TOHOKU UNIVERSITY

東北大學

Topological thermal responses in spin-nonconserving insulating magnets

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Tohoku University → Tokyo Metropolitan University

Topological magnons

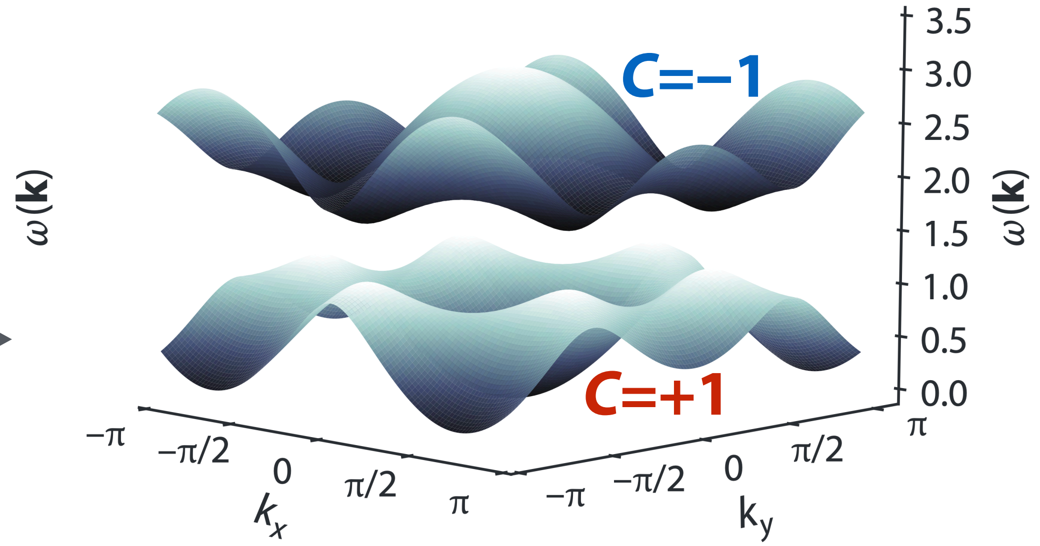
- Topological magnons

Nonzero Chern number (or Berry curvature) in each magnon band

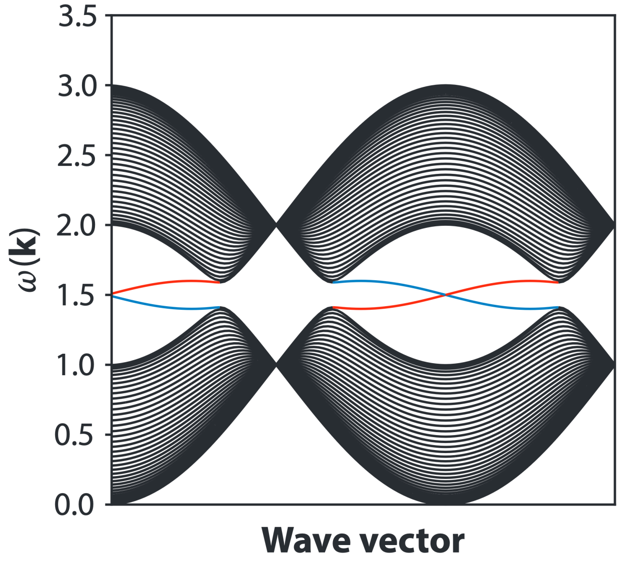
$$H = -|J| \sum_{\langle i,j \rangle_1} \boldsymbol{S}_i \cdot \boldsymbol{S}_j + D \sum_{\langle i,j \rangle_2} \hat{\boldsymbol{z}} \cdot (\boldsymbol{S}_i \times \boldsymbol{S}_j) - \sum_i \boldsymbol{b} \cdot \boldsymbol{S}_i$$

on honeycomb lattice

Band structure



Edge mode



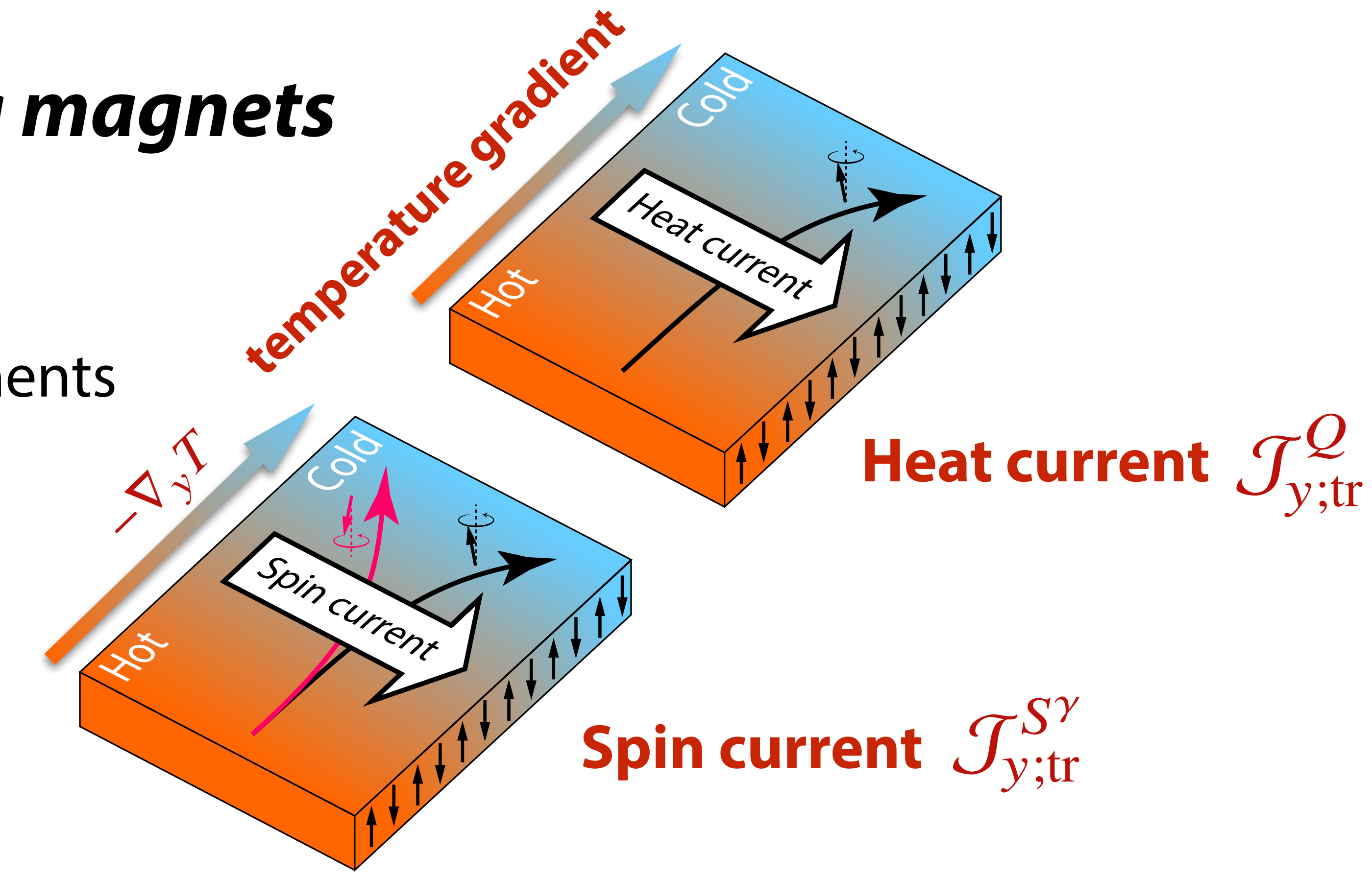
P. A. McClarty, Ann. Rev. Condens. Matt. Phys., **13**, 171 (2022).

- Topological transport due to magnons in ***insulating magnets***

Charge current = 0 ⟶ Heat current & spin current

Topologically nontrivial properties ⟶ Anti-symmetric components

- Thermal Hall effect $\mathcal{J}^{Q}_{y;\mathrm{tr}} = \kappa^{H}_{xy}(-\nabla_y T)$
- Spin Nernst effect $\mathcal{J}^{S^\gamma}_{y;\mathrm{tr}} = \kappa^{S^\gamma}_{xy}(-\nabla_y T)$



Contents

Formulation of thermal response using spin-wave theory

- Thermal Hall effect incorporating ***magnon damping***

S. Koyama and JN, Phys. Rev. B **109**, 174442 (2024).

Finite-temperature formulation of iDE approach & Green's function representation of *energy magnetization*

Conventional form

R. Matsumoto and S. Murakami, PRL **106**, 197202 (2011)
R. Matsumoto et al., PRB **89**, 054420 (2014)

$$\kappa_{xy}^{H(0)} = -\frac{k_B^2 T}{\hbar V} \sum_{\eta=1}^{N} \sum_{\boldsymbol{k}} \Omega_{\boldsymbol{k},\eta}^{xy} c_2[f_B(\varepsilon_{\boldsymbol{k},\eta})]$$

Berry curvature

Our results

$$\kappa_{xy}^{H} = -\frac{k_B^2 T}{\hbar V} \sum_{\eta=1}^{N} \sum_{\boldsymbol{k}} \Omega_{\boldsymbol{k},\eta}^{xy} \int_{-\infty}^{\infty} d\omega \rho_{\boldsymbol{k},\eta}(\omega) c_2[f_B(\omega)]$$

Spectral function of magnons

- Spin Nernst effect in ***spin-nonconserving systems***

S. Koyama and JN, arXiv:2503.10281.

Development of *bosonic* semiclassical theory & Formulation of spin Nernst coefficient *incorporating torque term*

Conventional form

$$\tilde{\kappa}_{xy}^{S^\gamma} = -\frac{k_B}{\hbar V} \sum_{\eta=1}^{N} \sum_{\boldsymbol{k}} (\tilde{\Omega}_{\boldsymbol{k},\eta}^{S^\gamma})_{xy} c_1[f_B(\varepsilon_{\boldsymbol{k},\eta})]$$

Spin Berry curvature

Valid only for ***spin-conserving systems***

R. Cheng, S. Okamoto, and D. Xiao, Phys. Rev. Lett. 117, 217202 (2016)
V. A. Zyuzin and A. A. Kovalev, Phys. Rev. Lett. 117, 217203 (2016)

Our results

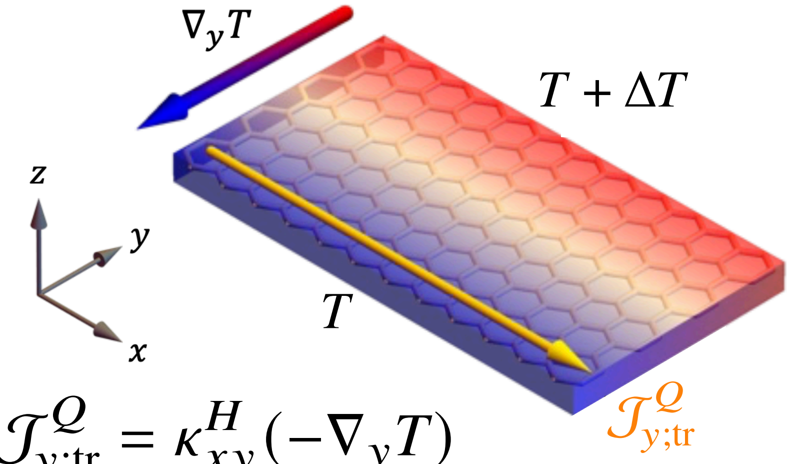
$$\kappa_{xy}^{S^\gamma} = -\frac{k_B}{\hbar V} \sum_{\eta=1}^{N} \sum_{\boldsymbol{k}} (\Upsilon_{\boldsymbol{k},\eta}^{S^\gamma})_{xy} c_1[f_B(\varepsilon_{\boldsymbol{k},\eta})]$$

$$(\Upsilon_{\boldsymbol{k},\eta}^{S^\gamma})_{xy} = -\Omega_{\boldsymbol{k},\eta}^{xy} (S_{\boldsymbol{k}}^{\gamma})_\eta + \frac{\partial}{\partial k_y} 2g_{\boldsymbol{k},\eta}^{k_x h_\gamma^\tau}$$

