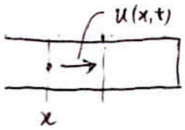
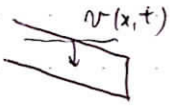
1. 格子振動とフォノン

1.1 固体の弾性



← 断面積A



訂正

応力 $\cancel{C_{12}}\ C_{44} \dfrac{\partial v}{\partial x}$

$$f(x,t) = C_{11} \frac{\partial u}{\partial x}(x,t)$$

(応力-ひずみ関係, フックの法則)

訂正

$C_{11} > \cancel{C_{12}}\ C_{44}$

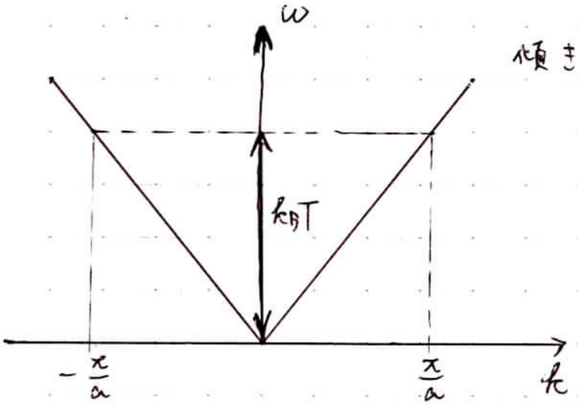
$$\rho \Delta x A \frac{\partial^2 u}{\partial t^2} = A\{f(x+\Delta x, t) - f(x,t)\} = C_{11} A \frac{\partial^2 u}{\partial x^2} \Delta x$$

$$\rho \frac{\partial^2 u}{\partial t^2} = C_{11} \frac{\partial^2 u}{\partial x^2}$$

$u \propto e^{i(kx - \omega t)}$ とすると,

$$\omega = \underbrace{\sqrt{\frac{C_{11}}{\rho}}}_{\text{音速}} |k| \qquad v = \frac{d\omega}{dk}$$

	C_{11} (GPa)	ρ (kg/m^3)	v (m·s^{-1})
Pb	50	11×10^3 (11 g/cm^3)	2.1×10^3
Cu	170	9×10^3 (9 g/cm^3)	4.3×10^3



傾き $v = 4 \times 10^3$ m/sec

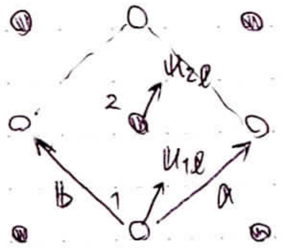
$T = 300$ K

$\to k_B T \sim 4 \times 10^{21}$ J

$\to \omega \sim 4 \times 10^{13}\ \mathrm{s}^{-1}$

$\to k = \dfrac{\omega}{v} \sim 10^{10}\ \mathrm{m}^{-1} \sim (1\text{Å})^{-1}$

1.2 結晶格子の動力学



$\mathbf{l} = l_a \mathbb{a} + l_b \mathbb{b}$; 並進ベクトル

$$K.E. = \frac{1}{2} \sum_{l,s} M_s |\dot{\mathbf{u}}_{sl}|^2$$, s : 原子数の index

$$V(\{\mathbf{u}_{sl}\})$$

$$= V_0 + \underbrace{\sum_{s l i} \frac{\partial V}{\partial u^i_{sl}} u^i_{sl}}_{=0} + \frac{1}{2} \sum_{\substack{s l i j \\ s' l'}} \frac{\partial^2 V}{\partial u^i_{sl} \partial u^j_{s'l'}} u^i_{sl} u^j_{s'l'} + \cdots$$

∵) ポテンシャル極少

$$M_s \ddot{u}^i_{sl} = - \sum_{s'l'} \frac{\partial^2 V}{\partial u^i_{sl} \partial u^j_{s'l'}} u^j_{s'l'}$$

$$= - \sum_{s'l'} G^{ij}_{sls'l'} u^j_{s'l'}$$

$$M_s \ddot{\mathbf{u}}_{sl} = - \sum_{s'l'} \mathbb{G}_{sls'l'} \cdot \mathbf{u}_{s'l'}$$

相対距離 $\mathbf{l}' - \mathbf{l} = \mathbf{h}$ のみに依存

$$M_s \ddot{\mathbf{u}}_{sl} = - \sum_{s'\mathbf{h}} \mathbb{G}_{ss'\mathbf{h}} \cdot \mathbf{u}_{s'\,l+\mathbf{h}}$$

$$u_{sl}(t) = U_{sq}\, e^{i(q\cdot l - \omega t)}$$ とすると、

$$-\omega^2 M_s U_{sq} = -\sum_{s'h} G_{ss'h}\, e^{iq\cdot h}\, U_{s'q}$$

$$= -\sum_{s'} G_{ss'}(q)\, U_{s'q}$$

$$\sum_{s'j'} \left[G_{ss'}(q)^{jj'} - \omega^2 M_s \delta_{ss'} \delta_{jj'} \right] U^{j}_{s'q} = 0 \quad , j = x, y, z$$

