CHIRAL PHONONS Workshop July 29th – 31st, 2025
WASEM Monastery, Ingelheim, Germany

Electron-chiral phonon coupling, crystal angular momentum, and phonon chirality

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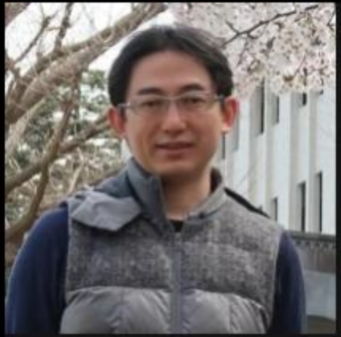

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Takuya Sato

Collaborative research at the Institute for Molecular Science, supported from OML (Open Mix Lab) at the National Institutes of Natural Sciences. Researchers in the field of condensed matter physics gather to conduct collaborative research on chirality in condensed matter.

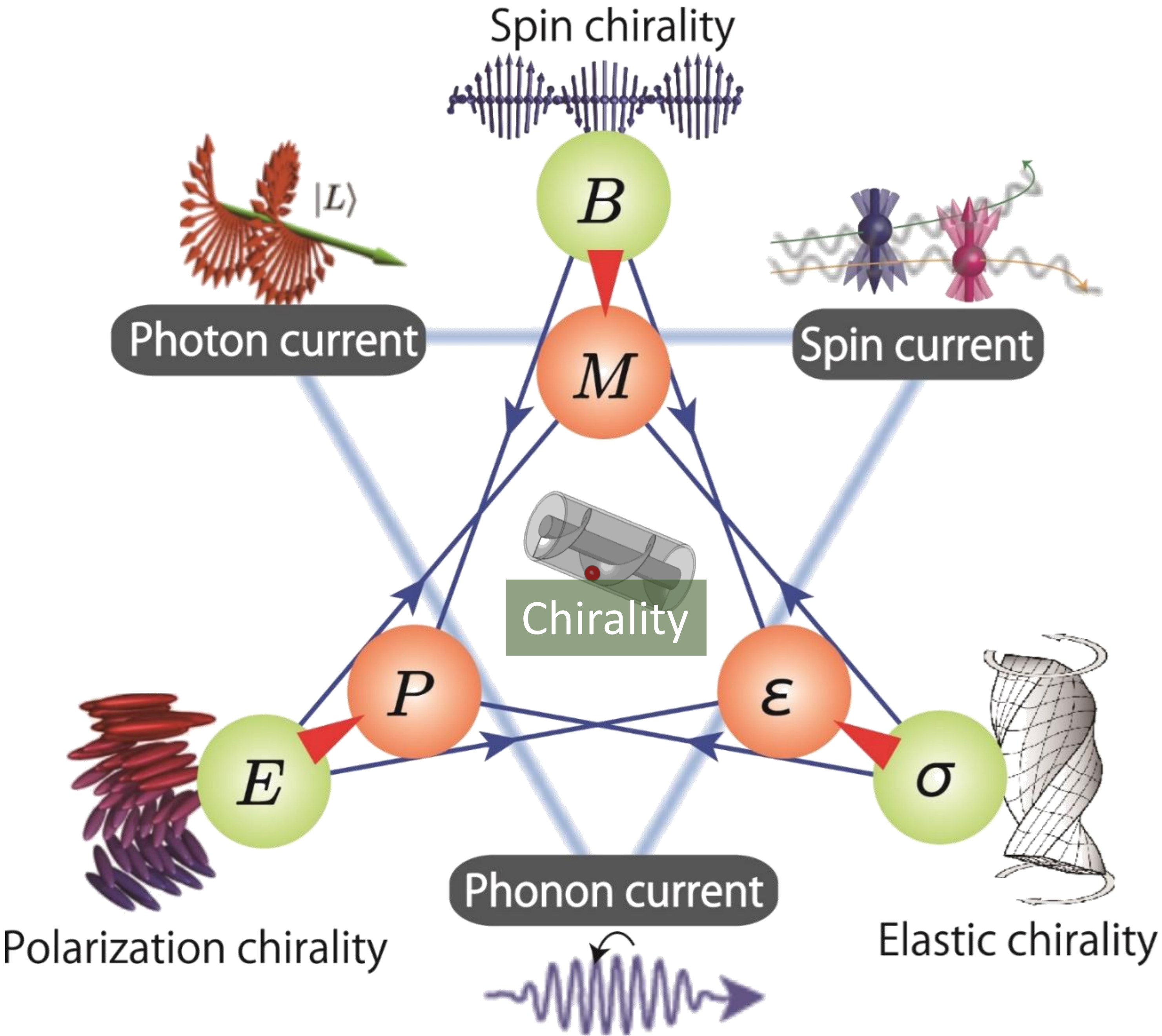
The perspective may change depending on whether the emphasis is placed on 'chiral' or 'phonon'.

CHIRAL **PHONONS**

CHIRAL PHONONS

I’m rather on this side …….

Chirality-selective cross-coupling = handshake



Contents

1. **Motivation: chirality-selective coupling (go very quickly)**
2. **Chiral Phonon: crystal angular momentum and phonon chirality**
3. **How to describe electron and chiral phonon interaction**

[1] T. Tateishi, A. Kato and JK, J. Phys. Soc. Jpn. 94, 053601 (2025)
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[7] JK, A. S. Ovchinikov, and A. A. Tereshchenko, Phys. Rev. Lett.125, 245302 (2020)

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Our definition of truly chiral phonon

Chiral phonons are the quantum of lattice vibrations where the rotational motion of atomic nuclei propagates as a wave with a finite wave number in the direction of rotation axis

AM (Axial) **Wave num. (Polar)**

$$\mathrm{R} : \boldsymbol{\ell} \cdot \boldsymbol{k} > 0$$

$$\mathrm{L} : \boldsymbol{\ell} \cdot \boldsymbol{k} < 0$$

T-even pseudo scalar

or electric toroidal monopole (G_0)