Berry curvature　　Quantum metric

Thermal Hall effect

- Thermal Hall effect within free magnon picture



$$\mathcal{J}^Q_{y;\mathrm{tr}} = \kappa^H_{xy}(-\nabla_y T)$$

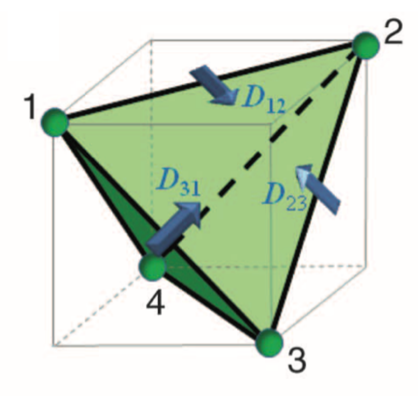
Linear spin-wave theory

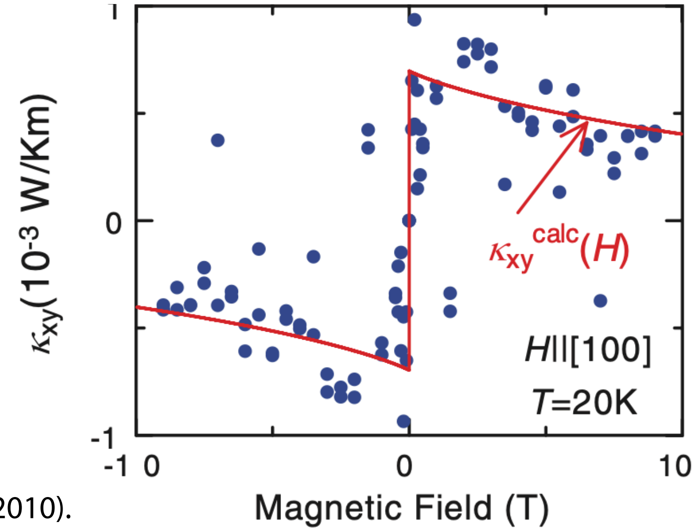
$$\kappa^{H(0)}_{xy} = -\frac{k_B^2 T}{\hbar V} \sum_{\eta=1}^{N} \sum_{\boldsymbol{k}} \Omega^{xy}_{\boldsymbol{k},\eta} c_2[f_B(\varepsilon_{\boldsymbol{k},\eta})]$$

Berry curvature

R. Matsumoto and S. Murakami, PRL **106**, 197202 (2011)
R. Matsumoto et al., PRB **89**, 054420 (2014)

- Observation of thermal Hall effect in $Lu_2V_2O_7$





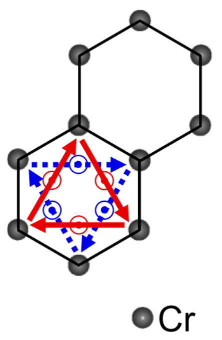
Y. Onose, et al., Science **329**, 297 (2010).

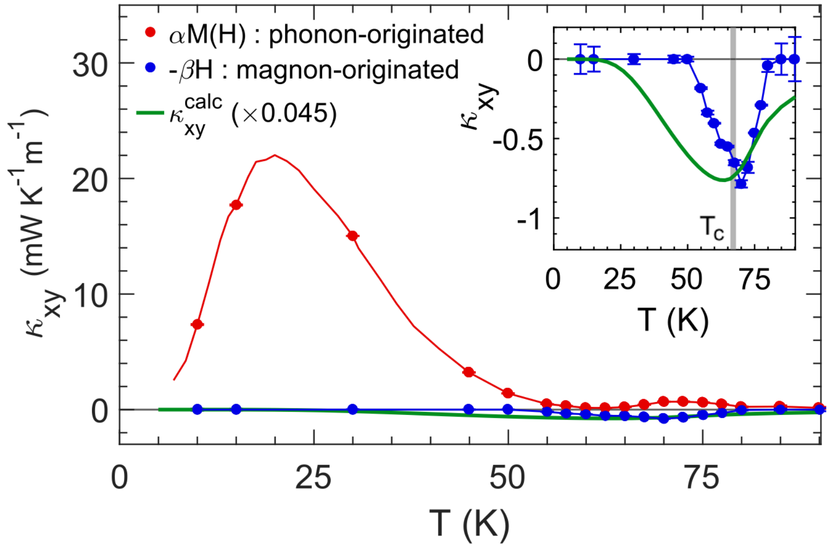
Consistent with theoretical prediction by <u>linear spin-wave theory</u>

- Recent progress

- S=3/2 Heisenberg + DM Honeycomb systems

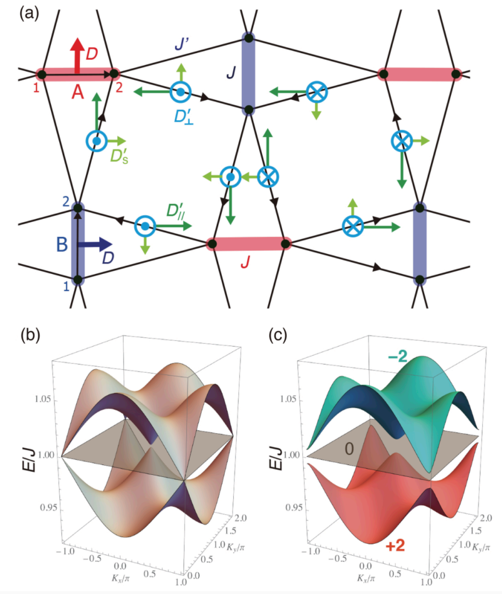
$Cr_2Ge_2Te_6$

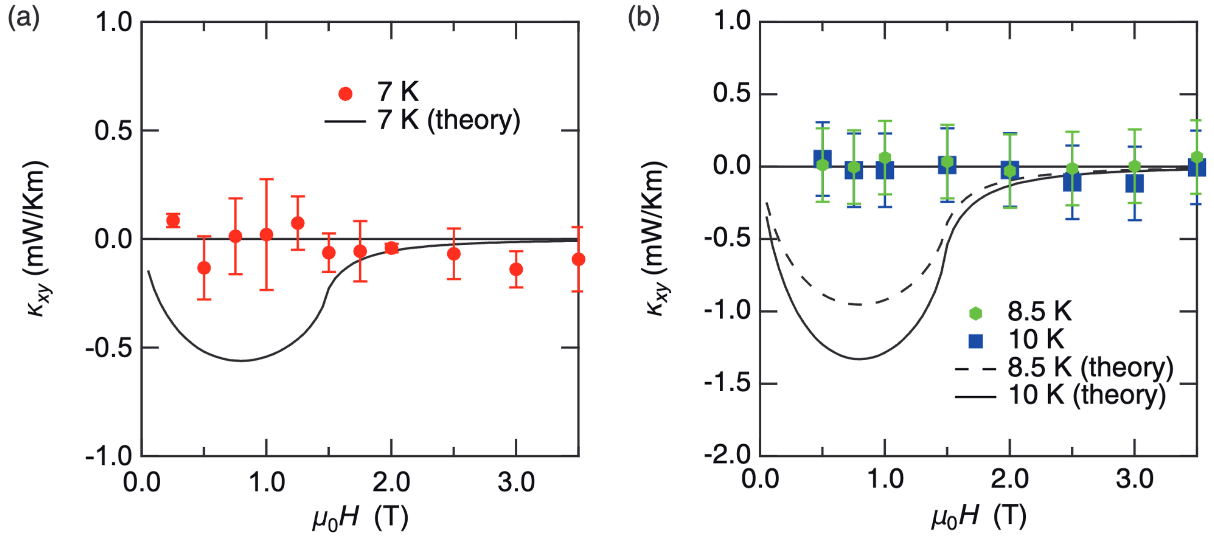




S. Spachmann et al., Phys. Rev. Research **4**, L022040 (2023)
Y. Choi et al., Phys. Rev. B **107**, 184434 (2023)

- Shastry-Sutherland systems with DM interactions





J. Romhányi, K. Penc and R. Ganesh, Nat. Commun. **6**, 6805 (2015)
S. Suetsugu et al., Phys. Rev. B **105**, 024415 (2022)

Discrepancy in *linear spin-wave theory* → Contributions from <u>*Nonlinear terms*</u>, disorder, or phonons ??

Nonlinear terms in spin-wave theory

- Holstein-Primakoff theory   1/S expansion & Bogoliubov transformation

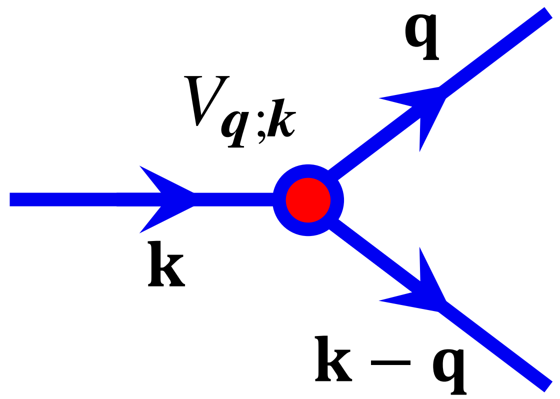
$$\mathcal{H} = \sum_{ij} \boldsymbol{S}_i \cdot \mathbf{J}_{ij} \cdot \boldsymbol{S}_j - \sum_i \boldsymbol{h} \cdot \boldsymbol{S}_i$$

$$S_i^z = S - a_i^\dagger a_i$$
$$S_i^+ = \sqrt{2S - a_i^\dagger a_i a_i}$$
$$S_i^- = a_i^\dagger \sqrt{2S - a_i^\dagger a_i}$$

$$\mathcal{H} = \sum_{\boldsymbol{k},\eta} \varepsilon_{\boldsymbol{k},\eta} b_{\boldsymbol{k},\eta}^\dagger b_{\boldsymbol{k},\eta} + \sum_{\eta\eta'\eta''} \sum_{\boldsymbol{qk}} \frac{V_{\boldsymbol{q};\boldsymbol{k}}^{\eta,\eta';\eta''}}{\sqrt{S}} b_{\boldsymbol{q},\eta}^\dagger b_{\boldsymbol{k}-\boldsymbol{q},\eta'}^\dagger b_{\boldsymbol{k},\eta''} + \cdots$$

Bilinear term   **Magnon-Magnon interactions**

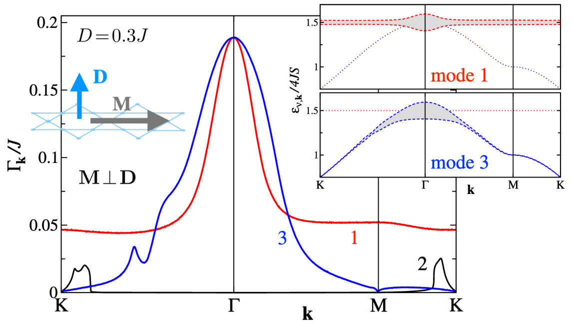
a_i : original magnon → $b_{\boldsymbol{k},\eta}$: Bogoliubov boson



Born approximation / **iDE** (imaginary Dyson Equation) approach / …

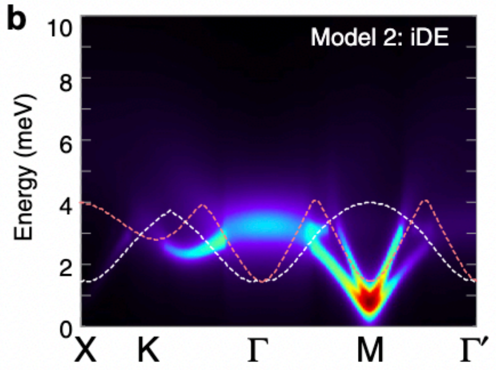
- Interaction effects on topological magnons

- Kagome systems



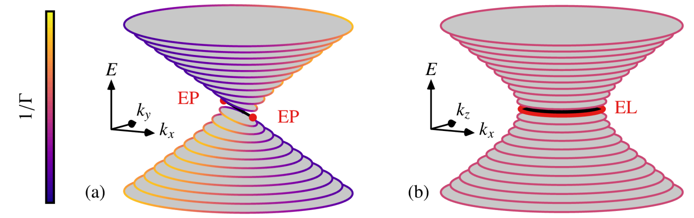
A. L. Chernyshev and P. A. Maksimov, Phys. Rev. Lett. **117**, 187203 (2016).

- Kitaev systems



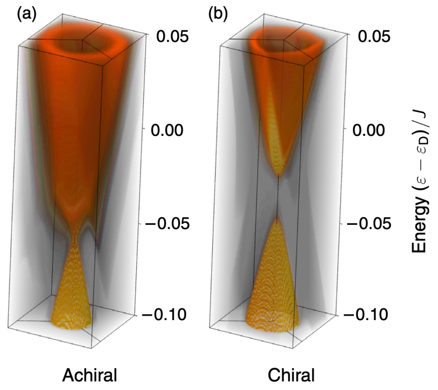
S. M. Winter et al., Nat. Commun. **8**, 1152 (2017).

- Non-harmitian systems



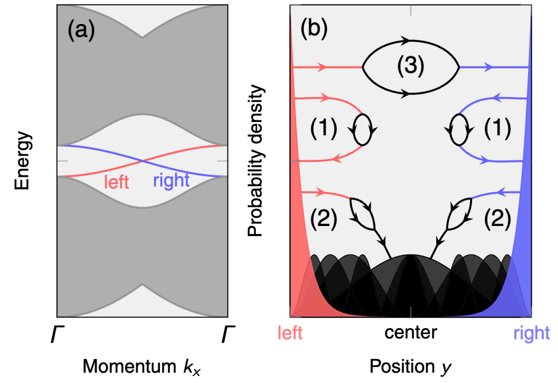
P. A. McClarty and J. G. Rau, Phys. Rev. B 100, 100405 (2019).

