On the Energy Level Crossing

(On the Conical Point Crossing)

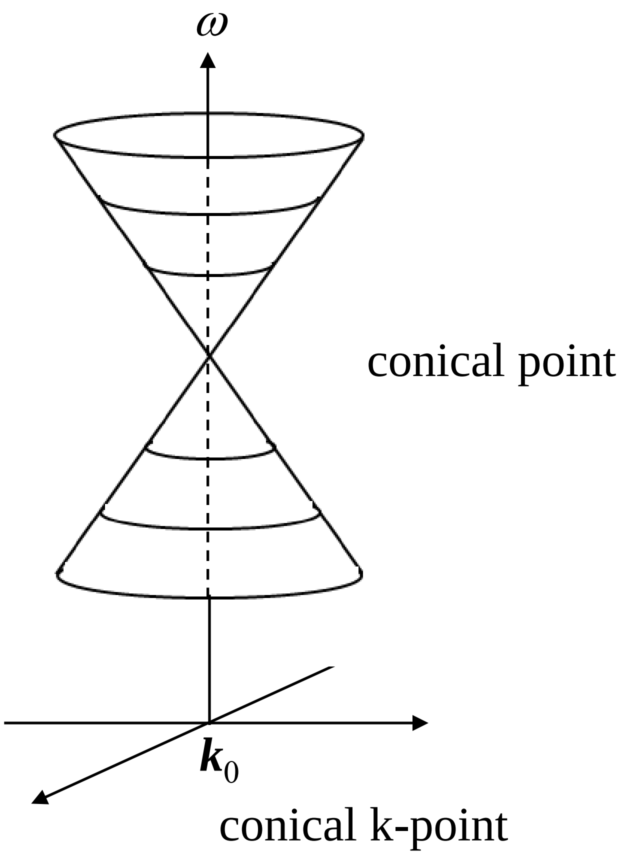
Y. Ishibashi, *Nagoya University*, yishi@kyudai.jp

M. Iwata, *Nagoya Insitute of Technology*, miwata@nitech.ac.jp

Y. Ishibashi and V. Dvorak: J. Phys. Soc. Jpn. **45** (1978) 1119.

Y. Ishibashi and M. Iwata: J. Phys. Soc. Jpn. 84 (2015) 67016.

The Conical Point Crossing--- a special form of energy level crossing



Y. Ishibashi and V. Dvorak: J. Phys. Soc. Jpn. **45** (1978) 1119.

Why now ?

(1) Graphene (hexagonal)

Dirac point------conical point

(2) Lu_2FeO_4 (rhombohedral)

electronic ferroelectrics

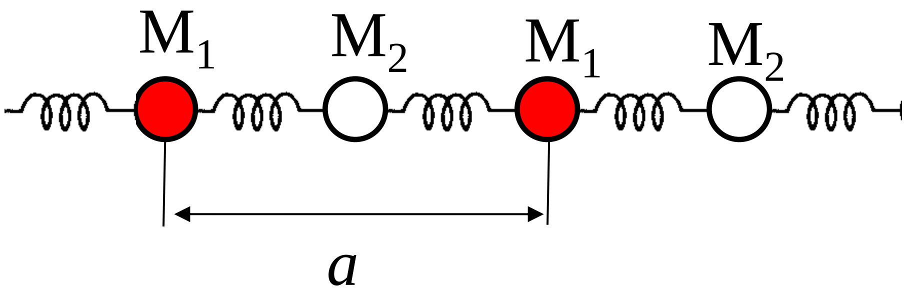
S. Ishihara: J. Phys. Soc. Jpn. **79**, 011010 (2010).

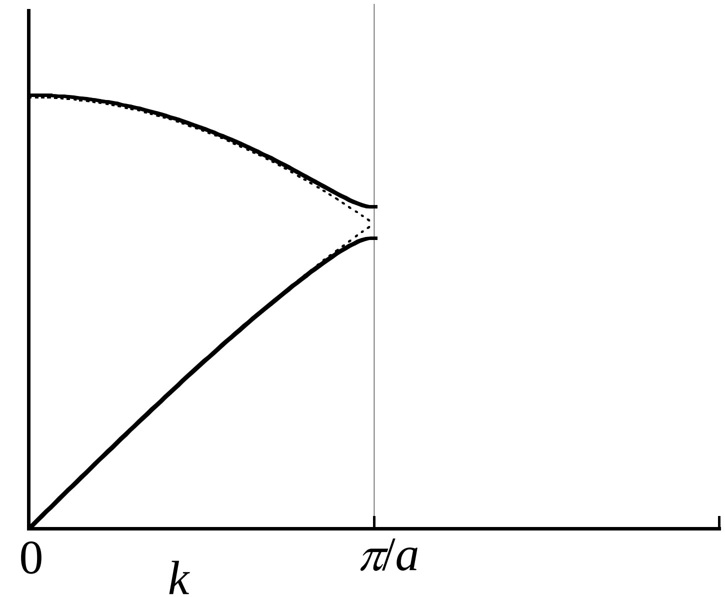
M. Iwata and Y. I.: JPSJ **81**, 114703 (2012).

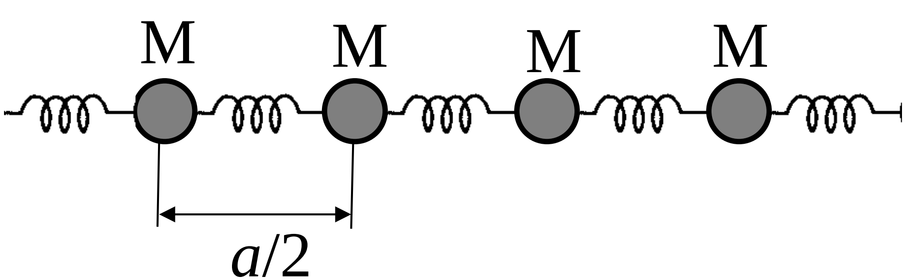
I. Simple level crossing

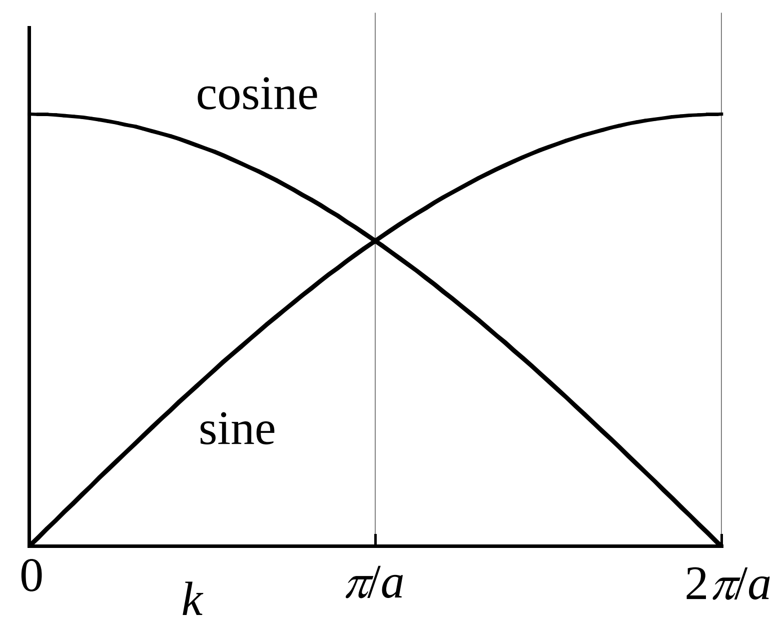
釈迦に説法

I. The level crossing









分散関係

a : 格子定数

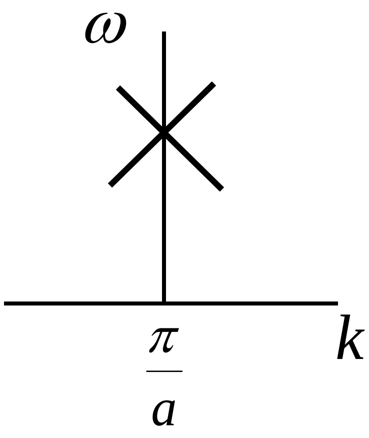
$$\omega^2 = \frac{K}{\mu} \pm K\sqrt{\frac{1}{\mu^2} - \frac{4}{M_1 M_2}\sin^2\frac{ka}{2}}$$

$$\frac{1}{\mu} = \frac{1}{M_1} + \frac{1}{M_2}$$ ： 換算質量

$$= \frac{K}{\mu} \pm K\sqrt{\left(\frac{1}{M_1} - \frac{1}{M_2}\right)^2 + \frac{4}{M_1 M_2}\cos^2\frac{ka}{2}}$$

$M_1 = M_2 = M$　とすると

$$\omega^2 = \frac{2K}{M}\left(1 \pm \cos\frac{ka}{2}\right)$$



原子の変位

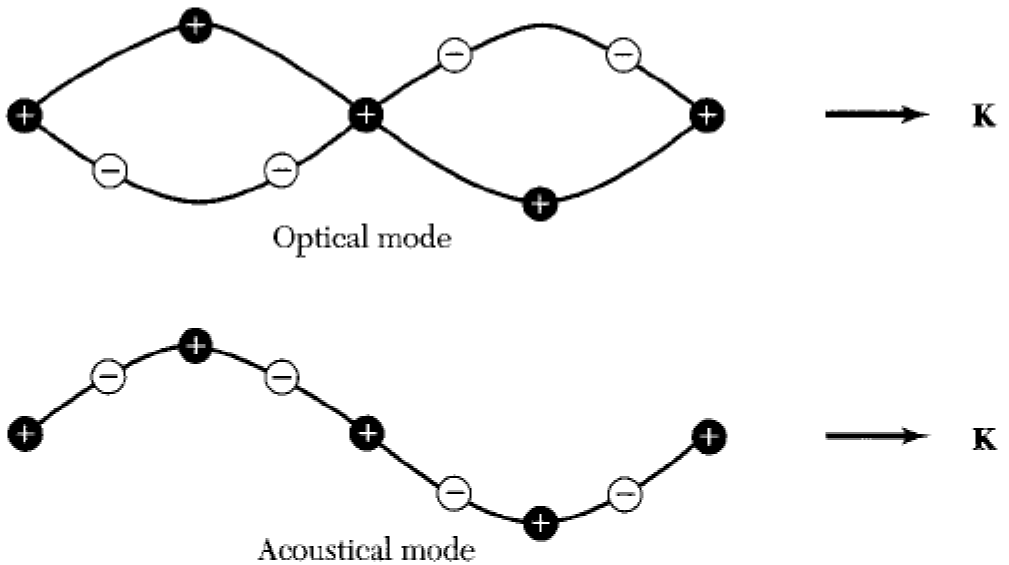
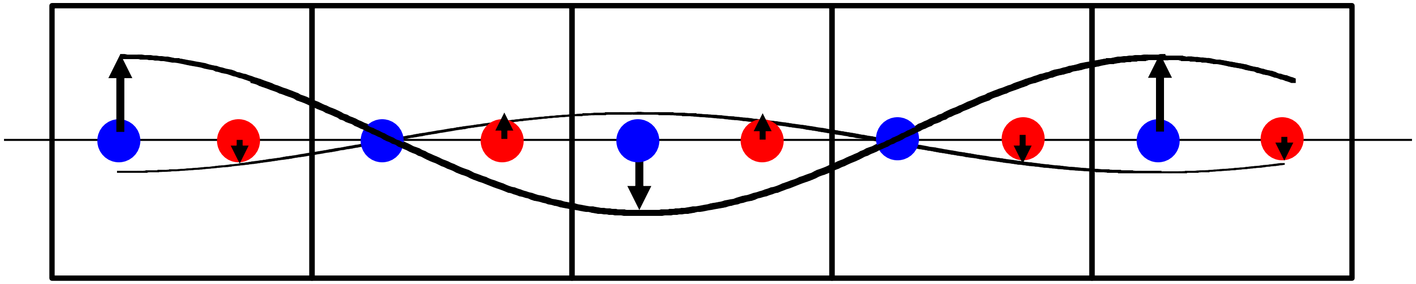


Figure 10 Transverse optical and transverse acoustical waves in a diatomic linear lattice, illustrated by the particle displacements for the two modes at the same wavelength.