nature physics

Letter https://doi.org/10.1038/s41567-022-01790-x

Truly chiral phonons in α-HgS

Received: 30 September 2021

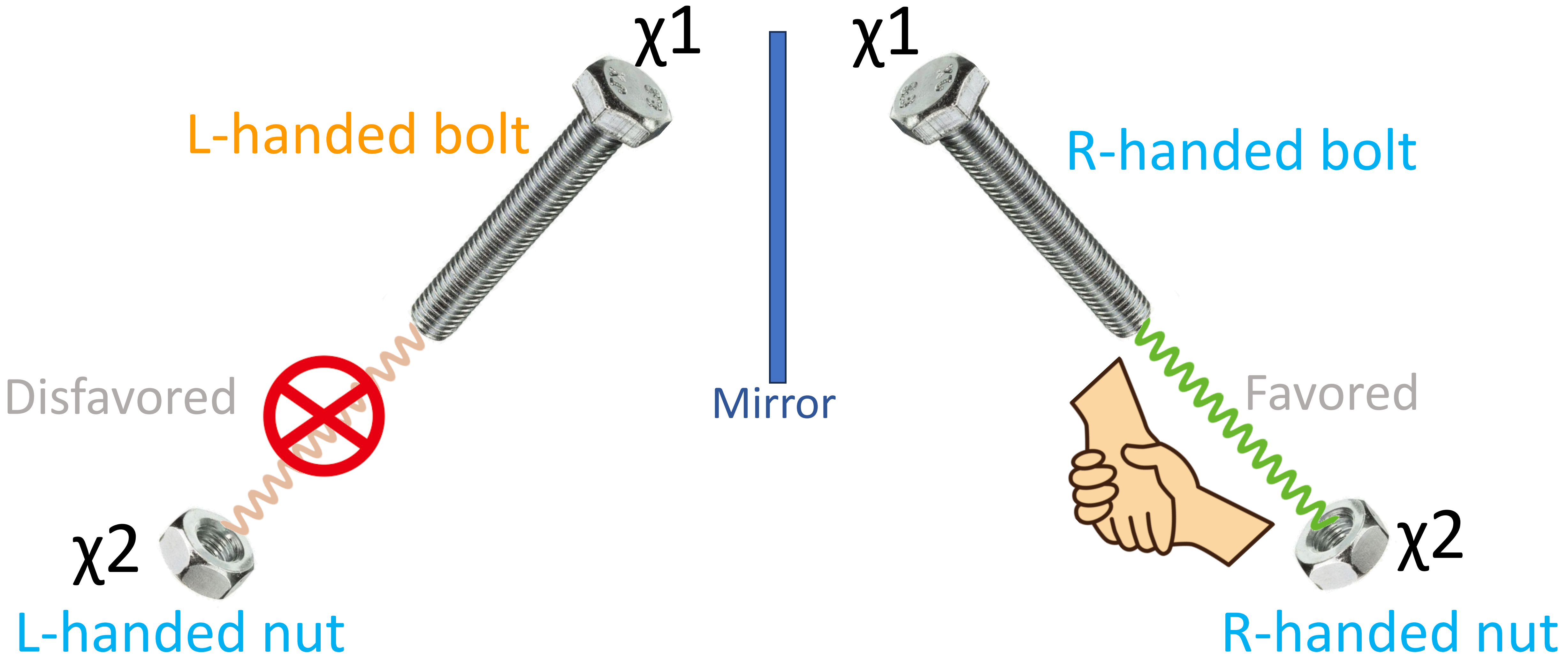
Accepted: 5 September 2022

Published online: 31 October 2022

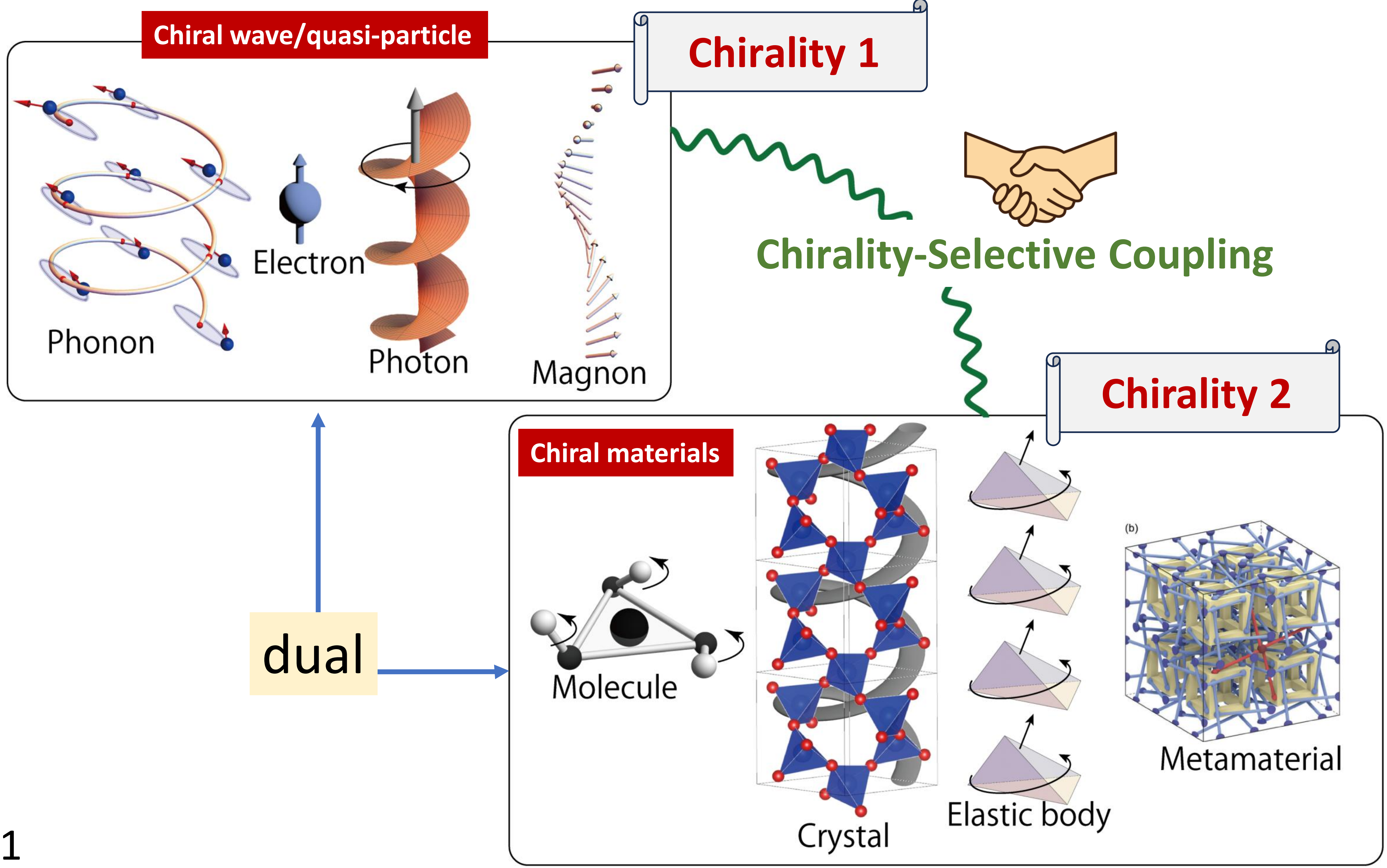
Kyosuke Ishito[1,7], Huiling Mao[1,7], Yusuke Kousaka[2,3], Yoshihiko Togawa[2], Satoshi Iwasaki[3], Tiantian Zhang[1,4], Shuichi Murakami[1,4], Jun-ichiro Kishine[5,6] & Takuya Satoh[1]

- JK, H. Kusunose, H.M. Yamamoto, Israel J.Chem.62, e202200049 (2022)
- H. Kusunose, JK. And H. M. Yamamoto, Appl. Phys. Lett. 124, 260501 (2024)

Chirality-selective coupling between two chiral dual entities



Chirality-selective coupling is quite robust!


Chiral wave/quasi-particle
Chirality 1
Phonon
Electron
Photon
Magnon
Chirality-Selective Coupling
Chirality 2
dual
Chiral materials
Molecule
Crystal
Elastic body
(b)
Metamaterial

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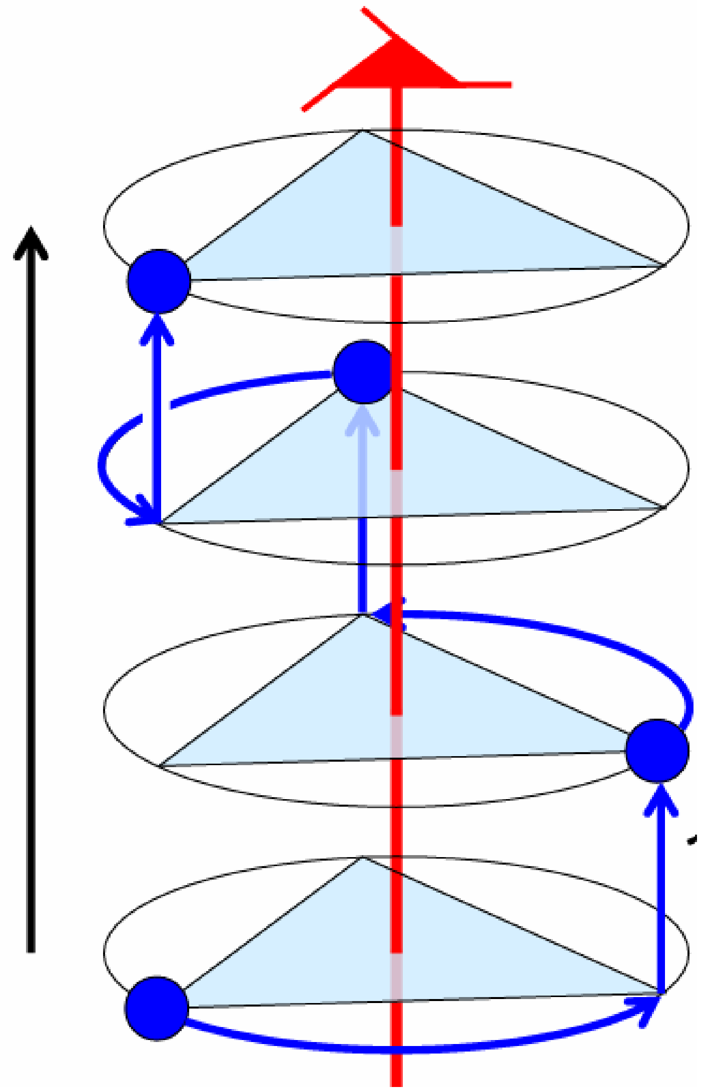
In chiral helical crystal, Not only CM but also CAM conserved