- Interaction-induced stability



A. Mook et al., Phys. Rev. X **11**, 021061 (2021).

- Edge mode damping



S. Koyama and JN, Phys. Rev. B **108**, 235162 (2023).
J. Habel et al., Phys. Rev. B **109**, 024441 (2024).
D. Malz et al., Nat. Commun. **10**, 3937 (2019).

Finite-temperature **framework is needed for thermal Hall effect**

Magnon damping at finite temperatures

Hamiltonian

$$\mathcal{H} = \sum_{\boldsymbol{k},\eta} \varepsilon_{\boldsymbol{k},\eta} b^\dagger_{\boldsymbol{k},\eta} b_{\boldsymbol{k},\eta} + \sum_{\eta\eta'\eta''} \sum_{\boldsymbol{qk}} \frac{V^{\eta,\eta';\eta''}_{\boldsymbol{q};\boldsymbol{k}}}{\sqrt{S}} b^\dagger_{\boldsymbol{q},\eta} b^\dagger_{\boldsymbol{k}-\boldsymbol{q},\eta'} b_{\boldsymbol{k},\eta''} + \cdots$$

- Green's function for Bogoliubov bosons

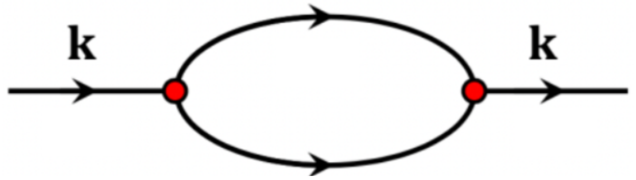
$$G^R_{\boldsymbol{k},\eta}(\omega) \simeq \frac{1}{(\omega + i0^+)\sigma_3 - \varepsilon_{\boldsymbol{k},\eta} + i\Gamma_{\boldsymbol{k},\eta}(\omega)}$$

with damping factor $\Gamma_{\boldsymbol{k},\eta}(\omega) = -\mathrm{Im}\,\Sigma^R_{\boldsymbol{k},\eta}(\omega)$

$$\sigma_3 = \begin{pmatrix} \mathbf{1}_{N\times N} & 0 \\ 0 & -\mathbf{1}_{N\times N} \end{pmatrix}$$

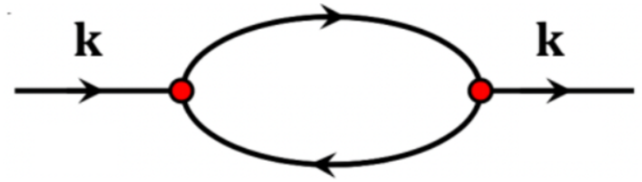
Lowest-order contribution to $\mathrm{Im}\,\Sigma^R_{\boldsymbol{k},\eta}(\omega)$ (Second order of $V^{\eta,\eta';\eta''}_{\boldsymbol{q};\boldsymbol{k}}/\sqrt{S}$)

Decay term



Contributing even at zero temperature

Collision term



Contributing ***only at finite temperature***

- imaginary self-consistent Dyson equation (iDE) approach

Γ is determined self-consistently
around the singularity of the Green's function.

A. L. Chernyshev and M. E. Zhitomirsky, Phys. Rev. B **79**, 144416 (2009).
P. A. Maksimov, M. E. Zhitomirsky, and A. L. Chernyshev, Phys. Rev. B **94**, 140407 (2016).
A. L. Chernyshev and P. A. Maksimov, Phys. Rev. Lett. **117**, 187203 (2016).
S. M. Winter et al., Nat Commun **8**, 1152 (2017).

$$z - \varepsilon_{\boldsymbol{k},\eta} + i\Gamma_{\boldsymbol{k},\eta}(z) = 0 \longrightarrow \Gamma_{\boldsymbol{k},\eta}(\omega) \simeq \tilde{\Gamma}_{\boldsymbol{k},\eta} = \Gamma_{\boldsymbol{k},\eta}(z^*)$$

Solve self-consistently $z = \varepsilon_{\boldsymbol{k},\eta} - i\tilde{\Gamma}_{\boldsymbol{k},\eta}$

Magnon damping at finite temperatures

- imaginary self-consistent Dyson equation (iDE) approach

Γ is determined self-consistently around the singularity of the Green's function.

A. L. Chernyshev and M. E. Zhitomirsky, Phys. Rev. B **79**, 144416 (2009).
P. A. Maksimov, M. E. Zhitomirsky, and A. L. Chernyshev, Phys. Rev. B **94**, 140407 (2016).
A. L. Chernyshev and P. A. Maksimov, Phys. Rev. Lett. **117**, 187203 (2016).
S. M. Winter et al., Nat Commun **8**, 1152 (2017).

$$z - \varepsilon_{\boldsymbol{k},\eta} + i\Gamma_{\boldsymbol{k},\eta}(z) = 0 \quad \longrightarrow \quad \Gamma_{\boldsymbol{k},\eta}(\omega) \simeq \tilde{\Gamma}_{\boldsymbol{k},\eta} = \Gamma_{\boldsymbol{k},\eta}(z^*)$$

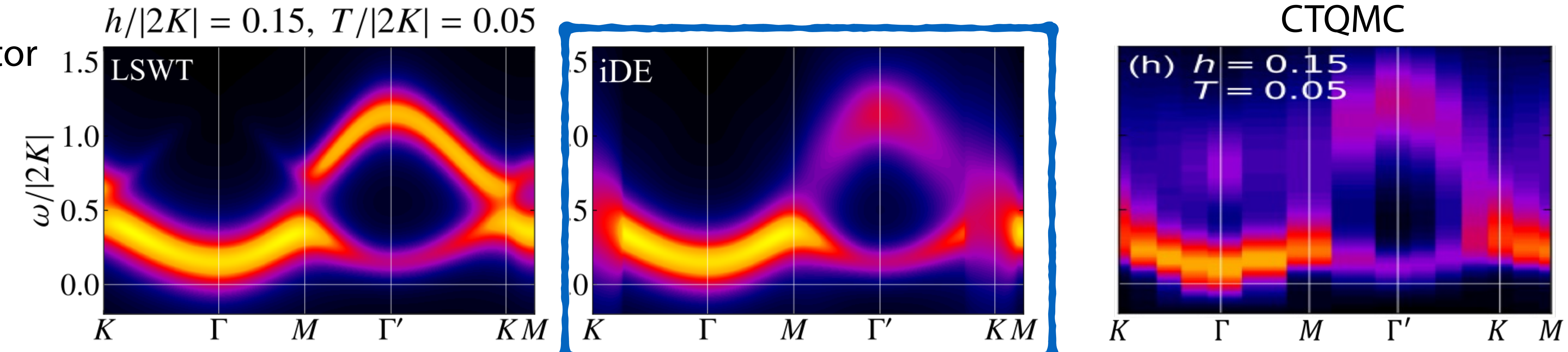
Solve self-consistently $\quad z = \varepsilon_{\boldsymbol{k},\eta} - i\tilde{\Gamma}_{\boldsymbol{k},\eta}$

- Demonstration $\mathcal{H} = 2K \sum_{\gamma=X,Y,Z} \sum_{\langle ij\rangle_\gamma} S_i^\gamma S_j^\gamma - \boldsymbol{h} \cdot \sum_i \boldsymbol{S}_i$

Ferromagnetic Kitaev model under magnetic fields

$2K < 0$

Dynamical spin correlator



Our finite-*T* iDE

J. Yoshitake, et al., Phys. Rev. B **101**, 100408 (2020).

Our finite-T result is consistent with that obtained by quantum Monte Carlo simulations

Formulation of thermal Hall conductivity

Thermal Hall conductivity

$$\kappa^H_{xy} = \frac{1}{T}\left(S_{xy} + \frac{2M^Q_z}{V}\right)$$

J. M. Luttinger, Phys. Rev. **135**, A1505 (1964).
L. Smrcka and P. Streda, J. Phys. C **10**, 2153 (1977).
R. Matsumoto and S. Murakami, PRL **106**, 197202 (2011)
R. Matsumoto et al., PRB **89**, 054420 (2014)

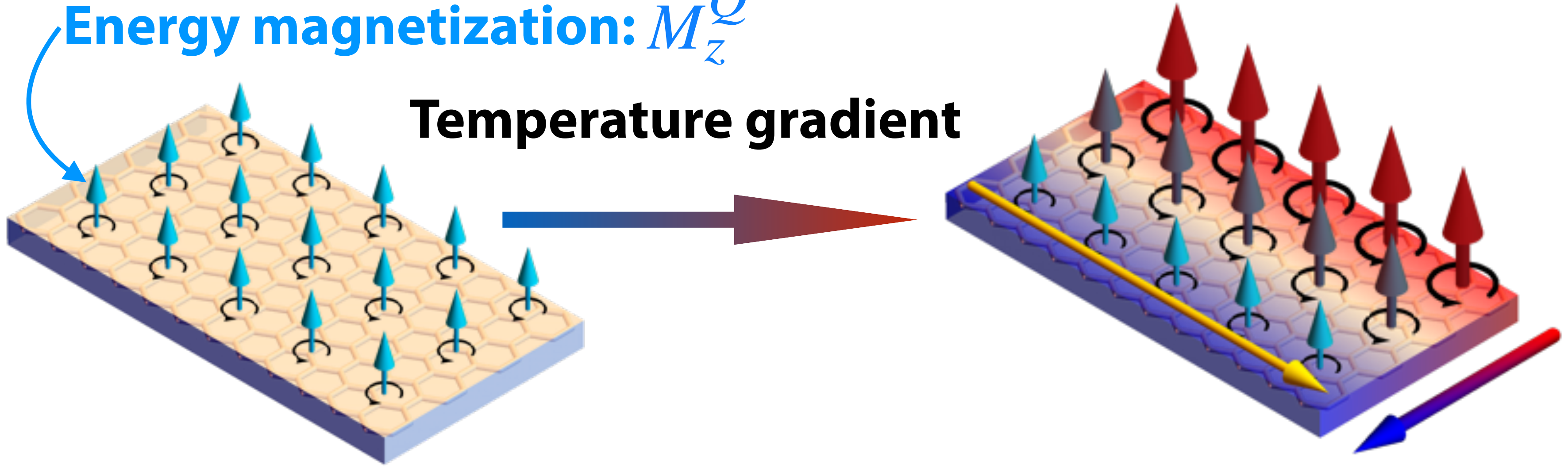
Contribution from Kobo formula: $S_{xy}(i\Omega) = \frac{\beta}{V}\int_0^\infty dt\, e^{-\delta t}\langle J^Q_y; J^Q_x\rangle_{\rm eq}$

Energy magnetization: $\frac{1}{\beta}\frac{\partial}{\partial\beta}\left(\beta^2 M^Q_z\right) = -\frac{\beta}{2i}\frac{\partial}{\partial q_y}\left\langle h_{-\boldsymbol{q}}; j_{\boldsymbol{q},x}\right\rangle_{\rm eq}\Big|_{\boldsymbol{q}\to\boldsymbol{0}} - (x \leftrightarrow y)$

D. Xiao, et al., PRL **97**, 026603 (2006).
T. Qin, et al., PRL **107**, 236601 (2011).

with $\lim_{\beta\to\infty}\beta\frac{\partial M^Q_z}{\partial\beta} = 0$

Energy magnetization: M^Q_z



Energy magnetization contributes to thermal Hall effect

Canonical correlation: $\langle X;Y\rangle_{\rm eq} = \frac{1}{\beta}\int_0^\beta d\tau\,\langle T_\tau X(\tau)Y\rangle_{\rm eq}$

Fourier transform of local Hamiltonian: $h_{\boldsymbol{q}}$

Fourier transform of local heat current: $j_{\boldsymbol{q}}$

Evaluation of M^Q_z is complicated…

All previous studies treated this within free-magnon picture.

L. Smrcka and P. Streda, J. Phys. C **10**, 2153 (1977).
T. Qin, et al., PRL **107**, 236601 (2011).
R. Matsumoto, et al, PRB **89**, 054402 (2014).

