Phonons and Electron-Phonon Couplings

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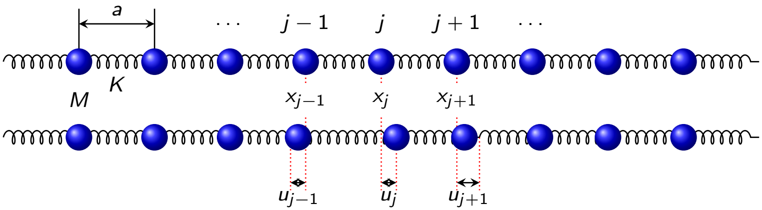
1 Introduction

A 1D chain of N equally spaced atoms at $R_j(t) = x_j + u_j(t)$



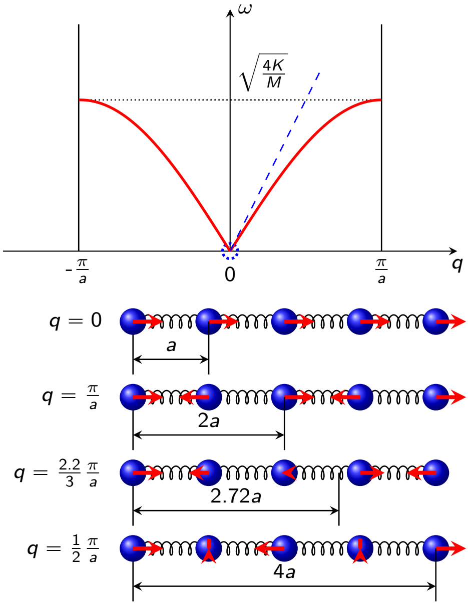
The Newton's Equation

$$M \frac{\mathrm{d}^2 u_j}{\mathrm{d}t^2} = K(u_{j+1} + u_{j-1} - 2u_j) \qquad j = 1, \ldots, N$$

Assume the solution has the form $u_j(t) = \frac{A_q}{\sqrt{M}} e^{i(qx_j - \omega t)}$, then [1]

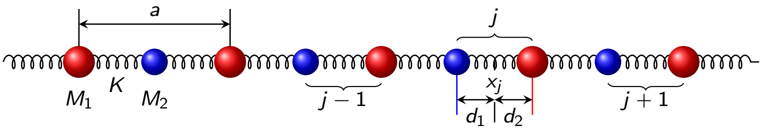
$$\begin{aligned} \omega^2 &= \frac{K}{M}(2 - e^{iqa} - e^{-iqa}) \\ &= \frac{2K}{M}(1 - \cos qa) \\ \Rightarrow \qquad \omega &= \sqrt{\frac{4K}{M}} \left| \sin \frac{qa}{2} \right| \end{aligned}$$

[1] $u_j(t)$ here is complex. In practice, take the real part, i.e. $\mathrm{Re}[u_j(t)]$.


ω
$\sqrt{\frac{4K}{M}}$
$-\frac{\pi}{a}$
0
$\frac{\pi}{a}$
q
$q = 0$
a
$q = \frac{\pi}{a}$
$2a$
$q = \frac{2.2}{3}\frac{\pi}{a}$
$2.72a$
$q = \frac{1}{2}\frac{\pi}{a}$
$4a$

1D Chain of Atoms — 2 Atoms per Unit

A 1D chain with 2 atoms in each unit: $R_j^s(t) = x_j + d_s + u_j^s(t); \quad s = 1, 2$



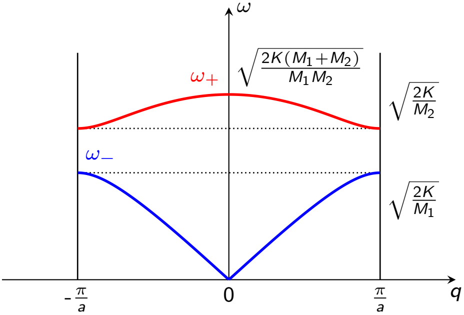
The Newton's Equation

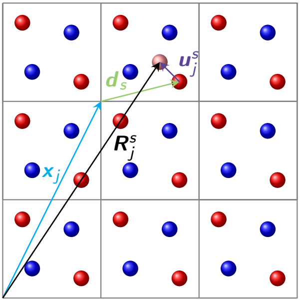
$$
\begin{aligned}
M_1 \frac{\mathrm{d}^2 u_j^1}{\mathrm{d}t^2} &= K(u_j^2 + u_{j-1}^2 - 2u_j^1) \\
M_2 \frac{\mathrm{d}^2 u_j^2}{\mathrm{d}t^2} &= K(u_j^1 + u_{j+1}^1 - 2u_j^2)
\end{aligned}
\quad \Longrightarrow \quad
\begin{cases}
u_j^1(t) = \dfrac{A_q}{\sqrt{M_1}} e^{i(qx_j - \omega t)} \\
u_j^2(t) = \dfrac{B_q}{\sqrt{M_2}} e^{i(qx_j - \omega t)}
\end{cases}
$$

