^2 = (\Omega_s^2 + \Omega_L^2) \pm \sqrt{\Omega_s^4 + \Omega_L^4 + 2\Omega_s^2\Omega_L^2 \cos qa}$$

4. Chaîne mono-atomique asymetrique 1D





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