Energy magnetization is given by ***canonical correlation***

→ **Formulation using Green's function is possible *in principle*.**

Approximation

Approximation / Simplification

1. Considering diagonal part of self-energy

$$G^R_{\boldsymbol{k},\eta}(\omega) \simeq \frac{1}{(\omega + i0^+)\sigma_3 - \varepsilon_{\boldsymbol{k},\eta} + i\Gamma_{\boldsymbol{k},\eta}(\omega)}$$

2. Assuming $\Gamma_{\boldsymbol{k},\eta}(\omega) \ll \varepsilon_{\boldsymbol{k},\eta}$
   and incorporating up to first order of $\Gamma_{\boldsymbol{k},\eta}(\omega)$

3. $\Gamma_{\boldsymbol{k},\eta}(\omega)$ is assumed to change slowly
   → Neglecting ω and T derivatives

4. $\Gamma_{\boldsymbol{k},\eta}(\omega)$ is evaluated by iDE approach
   → $\Gamma_{\boldsymbol{k},\eta}(\omega) \simeq \tilde{\Gamma}_{\boldsymbol{k},\eta}\theta(\omega)$

Our results

$$\kappa^H_{xy} = -\frac{k_B^2 T}{\hbar V}\sum_{\eta=1}^{N}\sum_{\boldsymbol{k}} \Omega^{xy}_{\boldsymbol{k},\eta}\int_{-\infty}^{\infty} d\omega \rho_{\boldsymbol{k},\eta}(\omega) c_2[f_B(\omega)]$$

Spectral function of magnons: $\rho_{\boldsymbol{k},\eta}(\omega) = \dfrac{\tilde{\Gamma}_{\boldsymbol{k},\eta}/\pi}{(\omega - \varepsilon_{\boldsymbol{k},\eta})^2 + \tilde{\Gamma}^2_{\boldsymbol{k},\eta}}\theta(\omega)$

Berry curvature: $\Omega^{xy}_{\boldsymbol{k},\eta} = -2\hbar^2 \sum_{\eta_1(\neq\eta)}^{2N} \sigma_{3,\eta}\sigma_{3,\eta_1} \dfrac{\mathrm{Im}\left[(v_{\boldsymbol{k},x})_{\eta\eta_1}(v_{\boldsymbol{k},y})_{\eta_1\eta}\right]}{\left(\bar{\varepsilon}_{\boldsymbol{k},\eta} - \bar{\varepsilon}_{\boldsymbol{k},\eta_1}\right)^2}$

Velocity: $\boldsymbol{v} = \dfrac{1}{\hbar}\dfrac{\partial H_{0,\boldsymbol{k}}}{\partial \boldsymbol{k}}$ $\qquad c_2(x) = \displaystyle\int_0^x dt \left(\ln\frac{1+t}{t}\right)^2$

Bose distribution function with μ=0: $f_B(\omega) = (e^{\beta\omega} - 1)^{-1}$

Free-magnon form

R. Matsumoto and S. Murakami, PRL **106**, 197202 (2011)
R. Matsumoto et al., PRB **89**, 054420 (2014)

$$\kappa^{H(0)}_{xy} = -\frac{k_B^2 T}{\hbar V}\sum_{\eta=1}^{N}\sum_{\boldsymbol{k}} \Omega^{xy}_{\boldsymbol{k},\eta} c_2[f_B(\varepsilon_{\boldsymbol{k},\eta})]$$

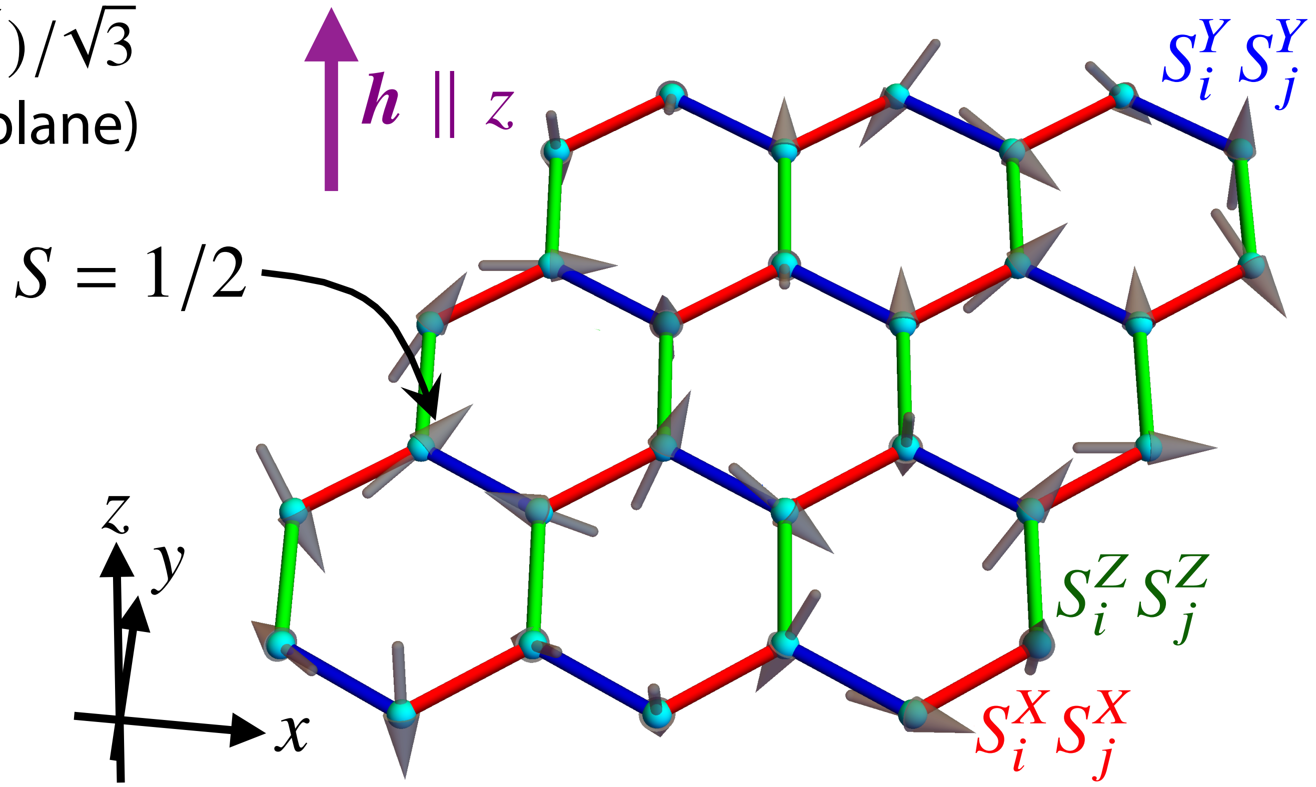
Berry curvature

Result: Kitaev model under magnetic field

Ferromagnetic Kitaev model under magnetic fields for $S^z = (S^X + S^Y + S^Z)/\sqrt{3}$ (perpendicular to honeycomb plane)

$2K < 0$

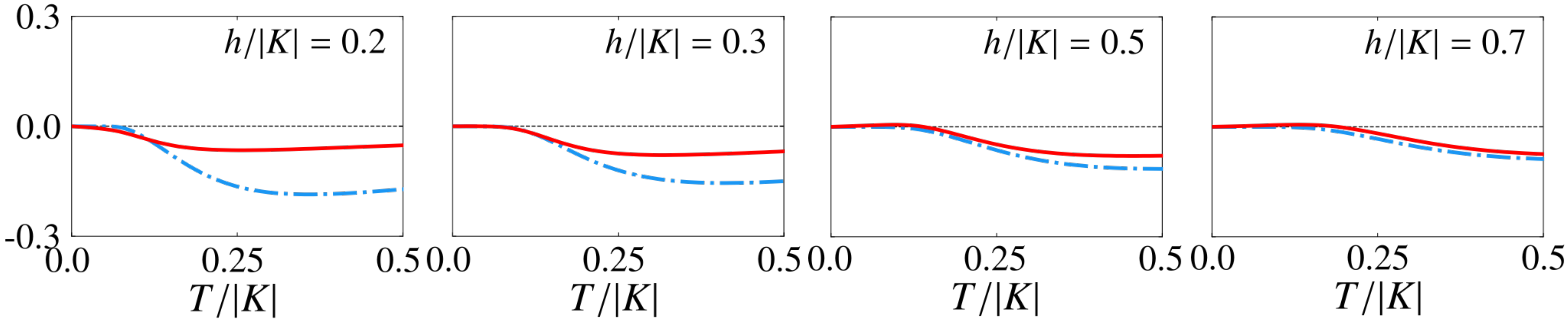
$$\mathcal{H} = 2K \sum_{\gamma=X,Y,Z} \sum_{\langle ij \rangle_\gamma} S_i^\gamma S_j^\gamma - \boldsymbol{h} \cdot \sum_i \boldsymbol{S}_i$$



Ground state: forced ferromagnetic along *z* direction

$\kappa_{xy}^{H(0)}/T$: for free magnons

κ_{xy}^{H}/T : with magnon damping



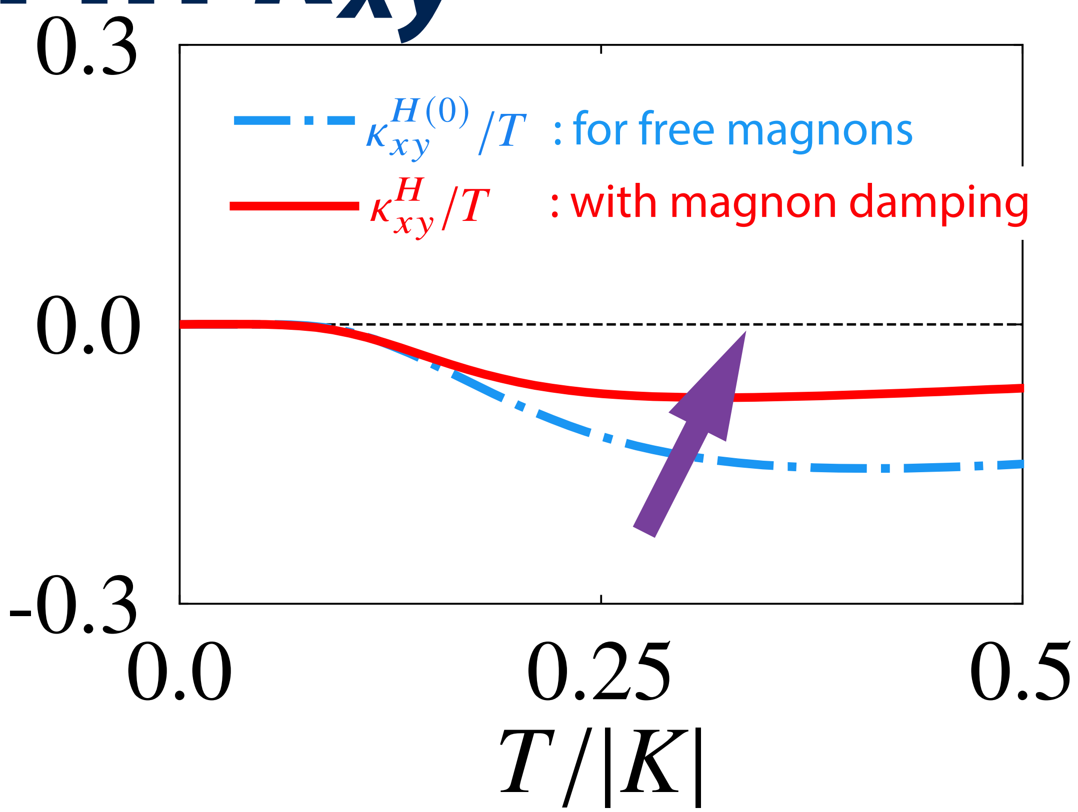
- Strong suppression of thermal Hall coefficient by magnon damping for small magnetic field.
- Impact of magnon damping becomes smaller as magnetic field increases.

Origin of suppression in κ_{xy}

<u>*Ferromagnetic*</u> Kitaev model under magnetic fields for $S^z = (S^X + S^Y + S^Z)/\sqrt{3}$ (perpendicular to honeycomb plane)

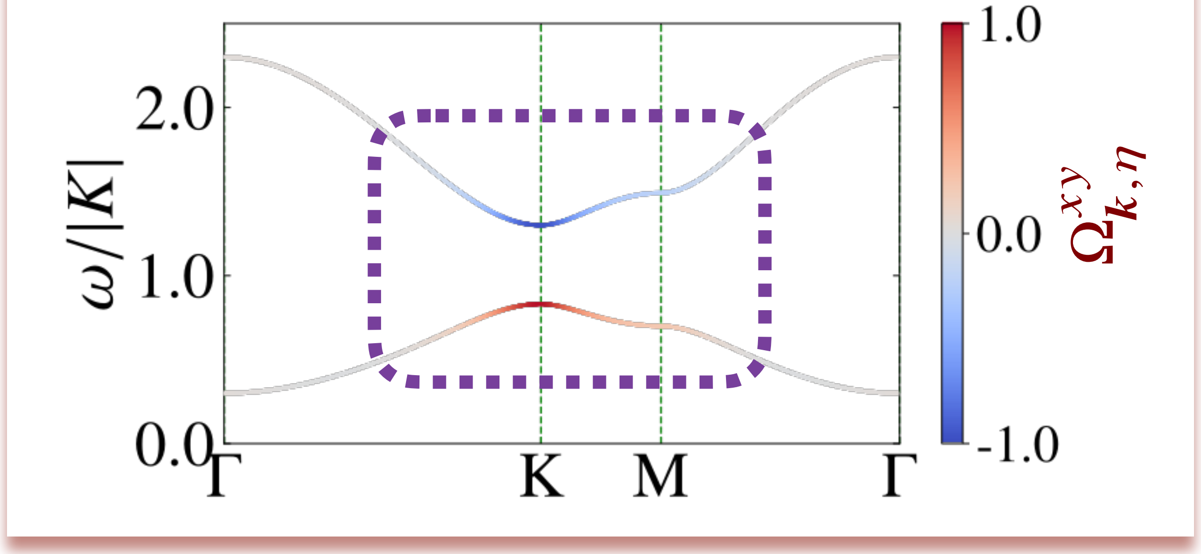
$2K < 0$

$$\mathcal{H} = 2K \sum_{\gamma=X,Y,Z} \sum_{\langle ij \rangle_\gamma} S_i^\gamma S_j^\gamma - \boldsymbol{h} \cdot \sum_i \boldsymbol{S}_i \qquad h/|K| = 0.3$$