Having screw symmetry is a narrower concept than being chiral, but it leads to a conserved angular momentum associated with the corresponding discrete rotational symmetry.



e.g., 3-fold as an example

- ✓ Continuous rotational symmetry broken ⇒ mechanical angular momentum (**MAM**) not conserved
- ✓ But discrete 3-fold ($2\pi/3$) rotational symmetry exists ⇒ crystal angular momentum (**CAM or PAM**) conserved

Wave Function of a Chiral Phonon

T. Tateishi, A. Kato and JK, J. Phys. Soc. Jpn. 94, 053601 (2025)

Chiral basis: $\boldsymbol{e}^{\pm} \equiv \frac{1}{\sqrt{2}}(\boldsymbol{e}^1 \mp i\boldsymbol{e}^2), \quad \boldsymbol{e}^0 \equiv \boldsymbol{e}^3$

Components of the chiral basis: $s = \pm 1, 0$

CM

CAM

Superposition of basis

Normal coordinate

$$u_l^s(t) = \frac{1}{\sqrt{3N}} \sum_{n=0}^{N-1} \sum_{m=\pm,0} e^{-i(l-1)[q_n \frac{c}{3} + \alpha(m - m_s)]} w_{nm}^s(t)$$

q_n : crystal momentum

m : crystal angular momentum

⟷

l : site number in real space

3N degrees of freedom

Chiral Phonon Dispersion

$$\Phi = \frac{M}{2} \sum_{n=0}^{N-1} \sum_{m=\pm 1,0} \boldsymbol{w}_{nm}^{\dagger} \mathbf{A}_{nm} \boldsymbol{w}_{nm}$$

$$\mathbf{A}_{nm} = \begin{pmatrix} |d_{nm}^{+}|^2 \Omega_{++} & (d_{nm}^{+})^* d_{nm}^{-} \Omega_{+-} & (d_{nm}^{+})^* d_{nm}^{0} \Omega_{+0} \\ (d_{nm}^{-})^* d_{nm}^{+} \Omega_{-+} & |d_{nm}^{-}|^2 \Omega_{--} & (d_{nm}^{-})^* d_{nm}^{0} \Omega_{-0} \\ (d_{nm}^{0})^* d_{nm}^{+} \Omega_{0+} & (d_{nm}^{0})^* d_{nm}^{-} \Omega_{0-} & |d_{nm}^{0}|^2 \Omega_{00} \end{pmatrix}$$

$$\omega_{nm}^{\lambda} = \sqrt{\frac{a_{nm} + b_{nm} + c_{nm} + 2\sqrt{\alpha_{nm}} \cos\left(\theta_{nm}^{\lambda}\right)}{3}} \equiv \sqrt{\zeta_{nm}^{\lambda}}$$

$$\alpha_{nm} \equiv a_{nm}^2 + b_{nm}^2 + c_{nm}^2 - a_{nm} b_{nm} - a_{nm} c_{nm} - b_{nm} c_{nm} + 3\left(|d_{nm}|^2 + |e_{nm}|^2 + |f_{nm}|^2\right)$$

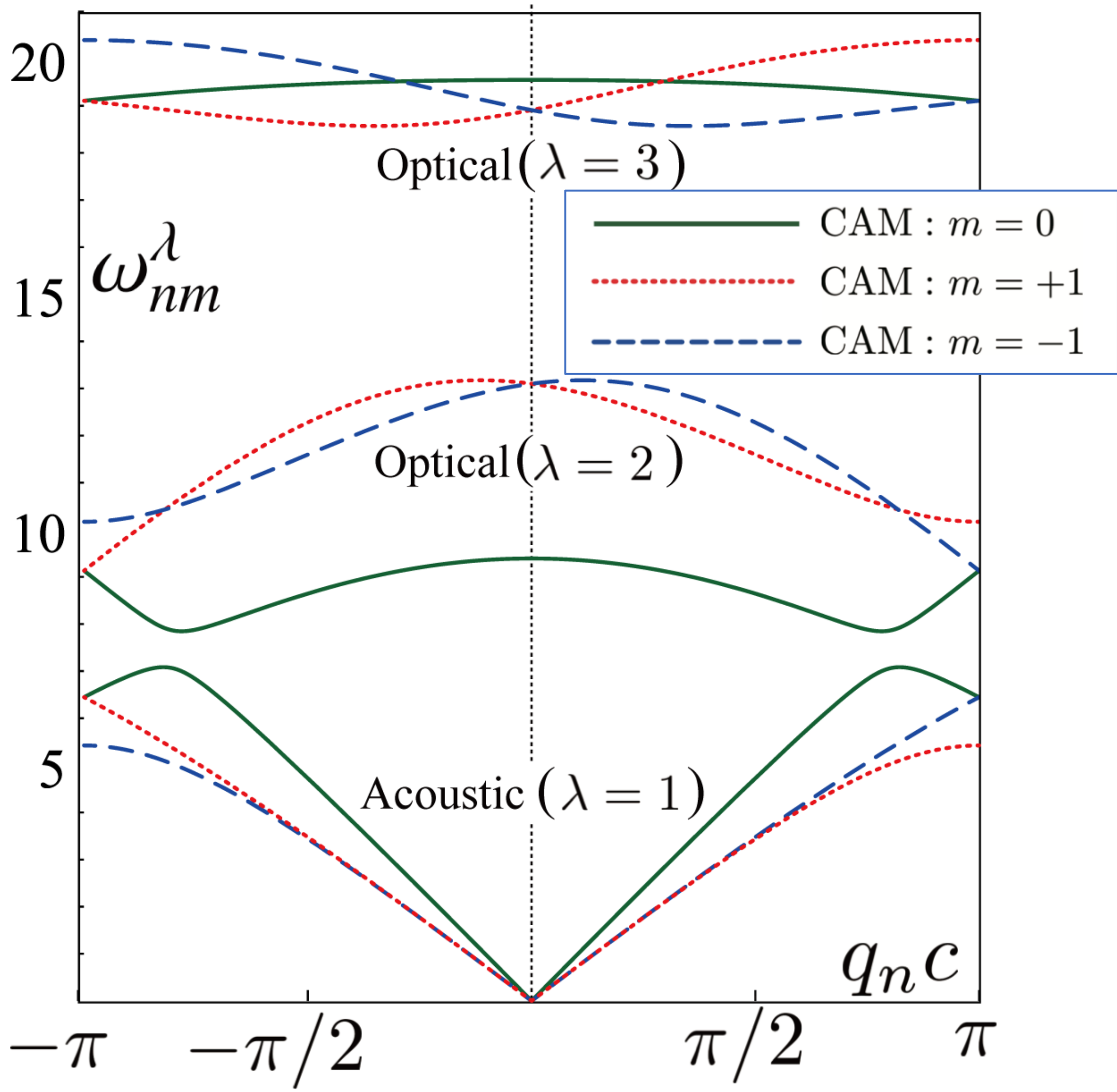
$$\beta_{nm} \equiv -(2a_{nm} - b_{nm} - c_{nm})(2b_{nm} - a_{nm} - c_{nm})(2c_{nm} - a_{nm} - b_{nm})$$

$$\theta_{nm}^{\lambda} = \begin{cases} \theta_{nm}^{1} = \frac{2\pi}{3} + \frac{1}{3} \arccos\left(-\frac{1}{2}(\alpha_{nm})^{-3/2} \beta_{nm}\right) \\ \theta_{nm}^{2} = \frac{2\pi}{3} - \frac{1}{3} \arccos\left(-\frac{1}{2}(\alpha_{nm})^{-3/2} \beta_{nm}\right) \\ \theta_{nm}^{3} = \frac{1}{3} \arccos\left(-\frac{1}{2}(\alpha_{nm})^{-3/2} \beta_{nm}\right) \end{cases}$$

$$a_{nm} \equiv |d_{nm}^{+}|^2 \Omega_{++}, \quad b_{nm} = |d_{nm}^{-}|^2 \Omega_{--},$$

$$c_{nm} \equiv |d_{nm}^{0}|^2 \Omega_{00}, \quad d_{nm} = (d_{nm}^{-})^* d_{nm}^{+} \Omega_{-+},$$

$$e_{nm} \equiv (d_{nm}^{0})^* d_{nm}^{-} \Omega_{0-}, \quad f_{nm} = (d_{nm}^{0})^* d_{nm}^{+} \Omega_{0+},$$

