2026.3.12　第13回 統計物理学懇談会

カイラリティによって誘起されるスピンフォノン変換

東京大学　物性研究所
加藤岳生

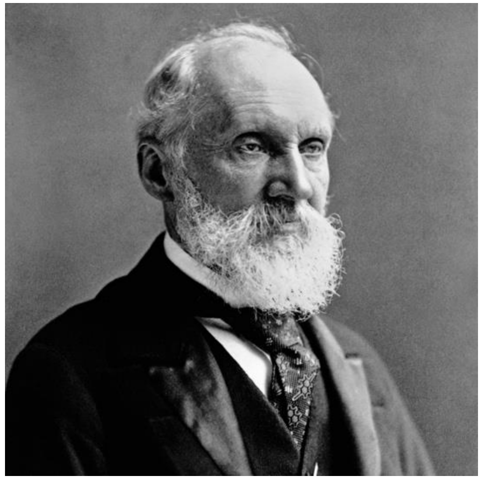
General Introduction

Thanks a lot!

Jun-Ichiro Kishine
(The Open University of Japan)

岸根順一郎（放送大学）

What is chirality?



Load Kelvin

1893

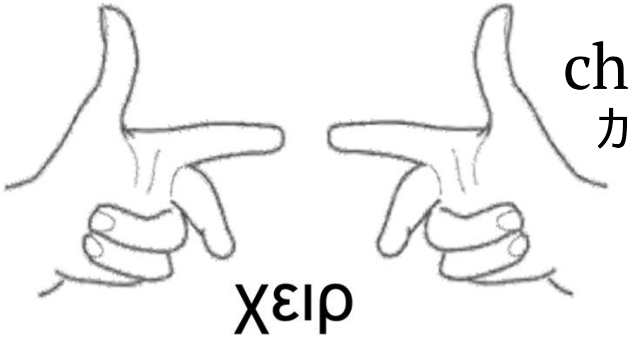
"... its image in a plane mirror, ideally realized, cannot be brought to coincide with itself."

Laurence Barron

1986

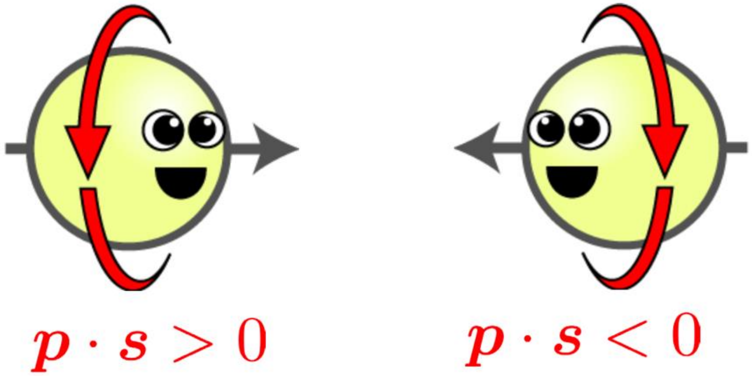
"The hallmark of a chiral system is that it can exhibit time-even pseudoscalar observables."

Truly chiral



cheir = hand
カイロ

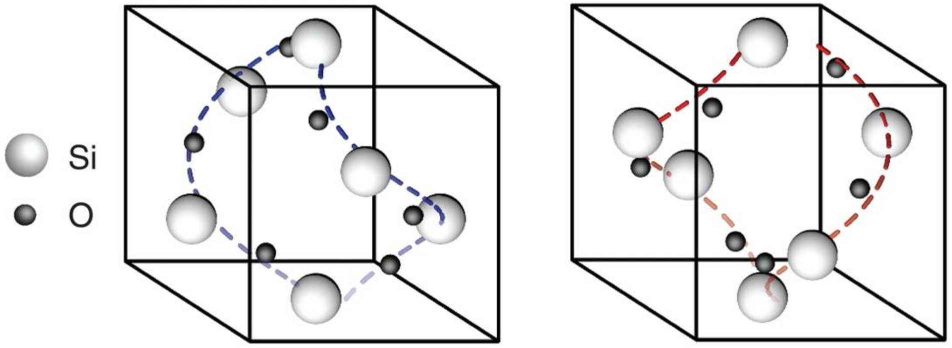
example:
Helicity



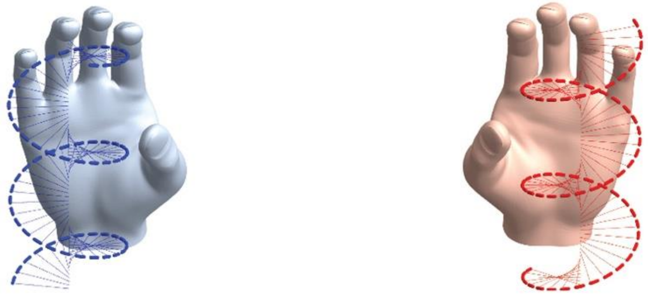
$\boldsymbol{p}\cdot\boldsymbol{s} > 0$ $\boldsymbol{p}\cdot\boldsymbol{s} < 0$

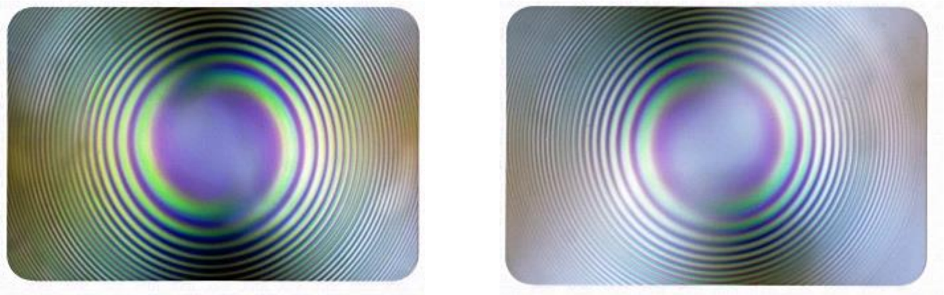
Structural chirality

SiO_2 (Quartz)

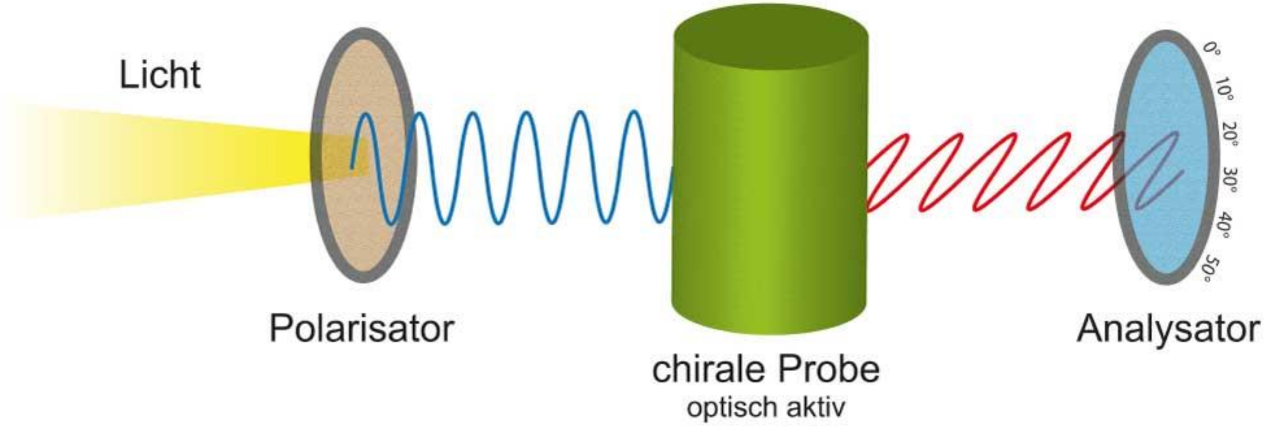


Right-handed α-Quartz   Left-handed α-Quartz





Natural optical activity



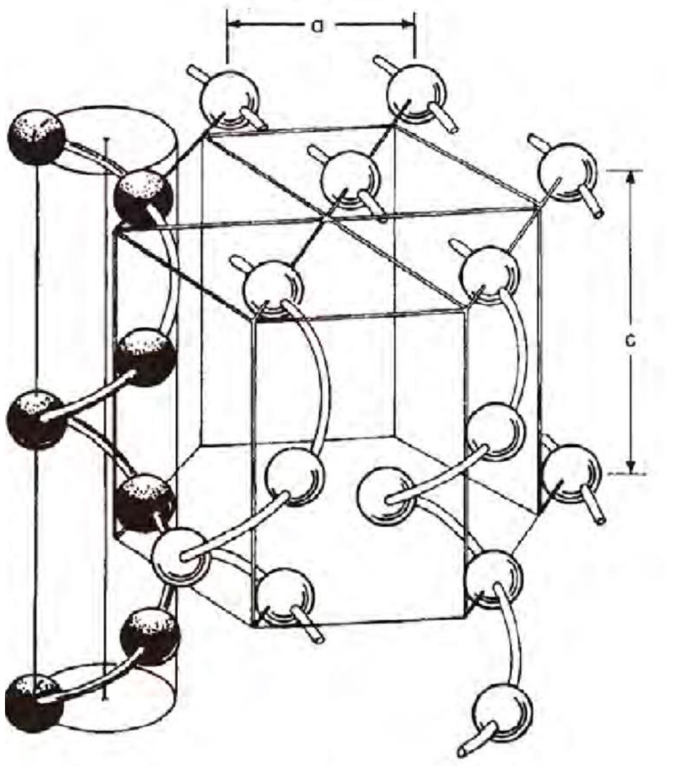
32 Crystallographic point groups

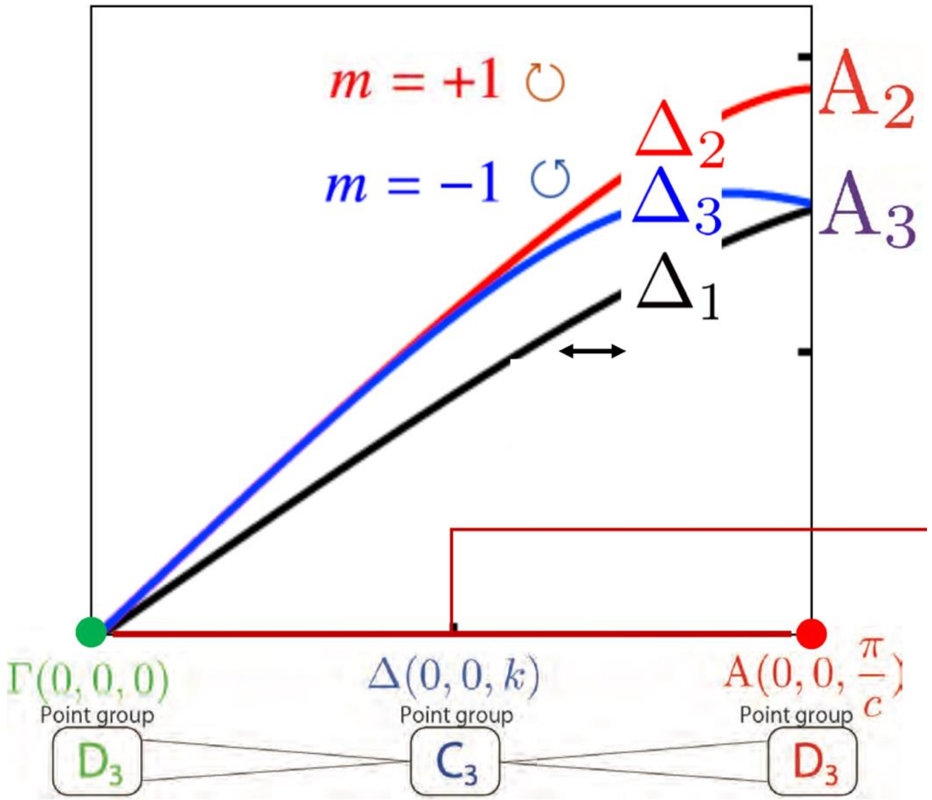
Cubic: O, T_d, T, T_h, O_h
Tetragonal: D_4, D_{2d}, C_{4v}, C_4, S_4, C_{4h}, D_{4h}
Orthogonal: D_2, C_{2v}, D_{2h}
Monoclinic: C_2, C_s, C_{2h}
Hexagonal: D_6, D_{3h}, C_{6v}, C_6, C_{3h}, C_{6h}, D_{6h}
Trigonal: D_3, C_{3v}, C_3, C_{3i}, D_{3d}
Triclinic: C_1, C_i

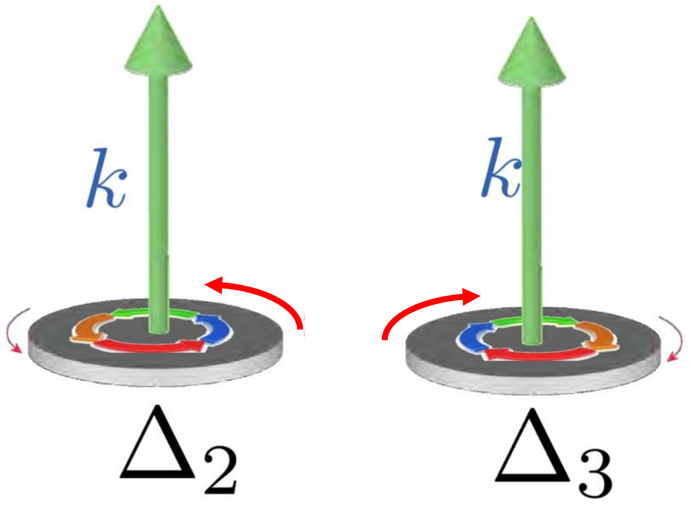
11 enantiomorphic point groups

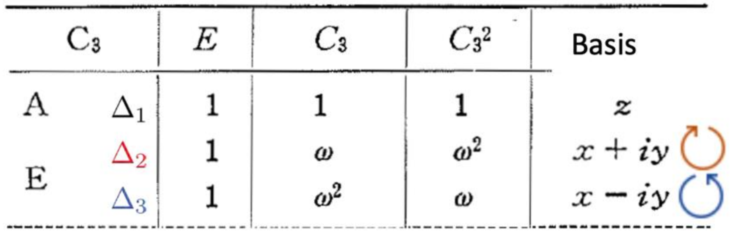
Dynamical chirality: chiral phonon

Example: Te









C_3		E	C_3	C_3^2	Basis
A	Δ_1	1	1	1	z
E	Δ_2	1	ω	ω^2	$x+iy$ ↻
	Δ_3	1	ω^2	ω	$x-iy$ ↺