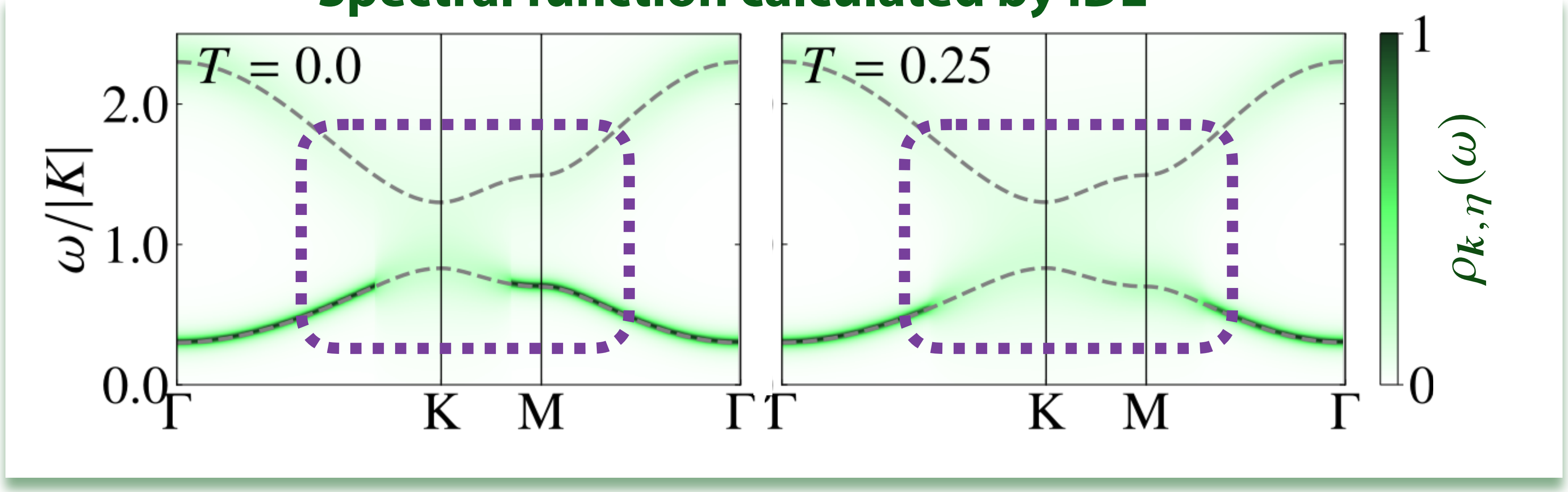


$$\kappa_{xy}^H = -\frac{k_B^2 T}{\hbar V} \sum_{\eta=1}^{N} \sum_{\boldsymbol{k}} \Omega_{\boldsymbol{k},\eta}^{xy} \int_{-\infty}^{\infty} d\omega \rho_{\boldsymbol{k},\eta}(\omega) c_2[f_B(\omega)]$$

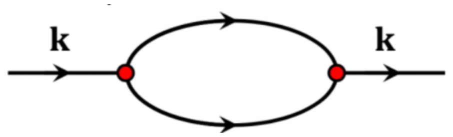
Berry curvature



Spectral function calculated by iDE



- Magnon damping around K point with large Berry curvature ⟶ Strong suppression at finite temperature
- Low-energy part is not smeared by magnon decay process



⟶ Low-T region of κ_{xy} remains nearly unaffected by magnon damping.

Spin Nernst effect

Previous theoretical studies

- Honeycomb antiferromagnet $MnPS_3$

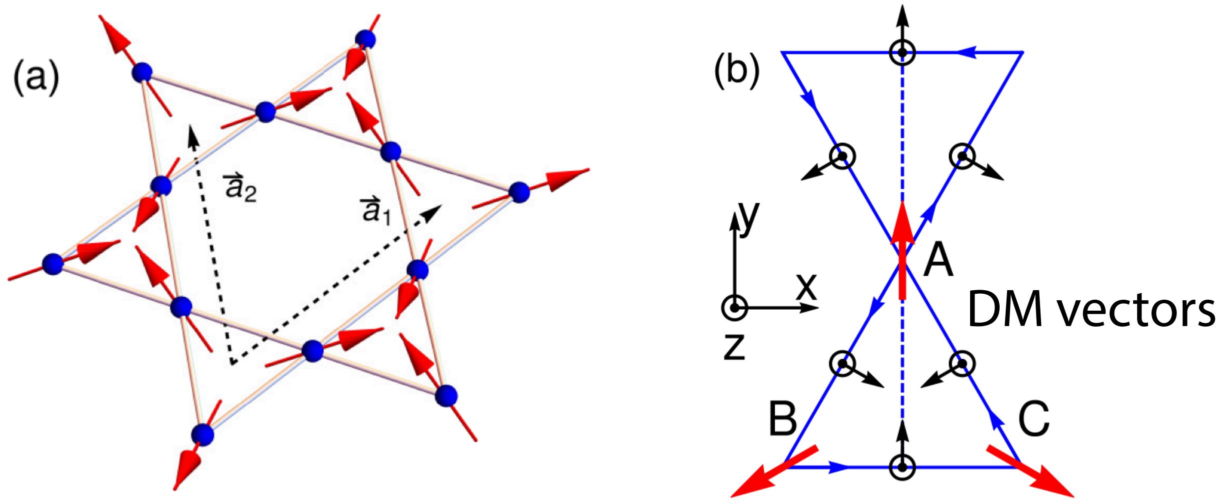
R. Cheng, S. Okamoto, and D. Xiao, Phys. Rev. Lett. 117, 217202 (2016)
V. A. Zyuzin and A. A. Kovalev, Phys. Rev. Lett. 117, 217203 (2016)

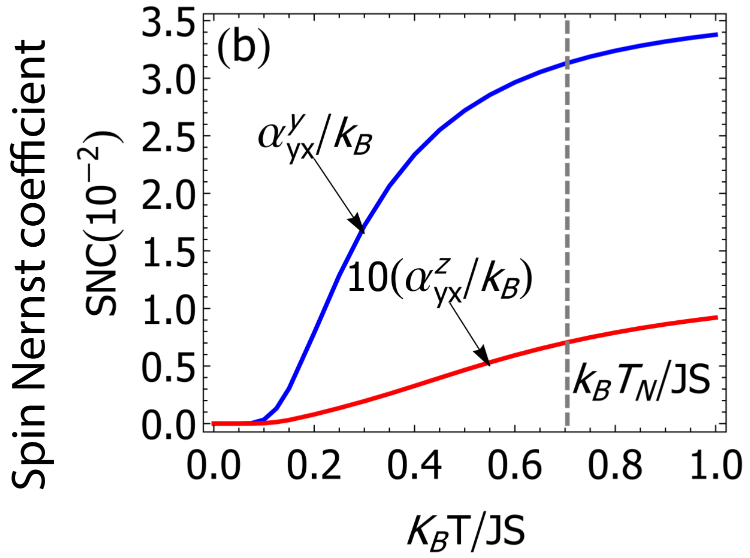
- Kagome antiferromagnet $KFe_3(OH)_6(SO_4)_2$

B. Li, S. Sandhoefner, and A. A. Kovalev, Phys. Rev. Research **2**, 013079 (2020)

Experiment in $MnPS_3$

Y. Shiomi, R. Takashima, and E. Saitoh, Phys. Rev. B **96**, 134425 (2017).





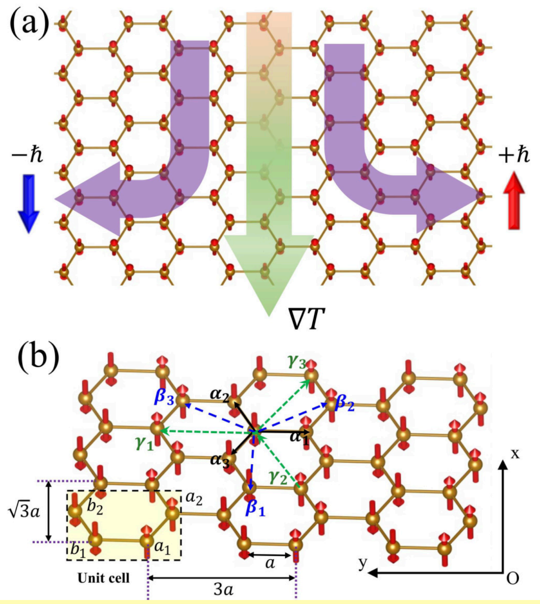
Presence of DM interactions

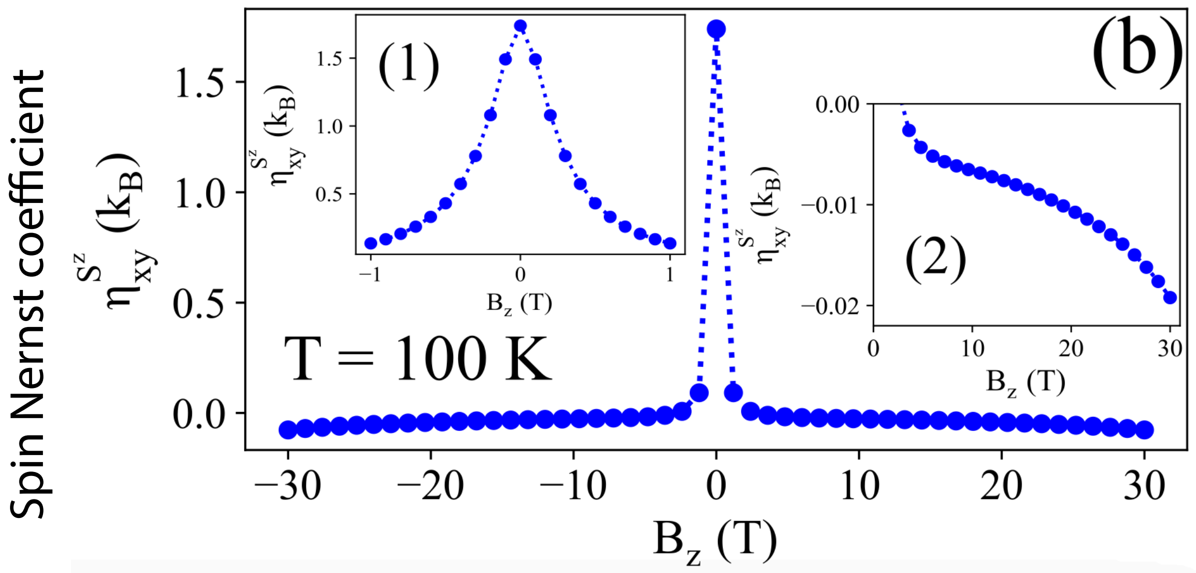
↓

Spin nonconserved

- Honeycomb Zigzag-ordered magnet $FePS_3$: Magnon-polaron

D.-Q. To et al., Phys. Rev. B **108**, 085435 (2023)





Magnon-phonon hybridization

↓

Spin nonconserved

$$\tilde{\kappa}^{S^\gamma}_{xy} = -\frac{k_B}{\hbar V}\sum_{\eta=1}^{N}\sum_{\boldsymbol{k}}(\tilde{\Omega}^{S^\gamma}_{\boldsymbol{k},\eta})_{xy}c_1[f_B(\varepsilon_{\boldsymbol{k},\eta})]$$ for ***spin-conserving*** systems was used even in ***spin-nonconserving systems***

→ Formula applicable to ***spin-nonconserving systems*** are highly desired.

Theoretical challenge for spin Nernst effect

Bosonic BdG Hamiltonian: $\mathcal{H}_0 = \frac{1}{2}\int d\boldsymbol{r}\mathcal{A}^\dagger(\boldsymbol{r})\hat{H}_0\mathcal{A}(\boldsymbol{r})$

Set of Bose operators: $\mathcal{A}(\boldsymbol{r}) = \{a_1(\boldsymbol{r}), a_2(\boldsymbol{r}), \ldots, a_N(\boldsymbol{r}), a_1^\dagger(\boldsymbol{r}), a_2^\dagger(\boldsymbol{r}), \ldots, a_N^\dagger(\boldsymbol{r})\}$

Equation of continuity: $\frac{\partial S^\gamma(\boldsymbol{r})}{\partial t} = \frac{i}{\hbar}[\mathcal{H}_0, S^\gamma(\boldsymbol{r})] = -\nabla\cdot\boldsymbol{j}^{S^\gamma}(\boldsymbol{r})$

holds when total spin commutes with (spin-wave) Hamiltonian.

