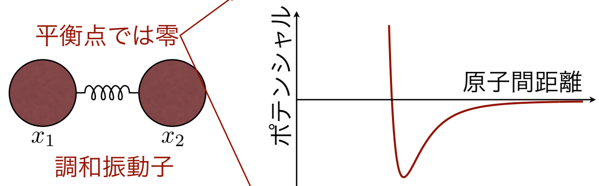
格子振動

一次元最隣接線型バネ模型

結晶中の原子間に働く力

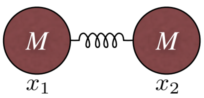
$$V(x_1-x_2)=V^{(0)}+\boxed{V^{(1)}(x_1-x_2)}+\frac{1}{2}V^{(2)}(x_1-x_2)^2+\cdots$$



$$F_1=-\frac{\partial}{\partial x_1}V(x_1-x_2)=-V^{(1)}-V^{(2)}(x_1-x_2)$$

$$F_2=-\frac{\partial}{\partial x_2}V(x_1-x_2)=V^{(1)}-V^{(2)}(x_2-x_1)$$

二原子分子の振動



調和振動子

$$M\frac{d^2}{dt^2}x_1=-K(x_1-x_2)$$

$$M\frac{d^2}{dt^2}x_2=K(x_1-x_2)$$

$$\begin{cases}x_1=x_{10}e^{-i\omega t}\\ x_2=x_{20}e^{-i\omega t}\end{cases}$$

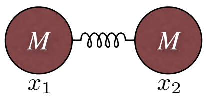
$$-M\omega^2x_{10}e^{-i\omega t}=-K\left(x_{10}e^{-i\omega t}-x_{20}e^{-i\omega t}\right)$$

$$-M\omega^2x_{20}e^{-i\omega t}=K\left(x_{10}e^{-i\omega t}-x_{20}e^{-i\omega t}\right)$$

$$\left(M\omega^2-K\right)x_{10}+Kx_{20}=0$$

$$Kx_{10}+\left(M\omega^2-K\right)x_{20}=0$$

二原子分子の振動



$$\left(M\omega^2-K\right)x_{10}+Kx_{20}=0$$

$$Kx_{10}+\left(M\omega^2-K\right)x_{20}=0$$

$$\begin{bmatrix}M\omega^2-K & K\\ K & M\omega^2-K\end{bmatrix}\begin{bmatrix}x_{10}\\ x_{20}\end{bmatrix}=0$$

$$\begin{vmatrix}M\omega^2-K & K\\ K & M\omega^2-K\end{vmatrix}=0$$

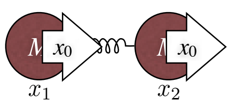
$$\left(M\omega^2-K\right)^2-K^2=M\omega^2\left(M\omega^2-2K\right)=0\Rightarrow\quad\omega=0\quad\omega=\sqrt{\frac{2K}{M}}$$

二原子分子の振動

$$\omega=0$$

$$\begin{bmatrix}-K & K\\ K & -K\end{bmatrix}\begin{bmatrix}x_{10}\\ x_{20}\end{bmatrix}=0$$

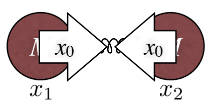
$$\Rightarrow\begin{bmatrix}x_{10}\\ x_{20}\end{bmatrix}=\begin{bmatrix}x_0\\ x_0\end{bmatrix}$$



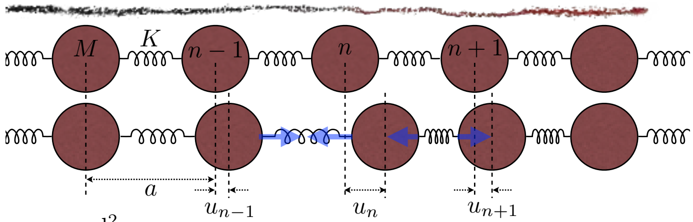
$$\omega=\sqrt{\frac{2K}{M}}$$

$$\begin{bmatrix}K & K\\ K & K\end{bmatrix}\begin{bmatrix}x_{10}\\ x_{20}\end{bmatrix}=0$$

$$\Rightarrow\begin{bmatrix}x_{10}\\ x_{20}\end{bmatrix}=\begin{bmatrix}x_0\\ -x_0\end{bmatrix}$$