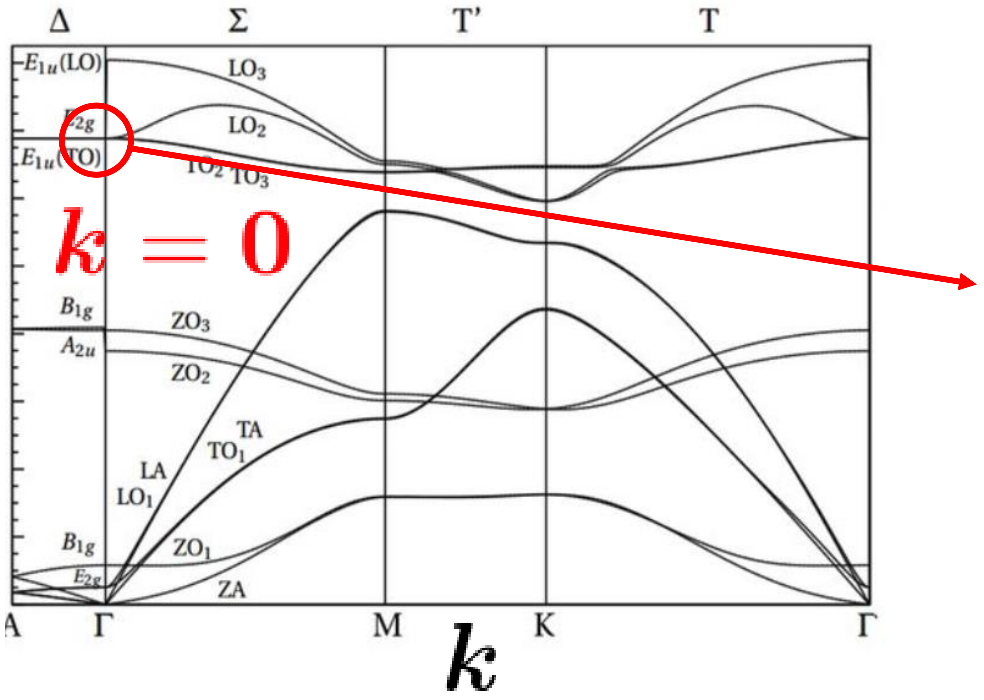
$\omega = \exp(-2\pi i/3)$

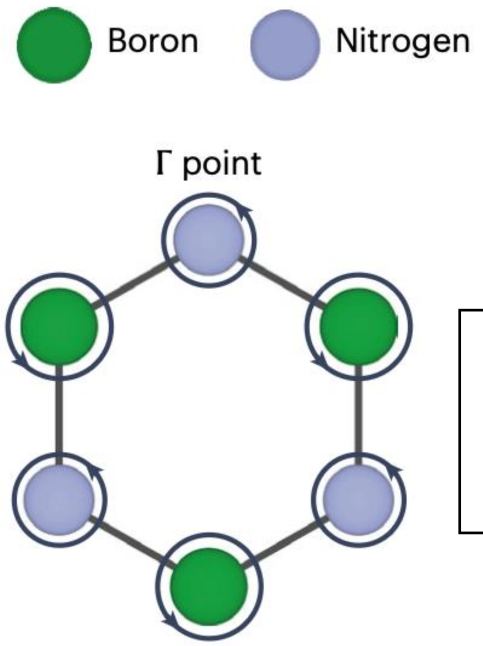
Pseudo angular momentum (PAM) from discrete rotational symmetry

I. Bozovic, Phys. Rev. B 84, 6586 (1984).

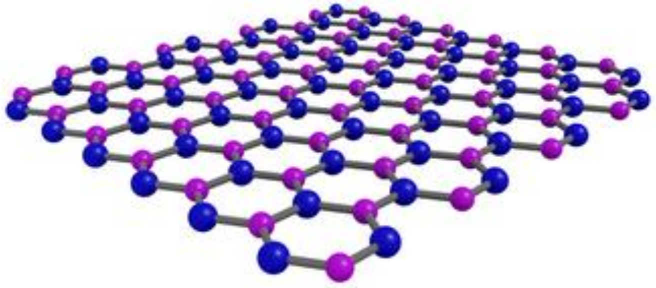
Phonon Angular Momentum

Example: BN atomic layer





Circular motion



Phonon angular momentum

$$\mathbf{J}_{\mathrm{ph}} = \sum_{l\alpha} m_\alpha \mathbf{u}_{l\alpha} \times \dot{\mathbf{u}}_{l\alpha},$$

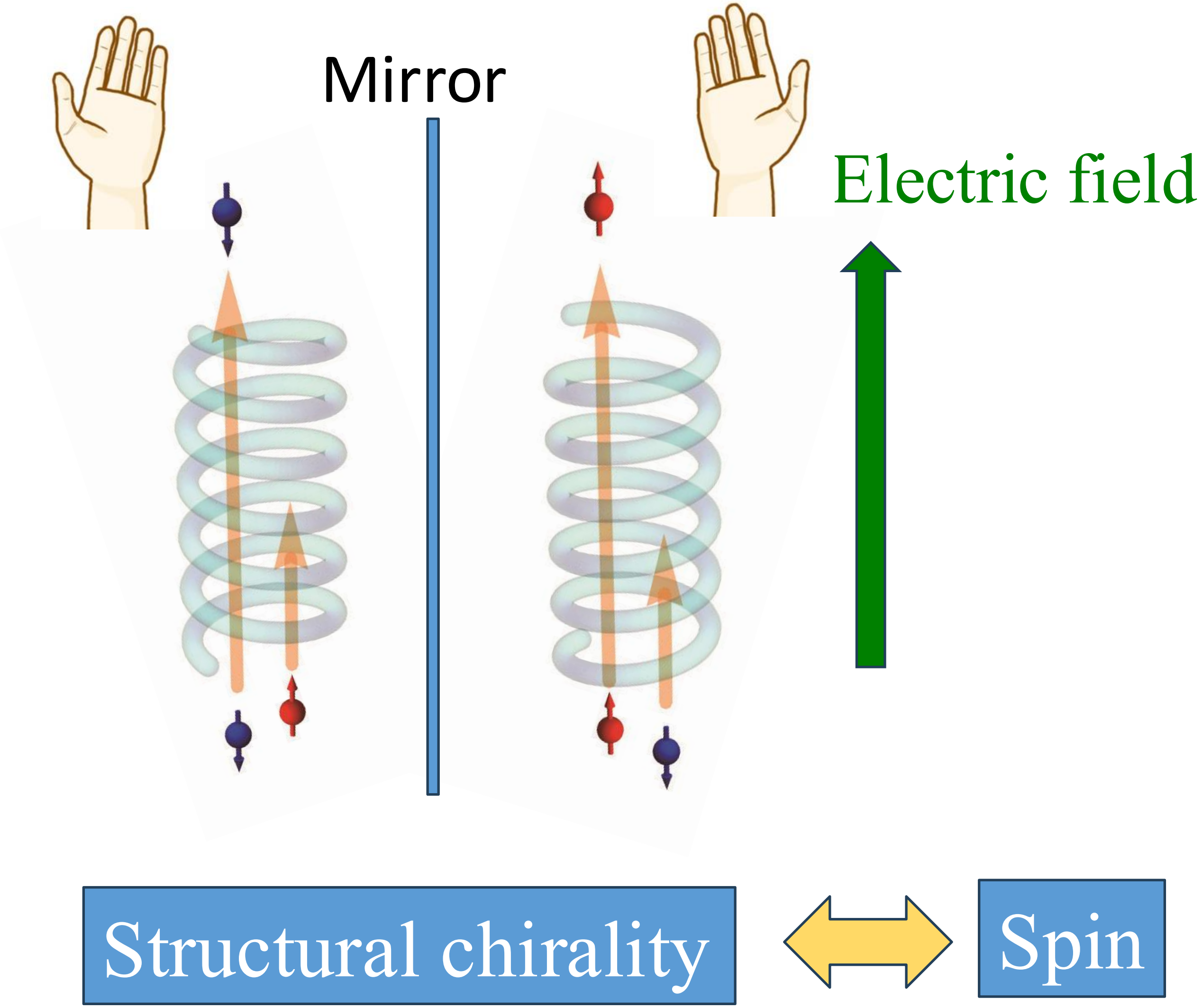
finite $\boldsymbol{J}_{\mathrm{ph}}$

≠ (truly) chiral phonon

[1962] S. V. Vonsovskii and M. S. Svirskii, Phonon Spin, Sov. Phys. Solid State 3, 1568 (1962).
[1962] A. T. Levine, A note concerning the spin of the phonon, Nuovo Cimento 26, 190 (1962).
[1984] Ivan Bozovic, Possible band-structure shapes of quasi-one-dimensional solids, PRB84, 6586 (1984).
[1988] A. G. McLellan, Angular momentum states for phonons, J. Phys. C Solid State Phys.21, 1177(1988).

[2014] L. Zhang and Q. Niu, Angular Momentum of Phonons and the Einstein–de Haas Effect, PRL 112, 085503 (2014).
[2015] L. Zhang and Q. Niu, Chiral Phonons at High-Symmetry Points in Monolayer Hexagonal Lattices, PRL115, 115502 (2015).

Introduction: Motivation



- Mechanism is unclear.
  - Spin-orbit (SO) interaction?
  - Chiral Phonons?
- Spin-rotation coupling (Micro Bernett effect)

⇩

No SO interaction is needed.
(Applicable to light elements)

1. Chiral-phonon/spin conversion at an interface of quartz (SiO_2)
2. Electron hopping in DNA

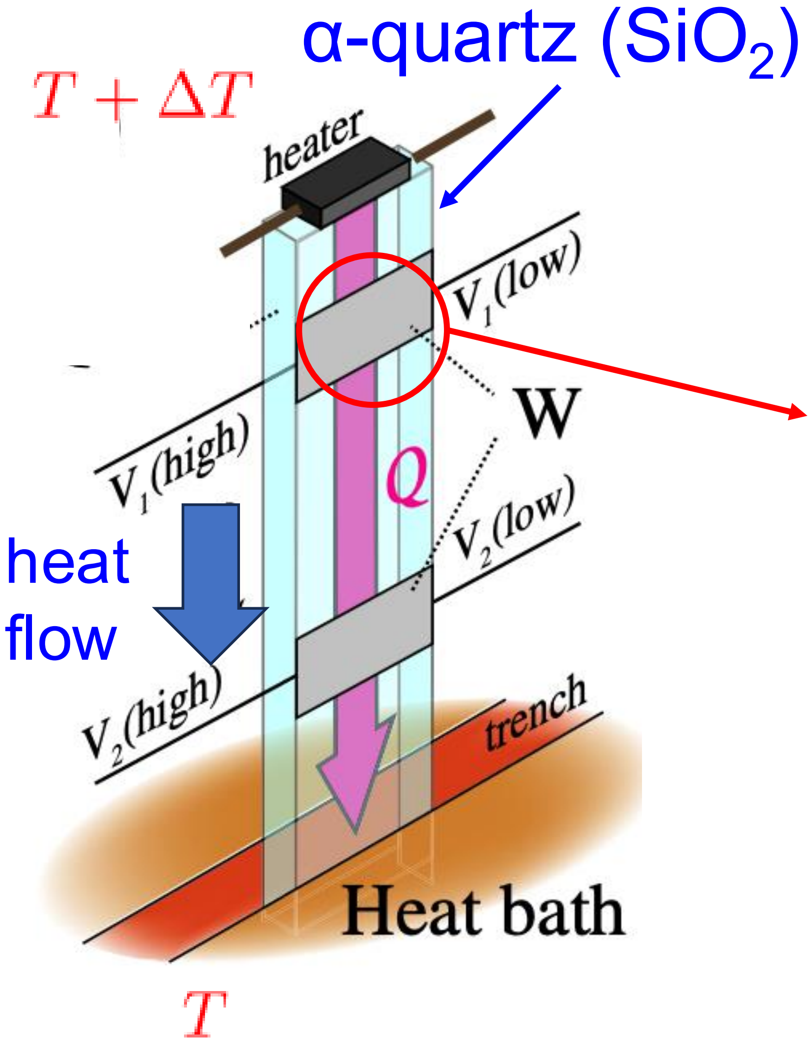
Takumi Funato
@JAEA（原研）

Mamoru Matsuo
@UCAS（北京）

Chiral phonon-spin conversion at an interface

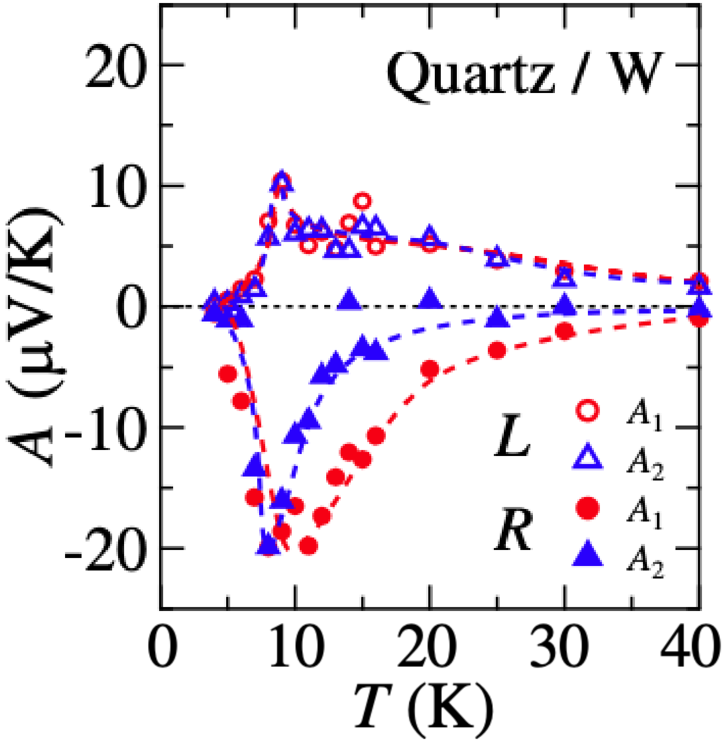
T. Funato, M. Matsuo, and T. Kato, Phys. Rev. Lett. **132**, 236201 (2024).