Our approach for *spin nonconserving systems*

Heisenberg Eq.: $\frac{\partial S^\gamma(\boldsymbol{r})}{\partial t} = \frac{i}{\hbar}[\mathcal{H}_0, S^\gamma(\boldsymbol{r})] = -\nabla\cdot\boldsymbol{j}^{S^\gamma}(\boldsymbol{r}) + \tau^{S^\gamma}(\boldsymbol{r})$ Torque term: deviation from equation of continuity

If torque is written by divergence form: $\langle\tau^{S^\gamma}(\boldsymbol{r})\rangle = -\nabla\cdot\boldsymbol{\pi}^{S^\gamma}(\boldsymbol{r})$ → $\frac{\partial\langle S^\gamma\rangle}{\partial t} = -\nabla\cdot\boldsymbol{\mathcal{J}}^{S^\gamma}$ with $\boldsymbol{\mathcal{J}}^{S^\gamma} = \langle\boldsymbol{j}^{S^\gamma}\rangle + \boldsymbol{\pi}^{S^\gamma}$

"equation of continuity" is recovered as expectation value.

Conserved spin current $\mathcal{J}^{S^\gamma} = \frac{1}{V}\int\boldsymbol{\mathcal{J}}^{S^\gamma}(\boldsymbol{r})d\boldsymbol{r}$ → $\mathcal{J}^{S^\gamma}_{y;\mathrm{tr}} = \kappa^{S^\gamma}_{xy}(-\nabla_y T)$

cf. *Fermion system*

C. Xiao, et al., PRB **104**, L241411 (2021).

Problems

Bosonic BdG Hamiltonian: $\mathcal{H}_0 = \frac{1}{2}\int d\boldsymbol{r}\mathcal{A}^\dagger(\boldsymbol{r})\hat{H}_0\mathcal{A}(\boldsymbol{r})$

Set of Bose operators:
$\mathcal{A}(\boldsymbol{r}) = \{a_1(\boldsymbol{r}), a_2(\boldsymbol{r}), \ldots, a_N(\boldsymbol{r}), a_1^\dagger(\boldsymbol{r}), a_2^\dagger(\boldsymbol{r}), \ldots, a_N^\dagger(\boldsymbol{r})\}$

Conserved spin current: $\mathcal{J}^{S^\gamma} = \langle \boldsymbol{j}^{S^\gamma}\rangle + \boldsymbol{\pi}^{S^\gamma}$ → Calculation of $\boldsymbol{\pi}^{S^\gamma}$ in the presence of temperature gradient

Conventional spin current: $\boldsymbol{j}^{S^\gamma} = \frac{1}{4}\mathcal{A}^\dagger(\boldsymbol{r})\left(\hat{\boldsymbol{v}}\sigma_3\hat{S}^\gamma + \hat{S}^\gamma\sigma_3\hat{\boldsymbol{v}}\right)\mathcal{A}(\boldsymbol{r}) =: \mathcal{A}^\dagger(\boldsymbol{r})\hat{\boldsymbol{j}}^{S^\gamma}\mathcal{A}(\boldsymbol{r})$

Velocity: $\hat{\boldsymbol{v}} = \frac{i}{\hbar}[\hat{H}_0, \hat{\boldsymbol{r}}]$

Torque: $\tau^{S^\gamma} = \frac{i}{2\hbar}\mathcal{A}^\dagger(\boldsymbol{r})\left(\hat{H}_0\sigma_3\hat{S}^\gamma - \hat{S}^\gamma\sigma_3\hat{H}_0\right)\mathcal{A}(\boldsymbol{r}) =: \mathcal{A}^\dagger(\boldsymbol{r})\hat{\tau}^{S^\gamma}\mathcal{A}(\boldsymbol{r})$

Para-unit matrix: $\sigma_3 = \begin{pmatrix} \mathbf{1}_{N\times N} & 0 \\ 0 & -\mathbf{1}_{N\times N}\end{pmatrix}$

are written by bosonic operators $\mathcal{A}(\boldsymbol{r})$

$\boldsymbol{\pi}^{S^\gamma}(\boldsymbol{r})$ is calculated within the first order of ∇T .

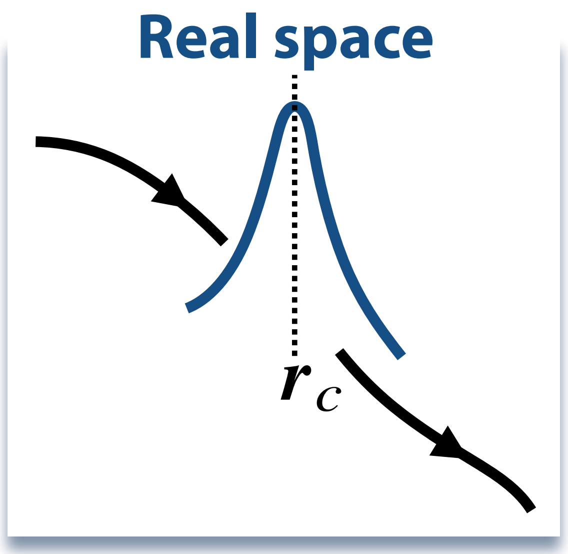
→ $\langle\tau^{S^\gamma}\rangle_{\nabla T} = -\nabla\cdot\boldsymbol{\pi}^{S^\gamma}$ should be evaluated up to the ***second order*** of spatial gradient.

Semiclassical theory on the dynamics of ***wave-packet***

This has been already applied to fermionic case.

→ Application to bosonic systems in the present study

D. Xiao, et al., RMP **82**, 1959 (2010).
C. Xiao, et al., PRB **104**, L241411 (2021).



Semiclassical theory

Conserved spin current: $\mathscr{J}^{S^\gamma} = \langle j^{S^\gamma} \rangle + \pi^{S^\gamma}$

$\langle \tau^{S^\gamma} \rangle = -\nabla \cdot \pi^{S^\gamma}$

Calculation of $\langle j^{S^\gamma}(r) \rangle$ and $\langle \tau^{S^\gamma}(r) \rangle$ in semiclassical theory $\hat{\theta} = \hat{j}^{S^\gamma}, \hat{\tau}^{S^\gamma}$

$$\hat{H} = \hat{H}_0 + \frac{\hbar}{2}\left[\hat{\theta} \cdot h(\hat{r}, t) + h(\hat{r}, t) \cdot \hat{\theta}\right] \longrightarrow \text{Lagrangian} \longrightarrow \langle \theta(r) \rangle \text{ from } \textit{functional derivative} \text{ of action}$$

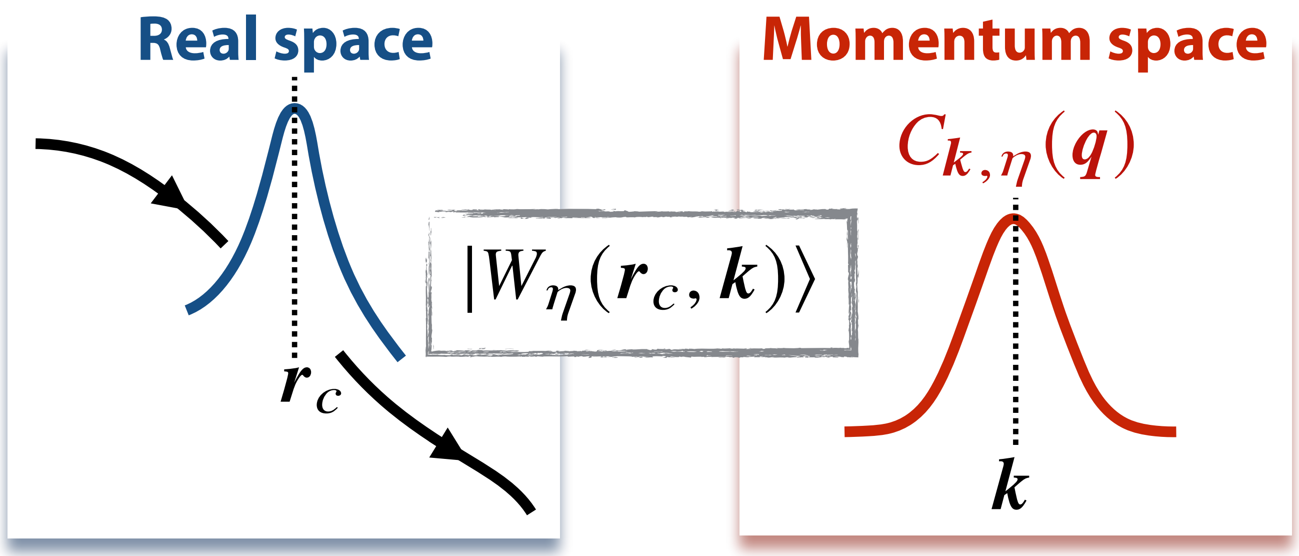
Virtual source field term

Wave packet = superposition of magnon Bloch states

$$|W_\eta(r_c, k)\rangle = \int dq C_{k,\eta}(q) e^{iq\cdot\hat{r}} |u_{q,\eta}\rangle$$

magnon Bloch states

D. Xiao, et al., RMP **82**, 1959 (2010).
X. Zhang, et al., PRL **123**, 167202 (2019).



Lagrangian: $\mathcal{L}_\eta = \dfrac{\langle W_\eta | \sigma_3 \left(i\hbar \frac{d}{dt} - \sigma_3 \hat{H}\right) | W_\eta \rangle}{\langle W_\eta | \sigma_3 | W_\eta \rangle}$ with virtual fields h^j, h^τ

$\longrightarrow$

$\langle j^{S^\gamma}(r) \rangle$ up to first order of **∇*T***

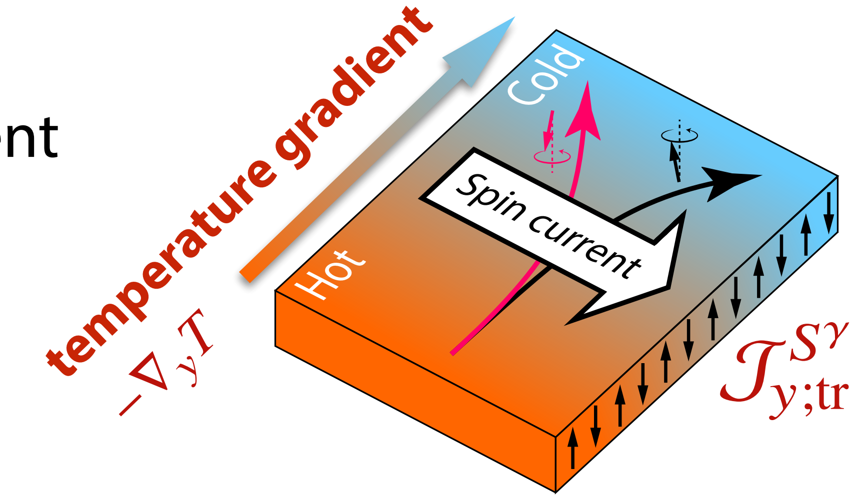
$\langle \tau^{S^\gamma}(r) \rangle$ up to first order of **∇*T*** and **∇**

(second order of spatial gradient)

Spin Nernst effect

Definition of spin Nernst coefficient

$$\mathcal{J}^{S^\gamma}_{y;\mathrm{tr}} = \kappa^{S^\gamma}_{xy}(-\nabla_y T)$$



Spin current

$\langle \tau^{S^\gamma}(\boldsymbol{r})\rangle$ up to first order of $\boldsymbol{\nabla} T$ and $\boldsymbol{\nabla}$

(up to second order of spatial gradient)

$$\langle \tau^{S^\gamma}\rangle_{\nabla T} = -\nabla\cdot\boldsymbol{\pi}^{S^\gamma}\Big|_{\nabla T} + \boldsymbol{F}\cdot\nabla T$$

$$H_{0,\boldsymbol{k}} = H_{0,-\boldsymbol{k}} \implies \boldsymbol{F} = 0$$

B. Li *et al.*, Phys. Rev. Res. **2**, 013079 (20220).

Spin current is introduced from **conserved spin current**.

$$\frac{\partial\langle S^\gamma\rangle}{\partial t} = -\nabla\cdot\mathcal{J}^{S^\gamma}$$ with **conserved spin current:** $\mathcal{J}^{S^\gamma} = \langle \boldsymbol{j}^{S^\gamma}\rangle + \boldsymbol{\pi}^{S^\gamma}$

$$\kappa^{S^\gamma}_{xy} = -\frac{k_B}{\hbar V}\sum_{\eta=1}^{N}\sum_{\boldsymbol{k}}\left(\Upsilon^{S^\gamma}_{\boldsymbol{k},\eta}\right)_{xy} c_1[f_B(\varepsilon_{\boldsymbol{k},\eta})] \quad \text{with} \quad \left(\Upsilon^{S^\gamma}_{\boldsymbol{k},\eta}\right)_{xy} = -\Omega^{xy}_{\boldsymbol{k},\eta}(S^\gamma_{\boldsymbol{k}})_\eta + \frac{\partial}{\partial k_y} 2g^{k_x h^\tau_\gamma}_{\boldsymbol{k},\eta}$$

$$f_B(\omega) = (e^{\beta\omega} - 1)^{-1}$$

$$c_1(x) = (1+x)\ln(1+x) - x\ln x$$

$$(S^\gamma_{\boldsymbol{k}})_\eta = \langle u_{\boldsymbol{k},\eta}|S^\gamma|u_{\boldsymbol{k},\eta}\rangle$$