格子振動(一次元バネ模型)



$$M\frac{\mathrm{d}^2u_n}{\mathrm{d}t^2}=F_n$$

$$F_n=-Ku_n+Ku_{n-1}-Ku_n+Ku_{n+1}$$

$$M\frac{\mathrm{d}^2}{\mathrm{d}t^2}u_n=K\left(u_{n-1}-u_n\right)-K\left(u_n-u_{n+1}\right)$$

$$M\frac{\mathrm{d}^2u_n}{\mathrm{d}t^2} = K\left(u_{n-1} - 2u_n + u_{n+1}\right)$$

$u_n = u_0\mathrm{e}^{i(kna-\omega t)}$ とおくと

$$-M\omega^2 u_0\mathrm{e}^{i(kna-\omega t)}$$
$$= K\left(u_0\mathrm{e}^{i(k(n-1)a-\omega t)} - 2u_0\mathrm{e}^{i(kna-\omega t)} + u_0\mathrm{e}^{i(k(n+1)a-\omega t)}\right)$$

$$\left(M\omega^2 + K\left(\mathrm{e}^{-ika} - 2 + \mathrm{e}^{ika}\right)\right)u_0\mathrm{e}^{i(kna-\omega t)} = 0$$

$$M\omega^2 - K\left(2 - \mathrm{e}^{ika} - \mathrm{e}^{-ika}\right) = 0$$

$\omega^2 = \frac{4K}{M}\sin^2\frac{ka}{2} \qquad \omega = \omega_c\left|\sin\frac{ka}{2}\right| \qquad$ ただし $\omega_c = 2\sqrt{\frac{K}{M}}$

周期境界条件と波数の範囲

$u_n = u_0 e^{i(kR_n - \omega t)} = u_0 e^{i(kna-\omega t)} \qquad R_n = na$

$u_N = u_0 e^{i(kNa-\omega t)} = u_0 e^{-i\omega t}$ 周期境界条件

$kNa = 2\pi m \Rightarrow k = \frac{2\pi}{a}\frac{m}{N} \qquad m = 0, \pm1, \pm2, \cdots$

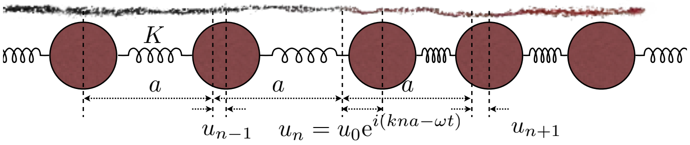
$u_n = u_0 e^{2\pi i \frac{m}{N} n}$

$m \geq N$ のとき $m = qN + m'$ $(0 \leq m' < N)$とおけばよい

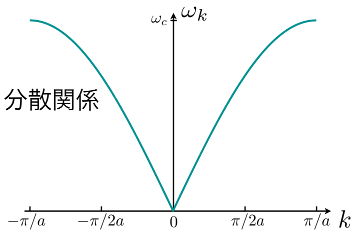
$k = \frac{2\pi}{a}\frac{m}{N}$ $(m = 0, 1, 2, \cdots, N-1)$

$N \to \infty \Rightarrow 0 \leq k < \frac{2\pi}{a}$ または $-\frac{\pi}{a} \leq k < \frac{\pi}{a}$

格子振動(一次元バネ模型)

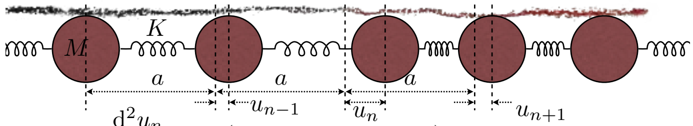


$\omega_k = \omega_c\left|\sin\frac{ka}{2}\right|$

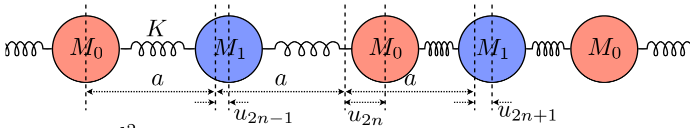


エネルギー $\hbar\omega_k$
運動量 $\hbar k$
の粒子(フォノン)

2 種類の原子を含む格子振動



$$M\frac{\mathrm{d}^2u_n}{\mathrm{d}t^2} = K\left(u_{n-1} - 2u_n + u_{n+1}\right)$$



$$M_0\frac{\mathrm{d}^2}{\mathrm{d}t^2}u_{2n} = K\left(u_{2n-1} - 2u_{2n} + u_{2n+1}\right)$$
$$M_1\frac{\mathrm{d}^2}{\mathrm{d}t^2}u_{2n+1} = K\left(u_{2n} - 2u_{2n+1} + u_{2n+2}\right)$$

$$M_0\frac{\mathrm{d}^2}{\mathrm{d}t^2}u_{2n} = K\left(u_{2n-1} - 2u_{2n} + u_{2n+1}\right)$$
$$M_1\frac{\mathrm{d}^2}{\mathrm{d}t^2}u_{2n+1} = K\left(u_{2n} - 2u_{2n+1} + u_{2n+2}\right)$$