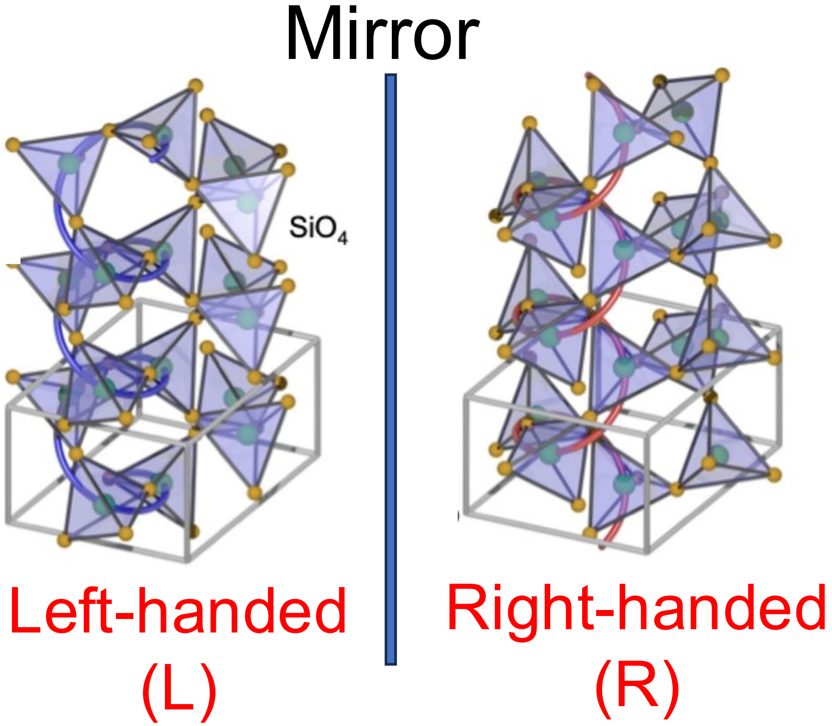
Phonon-Spin Conversion



Spin injection into W

(measured via inverse spin Hall effect at W)





α-quartz (SiO_2) is

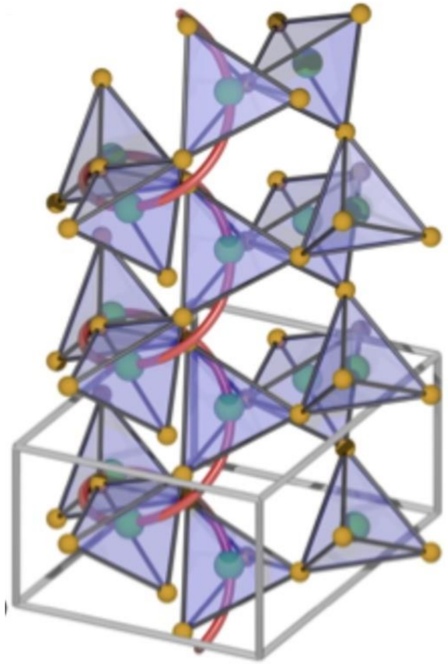
- ✓ band insulator
- ✓ non-magnetic
- ✓ no heavy elements

K. Ohe et al., Phys. Rev. Lett. **132,** 056302 (2024)

Phonon flow is converted into spins.

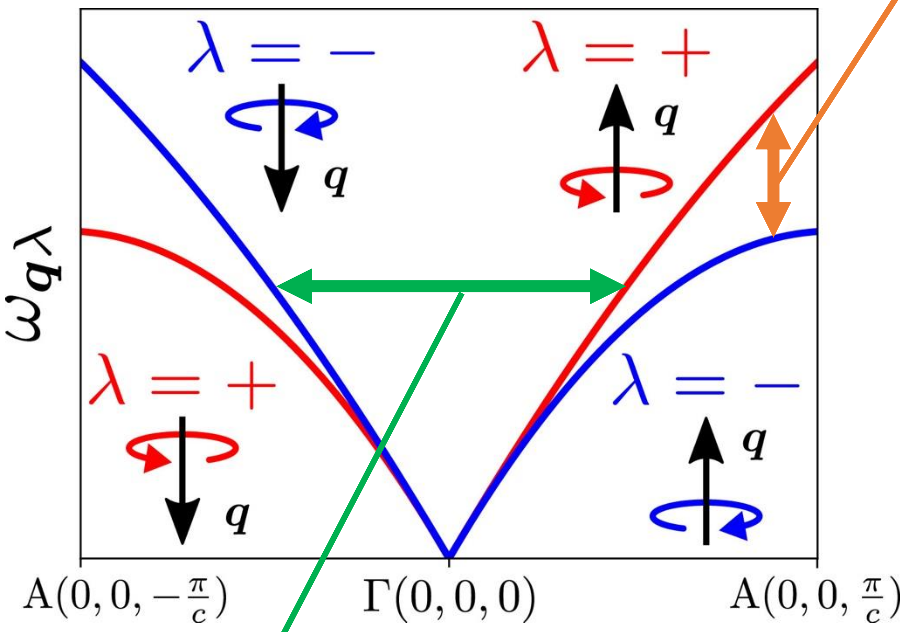
Chiral phonons

α-quartz (SiO_2)

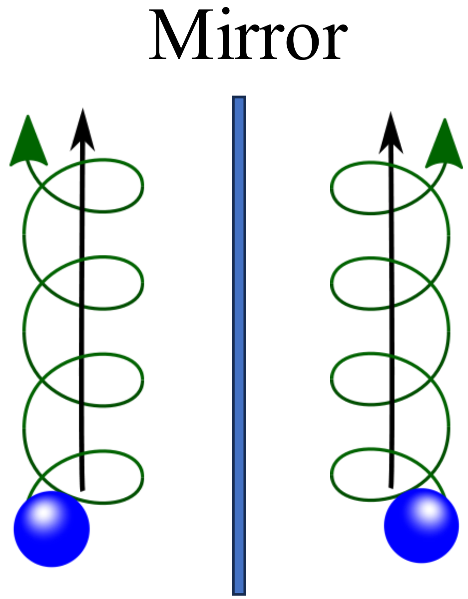


Chiral crystal structure

Phonon dispersion
(Transvers phonon)



No inversion symmetry



$$\omega_{\boldsymbol{q}\lambda} \neq \omega_{\boldsymbol{q}\bar{\lambda}}$$

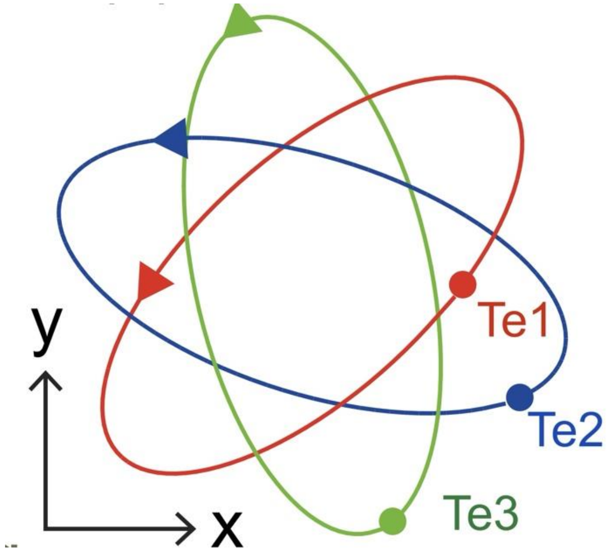
Time reversal symmetry

$$\omega_{\boldsymbol{q}\lambda} = \omega_{-\boldsymbol{q}\bar{\lambda}}$$

Main question: How chiral phonons are converted into spins?

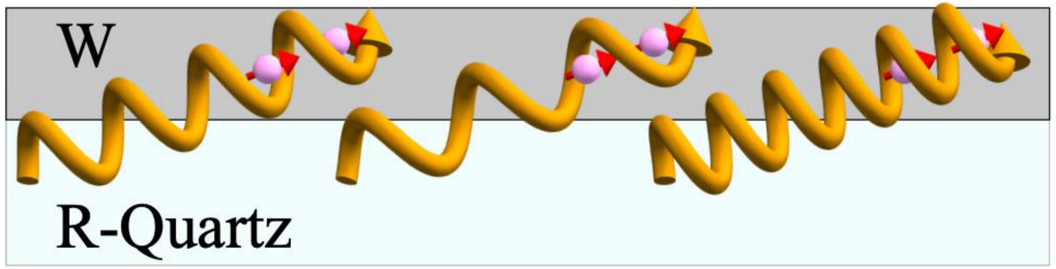
Theory of chiral-phonon spin conversion

$\boldsymbol{u}$: displacement



- ✓ Phonon angular momentum: $\propto \boldsymbol{u} \times \dot{\boldsymbol{u}}$
  Zhang-Niu, PRL **112**, 085503 (2014)
- ✓ Pseudo angular momentum
  Selection rule $m\hbar\,(m = 0, \pm 1)$
- ✓ Penetration of chiral modes + spin-orbit interaction
  Ohe et al., PRL **132**, 056302 (2024), Suzuki et al. PRB **107**, 115305 (2023)
  Yao-Murakami PRB **111**, 134414 (2025)
- ✓ Gyromagnetic effect (our study)

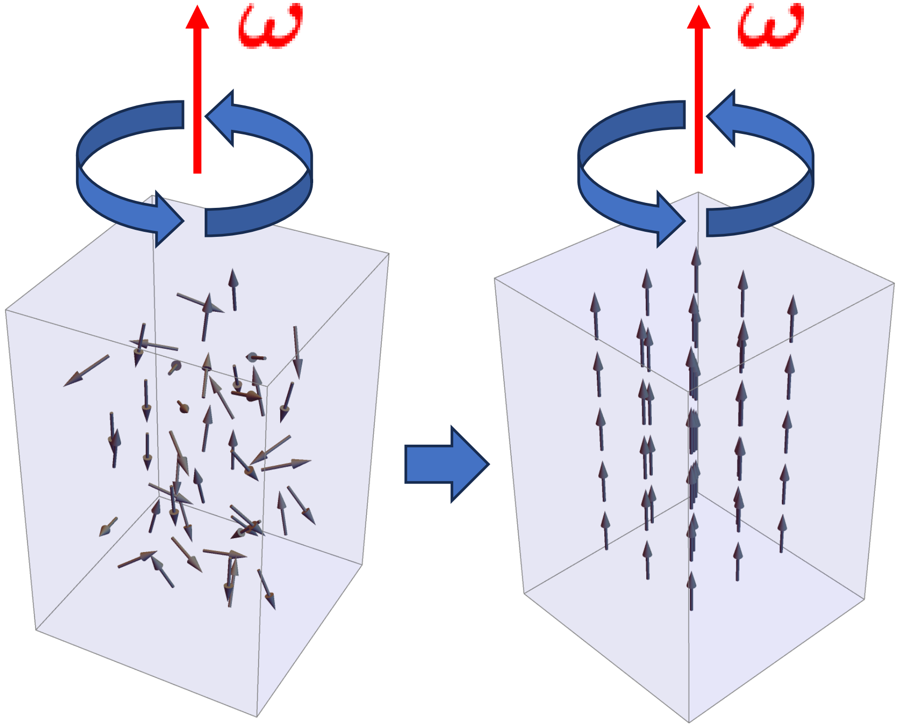
$$\boldsymbol{\Omega}(\boldsymbol{r}) = \nabla \times \dot{\boldsymbol{u}}(\boldsymbol{r})$$



Gyromagnetic Effect

Bernett effect

S.J. Barnett, PR 6, 239–270 (1915)



$$\mathcal{H}_{\mathrm{SR}} = -\boldsymbol{S}\cdot\boldsymbol{\omega}$$

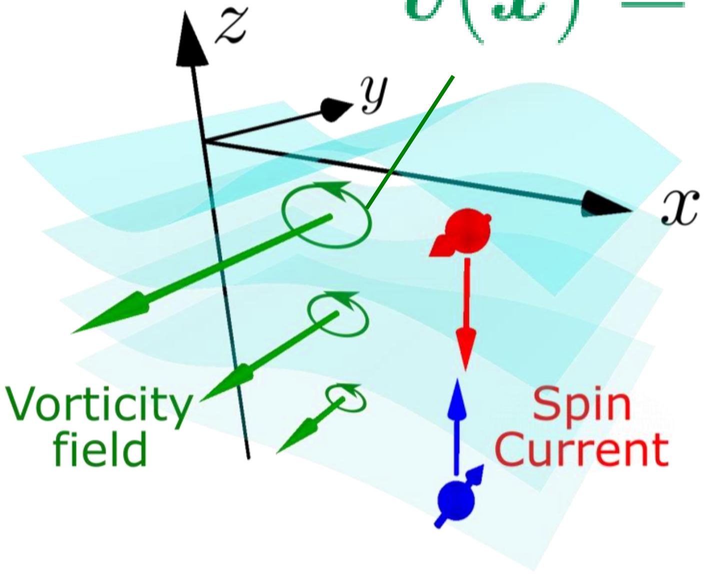
spin

angular velocity

Surface acoustic wave (SAW)