Bosonic quantum geometry in *mixed space* (***X***, ***Y***)

Quantum metric: $g^{X_\lambda Y_{\lambda'}}_{\boldsymbol{k},\eta} = \mathrm{Re}\left[\sigma_{3,\eta}\left\langle \partial_{X_\lambda} u_{\boldsymbol{k},\eta}\right|\sigma_3\left(\hat{1} - \sigma_{3,\eta}\left|u_{\boldsymbol{k},\eta}\right\rangle\left\langle u_{\boldsymbol{k},\eta}\right|\sigma_3\right)\left|\partial_{Y_{\lambda'}} u_{\boldsymbol{k},\eta}\right\rangle\right]$

Berry curvature: $\Omega^{X_\lambda Y_{\lambda'}}_{\boldsymbol{k},\eta} = -2\mathrm{Im}\left[\sigma_{3,\eta}\langle \partial_{X_\lambda} u_{\boldsymbol{k},\eta}|\sigma_3|\partial_{Y_{\lambda'}} u_{\boldsymbol{k},\eta}\rangle\right]$

$\boldsymbol{k}$ ⟵ $g^{k_x h^\tau_\gamma}_{\boldsymbol{k},\eta}$ ⟶ $(h^{\tau^S}_x, h^{\tau^S}_y, h^{\tau^S}_z)$

Virtual field for torque $(\tau^{S^x}, \tau^{S^y}, \tau^{S^z})$

Spin Nernst effect

Representation neglecting **torque** (valid only for *spin-conserving* systems) B. Li, et al., Phys. Rev. Res. **2**, 013079 (2020).

$$\tilde{\kappa}_{xy}^{S^\gamma} = -\frac{k_B}{\hbar V}\sum_{\eta=1}^{N}\sum_{\boldsymbol{k}}\left(\tilde{\Omega}_{\boldsymbol{k},\eta}^{S^\gamma}\right)_{xy} c_1[f_B(\varepsilon_{\boldsymbol{k},\eta})]$$ with

Spin Berry curvature $$\left(\tilde{\Omega}_{\boldsymbol{k},\eta}^{S^\gamma}\right)_{\lambda\lambda'} = -4\hbar^2 \sum_{\eta_1(\neq\eta)}^{2N} \sigma_{3,\eta}\sigma_{3,\eta_1}\frac{\mathrm{Im}\left[(v_{\boldsymbol{k},\lambda'})_{\eta\eta_1}(j_{\boldsymbol{k},\lambda}^{S^\gamma})_{\eta_1\eta}\right]}{(\bar{\varepsilon}_{\boldsymbol{k},\eta}-\bar{\varepsilon}_{\boldsymbol{k},\eta_1})^2}$$

$\left(\tilde{\Omega}_{\boldsymbol{k},\eta}^{S^\gamma}\right)_{\lambda\lambda'} = \left(\Upsilon_{\boldsymbol{k},\eta}^{S^\gamma}\right)_{\lambda\lambda'}$ only if spin is conserved.

Representation incorporating **torque**

$$\kappa_{xy}^{S^\gamma} = -\frac{k_B}{\hbar V}\sum_{\eta=1}^{N}\sum_{\boldsymbol{k}}\left(\Upsilon_{\boldsymbol{k},\eta}^{S^\gamma}\right)_{xy} c_1[f_B(\varepsilon_{\boldsymbol{k},\eta})]$$ with $$\left(\Upsilon_{\boldsymbol{k},\eta}^{S^\gamma}\right)_{xy} = -\Omega_{\boldsymbol{k},\eta}^{xy}(S_{\boldsymbol{k}}^{\gamma})_\eta + \frac{\partial}{\partial k_y}2g_{\boldsymbol{k},\eta}^{k_x h_\gamma^\tau}$$

$$f_B(\omega) = (e^{\beta\omega}-1)^{-1}$$

$$c_1(x) = (1+x)\ln(1+x) - x\ln x$$

$$(S_{\boldsymbol{k}}^{\gamma})_\eta = \langle u_{\boldsymbol{k},\eta}|S^\gamma|u_{\boldsymbol{k},\eta}\rangle$$

Bosonic quantum geometry in *mixed space* (***X***, ***Y***)

Quantum metric: $g_{\boldsymbol{k},\eta}^{X_\lambda Y_{\lambda'}} = \mathrm{Re}\left[\sigma_{3,\eta}\left\langle\partial_{X_\lambda}u_{\boldsymbol{k},\eta}\right|\sigma_3\left(\hat{1}-\sigma_{3,\eta}\left|u_{\boldsymbol{k},\eta}\right\rangle\left\langle u_{\boldsymbol{k},\eta}\right|\sigma_3\right)\left|\partial_{Y_{\lambda'}}u_{\boldsymbol{k},\eta}\right\rangle\right]$

Berry curvature: $\Omega_{\boldsymbol{k},\eta}^{X_\lambda Y_{\lambda'}} = -2\mathrm{Im}\left[\sigma_{3,\eta}\langle\partial_{X_\lambda}u_{\boldsymbol{k},\eta}|\sigma_3|\partial_{Y_{\lambda'}}u_{\boldsymbol{k},\eta}\rangle\right]$

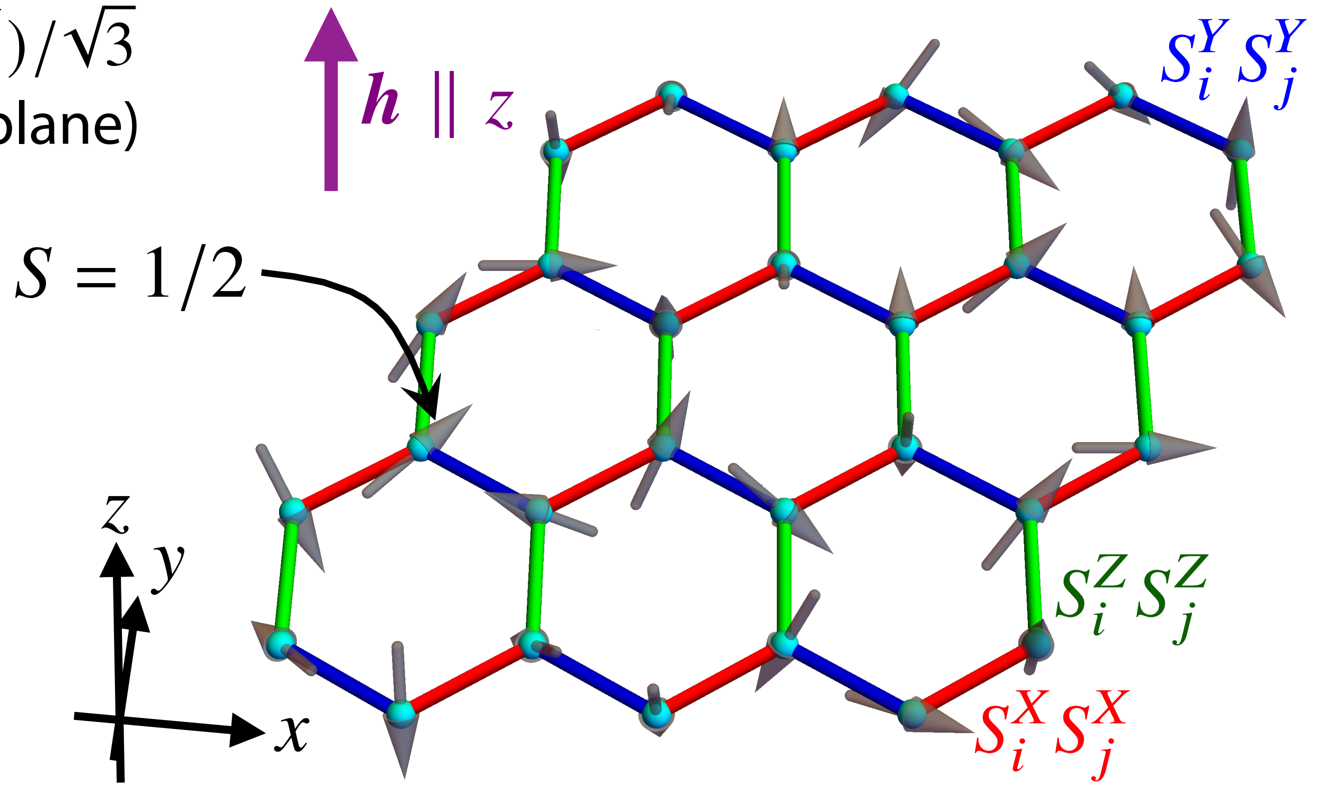
$\boldsymbol{k}$ ⟵ $g_{\boldsymbol{k},\eta}^{k_x h_\gamma^\tau}$ ⟶ $(h_x^{\tau^S}, h_y^{\tau^S}, h_z^{\tau^S})$ **Virtual field for torque** $(\tau^{S^x}, \tau^{S^y}, \tau^{S^z})$

Result: Kitaev model under magnetic field

Ferromagnetic Kitaev model under magnetic fields for $S^z = (S^X + S^Y + S^Z)/\sqrt{3}$ (perpendicular to honeycomb plane)

$2K < 0$

$$\mathcal{H} = 2K \sum_{\gamma=X,Y,Z} \sum_{\langle ij \rangle_\gamma} S_i^\gamma S_j^\gamma - \boldsymbol{h} \cdot \sum_i \boldsymbol{S}_i$$



Ground state: forced ferromagnetic along z direction

$H_{0,\boldsymbol{k}} = H_{0,-\boldsymbol{k}}$ is satisfied.

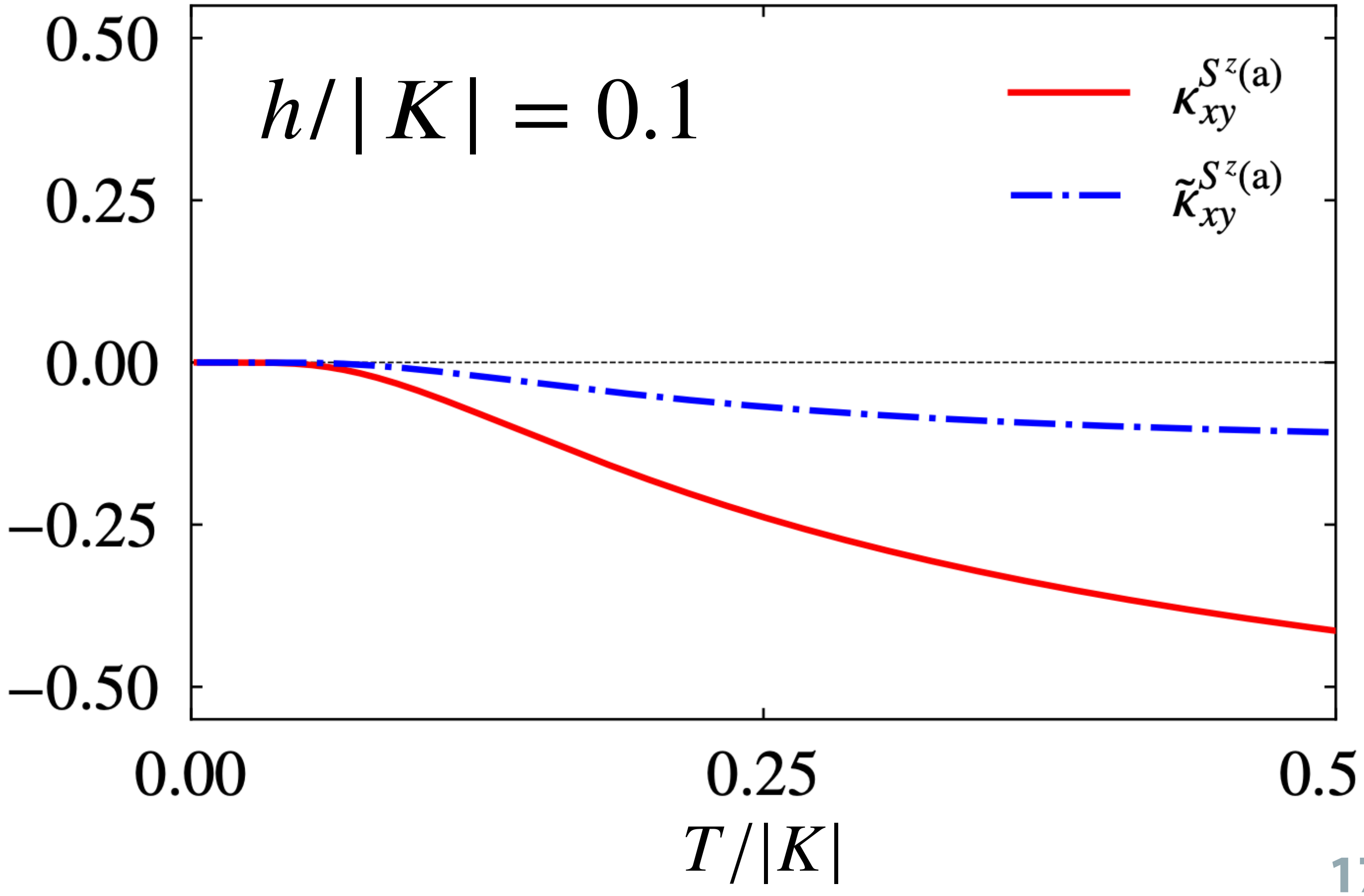
Anti-symmetrization

Spin Nernst coefficient w/ torque

$$\kappa_{xy}^{S^\gamma(\mathrm{a})} = \left(\kappa_{xy}^{S^\gamma} - \kappa_{yx}^{S^\gamma}\right)/2$$