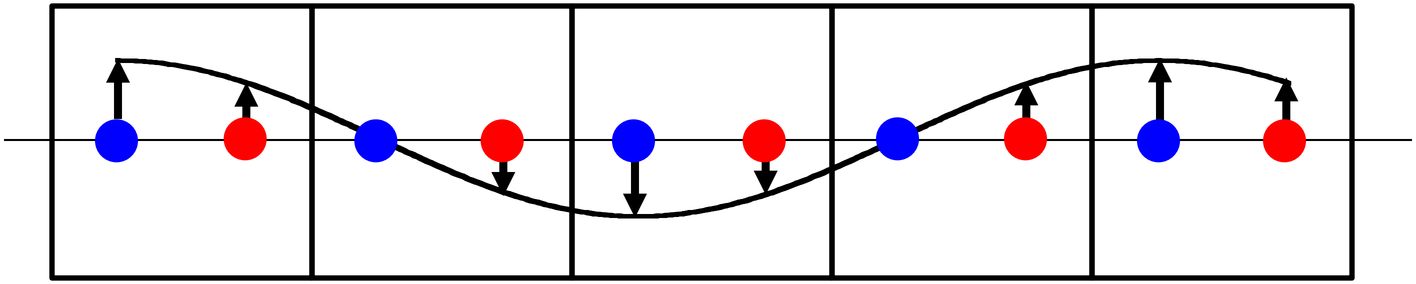
C. Kittel: 8th Ed. Introduction to Solid State Physics, John Wiley & Sons, Inc (2005).

半格子移動した図を考えると、$M_1=M_2$（特別の場合）であることがわかる

原子の変位



光学的モード



音響的モード

The Lifshitz invariant

$$p\frac{\mathrm{d}q}{\mathrm{d}x}-q\frac{\mathrm{d}p}{\mathrm{d}x}$$

The Lifshitz condition

The second order transition is prohibited,

when the Lifshitz invariant can be formed. (YI)

when the anti-symmetrized square contains the irreducible representation, to which the vector components belong. (LL)

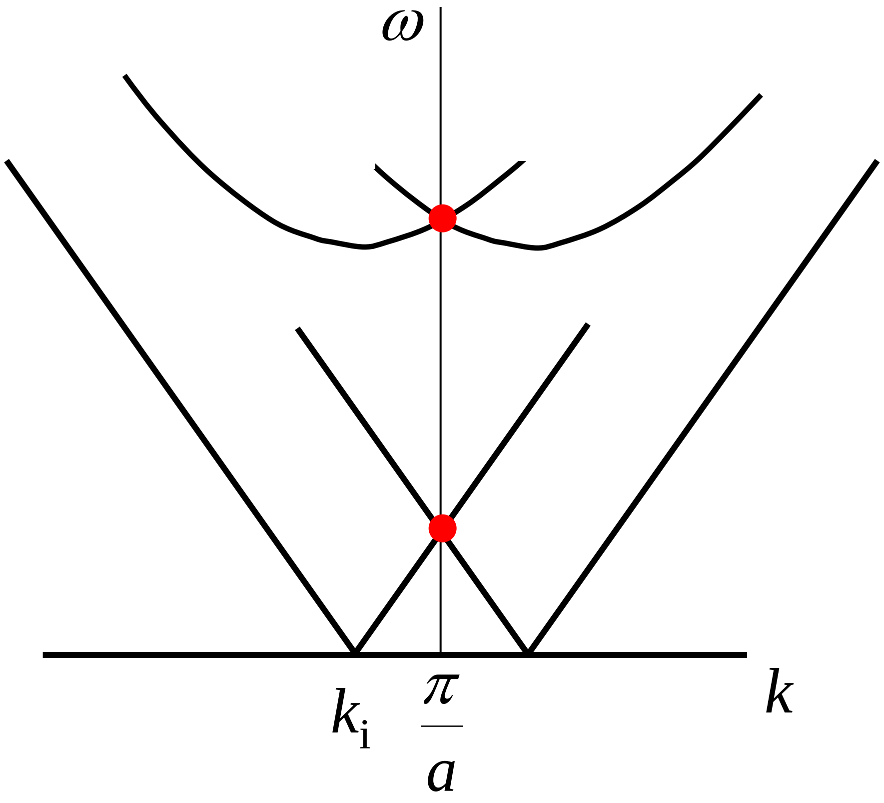
(underlined part) = the vector representation

Anti-symmetrized square

$$(p_1, q_1), (p_2, q_2)$$

$$p_1 q_2 - p_2 q_1$$

分散関係



r: the order parameter

$$p = r \cos kx, \quad q = r \sin kx$$

The Lifshitz (invariant) term = $2\, r^2 k\, \delta$

$$f = [a\,(T - T_0) + 2\,k\,\delta + \kappa\, k^2]\, r^2 + \ldots\ldots\ldots$$

[…..] を最初に 0 にする k と 温度

$$k_{\mathrm{inc}} = - \delta / \kappa$$

$$a\,(T_{\mathrm{inc}} - T_0) = \delta^2 / \kappa > 0$$

The Lifshitz invariant

(Rotation), Screw of the order parameters

Existence of the Lishitz invarinat in the space group

2_1, a, b, c, n

Existence of the Lifshitz invariant in the point group

$C_4(E)$, $D_4(E)$, $C_3(E)$, $D_3(E)$, $C_6(E_1)$, $C_6(E_2)$,

$D_6(E_1)$, $D_6(E_2)$, $T(F)$, $O(F_1)$, $O(F_2)$

Optical activity

II. The hexagonal lattice

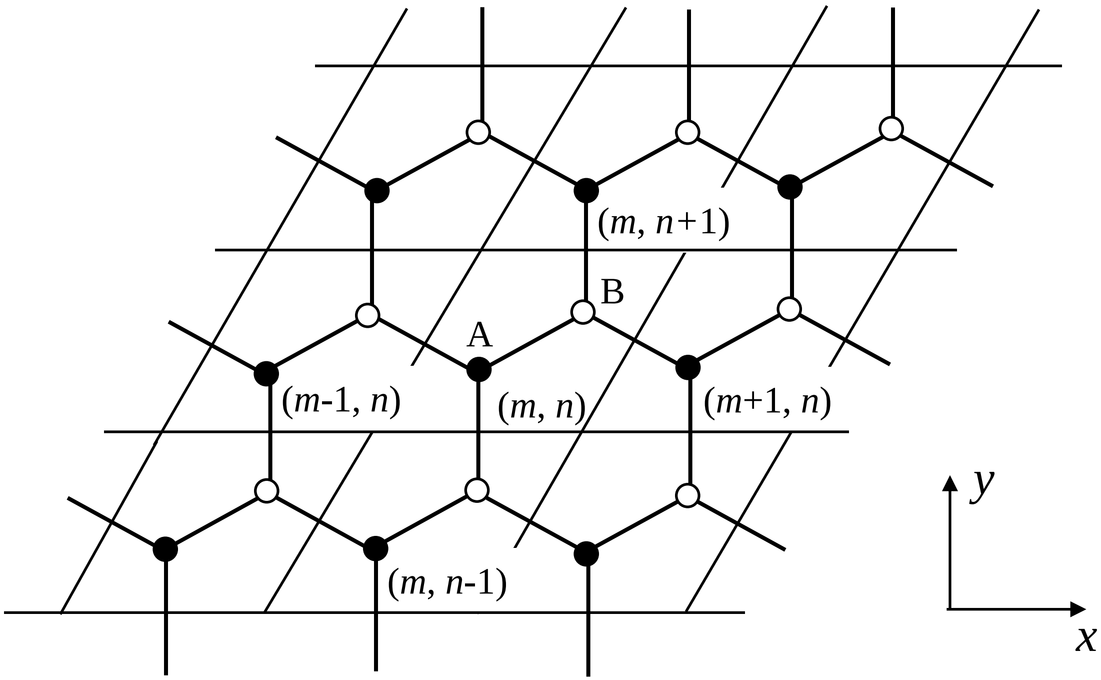


Fig. 2 M. Iwata and Y. Ishibshi

The displacement of A and B atoms in the (m, n) cell
(perpendicular to the plane)

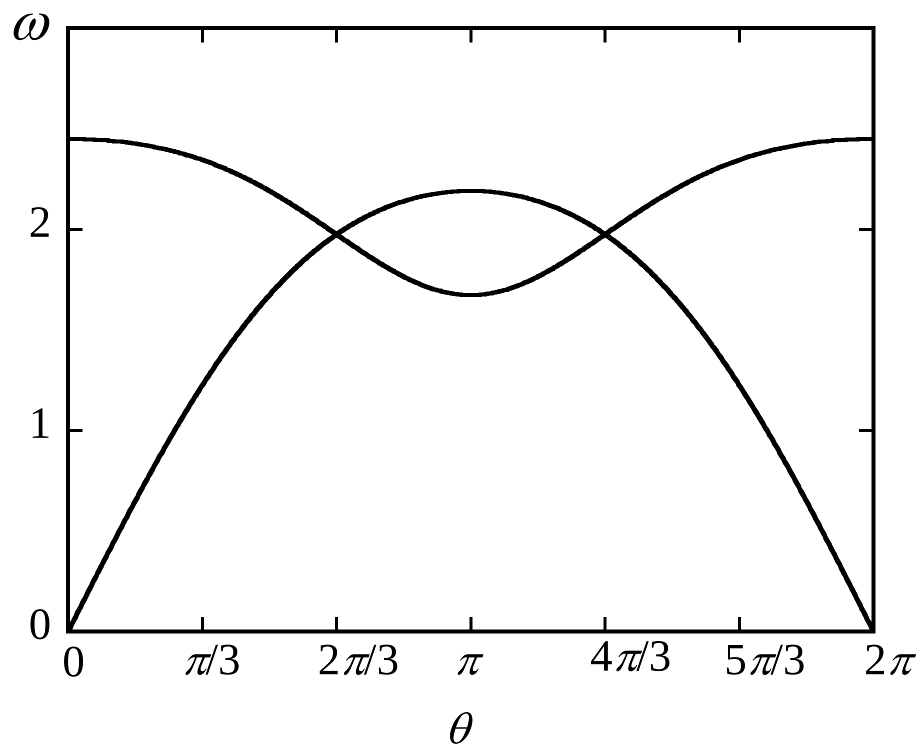
$$u_A(m, n) = p \exp[\, i(m\theta + n\chi)]$$
$$u_B(m, n) = q \exp[\, i(m\theta + n\chi)]$$

The dispersion relation

$$\omega^2 = \frac{1}{M}\left\{K\left(3 \pm \sqrt{3 + 2A}\right) + 2L(3 - A)\right\}$$

$$A = \cos\theta + \cos\chi + \cos(\theta - \chi).$$

Displacement perpendicular to the plane



L = 0

$\theta = 2\chi$

Symmetric at $\theta = \pi$ and locally symmetric at $\theta = 2\pi/3$.