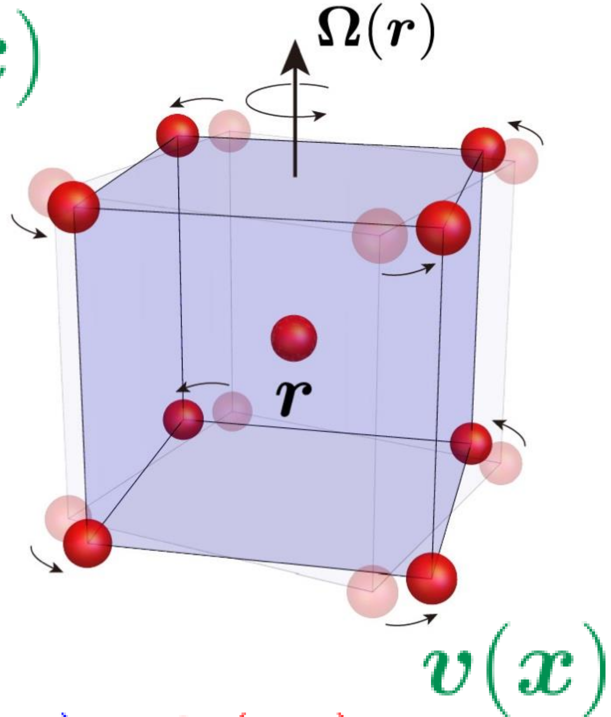
D. Kobayashi et al, PRL 119, 077202 (2017)

$$\boldsymbol{v}(\boldsymbol{x}) = \dot{\boldsymbol{u}}(\boldsymbol{x})$$



Chiral phonon

Our study



$$\mathcal{H}_{\mathrm{SR}} = -\frac{1}{2}\sum_i \boldsymbol{S}(\boldsymbol{x}_i)\cdot\boldsymbol{\Omega}(\boldsymbol{x}_i)$$

spin

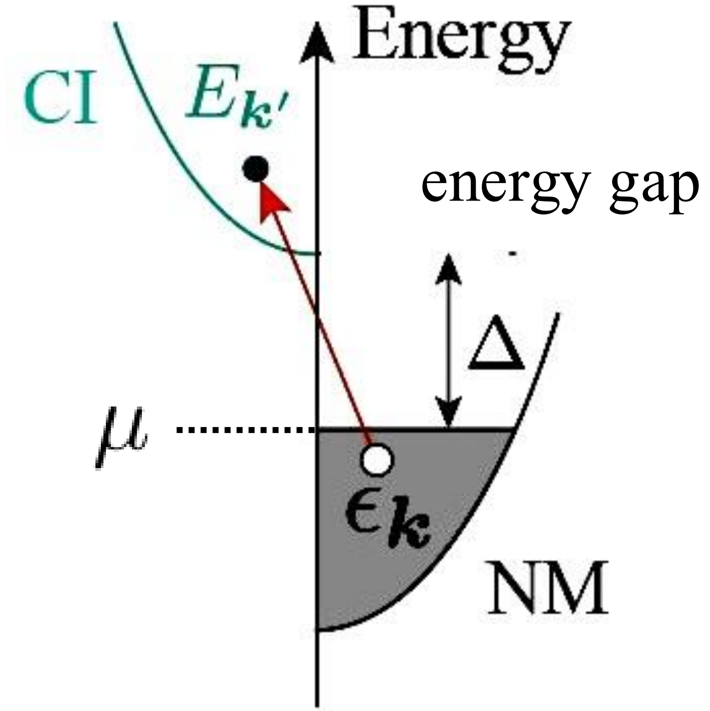
vorticity

$$\boldsymbol{\Omega}(\boldsymbol{x}) = \nabla\times\boldsymbol{v}(\boldsymbol{x})$$

velocity

Model

Hamiltonian: $\mathcal{H} = \mathcal{H}_{\mathrm{CI}} + \mathcal{H}_{\mathrm{NM}} + \mathcal{H}_{\mathrm{t}} + \mathcal{H}_{\mathrm{ph}} + \mathcal{H}_{\mathrm{SR}}$



Electrons in CI

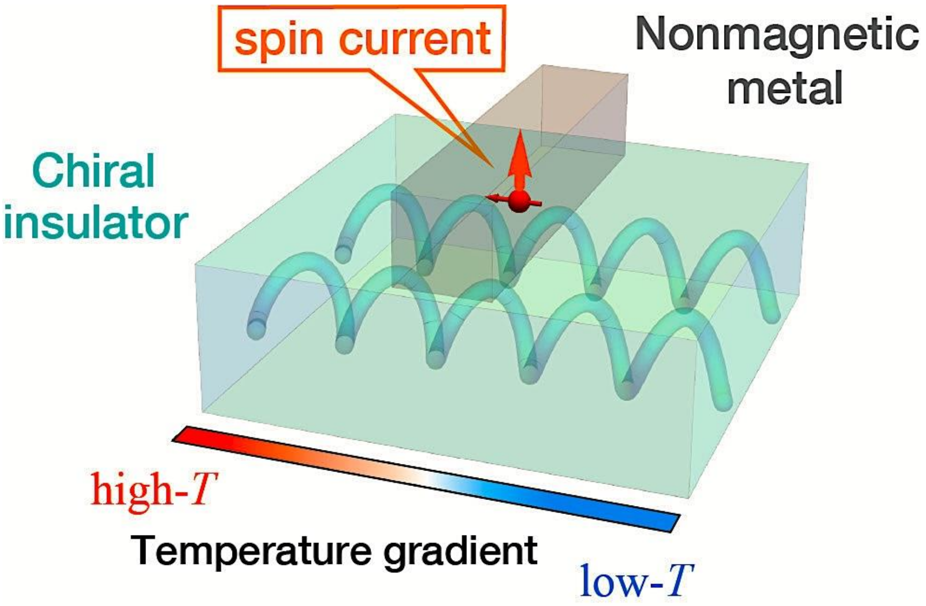
$$\mathcal{H}_{\mathrm{CI}} = \sum_{\boldsymbol{k}\sigma} E_{\boldsymbol{k}} d^{\dagger}_{\boldsymbol{k}\sigma} d_{\boldsymbol{k}\sigma}$$

Electrons in NM

$$\mathcal{H}_{\mathrm{NM}} = \sum_{\boldsymbol{k}\sigma} \epsilon_{\boldsymbol{k}} c^{\dagger}_{\boldsymbol{k}\sigma} c_{\boldsymbol{k}\sigma}$$

Interfacial tunneling

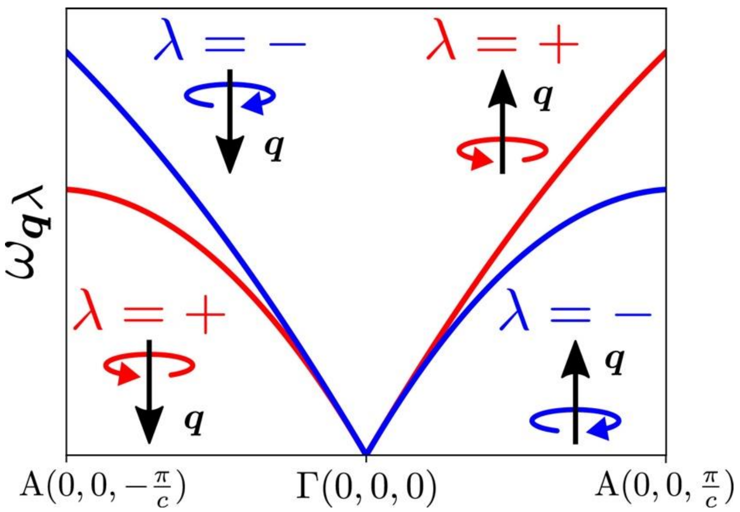
$$\mathcal{H}_{\mathrm{t}} = \sum_{\boldsymbol{k}\boldsymbol{k}'\sigma} \mathcal{T}_{\boldsymbol{k}',\boldsymbol{k}} d^{\dagger}_{\boldsymbol{k}'\sigma} c_{\boldsymbol{k}\sigma} + \mathrm{h.c}$$



Model

Hamiltonian: $\mathcal{H} = \mathcal{H}_{\mathrm{CI}} + \mathcal{H}_{\mathrm{NM}} + \mathcal{H}_{\mathrm{t}} + \mathcal{H}_{\mathrm{ph}} + \mathcal{H}_{\mathrm{SR}}$

Phonons in CI $\quad \mathcal{H}_{\mathrm{ph}} = \sum_{\boldsymbol{q}\lambda} \hbar\omega_{\boldsymbol{q}\lambda}(a^{\dagger}_{\boldsymbol{q}\lambda}a_{\boldsymbol{q}\lambda} + 1/2)$

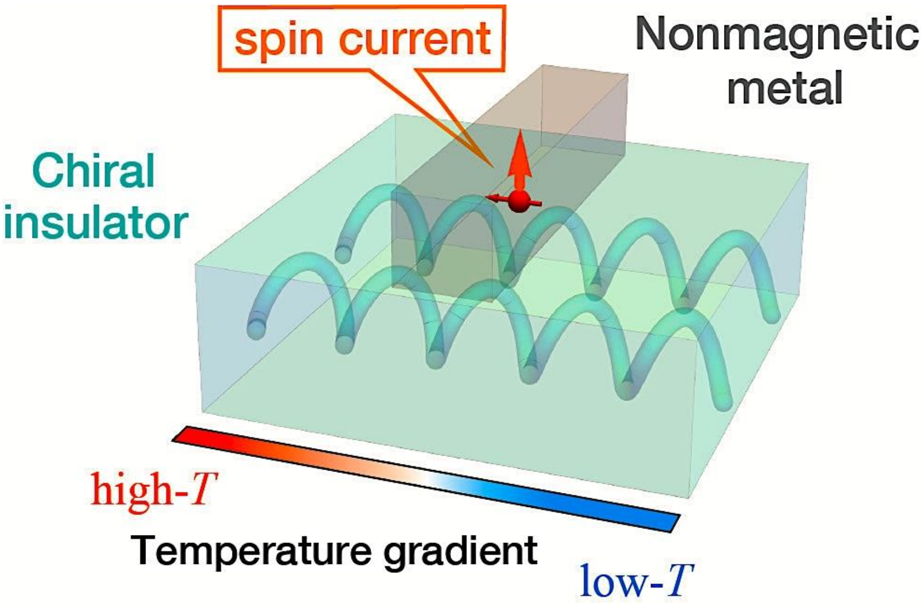


Time reversal

$$\omega_{\boldsymbol{q}+} = \omega_{-\boldsymbol{q}-}$$

Space inversion

$$\omega_{\boldsymbol{q}+} \neq \omega_{-\boldsymbol{q}+}$$



Spin-rotation coupling in CI

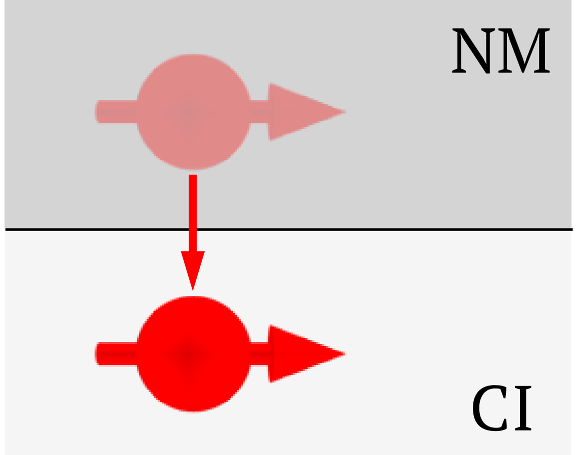
(Gyromagnetic effect)

$$\mathcal{H}_{\mathrm{SR}} = -\frac{\hbar}{2}\sum_{\boldsymbol{q}\lambda} \boldsymbol{S}_{-\boldsymbol{q}} \cdot \boldsymbol{\Omega}_{\boldsymbol{q}\lambda}$$

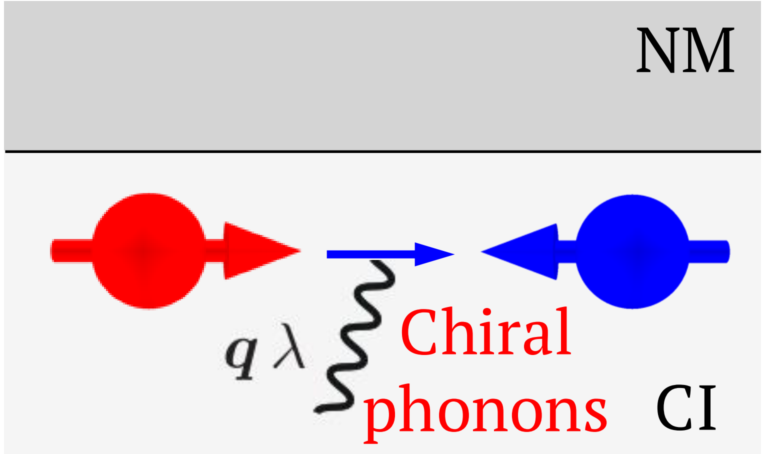
vorticity

Interfacial spin-phonon coupling

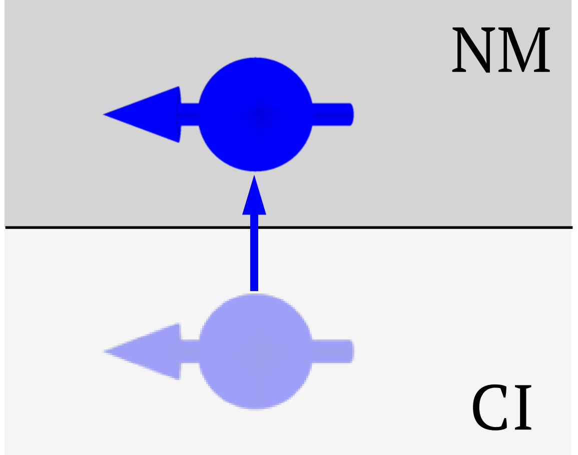
(1) Interfacial electron tunneling



(2) Spin-microrotation coupling in CI



(3) Interfacial electron tunneling



Interfacial spin-phonon coupling

$$\hat{\mathcal{H}}_{\text{e-ph}} = -\sum_{\boldsymbol{p}\boldsymbol{q}\lambda} \underbrace{J_{\boldsymbol{q},\boldsymbol{p}}}_{\text{Matrix element}} \Big(\underbrace{\Omega^{+}_{\boldsymbol{q}\lambda}}_{\text{Vorticity}} \hat{s}^{-}_{-\boldsymbol{p}} + \Omega^{-}_{-\boldsymbol{q}\bar{\lambda}} \underbrace{\hat{s}^{+}_{\boldsymbol{p}}}_{\text{Electron spin in NM}} \Big),$$

$$\hat{s}^{\pm}_{\boldsymbol{p}} = \hat{s}^{x}_{\boldsymbol{p}} \pm i\hat{s}^{y}_{\boldsymbol{p}}$$

$$\hat{s}^{\alpha}_{\boldsymbol{p}} = \frac{1}{2}\sum_{\boldsymbol{k}\sigma\bar{\sigma}} c^{\dagger}_{\boldsymbol{k}-\boldsymbol{p}\sigma}\sigma^{\alpha}_{\sigma\bar{\sigma}}c_{\boldsymbol{k}\bar{\sigma}}$$

$$\Omega^{\pm}_{\boldsymbol{q}\lambda} = \Omega^{x}_{\boldsymbol{q}\lambda} \pm \Omega^{y}_{\boldsymbol{q}\lambda}$$