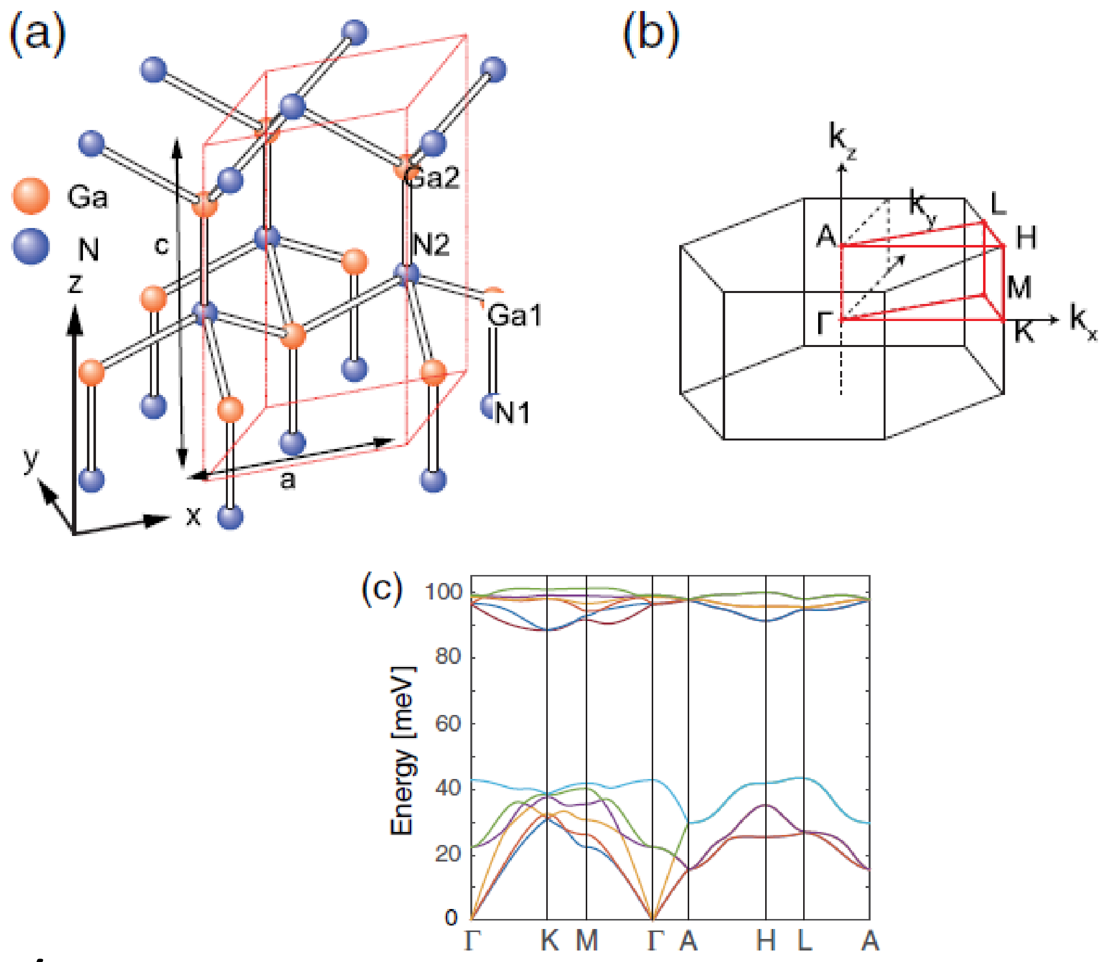


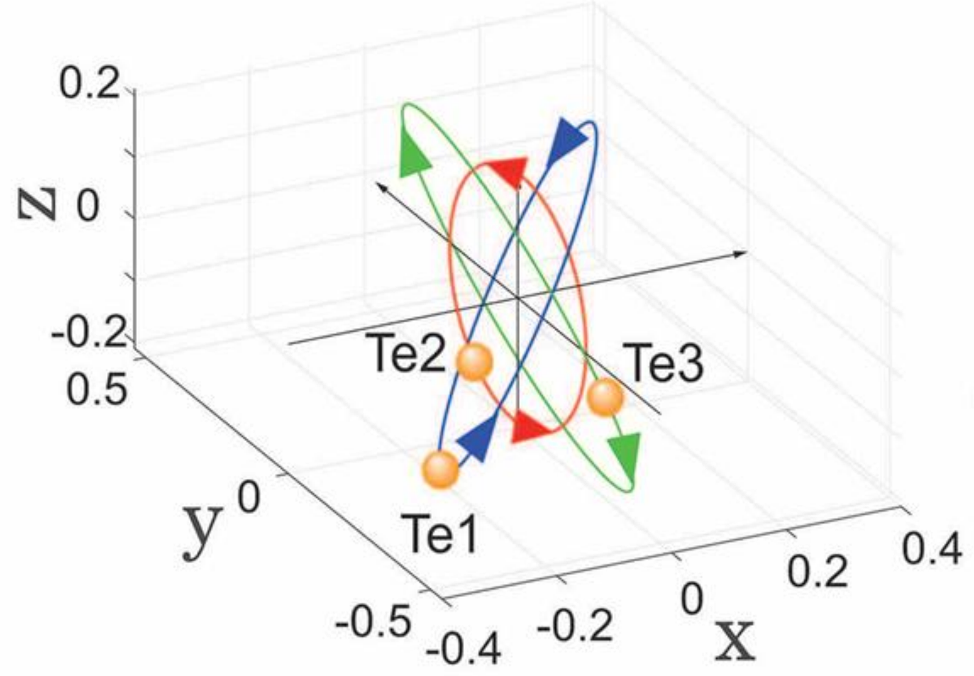
Chirality-selective coupling lifts degeneracy for non-zero wave number

PHYSICAL REVIEW LETTERS **121,** 175301 (2018)

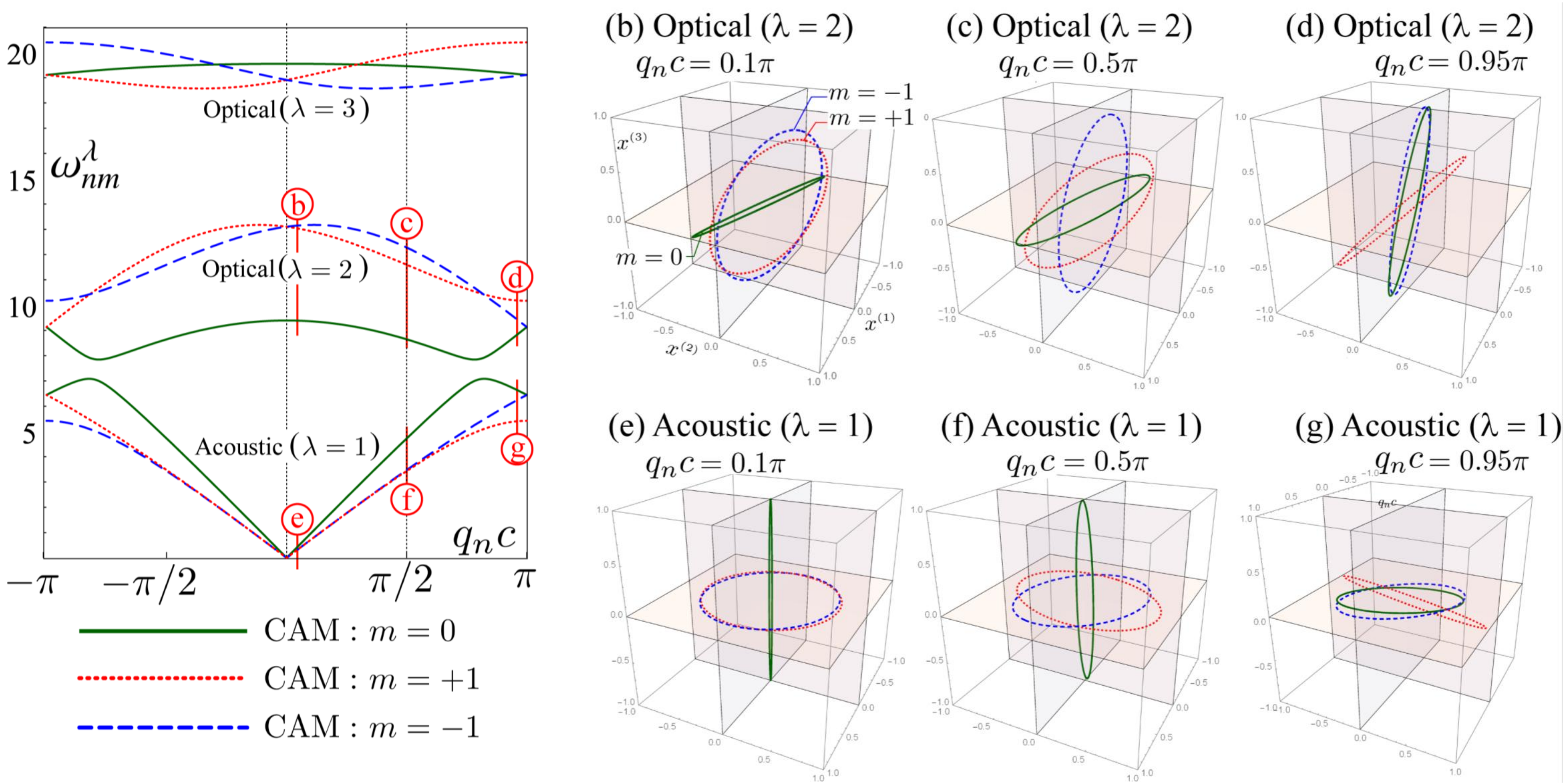
Phonon Angular Momentum Induced by the Temperature Gradient