$u_{2n} = u_0\mathrm{e}^{i(k(2n)a-\omega t)}$
$u_{2n+1} = u_1\mathrm{e}^{i(k(2n+1)a-\omega t)}$ とおくと

$$-M_0\omega^2 u_0\mathrm{e}^{i(k(2n)a-\omega t)}$$
$$= K\left(u_1\mathrm{e}^{i(k(2n-1)a-\omega t)} - 2u_0\mathrm{e}^{i(k(2n)a-\omega t)} + u_1\mathrm{e}^{i(k(2n+1)a-\omega t)}\right)$$

$$-M_1\omega^2 u_1\mathrm{e}^{i(k(2n+1)a-\omega t)}$$
$$= K\left(u_0\mathrm{e}^{i(k(2n)a-\omega t)} - 2u_1\mathrm{e}^{i(k(2n+1)a-\omega t)} + u_0\mathrm{e}^{i(k(2n+2)a-\omega t)}\right)$$

$$-M_0\omega^2 u_0 = K\left(u_1\mathrm{e}^{-ika} - 2u_0 + u_1\mathrm{e}^{ika}\right)$$
$$-M_1\omega^2 u_1 = K\left(u_0\mathrm{e}^{-ika} - 2u_1 + u_0\mathrm{e}^{ika}\right)$$

$$-M_0\omega^2 u_0 = K\left(u_1\mathrm{e}^{-ika} - 2u_0 + u_1\mathrm{e}^{ika}\right)$$
$$-M_1\omega^2 u_1 = K\left(u_0\mathrm{e}^{-ika} - 2u_1 + u_0\mathrm{e}^{ika}\right)$$

$$\left(M_0\omega^2 - 2K\right)u_0 + \left(2K\cos ka\right)u_1 = 0$$
$$\left(2K\cos ka\right)u_0 + \left(M_1\omega^2 - 2K\right)u_1 = 0$$

$$\begin{pmatrix} M_0\omega^2 - 2K & 2K\cos ka \\ 2K\cos ka & M_1\omega^2 - 2K \end{pmatrix}\begin{pmatrix} u_0 \\ u_1 \end{pmatrix} = 0$$

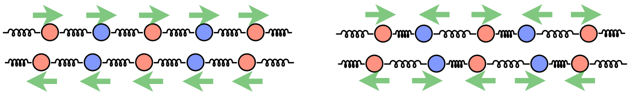
$$\begin{vmatrix} M_0\omega^2 - 2K & 2K\cos ka \\ 2K\cos ka & M_1\omega^2 - 2K \end{vmatrix} = 0 \Rightarrow \omega = \omega_k^{(+)}, \omega_k^{(-)}$$

$$\omega_k^{(\pm)} = \sqrt{\frac{K\left(M_0 + M_1\right) \pm K\sqrt{\left(M_0 - M_1\right)^2 + 4M_0M_1\cos^2 ka}}{M_0M_1}}$$

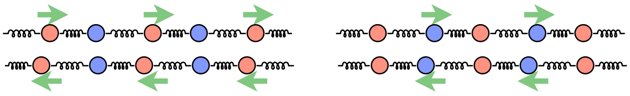
$$\begin{pmatrix} M_0\omega^2-2K & 2K\cos ka \\ 2K\cos ka & M_1\omega^2-2K \end{pmatrix}\begin{pmatrix} u_0 \\ u_1 \end{pmatrix}=0$$

$$\begin{vmatrix} M_0\omega^2-2K & 2K\cos ka \\ 2K\cos ka & M_1\omega^2-2K \end{vmatrix}=0$$

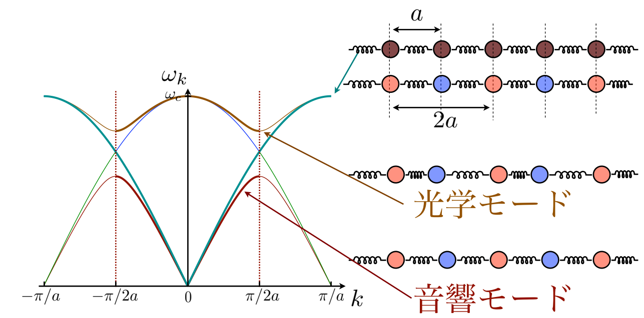
$$k=0,\ \frac{\pi}{a}\quad \Rightarrow \omega=0,\ \sqrt{2K\left(\frac{1}{M_0}+\frac{1}{M_1}\right)}$$



$$k=\frac{\pi}{2a}\quad \Rightarrow \omega=\sqrt{\frac{2K}{M_0}},\ \sqrt{\frac{2K}{M_1}}$$