Spin current (main result)

$$\langle \hat{I}_s^z \rangle \propto \sum_{\boldsymbol{q}\lambda} \omega^2_{\boldsymbol{q}\lambda} (\boldsymbol{q}\cdot\hat{\boldsymbol{z}})[\boldsymbol{q}\cdot \mathrm{Im}\,(\boldsymbol{e}^*_{\boldsymbol{q}\lambda}\times \boldsymbol{e}_{\boldsymbol{q}\lambda})]\left[f^{\mathrm{ph}}_{\boldsymbol{q}\lambda}(\omega_{\boldsymbol{q}\lambda}) - f_0(\omega_{\boldsymbol{q}\lambda})\right]$$

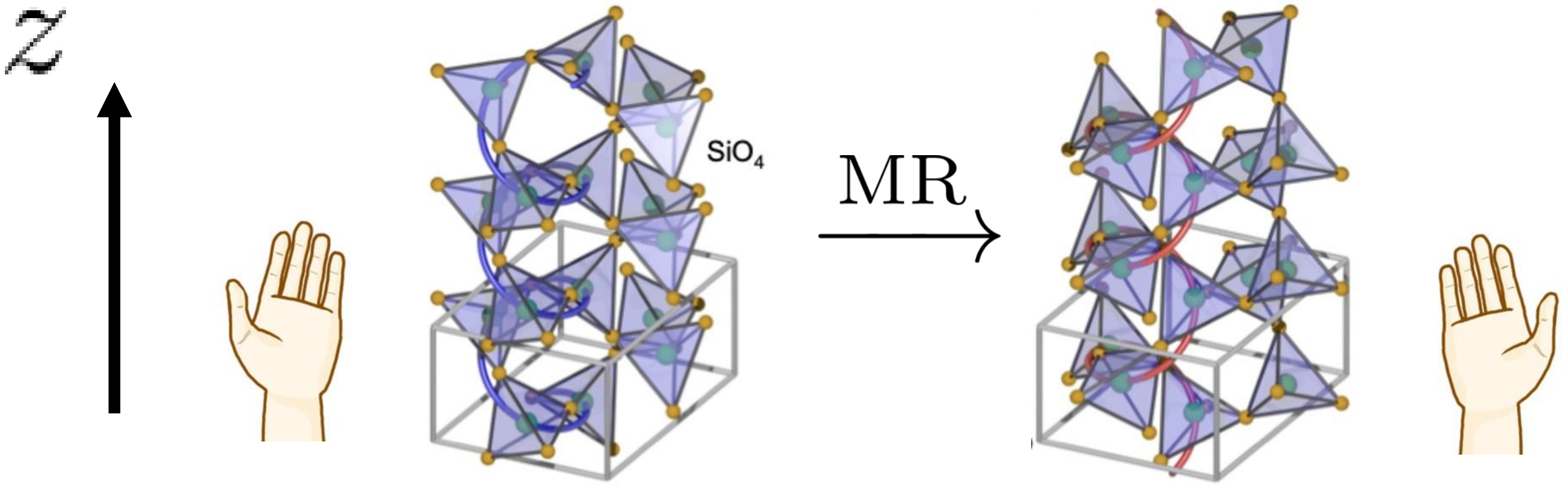
pseudo-scalar (chirality)

Mirror Reflection (MR)

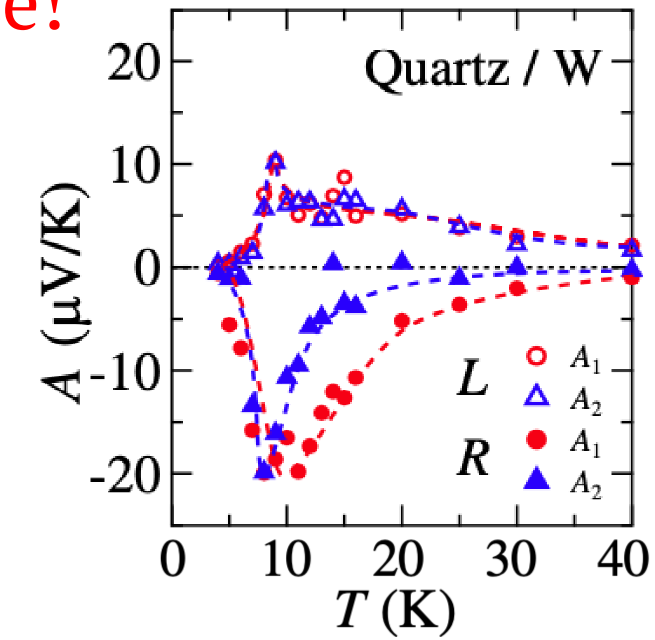
$$\boldsymbol{q}\cdot \mathrm{Im}\,(\boldsymbol{e}^*_{\boldsymbol{q}\lambda}\times \boldsymbol{e}_{\boldsymbol{q}\lambda}) \xrightarrow{\mathrm{MR}} -\,\boldsymbol{q}\cdot \mathrm{Im}\,(\boldsymbol{e}^*_{\boldsymbol{q}\lambda}\times \boldsymbol{e}_{\boldsymbol{q}\lambda})$$

$$\langle \hat{I}_s^\alpha \rangle \xrightarrow{\mathrm{MR}} -\langle \hat{I}_s^\alpha \rangle$$

Reverse!



Experiment



Spin current (main result)

$$\langle \hat{I}_s^z \rangle \propto \sum_{\boldsymbol{q}\lambda} \omega_{\boldsymbol{q}\lambda}^2 (\boldsymbol{q}\cdot\hat{\boldsymbol{z}})[\boldsymbol{q}\cdot \mathrm{Im}\,(\boldsymbol{e}^*_{\boldsymbol{q}\lambda}\times \boldsymbol{e}_{\boldsymbol{q}\lambda})]\left[f^{\mathrm{ph}}_{\boldsymbol{q}\lambda}(\omega_{\boldsymbol{q}\lambda}) - f_0(\omega_{\boldsymbol{q}\lambda})\right]$$

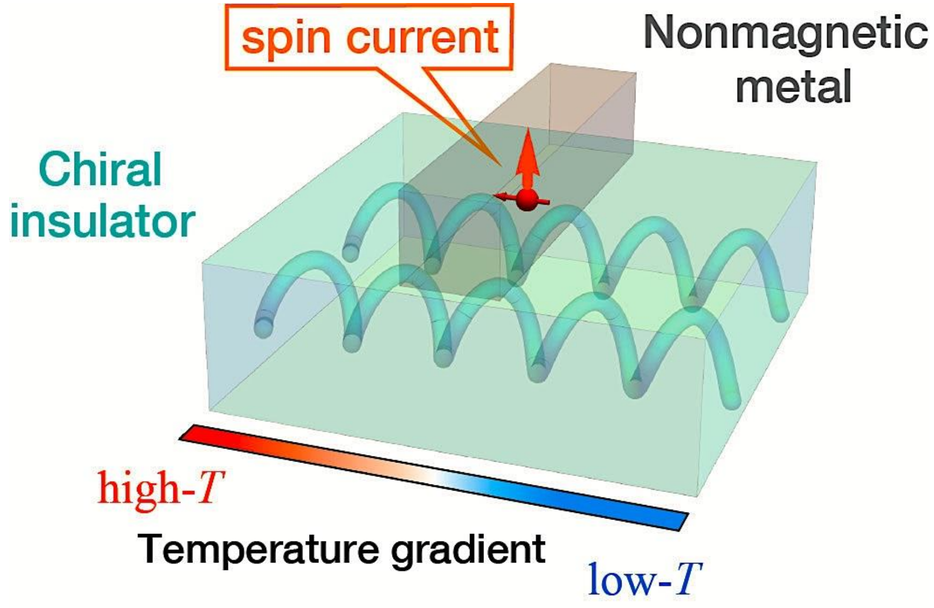
nonequilibrium distribution of phonons

Boltzmann equation

$$\boldsymbol{v}_{\boldsymbol{q}\lambda}\cdot\nabla f^{\mathrm{ph}}_{\boldsymbol{q}\lambda} = \frac{f^{\mathrm{ph}}_{\boldsymbol{q}\lambda} - f_0}{\tau_{\boldsymbol{q}\lambda}}$$

Velocity of phonons

Momentum relaxation



Parameters

Relaxation time: $\tau = 10^{-10}\mathrm{s}$

DOS of NM: $\nu_F = 10^{-2}\mathrm{eV}^{-1}$

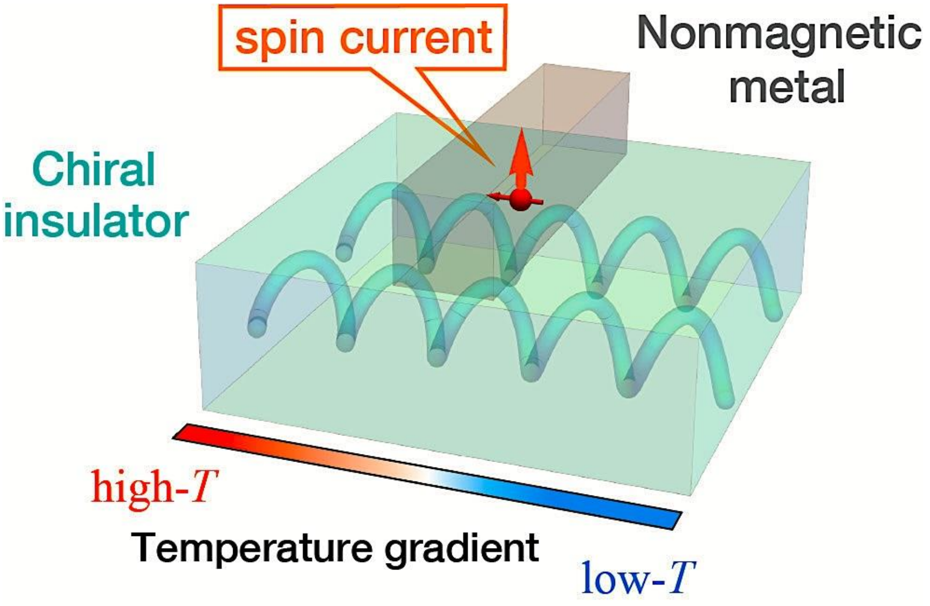
Interfacial hopping : $|T|/\Delta = 1/20$

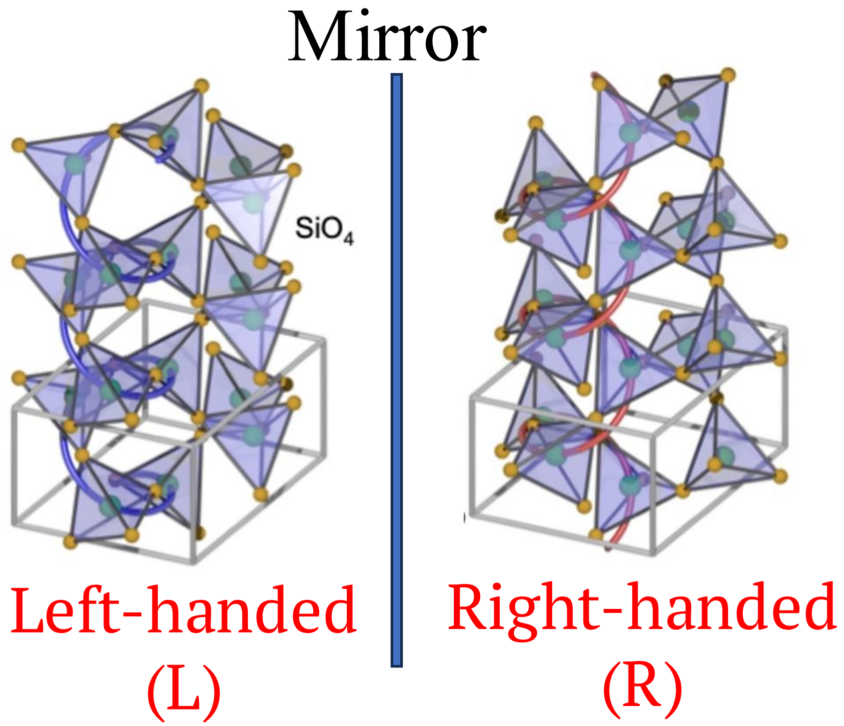
$$\langle \hat{I}_s^z \rangle \sim 10^2\,\mathrm{nA}$$

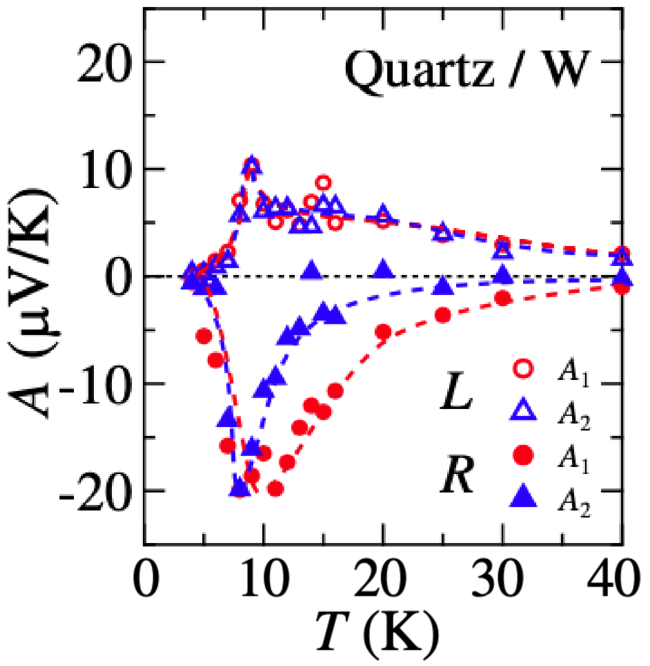
Observable!

Summary (the first part)

- ✓ Spin current is calculated from microscopic Hamiltonian of chiral phonons via spin-rotation coupling.
- ✓ The estimated spin current is consistent with the experiment.
- ✓ This study provides a comprehensive viewpoint for the CISS effect.