Masato Hamada,[1] Emi Minamitani,[2] Motoaki Hirayama,[1,3,4] and Shuichi Murakami[1,3]





Real-space trajectories of atomic motion



Longitudinal or transverse modes mixed!

⇒ Chiral nature of phonon comes up in electron-phonon interaction

MAM and CAM of chiral phonon

MAM of chiral phonons

$f(\omega^{\lambda}_{n,m})$: Bose-Einstein distribution function

$$J_z = M\sum_{l=1}^{3N}(x_l^{(1)}\dot{x}_l^{(2)} - x_l^{(2)}\dot{x}_l^{(1)})$$

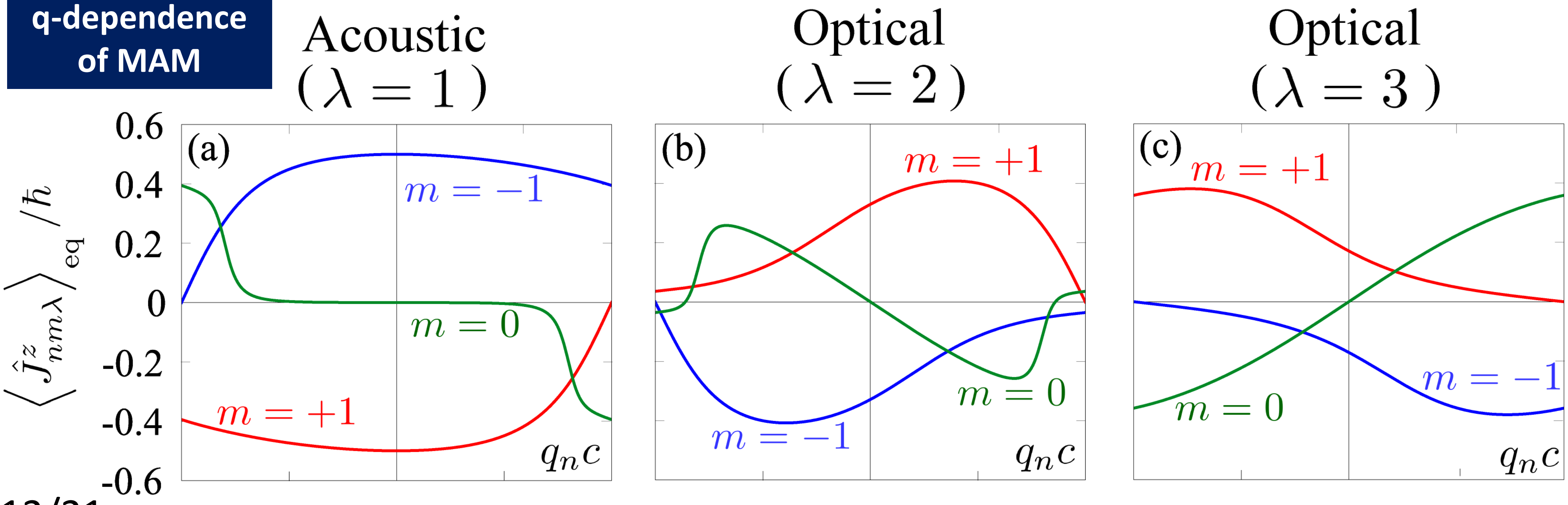
$$\langle \hat{J}^z\rangle_{eq} = -\sum_n\sum_m\sum_{\lambda=1,2,3}\hbar\left(\frac{1}{2}+f(\omega^{\lambda}_{n,m})\right)\left(|v^{\lambda(+)}_{nm}|^2 - |v^{\lambda(-)}_{nm}|^2\right)$$

Coherence factor

L.Zhang and Q.Niu: Phys.Rev.Lett.112(2014)085503:

$$J_z^{\mathrm{ph}} = \sum_{\sigma,\boldsymbol{k}} l^z_{\boldsymbol{k},\sigma}\left[f(\omega_{\boldsymbol{k},\sigma})+\frac{1}{2}\right],\ l^z_{\boldsymbol{k},\sigma} = (\epsilon^{\dagger}_{\boldsymbol{k},\sigma}M\epsilon_{\boldsymbol{k},\sigma})\hbar$$

q-dependence of MAM



Consistent with 1[st] principle computation (Ishito, Sato et al., Nat. Phys. 2022)

Phonon analogue of optical Zilch

Lipkin's Optical Chirality (Zilch)

D. M. Lipkin, Journal of Mathematical Physics 5, 696 (1964)

$$\rho_\chi = \frac{\varepsilon_0}{2}\boldsymbol{E}\cdot\boldsymbol{\nabla}\times\boldsymbol{E} + \frac{1}{2\mu_0}\boldsymbol{B}\cdot\boldsymbol{\nabla}\times\boldsymbol{B}$$