フォノンの分散関係

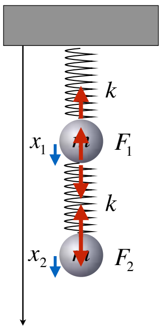


電子物性の基礎提出課題

図のように質量 m の球が二つ同じバネ定数 k のバネでつながっているときの球の振動の振動数を求めよ。
ただし、二つの球のそれぞれの平衡点からはかった変位をそれぞれ x_1, x_2 とせよ

$$F_1=-kx_1-kx_1+kx_2=m\frac{d^2}{dt^2}x_1$$

$$F_2=kx_1-kx_2=m\frac{d^2}{dt^2}x_2$$



$$m\frac{d^2}{dt^2}x_1=-2kx_1+kx_2$$

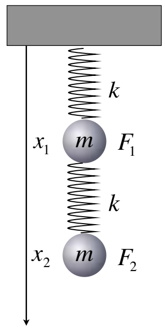
$$m\frac{d^2}{dt^2}x_2=kx_1-kx_2$$

$$\begin{cases} x_1(t)=x_{10}e^{-i\omega t} \\ x_2(t)=x_{20}e^{-i\omega t} \end{cases}$$

$$m\frac{d^2}{dt^2}x_1=-m\omega^2x_{10}e^{-i\omega t}$$

$$m\frac{d^2}{dt^2}x_2=-m\omega^2x_{20}e^{-i\omega t}$$

$$\begin{cases} -m\omega^2x_{10}e^{-i\omega t}=-2kx_{10}e^{-i\omega t}+kx_{20}e^{-i\omega t} \\ -m\omega^2x_{20}e^{-i\omega t}=kx_{10}e^{-i\omega t}-kx_{20}e^{-i\omega t} \end{cases}$$



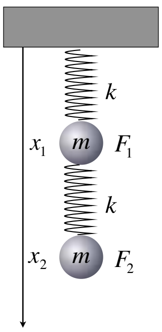
$$\begin{cases} -m\omega^2x_{10}e^{-i\omega t}=-2kx_{10}e^{-i\omega t}+kx_{20}e^{-i\omega t} \\ -m\omega^2x_{20}e^{-i\omega t}=kx_{10}e^{-i\omega t}-kx_{20}e^{-i\omega t} \end{cases}$$

$$\omega_0^{\ 2}=\frac{k}{m}$$

$$\begin{cases} 2\omega_0^{\ 2}x_{10}-\omega_0^{\ 2}x_{20}=\omega^2x_{10} \\ -\omega_0^{\ 2}x_{10}+\omega_0^{\ 2}x_{20}=\omega^2x_{20} \end{cases}$$

$$\begin{bmatrix} 2\omega_0^{\ 2}-\omega^2 & -\omega_0^{\ 2} \\ -\omega_0^{\ 2} & \omega_0^{\ 2}-\omega^2 \end{bmatrix}\begin{bmatrix} x_{10} \\ x_{20} \end{bmatrix}=0$$

$$\begin{vmatrix} 2\omega_0^{\ 2}-\omega^2 & -\omega_0^{\ 2} \\ -\omega_0^{\ 2} & \omega_0^{\ 2}-\omega^2 \end{vmatrix}=0$$



$$\begin{vmatrix} 2\omega_0^{\ 2}-\omega^2 & -\omega_0^{\ 2} \\ -\omega_0^{\ 2} & \omega_0^{\ 2}-\omega^2 \end{vmatrix}=0$$

$$\left(2\omega_0^{\ 2}-\omega^2\right)\left(\omega_0^{\ 2}-\omega^2\right)-\omega_0^{\ 4}=0$$

$$\omega^4-3\omega_0^{\ 2}\omega^2+\omega_0^{\ 4}=0$$

$$\omega^2=\frac{3\pm\sqrt{5}}{2}\omega_0^{\ 2}$$

$$=\frac{6\pm2\sqrt{5}}{4}\omega_0^{\ 2}=\frac{\left(\sqrt{5}\pm1\right)^2}{2^2}\omega_0^{\ 2}$$

$$\omega=\frac{\sqrt{5}\pm1}{2}\omega_0$$