T. Funato, M. Matsuo, and T. Kato, Phys. Rev. Lett. **132**, 236201 (2024).

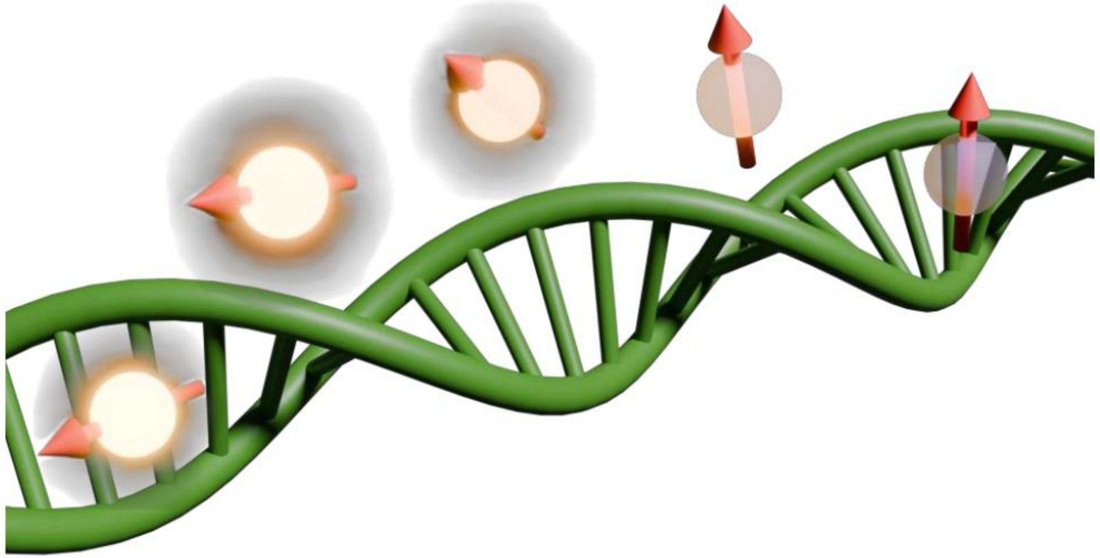
佐野涼太郎 助教
（物性研加藤研究室）

Hopping transport in DNA

R. Sano and T. Kato, arXiv:2404.19000

Chirality-Induced Spin Selectivity (CISS) in DNA

[B. Göhler *et al.*, Science (2011)]
[Z. Xie *et al.*, Nano Lett. (2011)]

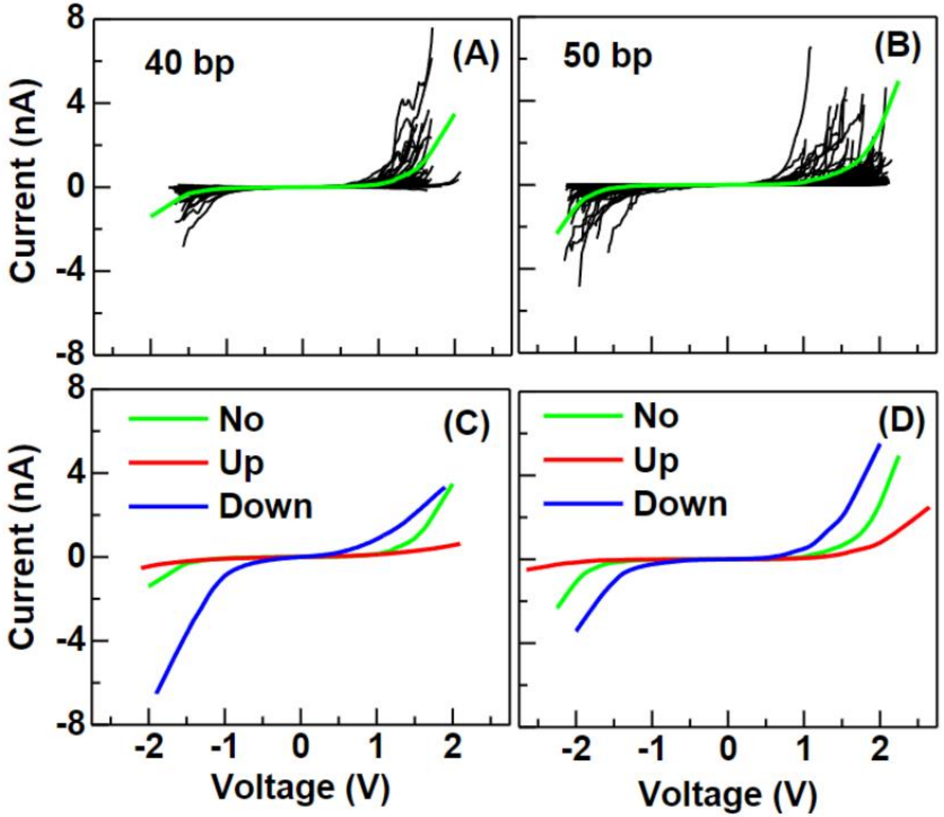


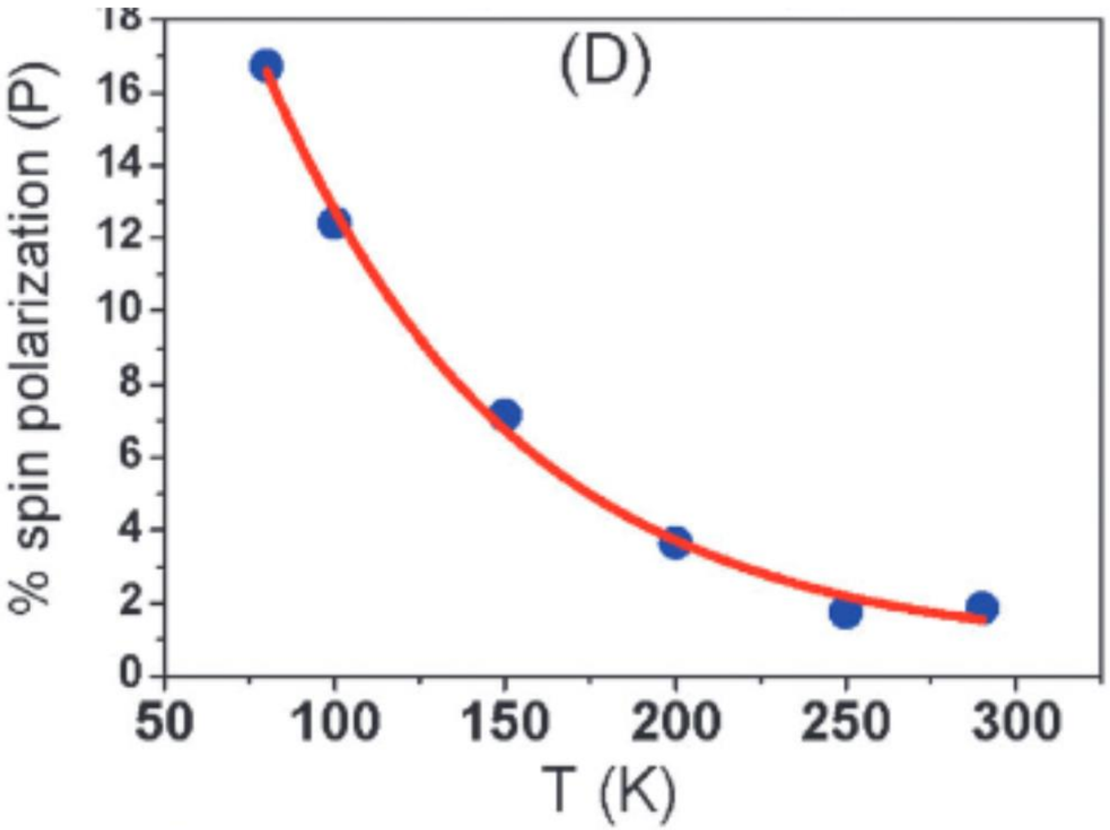
- ➢ Organic Spintronics
- ➢ Enantiomer Separation
- ➢ Clues to the homochirality
- ➢ Quantifying Chirality

「Spin aligns with ascending the spiral stairs」

- No need of magnets/magnetic field & SOC
- Multiscaleness: from DNA to Solids
- Non-Equilibrium Phenomena

To know the mechanism of unknown phenomena
☞ Investigate its Temperature dependence



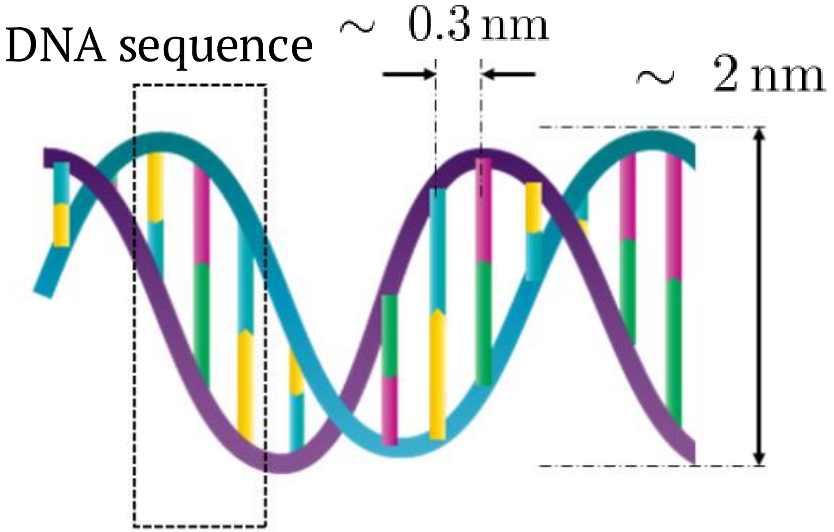


[R. Naaman, Waldeck, Annu. Rev. Phys. Chem. (2015)]
[K. S. Kumar *et al*., Phys. Chem. Chem. Phys. (2013)]
[S. Alwan *et al*., J. Chem. Phys. (2023)]

✓ Spin polarization increases
@ Low temperature

Summary of our study

Anderson localization



$$\mathcal{H} = -t\sum_i (c^\dagger_{i+1\sigma}c_{i\sigma} + \mathrm{h.c.}) + \sum_i \epsilon_i c^\dagger_{i\sigma}c_{i\sigma}$$

$$+\frac{\hbar}{2}\sum_i\sum_{\sigma,\sigma'} c^\dagger_{i\sigma}(\boldsymbol{\sigma})_{\sigma\sigma'}c_{i\sigma'} \cdot \boldsymbol{\Omega}_i$$

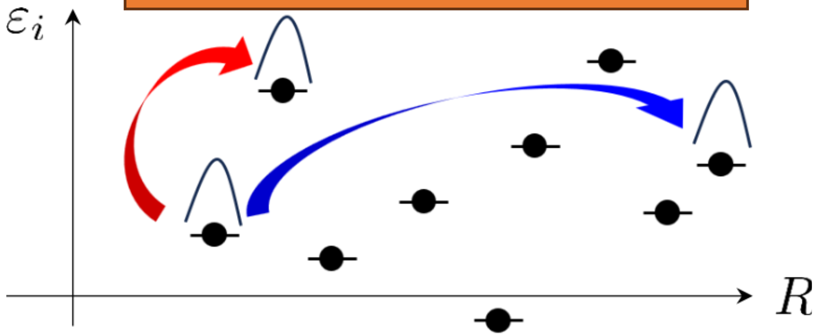
$\boldsymbol{S}_i$

random potential

vorticity (phonon)

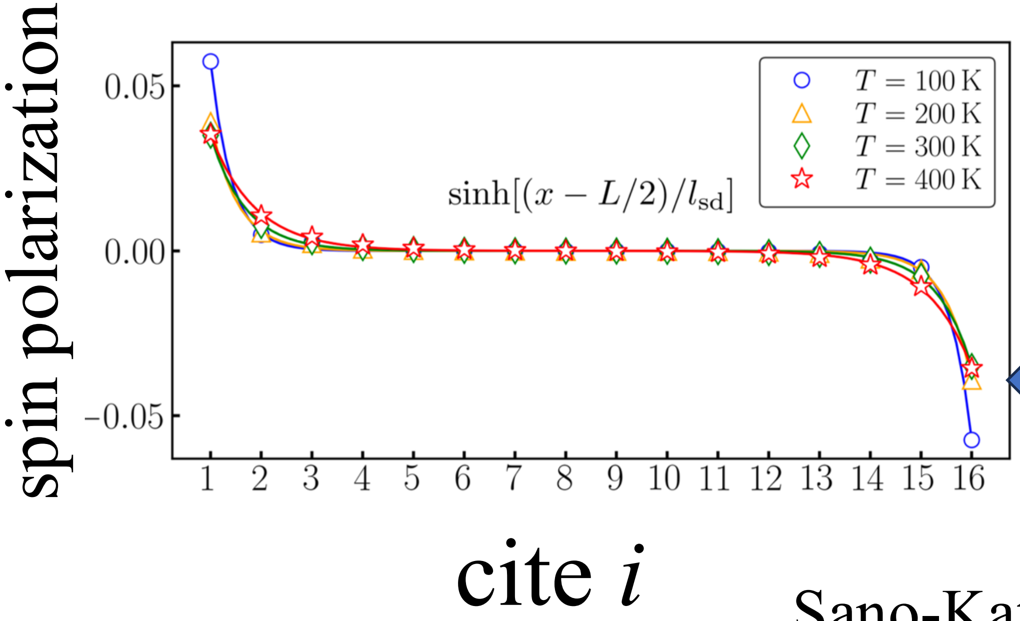
spin-rotation coupling

Hopping transport



Hop into NN sites @ High T

Hop into remote sites @ Low T



At low-T

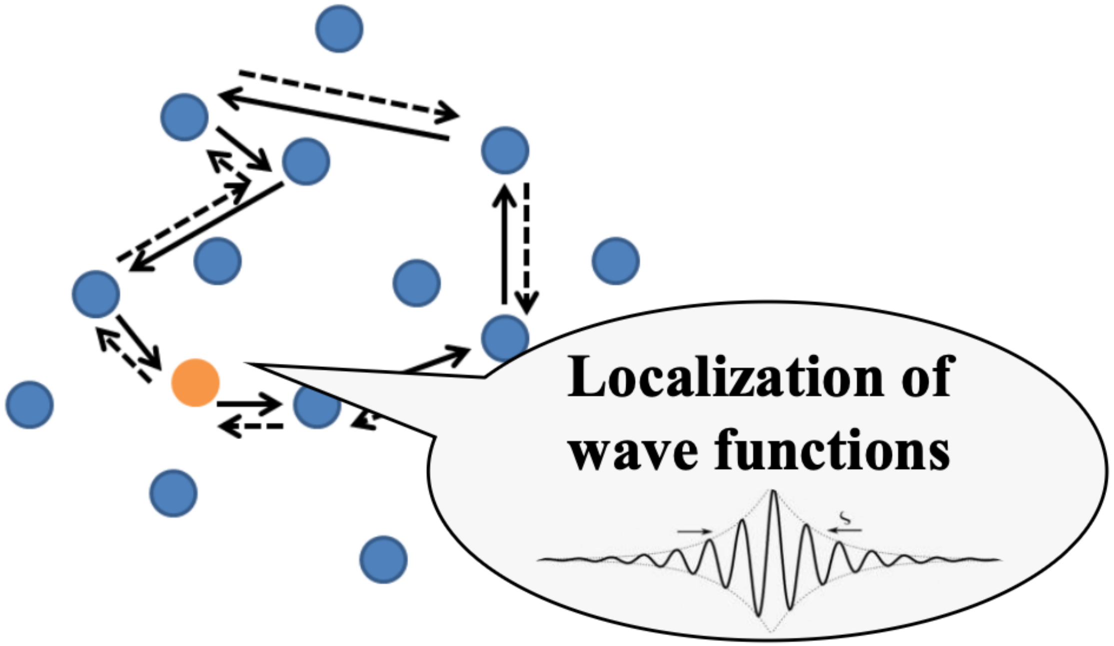
$> 10\,\%$

Sano-Kato, arXiv:2404.19000

Variable-Range Hopping (VRH)