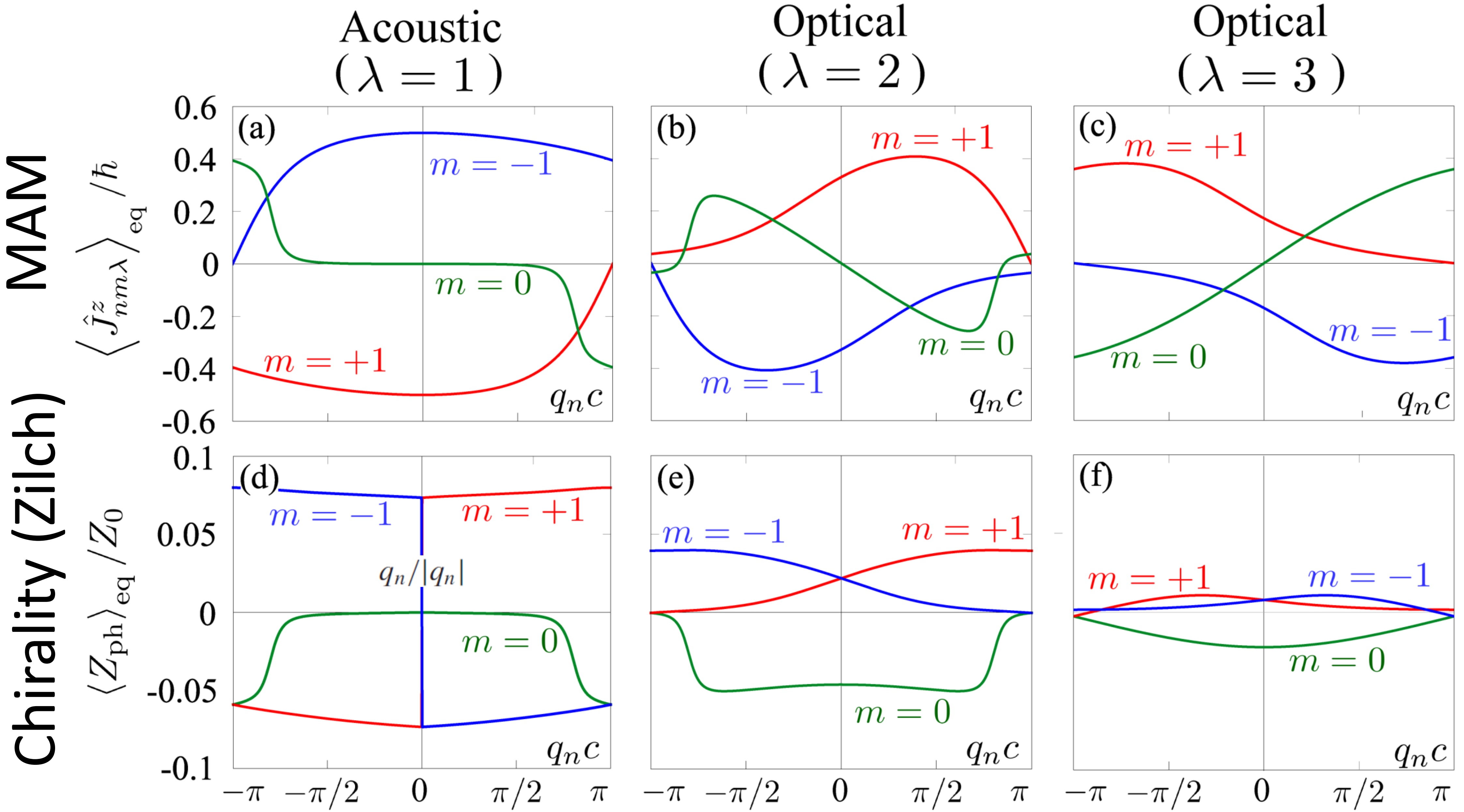
MAM, CAM and phonon Zilch

Zilch of chiral phonons (as a trial....)

$$Z_{ph} \equiv \sum \boldsymbol{u}_l\cdot\nabla\times\boldsymbol{u}_l$$

$$\langle Z_{ph}\rangle_{eq} = \frac{3}{c}\sum_n\sum_m\sum_\lambda \frac{\hbar}{M\omega^\lambda_{n,m}}\left(\frac{1}{2}+f(\omega^\lambda_{n,m})\right) \times\left(\sin[q_n\frac{c}{3}+\alpha(m-1)]|v^{\lambda(+)}_{nm}|^2 - \sin[q_n\frac{c}{3}+\alpha(m+1)]|v^{\lambda(-)}_{nm}|^2\right)$$

Phonon analogue of optical Zilch



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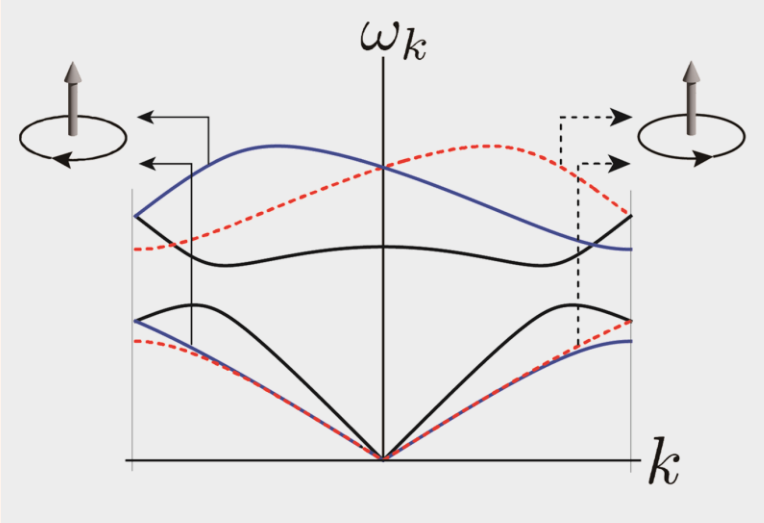
Electron and Phonon operators

Phonon operator

$$u_l^s(t) = \frac{1}{\sqrt{3N}} \sum_{n=-\frac{N-1}{2}}^{\frac{N-1}{2}} \sum_{m=\pm,0} e^{-i(l-1)[q_n \frac{c}{3} + \alpha(m-m_s)]} w_{nm}^s(t)$$

Quantization of lattice vib.

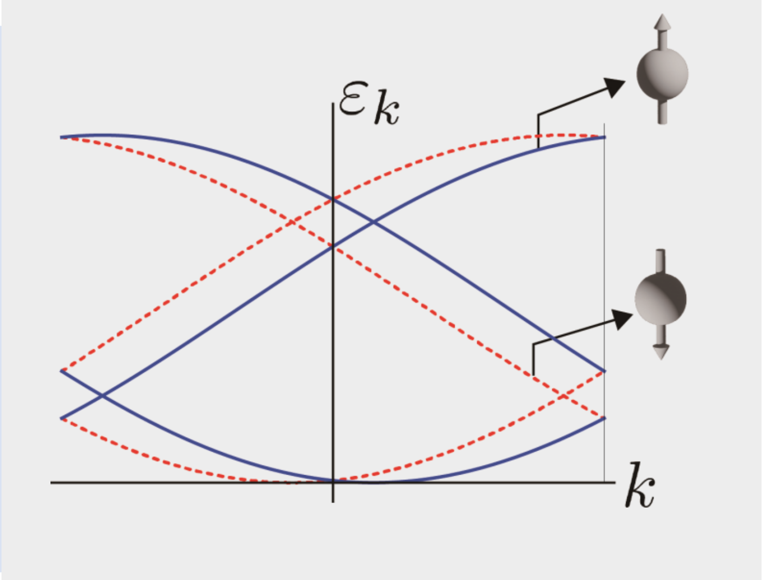
$$\hat{\boldsymbol{w}}_{nm}(t) = \sum_{\lambda=1,2,3} \left(\frac{\hbar}{2M\omega_{nm}^{\lambda}} \right)^{\frac{1}{2}} \left(\hat{a}_{n,m}^{\lambda}(t) + \hat{a}_{-n,-m}^{\lambda\dagger}(t) \right) \boldsymbol{v}_{nm}^{\lambda}$$



Electron operator

$\sigma = \uparrow, \downarrow$: spin index

$$\hat{c}_{l,\sigma} = \frac{1}{\sqrt{3N}} \sum_{n',m'} e^{-i(l-1)\left(k_{n'} \frac{c}{3} + \alpha m'\right)} \hat{c}_{n',m',\sigma}$$



I. Božović: Phys. Rev. B **29** (1984) 6586

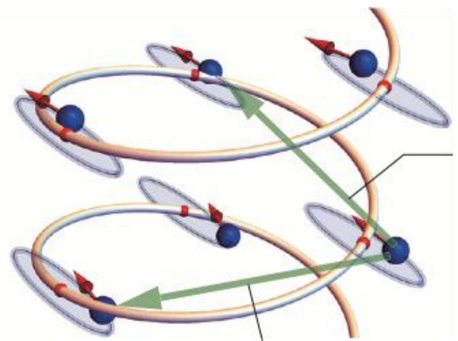
Electron-chiral phonon coupling Hamiltonian

Modified tight-binding approximation:

$$\mathscr{H}_{\mathrm{el}} = -\sum_{\langle l,l'\rangle}\sum_{\sigma} t\left(\boldsymbol{r}_l - \boldsymbol{r}_{l'}\right)\hat{c}^{\dagger}_{l,\sigma}\hat{c}_{l',\sigma}$$

$\sigma = \uparrow,\downarrow$:spin index

S.Barišić ,J.Labbé,andJ.Friedel:Phys.Rev.Lett.25(1970)919.



$$t\left(\boldsymbol{r}_l - \boldsymbol{r}_{l'}\right) = t_0 + \left.\frac{\partial t\left(\boldsymbol{r}\right)}{\partial \boldsymbol{r}}\right|_{\boldsymbol{r}=\boldsymbol{R}_l-\boldsymbol{R}_{l'}} \cdot \left[\boldsymbol{u}_l(t) - \boldsymbol{u}_{l'}(t)\right],$$

$$-\zeta t_0\left(\frac{\boldsymbol{R}_l - \boldsymbol{R}_{l'}}{\left|\boldsymbol{R}_l - \boldsymbol{R}_{l'}\right|}\right)$$

ζ :Slater coefficient describing exponential decay $e^{-\zeta r}$ of the electron