Two zone boundaries

Fig. 3 Y. Ishibshi and M. Iwata

(a)

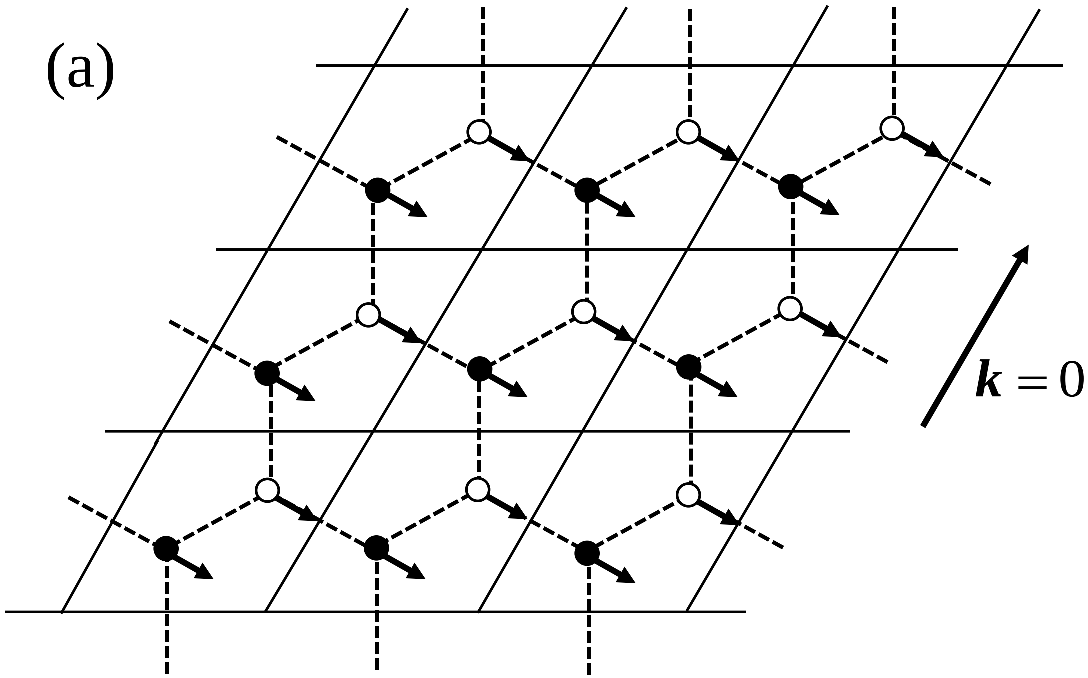


Fig. 5(a) M. Iwata and Y. Ishibshi

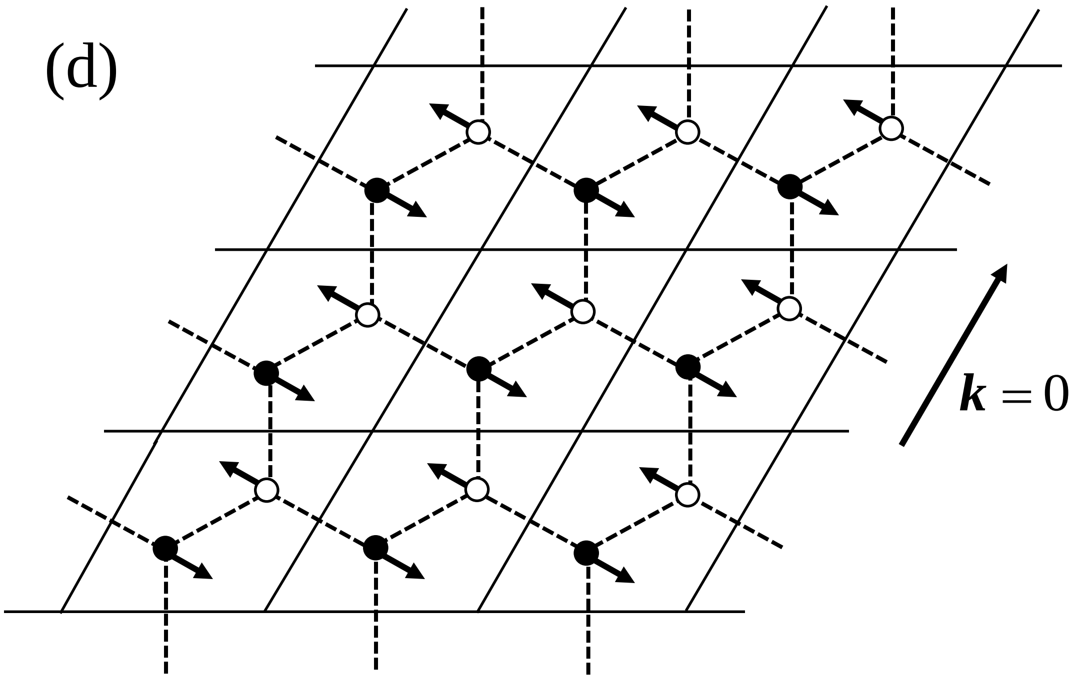


Fig. 5(d)   M. Iwata and Y. Ishibshi

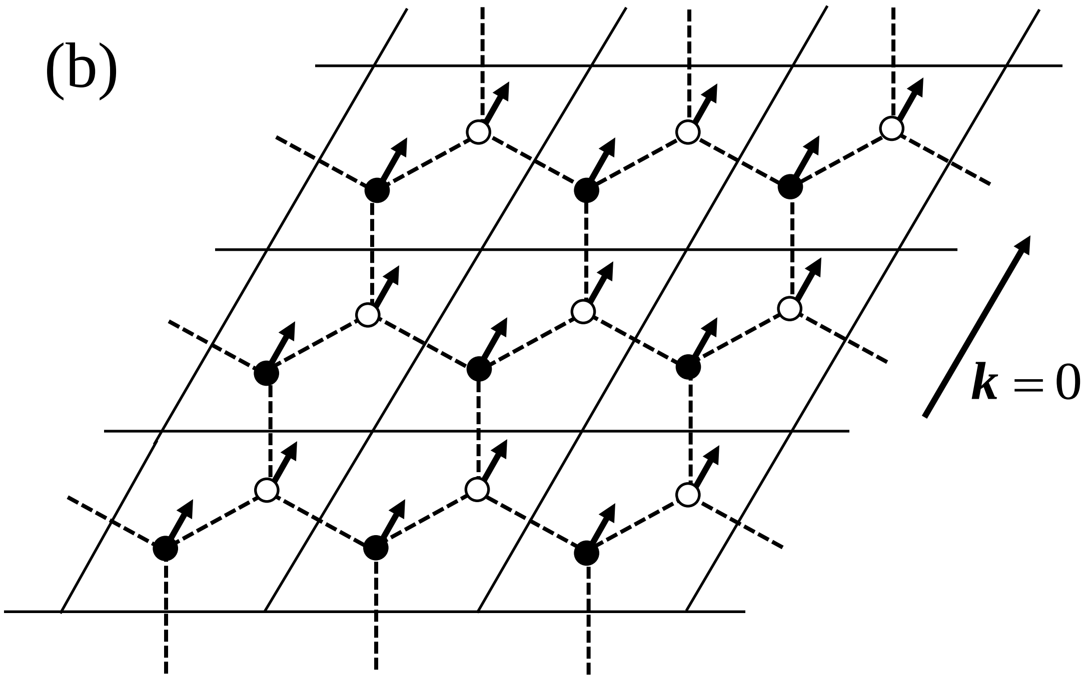


Fig. 5(b) M. Iwata and Y. Ishibshi