A transport mechanism specific to strongly disordered systems

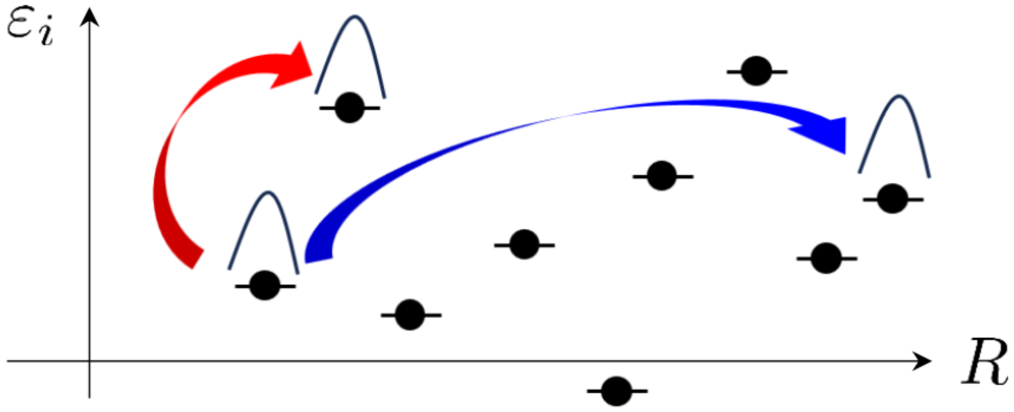
$T = 0$



Localization of wave functions

"Phase interference effects"
in random systems

$T \neq 0$

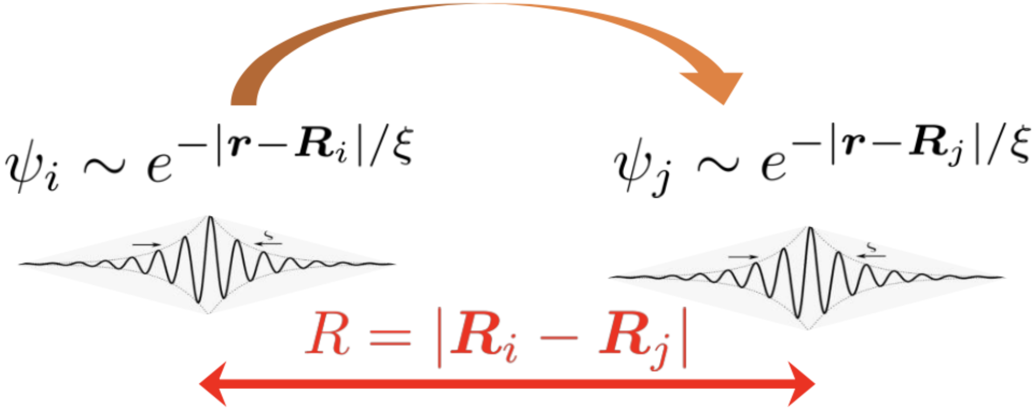


Hop into NN sites @ High *T*
Hop into remote sites @ Low *T*

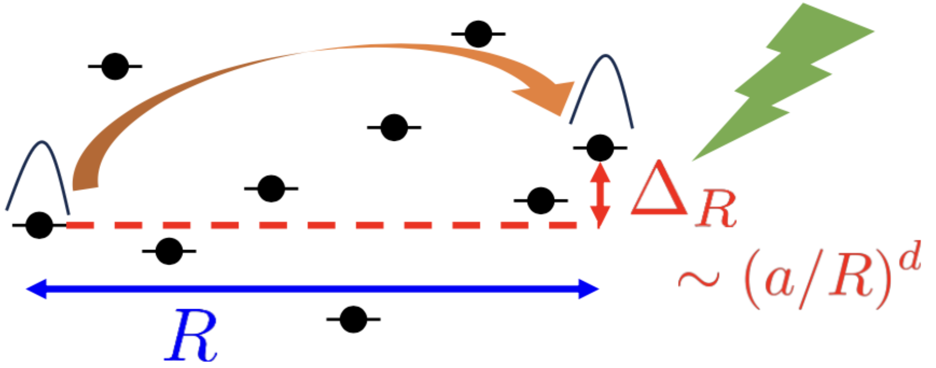
☞ **Unique *T*-dependence in Resistance**

Variable-Range Hopping (VRH)

Overlap of Wave Functions v.s. **Energy Compensation by phonons**



$$\int \mathrm{d}\boldsymbol{r}\, \psi_i^* \psi_j \sim e^{-R/\xi}$$



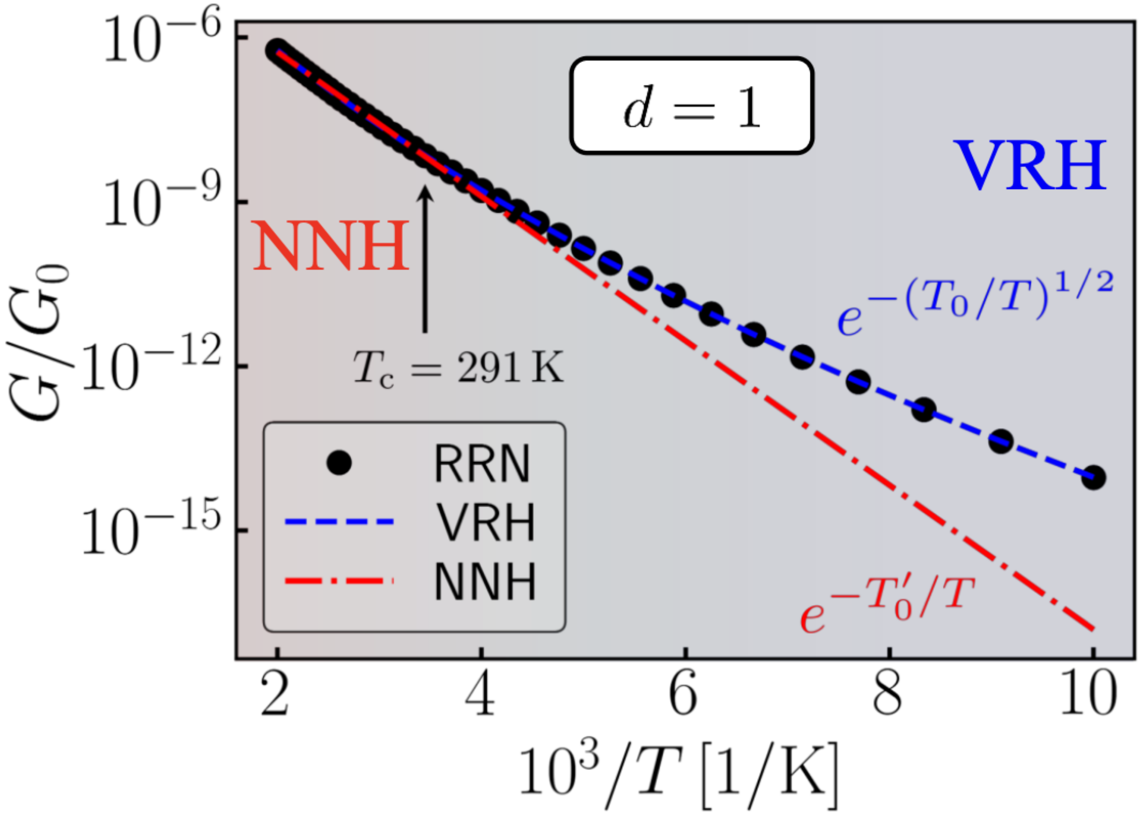
$$e^{-\Delta_R/k_\mathrm{B}T} \nu(\Delta_R)$$

Transition Rate for Electrons

$$\frac{1}{\tau_\mathrm{VRH}} \sim g^2 \nu(\Delta_\mathrm{opt}) e^{-R_\mathrm{opt}(T)/\xi} \propto e^{-1/T^{\frac{1}{d+1}}}$$

Optimzaed Hopping Distance

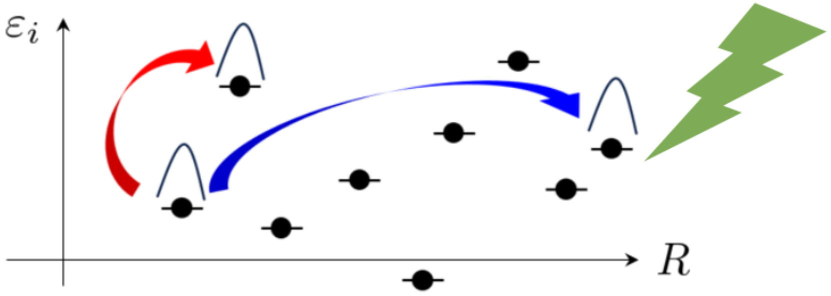
$$R_{\mathrm{opt}} = \begin{cases} a\left(\dfrac{T_{\mathrm{c}}}{T}\right)^{1/(d+1)} & (T < T_{\mathrm{c}}) : \text{Variable-Range Hopping (VRH)} \\ a & (T > T_{\mathrm{c}}) : \text{Nearest-Neighbor Hopping (NNH)} \end{cases}$$



By supplying energy from **Phonons**,

Hopping distance changes

☞ Unique T-dependence of conductance

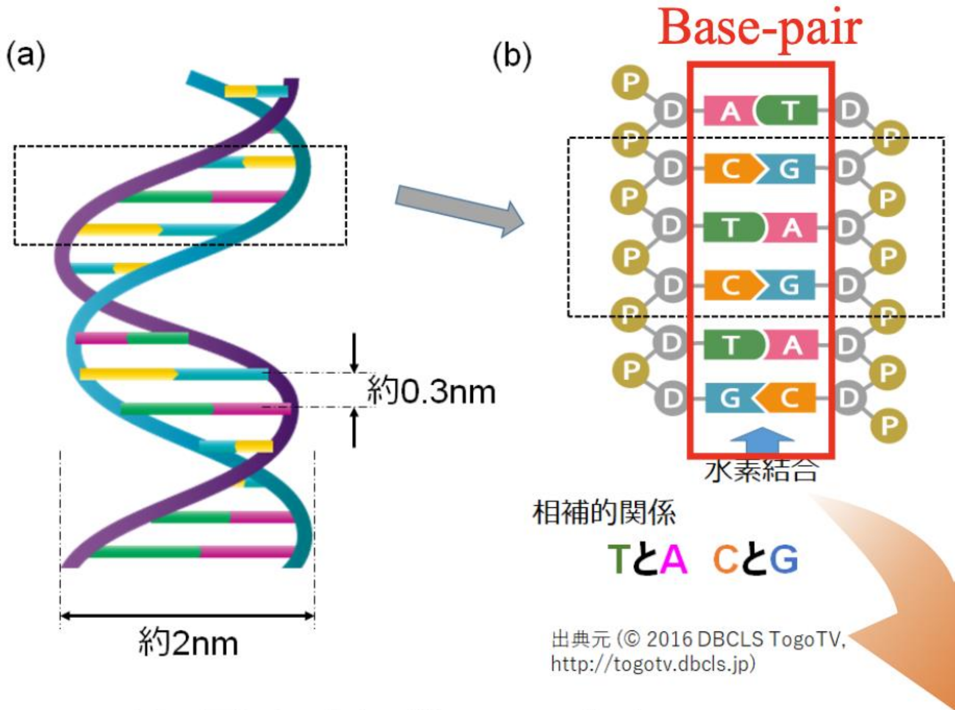


Hop into NN sites @ High T

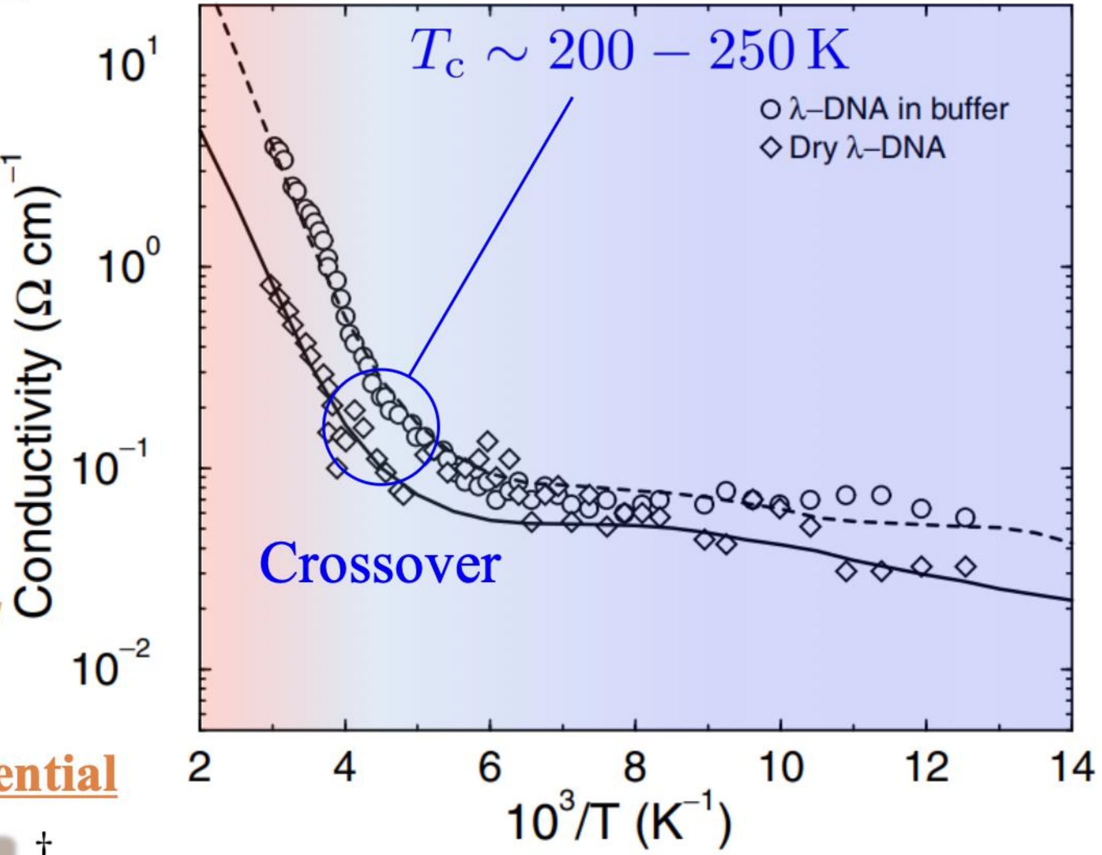
Hop into remote sites @ Low T

Charge Current (Conductivity)

- Strongly disordered system （☞ Anderson Localization）



出典元 (© 2016 DBCLS TogoTV, http://togotv.dbcls.jp)



[Z. G. Yu & X. Song, PRL **86**, 6018 (2000)]

1D Tight binding model + **Random Potential**

$$H = -t\sum_i (c^\dagger_{i+1} c_i + \mathrm{h.c.}) + \sum_i \epsilon_i c^\dagger_i c_i$$

Temperature dependence is well described by VRH !