Electron-chiral phonon coupling Hamiltonian

$$\mathcal{H}_{\mathrm{el}-\chi\mathrm{ph}} = \zeta t_0 \sum_{\langle l,l'\rangle}\sum_{\sigma}\left(\frac{\boldsymbol{R}_l - \boldsymbol{R}_{l'}}{\left|\boldsymbol{R}_l - \boldsymbol{R}_{l'}\right|}\right)\cdot\left[\hat{\boldsymbol{u}}_l(t) - \hat{\boldsymbol{u}}_{l'}(t)\right]\hat{c}^{\dagger}_{l,\sigma}\hat{c}_{l',\sigma}$$

$$= \sum_{n.n'}\sum_{m.m'}\sum_{\lambda}\sum_{\sigma}\Gamma^{\lambda}_{nn'mm'}\left(\hat{a}^{\lambda}_{n,m} + \hat{a}^{\lambda\dagger}_{-n,-m}\right)\hat{c}^{\dagger}_{n+n',m+m',\sigma}\hat{c}_{n',m',\sigma}$$

Electron-chiral phonon coupling vertex

T. Tateishi, A. Kato and JK, J. Phys. Soc. Jpn. 94, 053601 (2025)

$$\Gamma^{\lambda}_{nn'mm'} = \left(\frac{\hbar}{6MN\omega^{\lambda}_{nm}}\right)^{\frac{1}{2}} \frac{\zeta t_0}{\sqrt{3\rho^2+\frac{c^2}{9}}}$$

$$\times\left[\sqrt{6}\rho\left\{\sin\left[k_{n'}\frac{c}{3}+\alpha\left(m'+\frac{1}{2}\right)\right]-\sin\left[(q_n+k_{n'})\frac{c}{3}+\alpha\left(m+m'-\frac{1}{2}\right)\right]\right\}v^{\lambda(+)}_{nm}\right.$$

$$-\sqrt{6}\rho\left\{\sin\left[k_{n'}\frac{c}{3}+\alpha\left(m'-\frac{1}{2}\right)\right]-\sin\left[(q_n+k_{n'})\frac{c}{3}+\alpha\left(m+m'+\frac{1}{2}\right)\right]\right\}v^{\lambda(-)}_{nm}$$

$$\left.+\frac{2i}{3}c\left\{\sin\left[k_{n'}\frac{c}{3}+\alpha m'\right]-\sin\left[(q_n+k_{n'})\frac{c}{3}+\alpha(m+m')\right]\right\}v^{\lambda(0)}_{nm}\right]$$

Satisfying time-re

$\Gamma^{\lambda}_{-n,-n'-m-,n}$

TIGHT BINDING AND TRANSITION-METAL SUPERCONDUCTIVITY*

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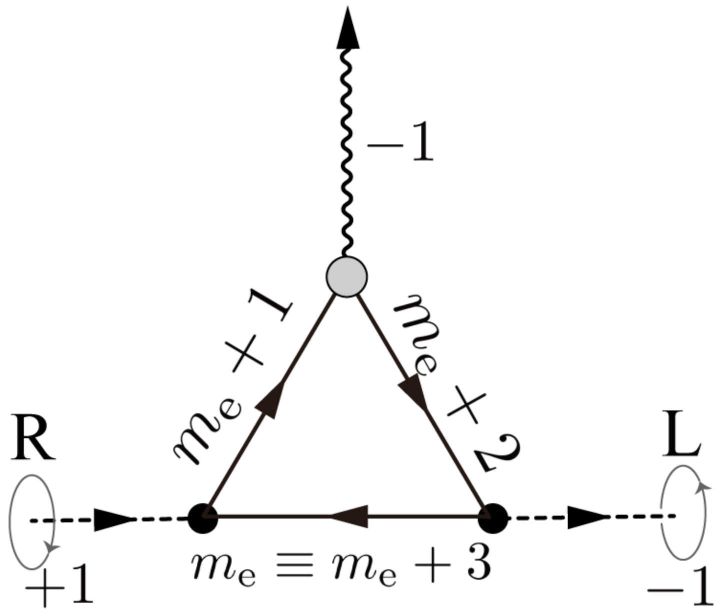
Laboratoire de Physique des Solides,‡ Faculté des Sciences de l'Université de Paris, 91 Orsay, France

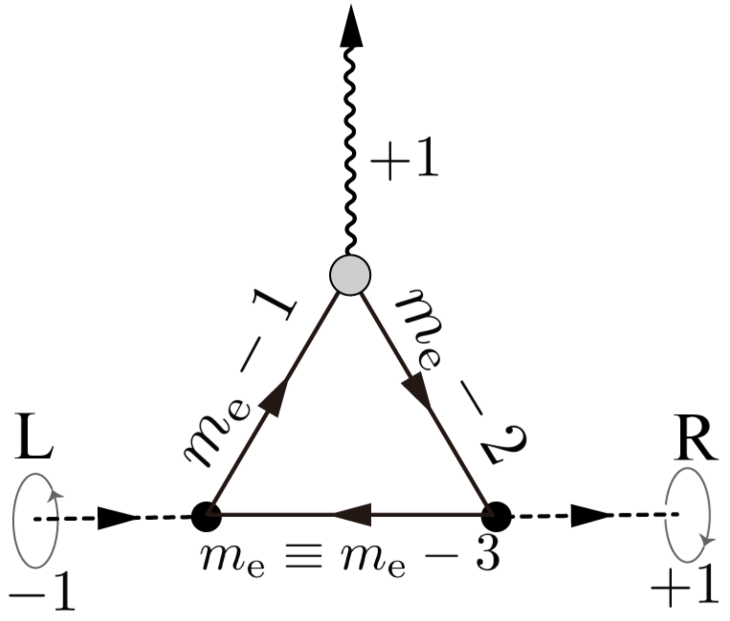
(Received 6 July 1970)

$$I_{kk'}{}^{\nu} = 2iq_0\sum_{\alpha} J(\vec{a}_{\alpha})\frac{\vec{a}_{\alpha}\cdot\vec{\epsilon}_{\alpha}{}^{\nu}}{a_{\alpha}}(\sin k_{\alpha}a_{\alpha}-\sin k_{\alpha}'a_{\alpha}).$$

Stokes Raman



Anti-Stokes Raman



All process reflect **CAM** conservation (modulo 3) at the vertex

nature physics

Quantum description of experimental findings

Letter

https://doi.org/10.1038/s41567-022-01790-x

Truly chiral phonons in α-HgS

Received: 30 September 2021

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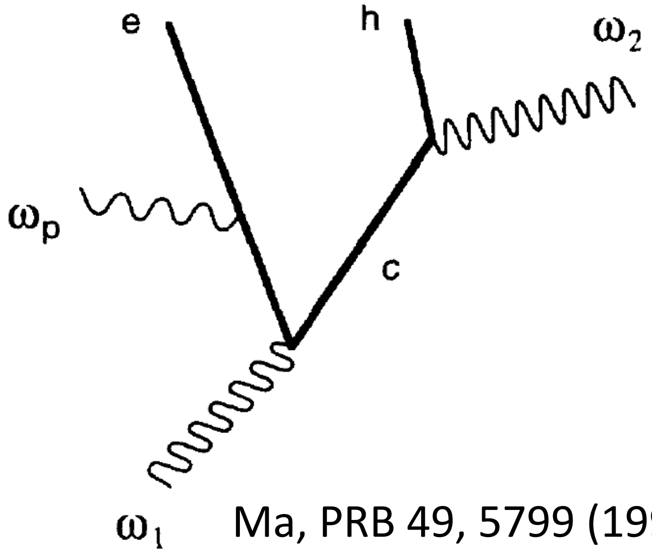
Kyosuke Ishito[1,7], Huiling Mao[1,7], Yusuke Kousaka[2,3], Yoshihiko Togawa[2], Satoshi Iwasaki[3], Tiantian Zhang[1,4], Shuichi Murakami[1,4], Jun-ichiro Kishine[5,6] & Takuya Satoh[1]

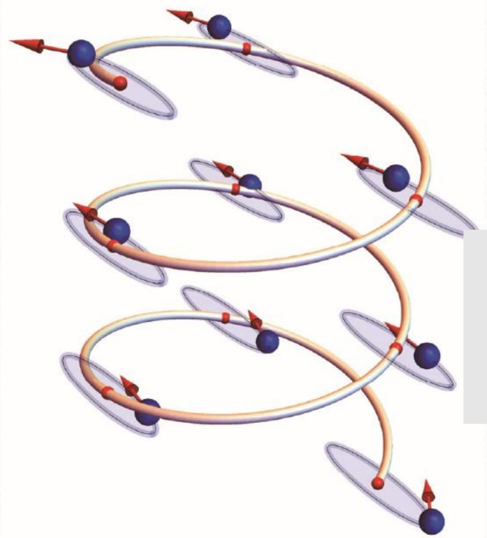
How about X-rays:?
Ueda et al., Nature (2023)



