Intrinsic Thermal Hall Effect in **Mott Insulators**

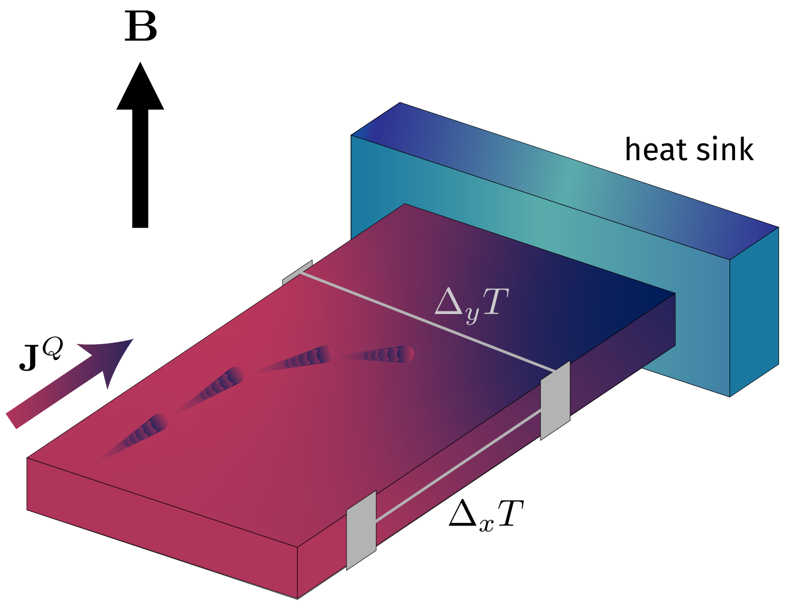
Emily Z Zhang*

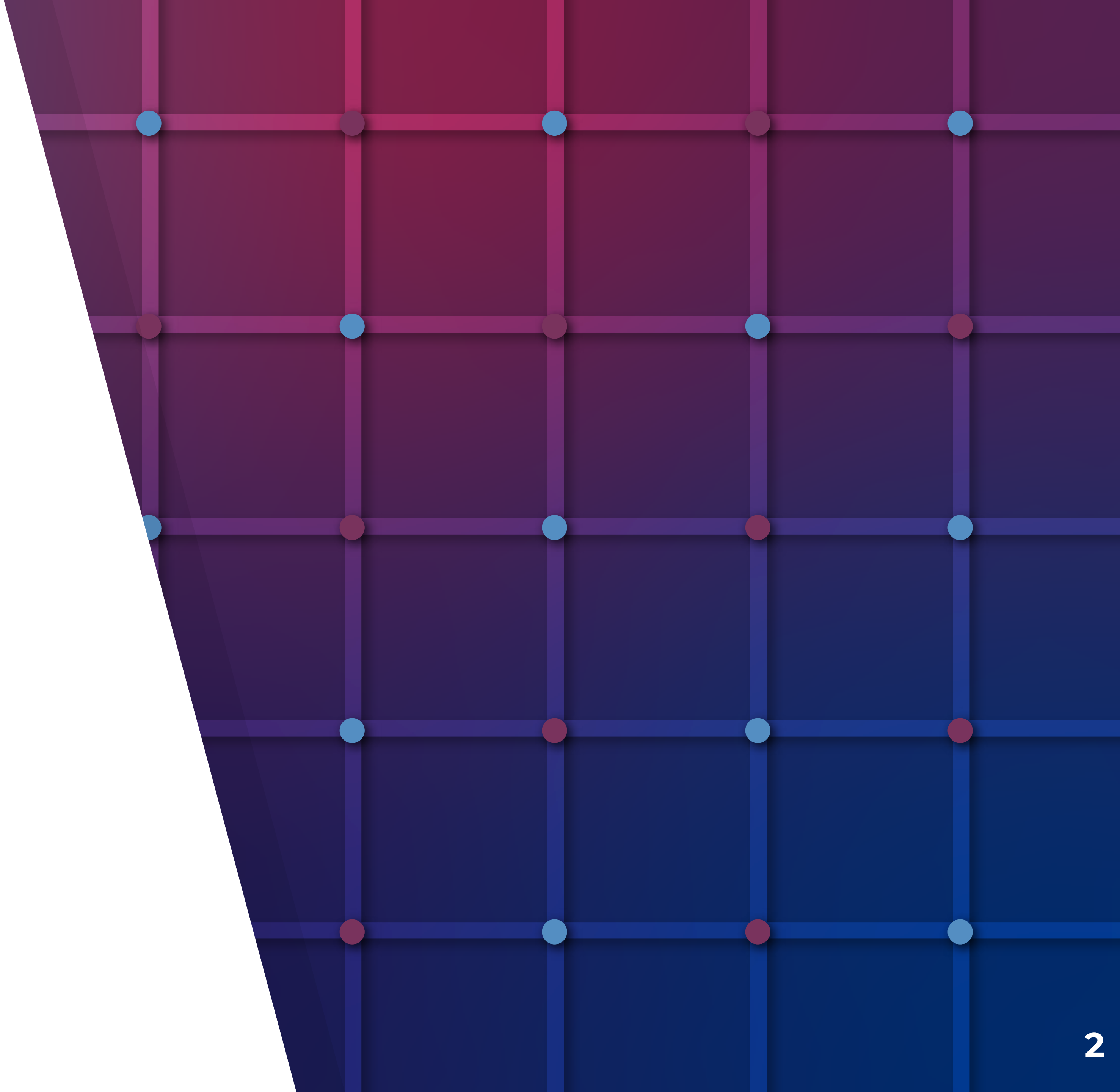
Jixun K. Ding*, Wen O. Wang, Tessa Cookmeyer, Brian Moritz, Yong Baek Kim, Thomas P. Devereaux