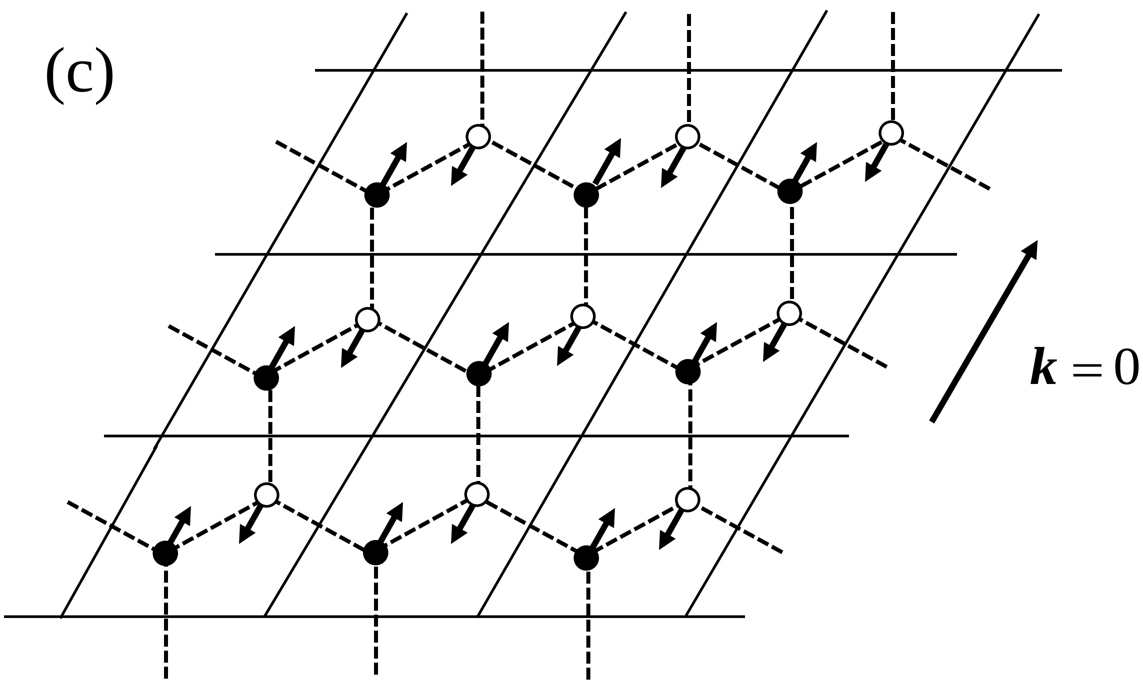
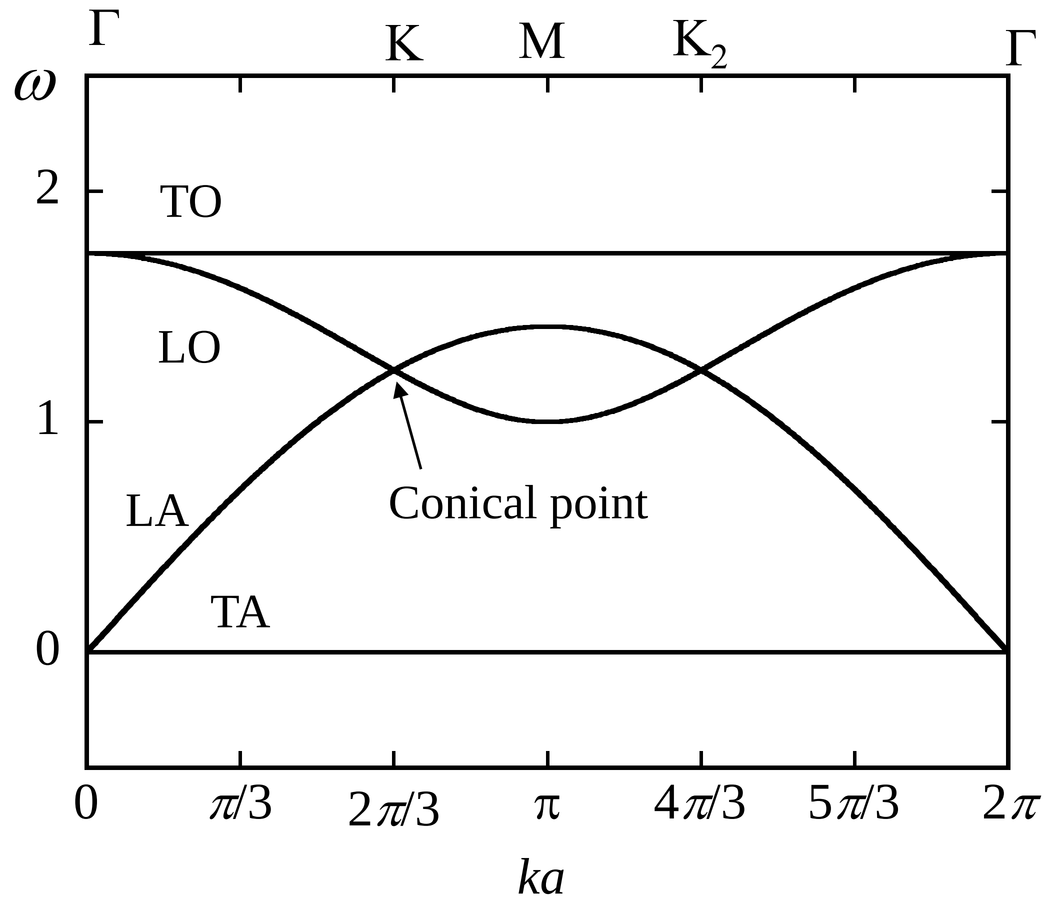


Fig. 5(c) M. Iwata and Y. Ishibshi

Displacement in the plane

$K_1 \equiv K_3 \quad K_2 \equiv K_4$



Only with the nearest neighbor interaction

２次元交差

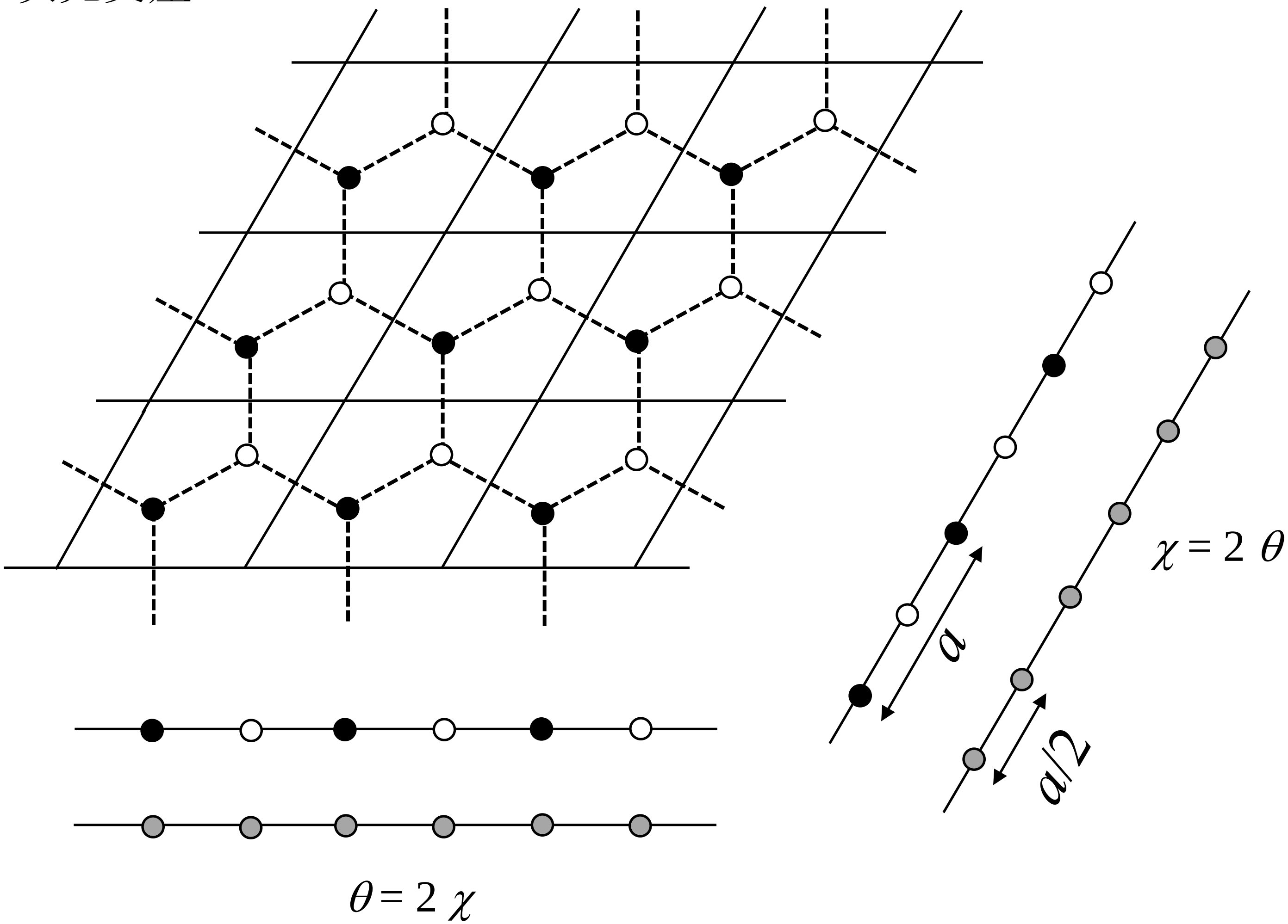


Fig. 5　Y. Ishibshi and M. Iwata

(a)