Spin Nernst coefficient w/o torque

$$\tilde{\kappa}_{xy}^{S^\gamma(\mathrm{a})} = \left(\tilde{\kappa}_{xy}^{S^\gamma} - \tilde{\kappa}_{yx}^{S^\gamma}\right)/2$$



- Torque term significantly affects spin Nernst coefficient
- Enhancement of spin Nernst coefficient due to torque term

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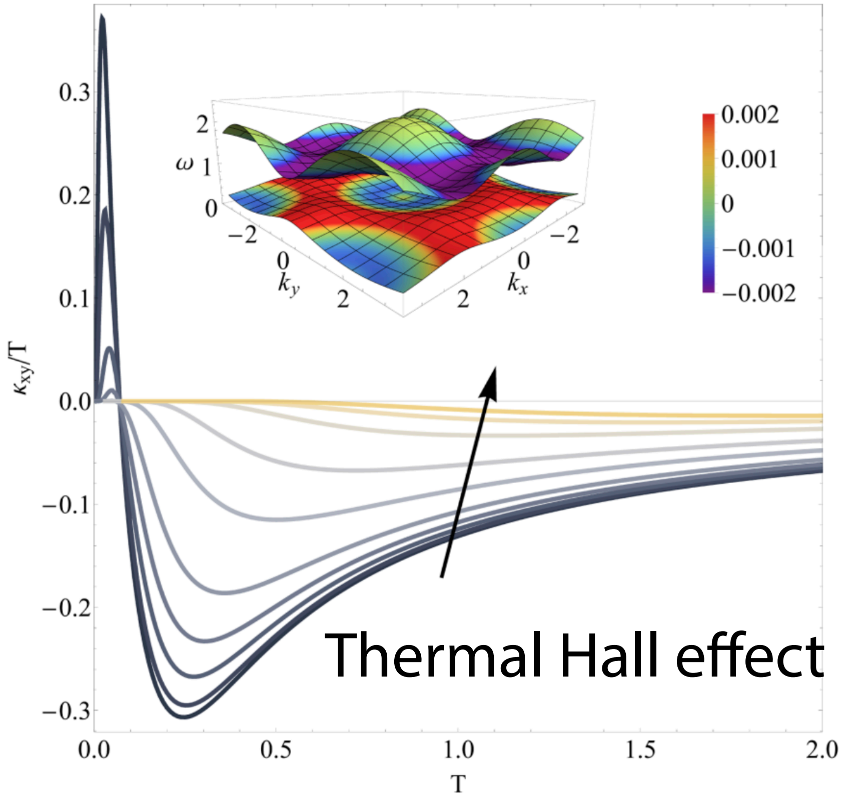
Effect of quantum metric

Anti-symmetrized spin Nernst coefficient

$$\kappa_{xy}^{S^\gamma(\mathrm{a})} = -\frac{k_B}{\hbar V}\sum_{\eta=1}^{N}\sum_{\boldsymbol{k}} (\Upsilon_{\boldsymbol{k},\eta}^{S^\gamma})_{xy}^{(\mathrm{a})} c_1[f_B(\varepsilon_{\boldsymbol{k},\eta})] \quad \text{with} \quad (\Upsilon_{\boldsymbol{k},\eta}^{S^\gamma})_{xy}^{(\mathrm{a})} = -\Omega_{\boldsymbol{k},\eta}^{xy}(S_{\boldsymbol{k}}^{\gamma})_\eta + (D_{\boldsymbol{k},\eta}^{S^\gamma})_{xy}^{(\mathrm{a})}$$

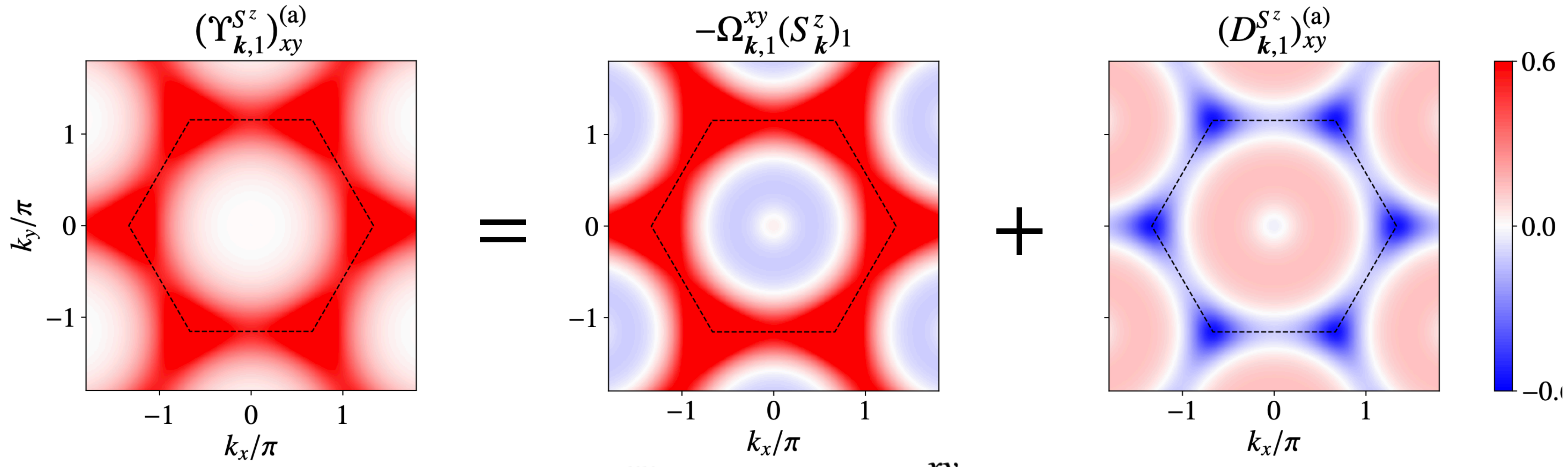
Antisymmetric component

$$(D_{\boldsymbol{k},\eta}^{S^\gamma})_{xy}^{(\mathrm{a})} = \partial_{k_y} g_{\boldsymbol{k},\eta}^{k_x h_\gamma^\tau} - \partial_{k_x} g_{\boldsymbol{k},\eta}^{k_y h_\gamma^\tau}$$

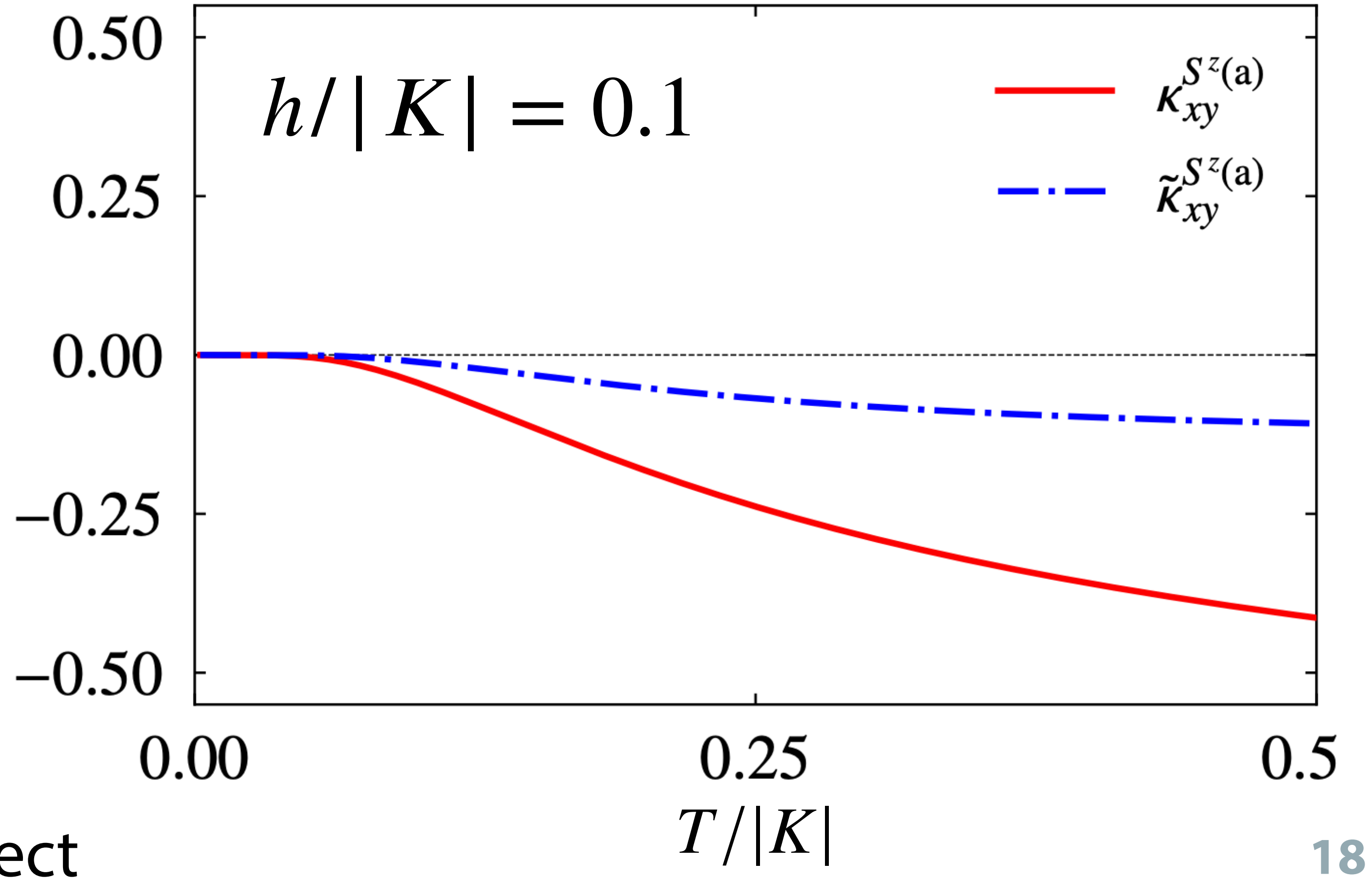


P. A. McClarty et al., Phys Rev B **98**, 060404 (2018).

Momentum dependence for lowest energy branch



$$-\Omega_{\boldsymbol{k},1}^{xy}(S_{\boldsymbol{k}}^z)_1 \sim \Omega_{\boldsymbol{k},1}^{xy}$$



- Negative region around Γ point in $\Omega_{\boldsymbol{k},1}^{xy}$ leads to sign change in κ_{xy}^{H}
- Sign change feature disappears in $(\Upsilon_{\boldsymbol{k},\eta}^{S^\gamma})_{xy}^{(\mathrm{a})}$ due to cancellation
- Quantum metric part $(D_{\boldsymbol{k},\eta}^{S^\gamma})_{xy}^{(\mathrm{a})}$ results in absence of low-T peak in spin Nernst effect

Summary

Formulation of thermal response using spin-wave theory

- Thermal Hall conductivity incorporating ***magnon damping***

S. Koyama and JN, Phys. Rev. B **109**, 174442 (2024).

Finite-temperature formulation of iDE approach & Green' function representation of *energy magnetization*

Our results

$$\kappa^{H}_{xy} = -\frac{k_B^2 T}{\hbar V}\sum_{\eta=1}^{N}\sum_{\boldsymbol{k}}\Omega^{xy}_{\boldsymbol{k},\eta}\int_{-\infty}^{\infty} d\omega \underline{\rho_{\boldsymbol{k},\eta}(\omega)} c_2[f_B(\omega)]$$

Spectral function of magnons

- Magnon damping significantly suppresses thermal Hall conductivity at finite temperature.

- Spin Nernst effect in ***spin-nonconserving systems***

S. Koyama and JN, arXiv:2503.10281.

Development of *bosonic* semiclassical theory & Formulation of spin Nernst coefficient *incorporating torque term*

Our results

$$\kappa^{S^\gamma}_{xy} = -\frac{k_B}{\hbar V}\sum_{\eta=1}^{N}\sum_{\boldsymbol{k}}\underline{(\Upsilon^{S^\gamma}_{\boldsymbol{k},\eta})_{xy}} c_1[f_B(\varepsilon_{\boldsymbol{k},\eta})]$$

$$(\Upsilon^{S^\gamma}_{\boldsymbol{k},\eta})_{xy} = -\underline{\Omega^{xy}_{\boldsymbol{k},\eta}}(S^\gamma_{\boldsymbol{k}})_\eta + \frac{\partial}{\partial k_y} 2\underline{g^{k_x h^\tau_\gamma}_{\boldsymbol{k},\eta}}$$

Berry curvature Quantum metric

- Quantum metric part can substantially contributes to spin Nernst effect.