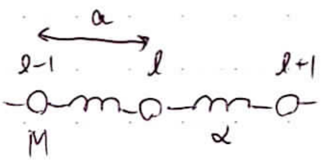
$$\det[\quad] = 0 \longrightarrow \omega_q \text{ 決まる}$$

$\underbrace{3}_{\text{空間の次元}}\underbrace{S}_{\text{原子数}}$ 個の固有モード

1.3 一次元単原子格子

$$V = \frac{1}{2} \Sigma_l \underset{\uparrow}{\alpha} (u_l - u_{l+a})^2$$

バネ定数



$$M \ddot{u}_l = -\alpha \{ (u_l - u_{l+a}) - (u_{l-a} - u_l) \}$$

$$= -\alpha (2u_l - u_{l+a} - u_{l-a})$$

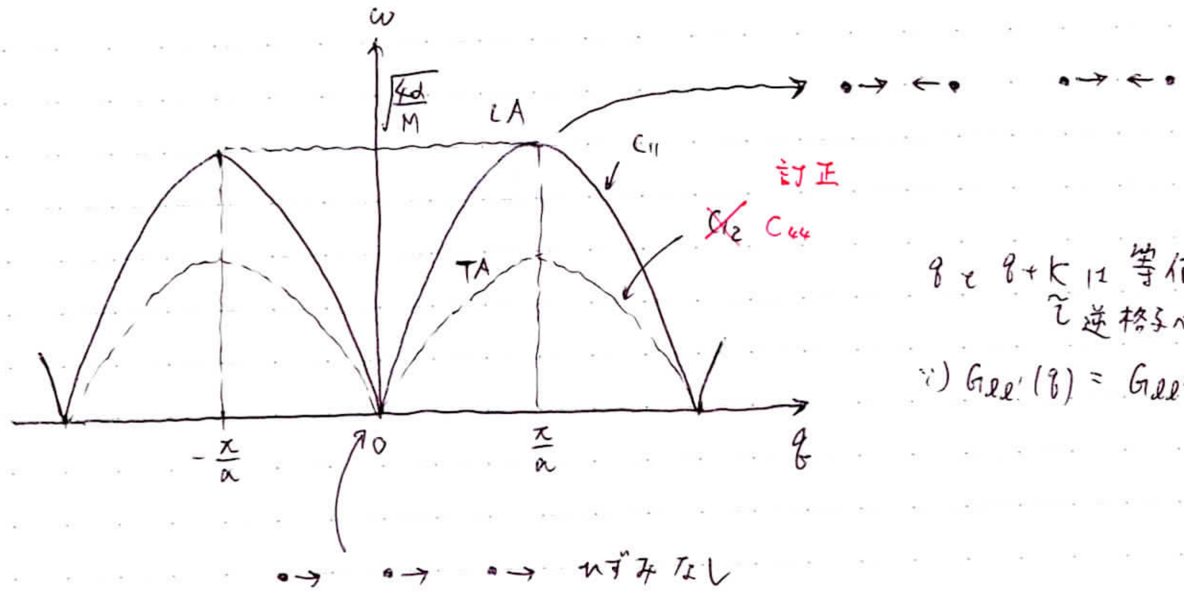
$$\frac{\partial^2 V}{\partial u_l^2} \qquad \frac{\partial^2 V}{\partial u_l \partial u_{l+a}} \qquad \frac{\partial^2 V}{\partial u_l \partial u_{l-a}}$$

$u_l = U_q e^{i(ql - \omega t)}$ とすると、

$$-M\omega^2 U_q = -\alpha (2 - e^{iqa} - e^{-iqa}) U_q$$

$$= \underbrace{-2\alpha (1 - \cos qa)}_{G(q)} U_q$$

$$\omega = \sqrt{\frac{4\alpha}{M}} \left| \sin \frac{qa}{2} \right|$$



q と $q+K$ は 等価
$\tilde{}$ 逆格子ベクトル

$\because$) $G_{ll'}(q) = G_{ll'}(q+K)$

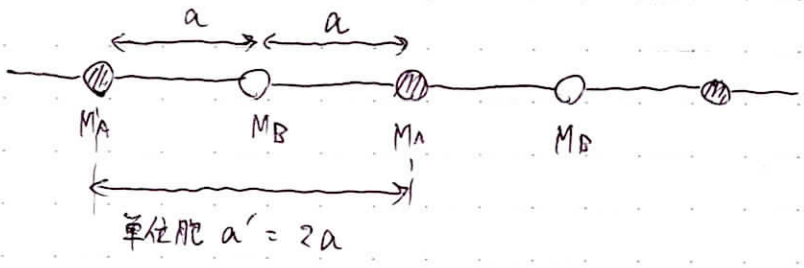
$q \to 0$

$$\omega = \sqrt{\frac{4\alpha}{M}}\,\frac{qa}{2} = \sqrt{\frac{\alpha a^2}{M}}\,q$$