Ma, PRB 49, 5799 (1994)

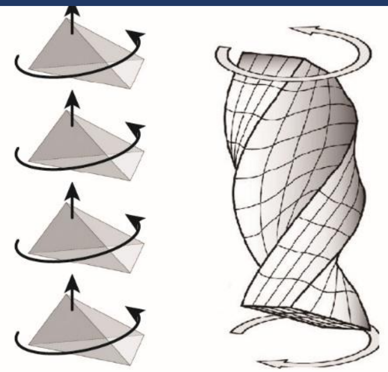
Sometimes, continuum field theory is useful

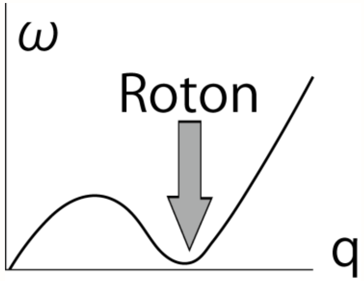
Chiral lattice vib.



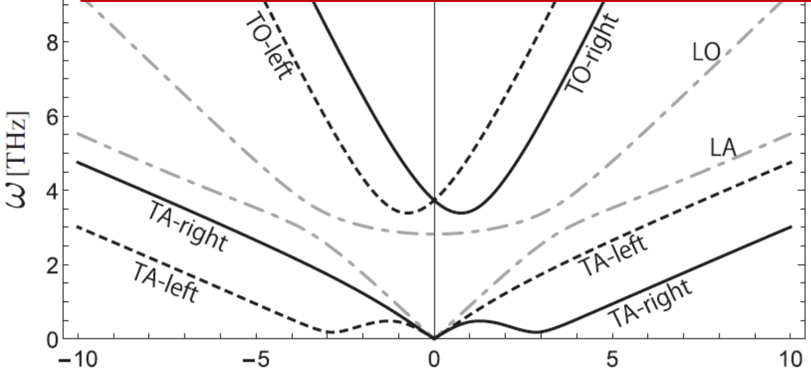
Micropolar elasticity theory

Chiral elastic wave



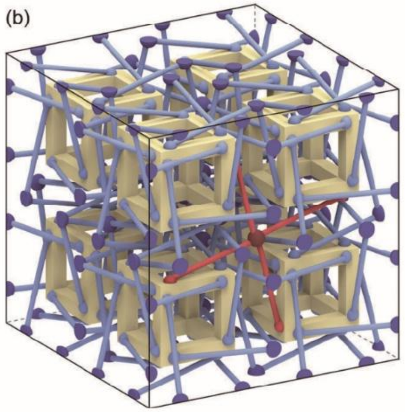


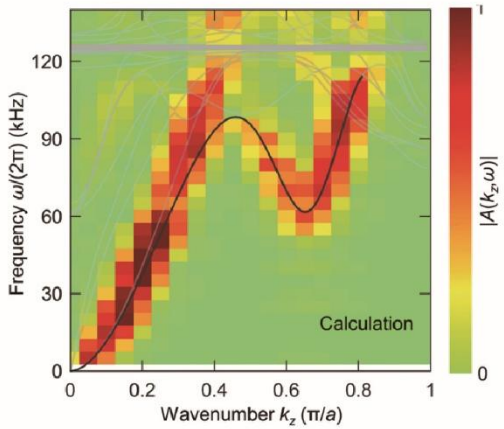
JK, A. S. Ovchinnikov, A. A. Tereshchenko,
Phys. Rev. Lett. 125, 245302 (2020)



Meta material

Chiral metamateroal





RESEARCH ARTICLE Adv. Funct. Mater. 2023, 2302699

ADVANCED FUNCTIONAL MATERIALS
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Observation of Chirality-Induced Roton-Like Dispersion in a 3D Micropolar Elastic Metamaterial

Yi Chen, Jonathan L. G. Schneider, Michael F. Groß, Ke Wang, Sebastian Kalt, Philip Scott, Muamer Kadic, and Martin Wegener**

Phonon: CAM to MAM

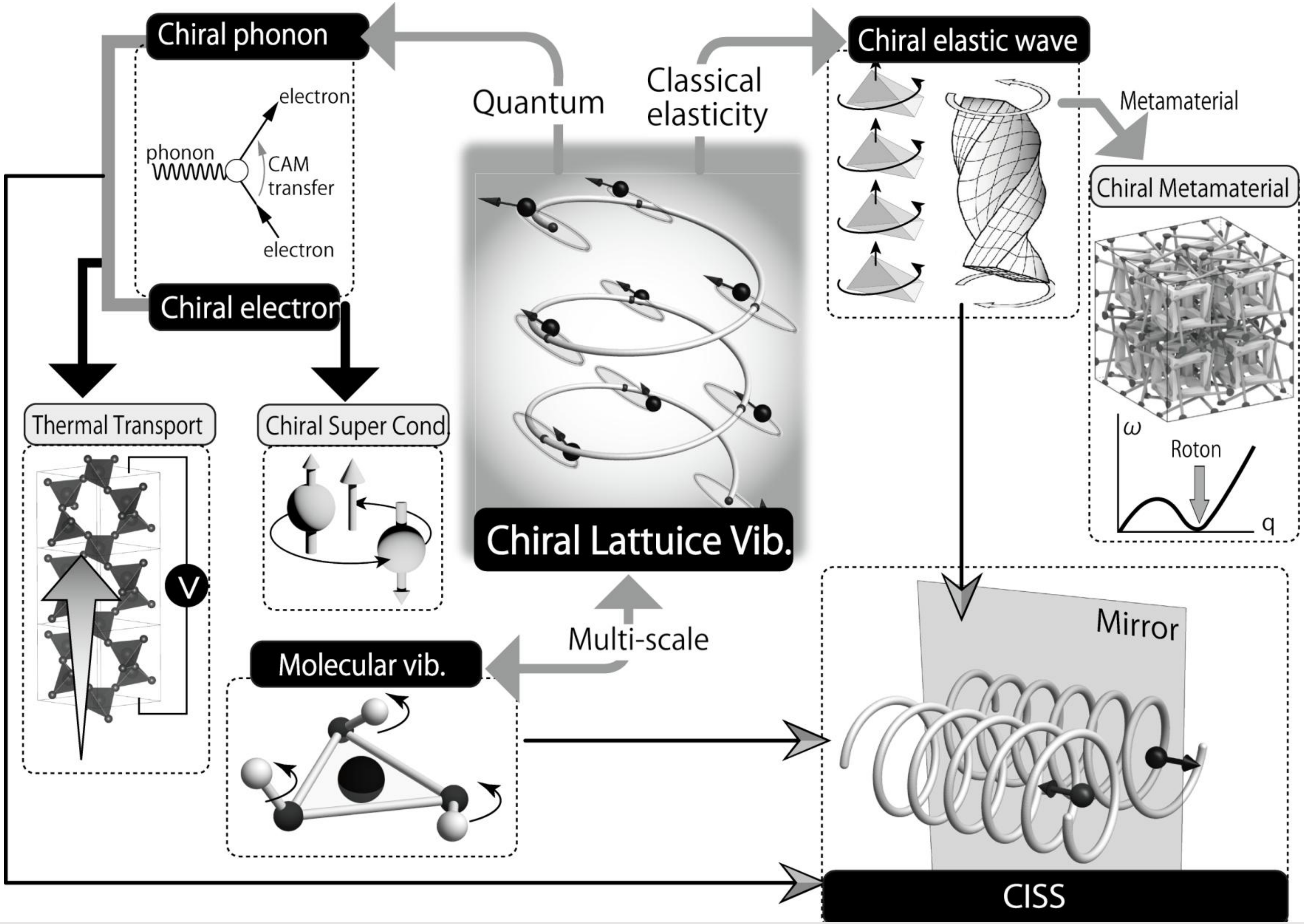
$\Downarrow$

Electron orbital

$\Downarrow$

Electron spin

Summary and Outlook: From Chiral Lattice Vibrations to Broader Phenomena



How to control chirality-selective cross-coupling based on "chiralization"