☞ VRH is a good starting point to analyze CISS in DNA

Spin-dependent Transition rate

$$H_{\text{svc}} = \frac{\hbar}{2}\sum_{i}\sum_{\sigma,\sigma'} \underbrace{c^{\dagger}_{i\sigma}(\boldsymbol{\sigma})_{\sigma\sigma'}c_{i\sigma'}}^{\boldsymbol{S}_i} \cdot \boldsymbol{\Omega}_i$$

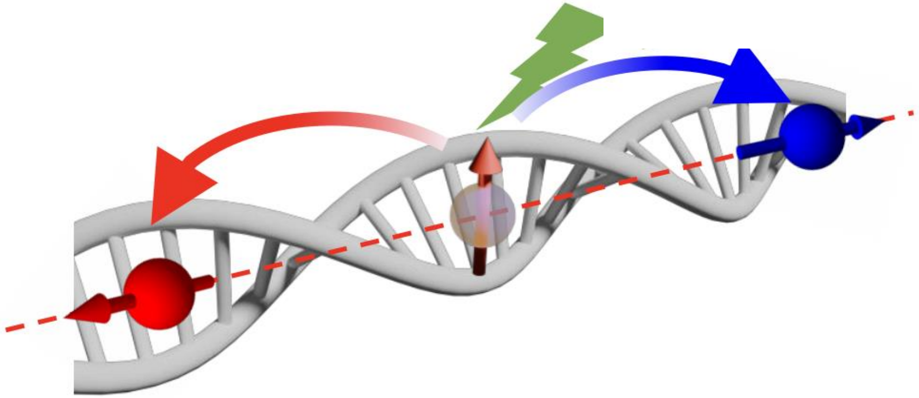
spin-rotation coupling

vorticity
(phonon)

[M. Matsuo *et al.*, JPSJ (2017)]
[T. Funato *et al.*, PRL (2024)]

$$\Gamma_{i\to j} = \sum_{\beta=\uparrow,\downarrow} |\langle i,\alpha|H_{\text{svc}}|j,\beta\rangle|^2 \propto \sum_{\beta=\uparrow,\downarrow} |\boldsymbol{\sigma}_{\alpha\beta}\cdot(\boldsymbol{q}\times\boldsymbol{\epsilon}_q)|^2$$

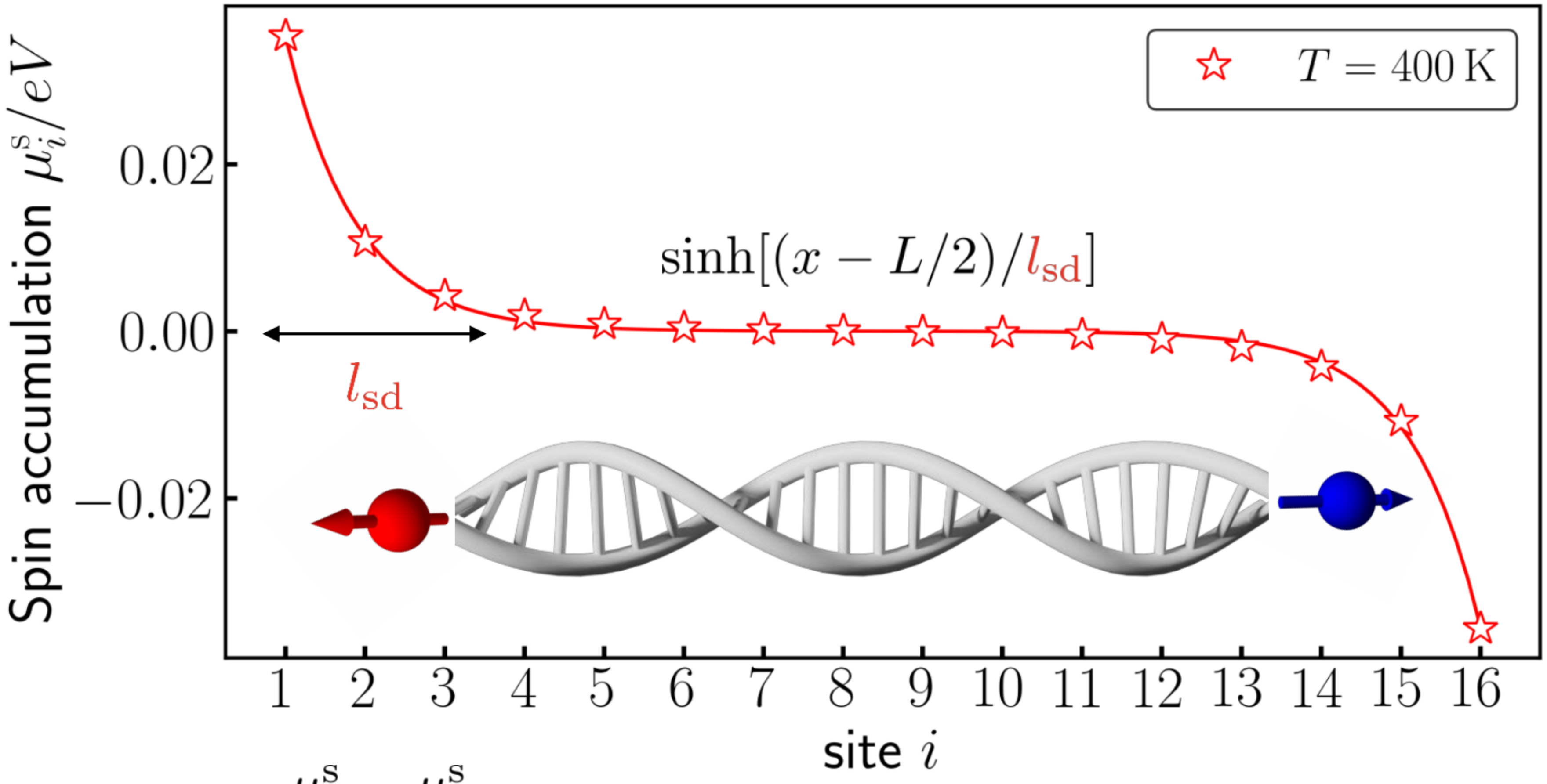
$$= \delta_{\alpha\alpha}[\boldsymbol{q}^2 - (\boldsymbol{q}\cdot\boldsymbol{\epsilon}_q)(\boldsymbol{q}\cdot\boldsymbol{\epsilon}^*_q)] + (\boldsymbol{q}\cdot\boldsymbol{\sigma}_{\alpha\alpha})[\boldsymbol{q}\cdot\text{Im}(\boldsymbol{\epsilon}^*_q\times\boldsymbol{\epsilon}_q)]$$



Chiral Phonon is important !!

☞ Spin Dependences in transition rate

Main Result: Spin Accumulation

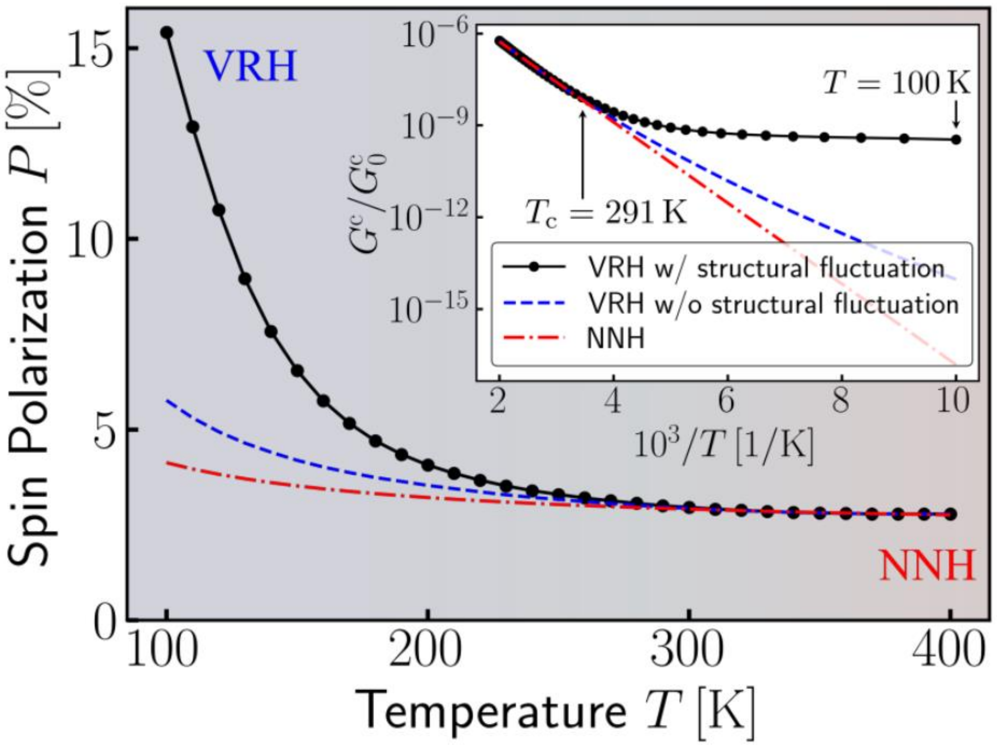


$$P = \frac{\mu_1^{\mathrm{s}} - \mu_{\mathrm{N}}^{\mathrm{s}}}{V} \times 100\,[\%]$$

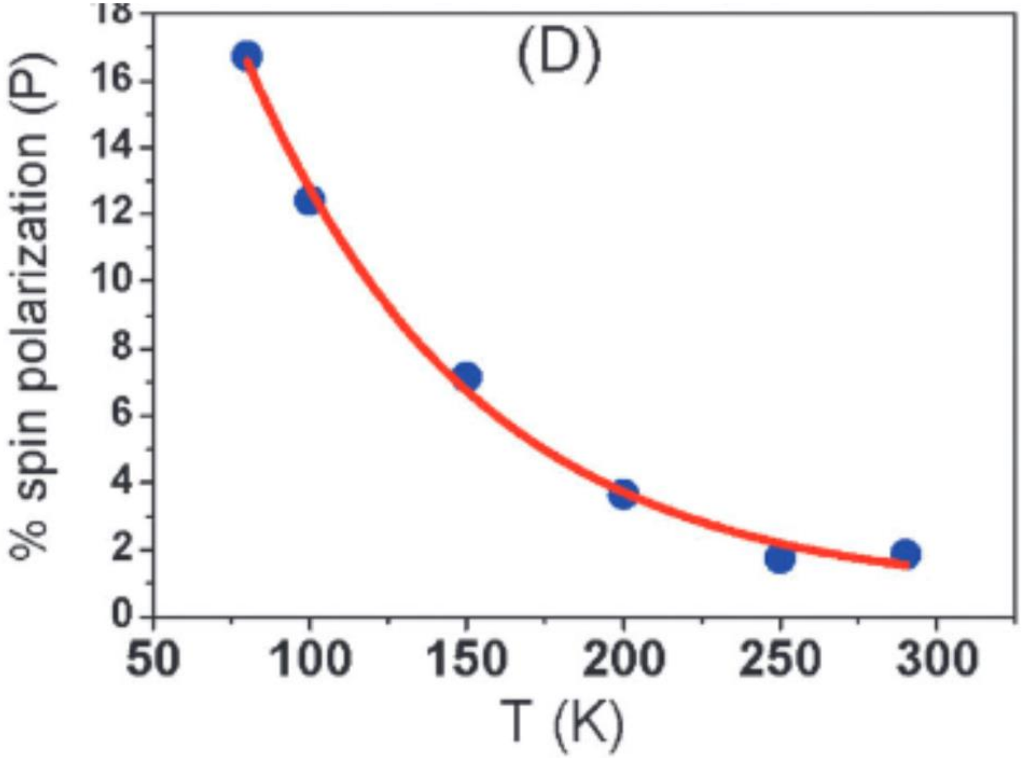
Formation of Anti-parallel Spin Pair

Main Result: Temperature Dependence

- <u>Our Theory</u> (VRH + Chiral phonon)



- <u>Experiment</u>



[R. Naamann, Waldeck, Annu. Rev. Phys. Chem. (2015)]
[K. S. Kumar et al., Phys. Chem. Chem. Phys. (2013)]

☞ Variable-range hopping governs *T*-dependence of CISS in DNA

Summary (the second part)

- ✓ DNA double helix + chiral phonon (spin-rotation coupling)
- ✓ Spin accumulation is calculated from microscopic Hamiltonian of chiral phonons via spin-rotation coupling.
- ✓ The estimated spin accumulation is consistent with the experiment.
- ✓ This study may provide a direct explanation of the CISS effect by light elements.