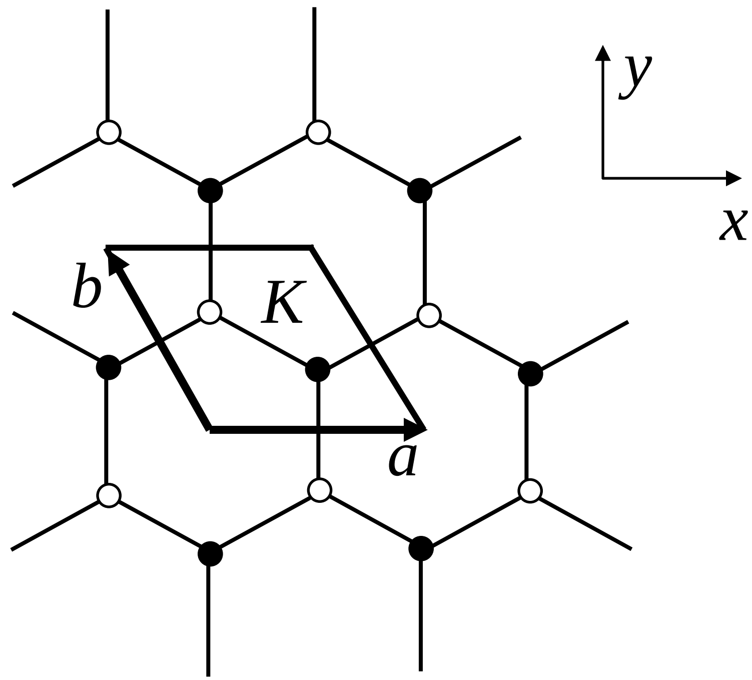


Fig. 1 (a)   Y. Ishibshi and M. Iwata

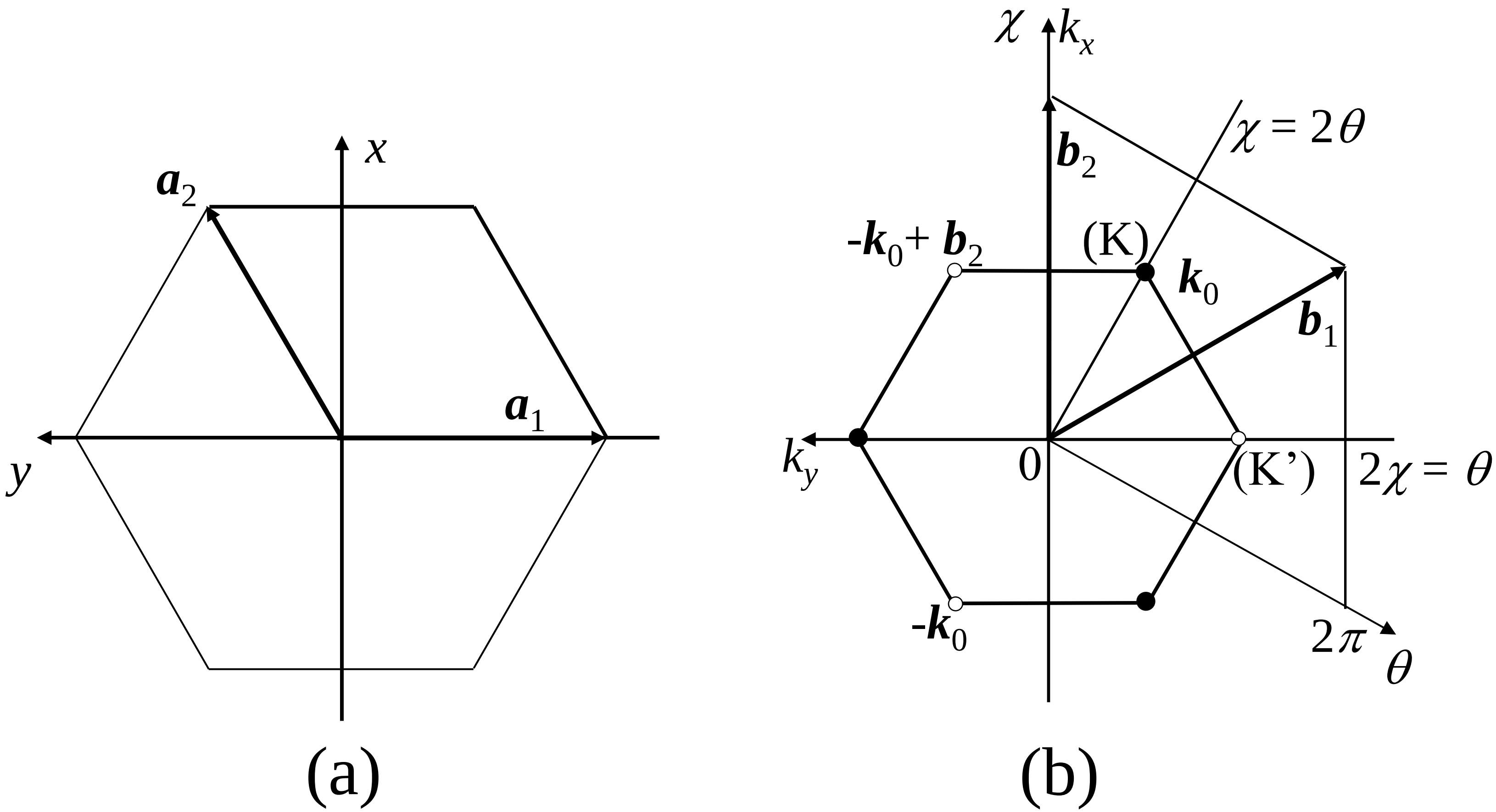


Fig. 4 Y. Ishibshi and M. Iwata

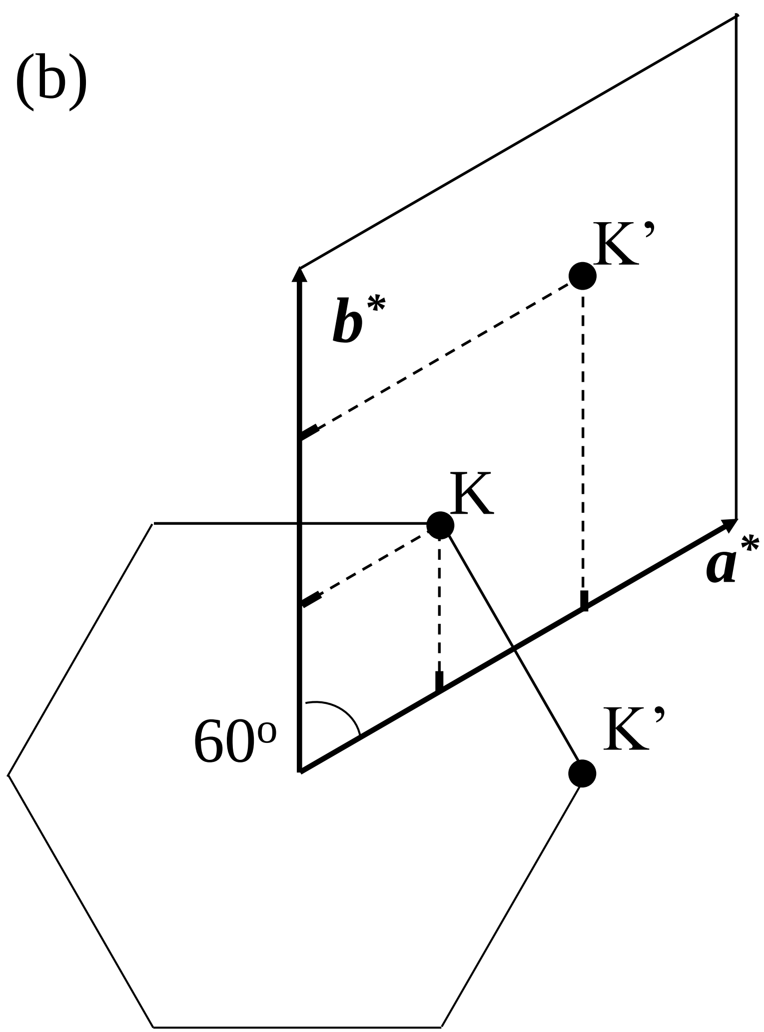


Fig. 1 (b) Y. Ishibshi and M. Iwata

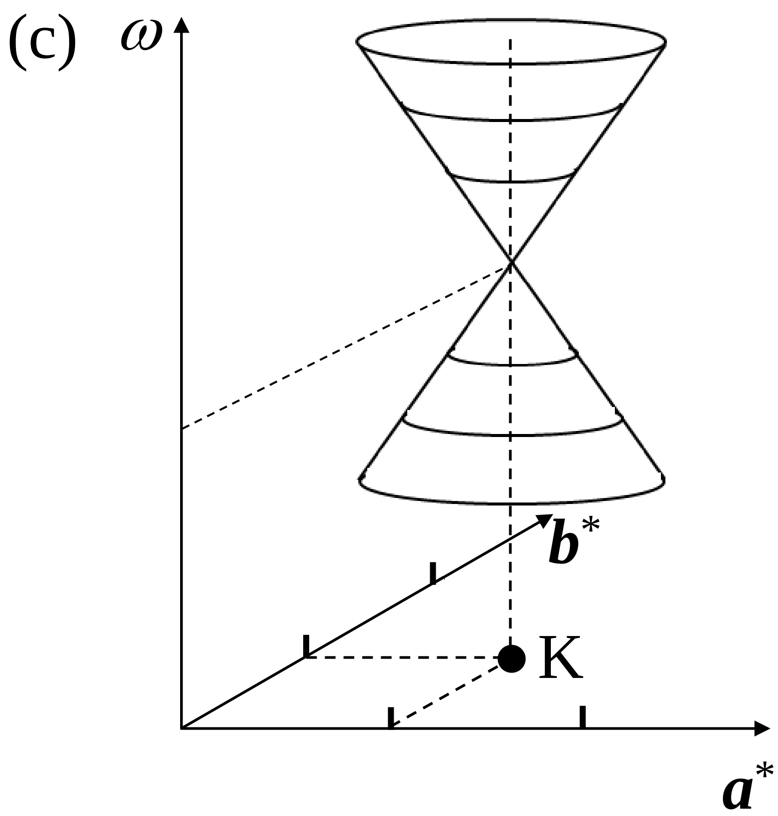
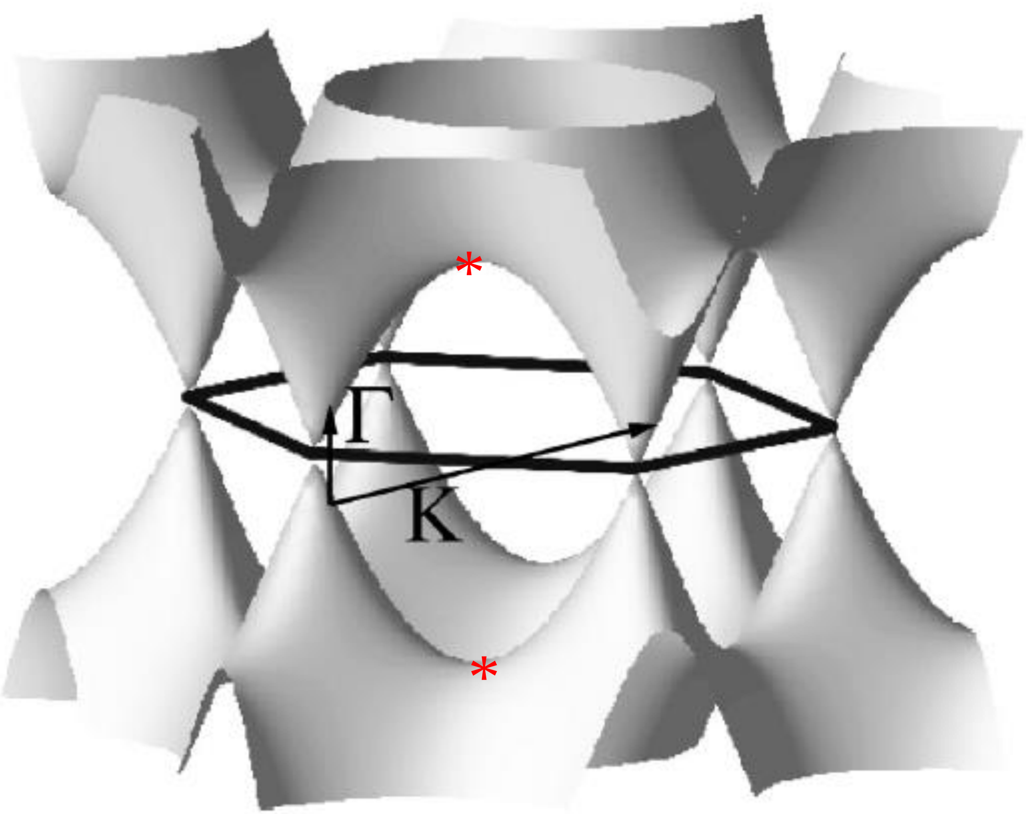