We then have

$$
\begin{pmatrix}
\frac{2K}{M_1} & \frac{-K}{\sqrt{M_1 M_2}}(1 + e^{-iqa}) \\
\frac{-K}{\sqrt{M_1 M_2}}(1 + e^{iqa}) & \frac{2K}{M_2}
\end{pmatrix}
\begin{pmatrix} A_q \\ B_q \end{pmatrix}
= \omega^2 \begin{pmatrix} A_q \\ B_q \end{pmatrix}
$$

$$
\Longrightarrow \quad \omega_\pm^2 = \frac{K}{M_1 M_2}\left((M_1 + M_2) \pm \sqrt{M_1^2 + M_2^2 + 2M_1 M_2 \cos qa}\right)
$$


ω
ω_+
$\sqrt{\frac{2K(M_1+M_2)}{M_1 M_2}}$
$\sqrt{\frac{2K}{M_2}}$
ω_-
$\sqrt{\frac{2K}{M_1}}$
$-\frac{\pi}{a}$
0
$\frac{\pi}{a}$
q



- $\boldsymbol{x}_j$: the position of unit cell j
- $\boldsymbol{d}_s$: the equilibrum position of the atom s in the cell
- $\boldsymbol{u}_j^s$: displacement from the equilibrum positon for the atom s in the cell j
- $\boldsymbol{R}_j^s$: the position of the atom s in the cell j

$$
\begin{aligned}
\boldsymbol{R}_j^s(t) &= \boldsymbol{x}_j + \boldsymbol{d}_s + \boldsymbol{u}_j^s(t) \\
&= \boldsymbol{r}_j^s + \boldsymbol{u}_j^s(t) \\
R_{j\alpha}^s(t) &= r_{j\alpha}^s + u_{j\alpha}^s(t) \quad (\alpha = x, y, z)
\end{aligned}
$$

The total energy can be written as

$$
E_{\text{tot}}\left(\{\boldsymbol{R}_j^s(t)\}\right) = E_{\text{tot}}^0\left(\{\boldsymbol{r}_j^s\}\right) + \sum_{js\alpha} \frac{\partial E_{\text{tot}}^0}{\partial u_{j\alpha}^s} u_{j\alpha}^s + \frac{1}{2} \sum_{\substack{js\alpha \\ kt\beta}} \frac{\partial^2 E_{\text{tot}}^0}{\partial u_{j\alpha}^s \partial u_{k\beta}^t} u_{j\alpha}^s u_{k\beta}^t + \ldots
$$

- The expression is exact if we take all the orders in the expansion.
- All the derivatives are taken at the equilibrium positions $\{\boldsymbol{r}_j^s\}$, i.e. $\frac{\partial E_{\text{tot}}^0}{\partial u_{j\alpha}^s} = 0$.
- Harmonic approximation: truncated at *second* order.

Within the harmonic approximation, the Newton's equation for the atom s in cell j

$$M_s \frac{\mathrm{d}^2 u^s_{j\alpha}(t)}{\mathrm{d}t^2} = -\frac{\partial E_{\text{tot}}}{\partial u^s_{j\alpha}} = -\sum_{kt\beta} \frac{\partial^2 E^0_{\text{tot}}}{\partial u^s_{j\alpha} \partial u^t_{k\beta}} u^t_{k\beta} = -\sum_{kt\beta} C_{s\alpha,t\beta}(k-j)\, u^t_{k\beta} \tag{1}$$

The ansatz of the solution

$$u^s_{j\alpha}(t) = \frac{\eta^s_\alpha(\boldsymbol{q})}{\sqrt{M_s}}\, e^{i\boldsymbol{q}\boldsymbol{x}_j}\, e^{-i\omega t} \tag{2}$$

Substitute Eq. 2 into Eq. 1

$$\omega^2(\boldsymbol{q})\, \eta^s_\alpha = \sum_{t\beta} \left[\sum_k \frac{1}{\sqrt{M_s M_t}} \frac{\partial^2 E^0_{\text{tot}}}{\partial \boldsymbol{u}^s_{j\alpha} \partial \boldsymbol{u}^t_{k\beta}}\, e^{i\boldsymbol{q}(\boldsymbol{x}_k - \boldsymbol{x}_j)} \right] \eta^t_\beta = \sum_{t\beta} D_{s\alpha,t\beta}(\boldsymbol{q})\, \eta^t_\beta$$

In matrix form

$$\underbrace{\begin{pmatrix} \ddots & & \\ & D_{s\alpha,t\beta}(\boldsymbol{q}) & \\ & & \ddots \end{pmatrix}}_{3N_a \times 3N_a} \begin{pmatrix} \vdots \\ \eta^t_\beta(\boldsymbol{q}) \\ \vdots \end{pmatrix} = \omega^2(\boldsymbol{q}) \underbrace{\begin{pmatrix} \vdots \\ \eta^t_\beta(\boldsymbol{q}) \\ \vdots \end{pmatrix}}_{3N_a}$$

where N_a is the number of atoms in a cell.

Thank you!