$$v = \sqrt{\frac{\alpha a^2}{M}} = \sqrt{\frac{\alpha a}{M/a}} = \sqrt{\frac{C_{11}}{\rho}}$$

$$C_{11} = \alpha a$$
$$\rho = M/a$$

1.4 一次元二原子格子



$$-\omega^2 M_A \bar{U}_{Aq} = -\alpha\left(2\bar{U}_{Aq} - 2\cos qa\, \bar{U}_{Bq}\right)$$
$$-\omega^2 M_B \bar{U}_{Bq} = -\alpha\left(-2\cos qa\, \bar{U}_{Aq} + 2\bar{U}_{Bq}\right)$$

$$\begin{pmatrix} -2\alpha + M_A\omega^2 & 2\alpha\cos qa \\ 2\alpha\cos qa & -2\alpha + M_B\omega^2 \end{pmatrix}\begin{pmatrix} \bar{U}_{Aq} \\ \bar{U}_{Bq} \end{pmatrix} = 0$$

$G_{ss'}(q)$

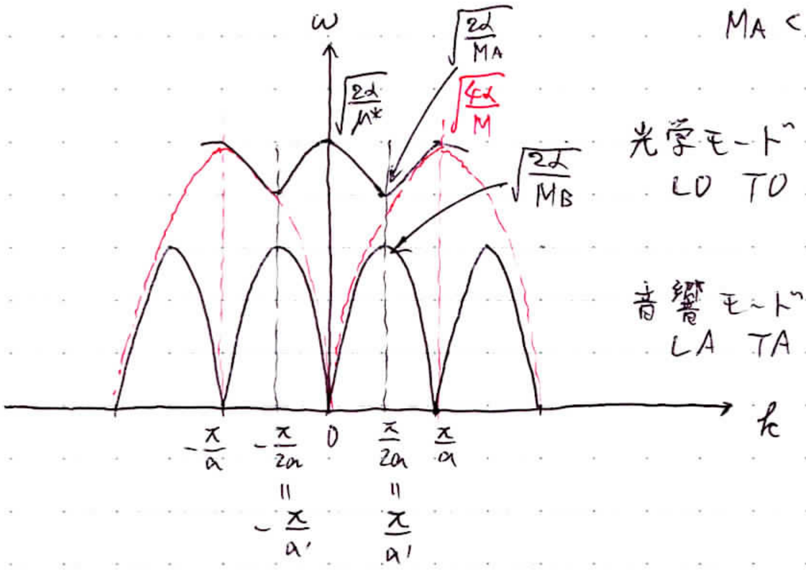
$$\det = (M_A\omega^2 - 2\alpha)(M_B\omega^2 - 2\alpha) - 4\alpha^2\cos^2 qa = 0$$
$$M_A M_B \omega^4 - 2\alpha(M_A + M_B)\omega^2 + 4\alpha^2 \sin^2 qa = 0$$

$$\frac{1}{\mu^*} = \frac{1}{M_A} + \frac{1}{M_B}$$

$$\omega^4 - \frac{2\alpha}{\mu^*}\omega^2 + \frac{4\alpha^2}{M_A M_B}\sin^2 qa = 0$$

$$\omega^2 = \frac{\alpha}{\mu^*} \pm \sqrt{\left(\frac{\alpha}{\mu^*}\right)^2 - \frac{4\alpha^2}{M_A M_B}\sin^2 qa}$$

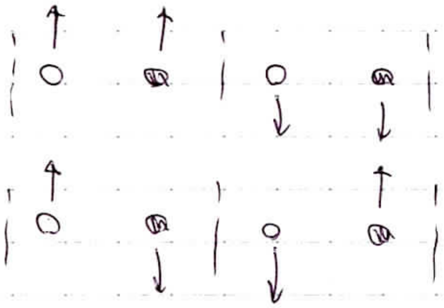
$M_A < M_B$



$M_A = M_B = M$

$\sqrt{\frac{2\alpha}{M^*}} = \sqrt{\frac{4\alpha}{M}}$

$k = \frac{\pi}{2a}$

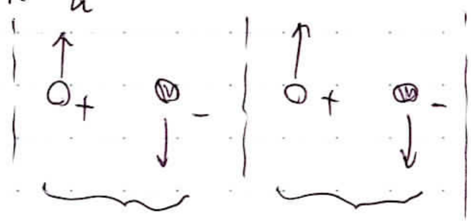


反位相

同じ

$k = 0$

$k = \frac{\pi}{a}$



分子内モード

$k=0$と等価

分極して光学活性になり得る

→ 光学モード