Fig. 1 (c)   Y. Ishibshi and M. Iwata

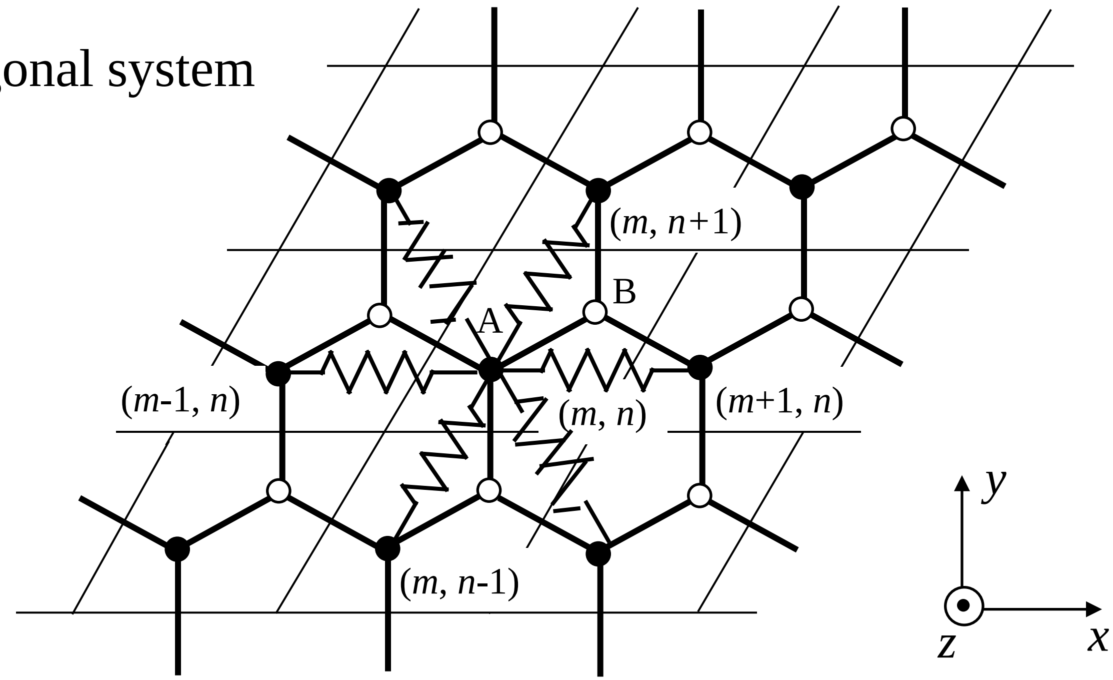
III. The conical point crossing



O. Dubay and G. Kresse: PRB67 (2003) 035401

２種類のZone boundary があることを示す簡単なモデル

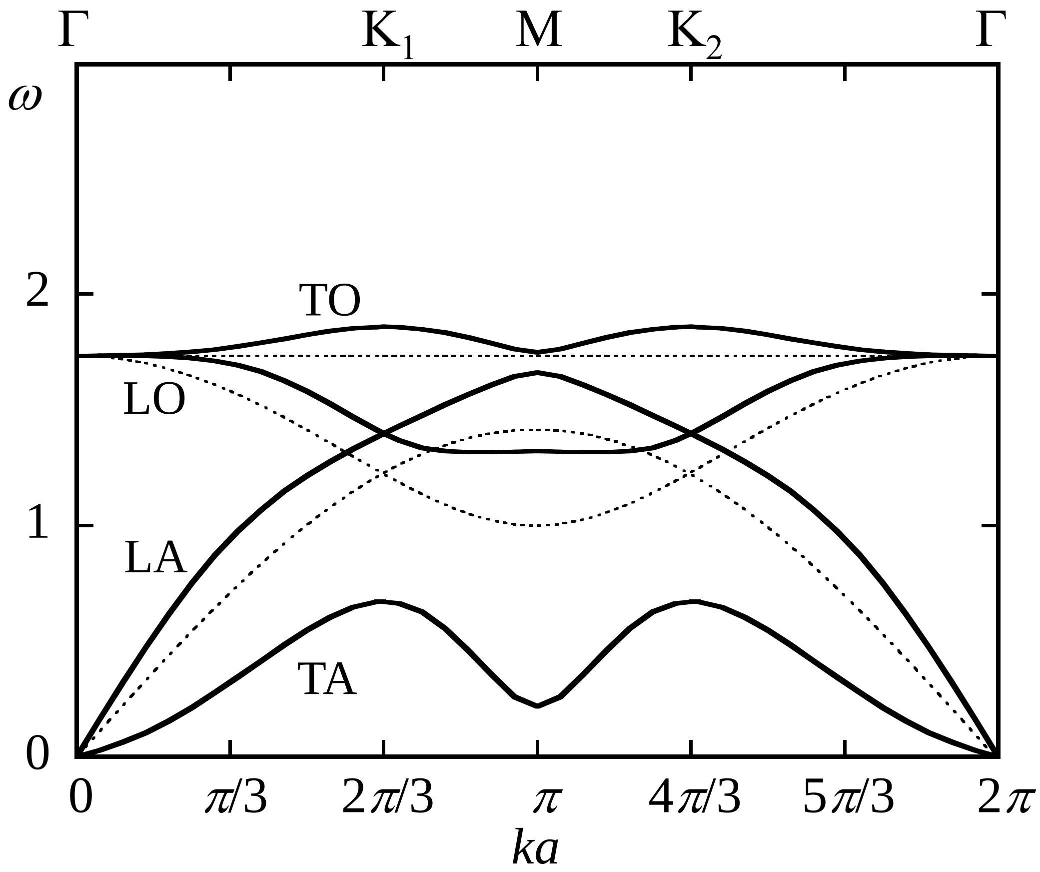
Hexagonal system



K: nn interaction

L: nnn interaction

Fig. 2　Y. Ishibshi and M. Iwata



極大極小の位置に注意

Iwata and Ishibashi: JPSJ **81** (2012)114703

The conical point crossing

the double degeneracy at 2 *unequal* points K and K'

the small representation is 2-dimensional

2 x 2 = 4,   4-dimensional representation
(the fourfold degeneracy)

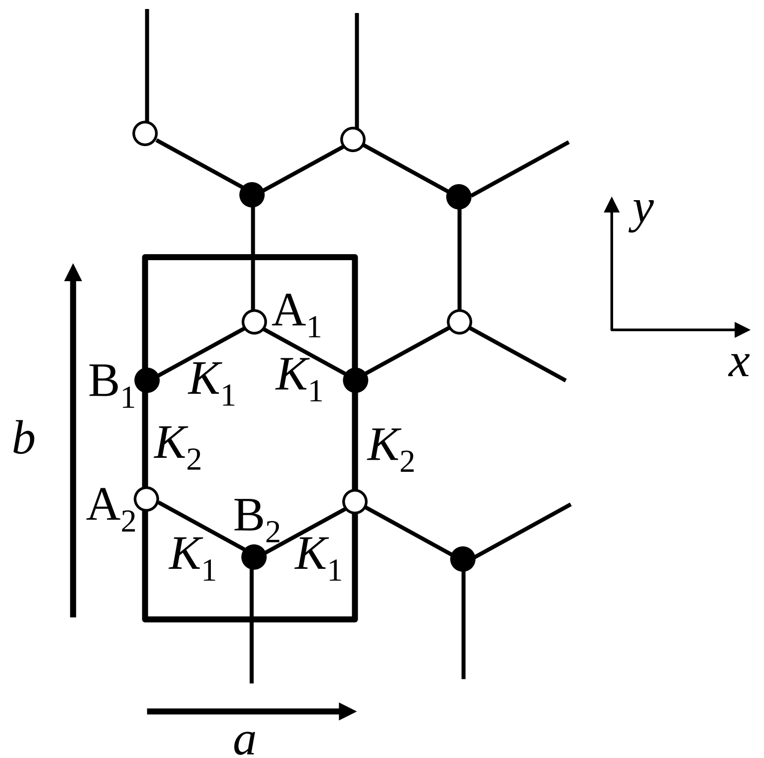
no conical point at Γ-point

characteristic to the space group
(the point group up to 3-dimensional)

III. The conical point crossing in the orthorhombic lattices

相互作用のnetwork と単位胞の形は別物

相互作用のnetwork は結晶系（対称性）を反映している



The network of the interaction is topologically the same as in the hexagonal lattice

例：K_2SeO_4, K_2SeO_4,……(improper ferroelastic)

Fig. 2 Y. Ishibshi and M. Iwata

An orthorhombic lattice

$$D = \begin{pmatrix} 2K_1 + K_2 - \omega^2 & -K_1\left(1+e^{\mathrm{i}k_a a}\right) & 0 & -K_2 e^{\mathrm{i}k_b b} \\ -K_1\left(1+e^{-\mathrm{i}k_a a}\right) & 2K_1 + K_2 - \omega^2 & -K_2 & 0 \\ 0 & -K_2 & 2K_1 + K_2 - \omega^2 & -K_1\left(1+e^{-\mathrm{i}k_a a}\right) \\ -K_2 e^{-\mathrm{i}k_b b} & 0 & -K_1\left(1+e^{\mathrm{i}k_a a}\right) & 2K_1 + K_2 - \omega^2 \end{pmatrix}$$

The eigenvalues are obtained as

$$\omega_i^2 = 2K_1 + K_2 \pm \left[4K_1^2 \cos^2 \frac{k_a a}{2} + K_2^2 \pm 4K_1 K_2 \cos \frac{k_a a}{2} \cos \frac{k_b b}{2} \right]^{1/2} \quad (i = 1 \sim 4)$$

At the conical k-point the $[\ldots\ldots]^{1/2}$-term in eq. (5) must vanish, i.e.,

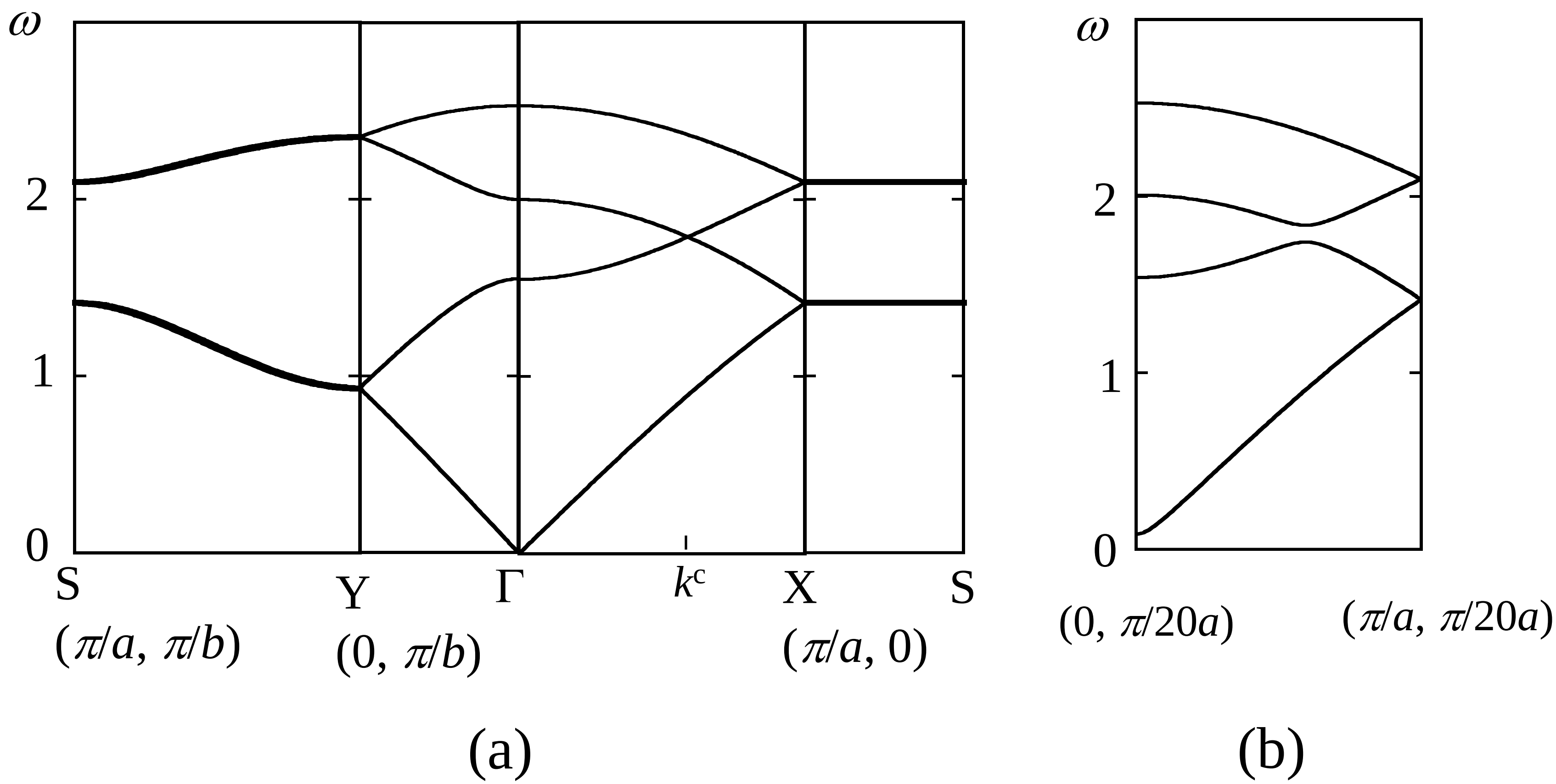
$$4K_1^2 \cos^2 \frac{k_a a}{2} + K_2^2 \pm 4K_1 K_2 \cos \frac{k_a a}{2} \cos \frac{k_b b}{2} = 0.$$

The dispersion relation around the conical k-points

$$\omega^2 = 2K_1 + K_2 \pm \sqrt{\frac{A}{2}\kappa_a^2 + \frac{B}{2}\kappa_b^2 + O\left(\kappa^4\right)}$$

$$\kappa_a = k_a - k_a^{\mathrm{c}}, \quad \kappa_b = k_b - k_b^{\mathrm{c}}, \quad \kappa^2 = \kappa_a^2 + \kappa_b^2$$

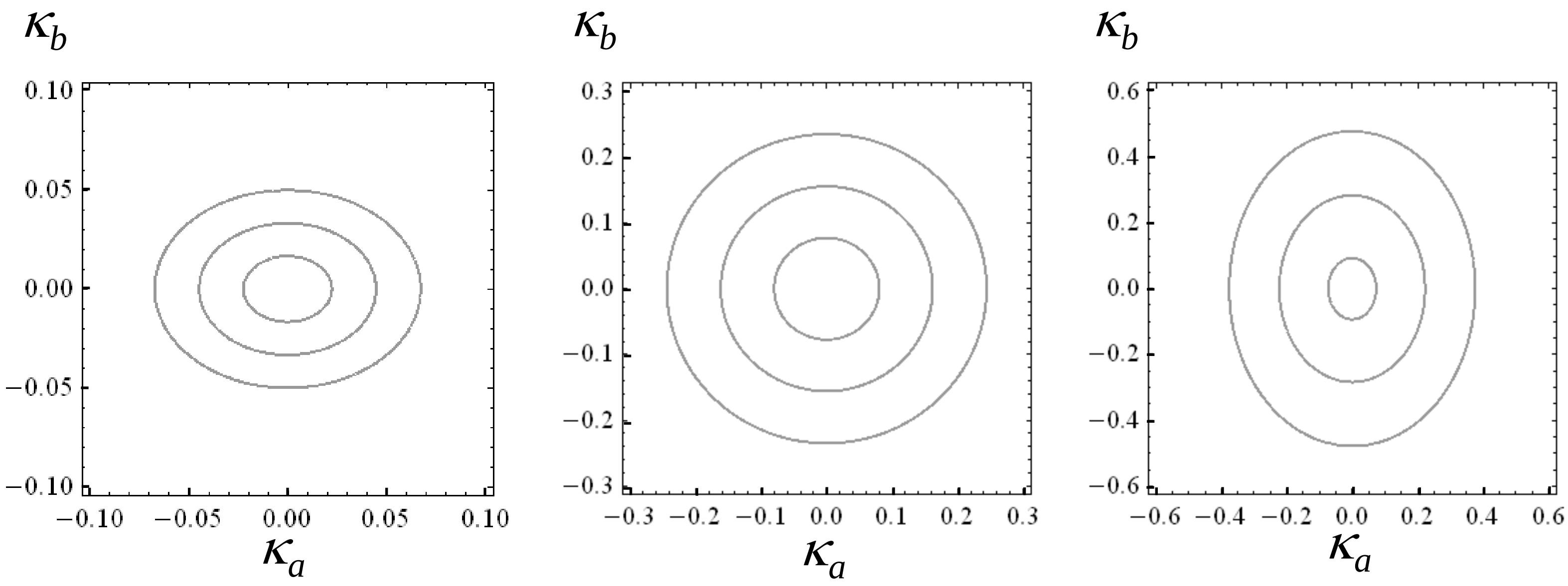
$$\cos k_b b = 1, \quad \cos \frac{k_a a}{2} = \frac{K_2}{2K_1}$$



The conical point crossing occurs at the general point inside the Brillouin zone !

Fig. 3 Y. Ishibshi and M. Iwata

Equal-frequency lines on the upper and the lower cones



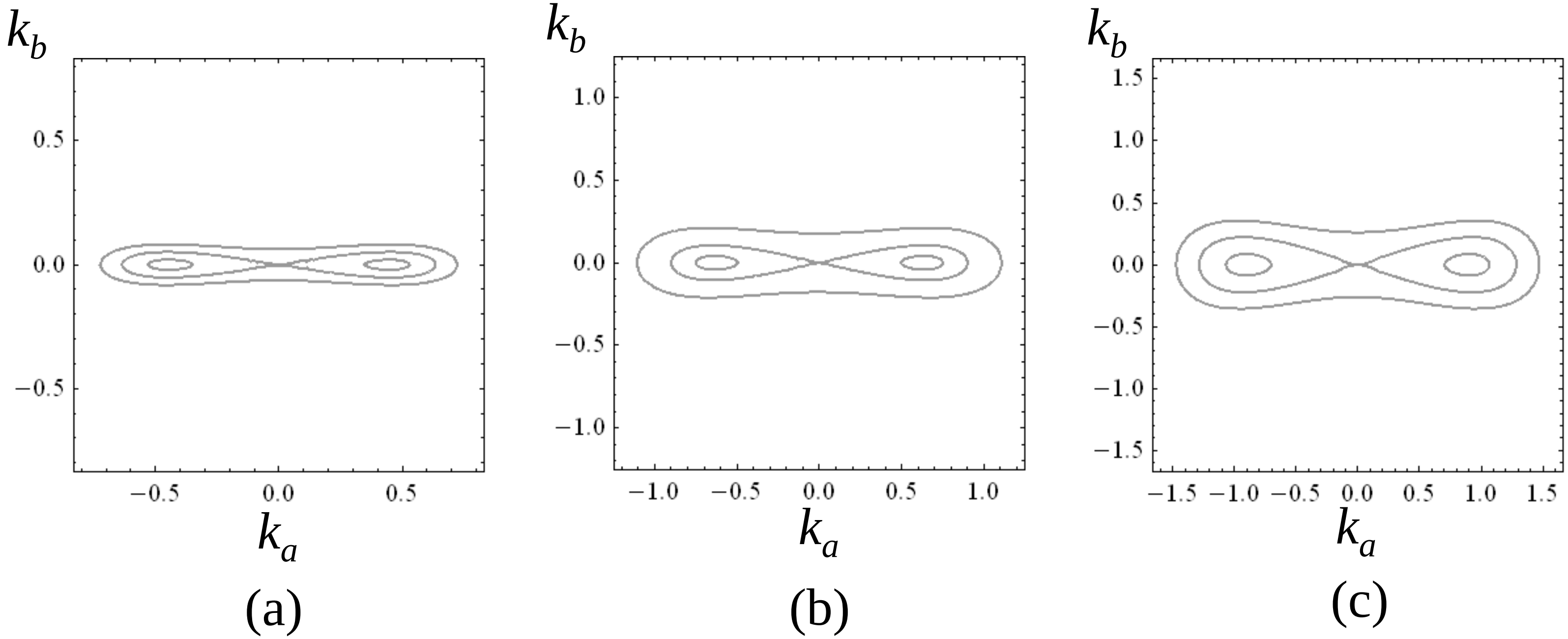
(a) (b) (c)

The oblique conical *k*-point

towards the Γ point — $\cos\theta = ½$ — towards the zone boundary

the z. b. in hexagonal lattice

Fig. 4 Y. Ishibshi and M. Iwata



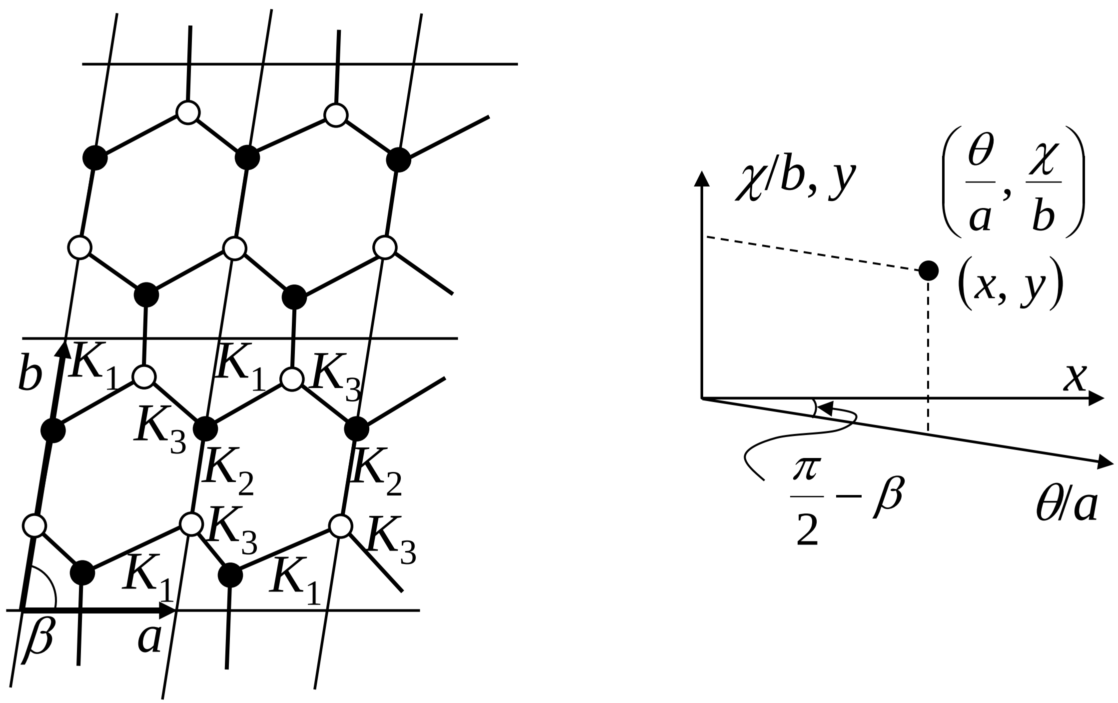
close to the Γ point

far from the Γ point

small slope

Fig. 9 Y. Ishibshi and M. Iwata

IV. The conical point crossing in the monoclinic lattices



(a) (b)

Fig. 5 Y. Ishibshi and M. Iwata

A monoclinic lattice

$$D=\begin{pmatrix} K_1+K_2+K_3-\omega^2 & -J & 0 & -K_2\zeta \\ -J^* & K_1+K_2+K_3-\omega^2 & -K_2 & 0 \\ 0 & -K_2 & K_1+K_2+K_3-\omega^2 & -J\xi^* \\ -K_2\zeta^* & 0 & -J^*\xi & K_1+K_2+K_3-\omega^2 \end{pmatrix}$$

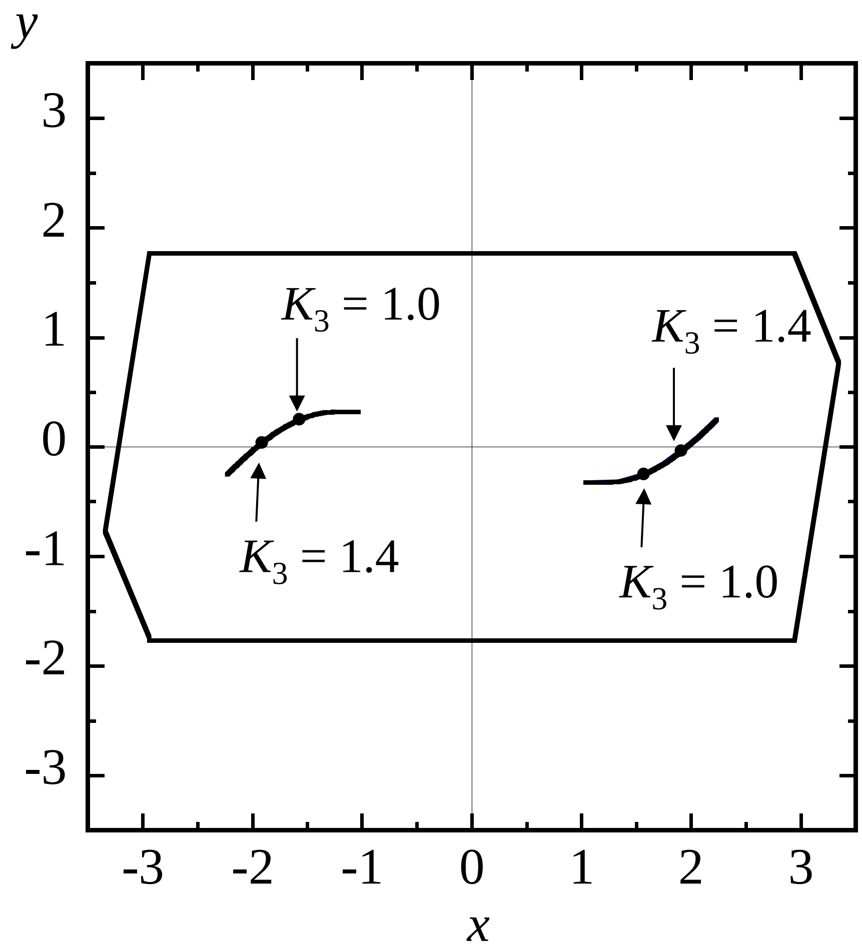
$$\xi=\mathrm{e}^{\mathrm{i}\theta},\quad \zeta=\mathrm{e}^{\mathrm{i}\chi}\qquad J=K_1+K_3\xi.$$

Then, we obtain four eigen-frequencies as

$$\left(\omega^2-\omega_0^2\right)^2=JJ^*+K_2^2\pm K_2\sqrt{2JJ^*+J^{*2}\xi\varsigma+J^2\xi^*\varsigma^*}\ .$$

At the conical k-point, (θ, χ) is given by

$$\cos\theta^{\mathrm{c}}=\frac{K_2^2-K_1^2-K_3^2}{2K_1K_3},\qquad \cos\chi^{\mathrm{c}}=\frac{\left(K_1^2+K_3^2\right)K_2^2-\left(K_1^2-K_3^2\right)^2}{2K_1K_3K_2^2},$$



The conical point crossing occurs at the general point inside the Brillouin zone !

Fig. 6 Y. Ishibshi and M. Iwata

A Primitive Monoclinic Cell

$$D = \begin{pmatrix} K_1 + K_2 + K_3 - \omega^2 & -\left(K_1 + K_3 e^{i\theta}\right) - K_2 e^{i\chi} \\ -\left(K_1 + K_3 e^{-i\theta}\right) - K_2 e^{-i\chi} & K_1 + K_2 + K_3 - \omega^2 \end{pmatrix}$$

The eigen-frequencies are given as

$$\omega^2 = K_1 + K_2 + K_3 \pm \sqrt{W},$$

$$W = K_1^2 + K_2^2 + K_3^2 + 2K_1K_2 \cos\chi + 2K_1K_3 \cos\theta + 2K_2K_3 \cos(\chi - \theta).$$

The conical k-points

$$\cos\theta^{c} = \frac{K_2^2 - K_1^2 - K_3^2}{2K_1K_3},$$

$$\cos\chi^{c} = \frac{K_3^2 - K_1^2 - K_2^2}{2K_1K_2},$$

$$\cos\left(\theta^{c} - \chi^{c}\right) = \frac{K_1^2 - K_2^2 - K_3^2}{2K_2K_3}.$$

	Monoclinic	Orthorhombic	Hexagonal
	K_1, K_2, K_3	$K_1, K_2 = K_3$	$K_1 = K_2 = K_3$
	$\cos\theta^{c} = \dfrac{K_2^2 - K_1^2 - K_3^2}{2K_1K_3}$,	$-\dfrac{K_1}{2K_2}$	$-\dfrac{1}{2}$
	$\cos\chi^{c} = \dfrac{K_3^2 - K_1^2 - K_2^2}{2K_1K_2}$,	$-\dfrac{K_1}{2K_2}$	$-\dfrac{1}{2}$
	$\cos\left(\theta^{c} - \chi^{c}\right) = \dfrac{K_1^2 - K_2^2 - K_3^2}{2K_2K_3}$.	$-\dfrac{K_1^2 - 2K_2^2}{2K_2^2}$	$\dfrac{1}{2}$

Conical point crossing 型縮退の解け方

* Robust against the perturbation.

* Not resolved at the conical k point, wherever it exists.

* The conical k point moves by the perturbation.

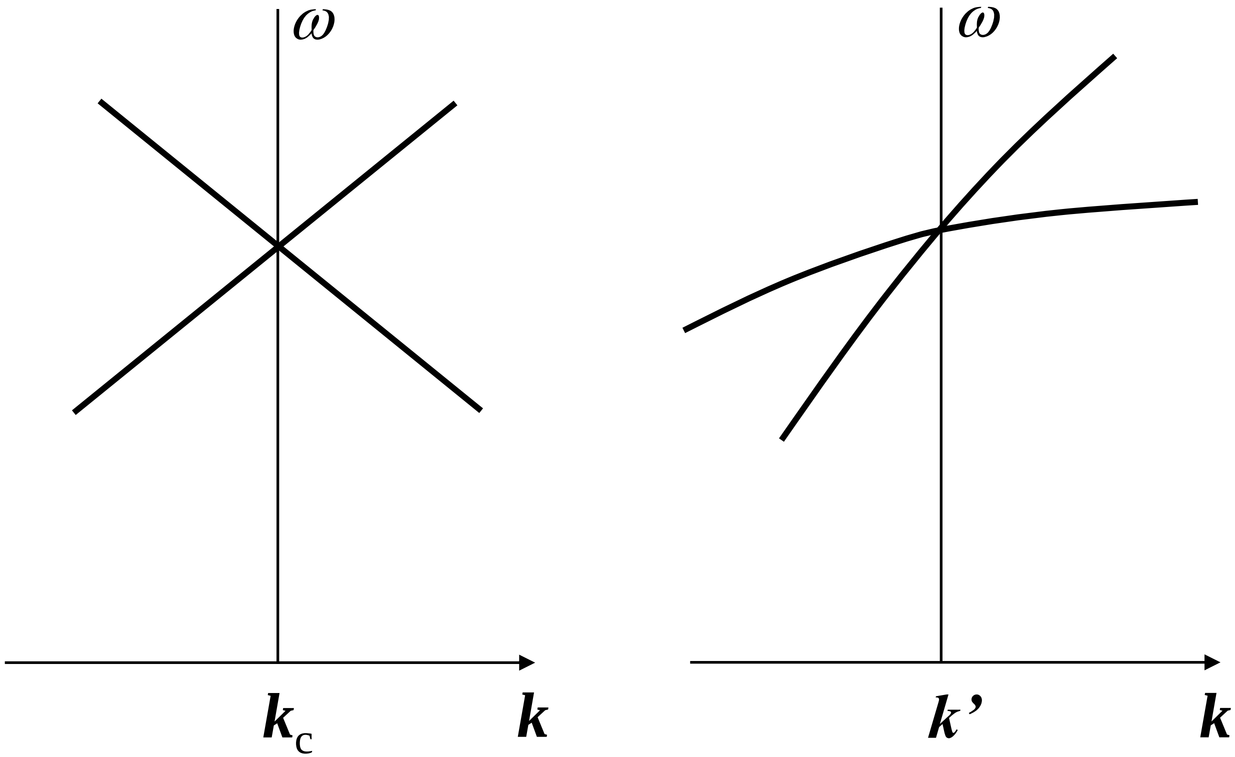
*When moving towards the zone boundary ($k_x = \pi/a$), flatter along the k_y axis. The crossing along the k_x axis remains.

* When moving towards the Γ point ($k_x = 0$), flatter along the k_x axis. The degeneracy is resolved at the Γ point.

The methodological comments

1. For the conical point crossing in the hexagonal lattice: The group theory is useful (as it should).

2. For the conical point crossing in the orthorhombic and the monoclinic lattices:
   (1) Models are needed, because the conical point crossing occurs at the general point inside the Brillouin zone.
   (2) Models should be simple and include all substantial symmetry aspects of the lattices.



(a)

Crossing by symmetry.
Symmetric

(b)

Accidental crossing (degeneracy)
Asymmetric

Fig. 10 Y. Ishibshi and M. Iwata

Thank you very much for your attention