*Contributed equally to this work

Thermal Hall Transport for Mott Insulators

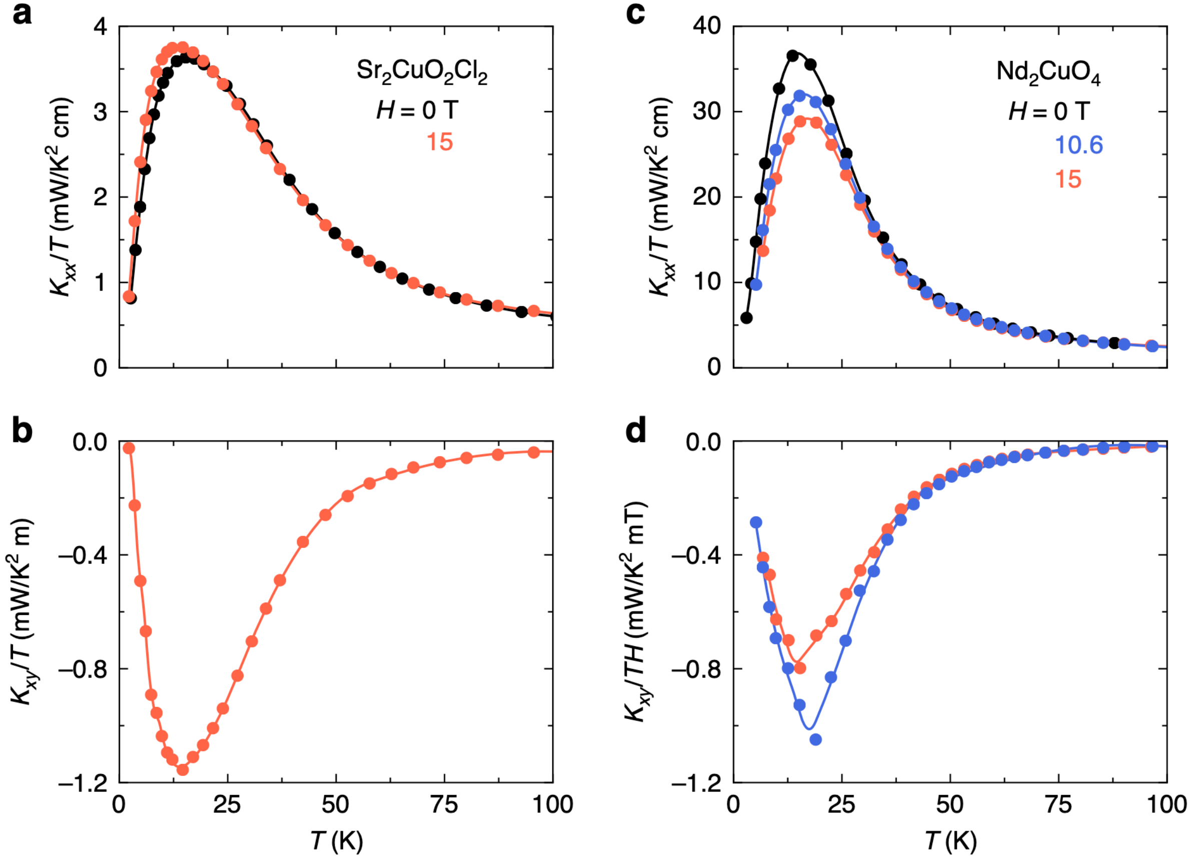
- Electrons localized, **no charge transport**
- Collective excitations **carry heat**
- Sensitive to **nontrivial topologies** of the heat carriers

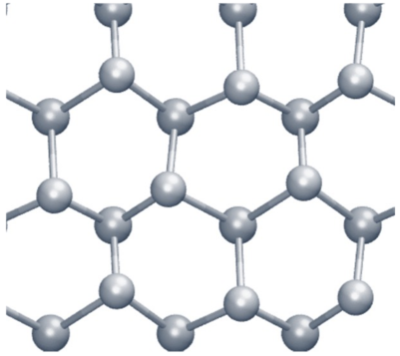




Phonon Thermal Hall Transport

Large thermal Hall conductivity in the undoped cuprates attributed to **phonons**





Hanyu Zhu, et al., Berkeley Lab

How do phonons acquire chirality?

Intrinsic:

Berry curvature, coupling to topological quasiparticle,...

Extrinsic:

Impurity scattering, scattering off domain boundaries,...

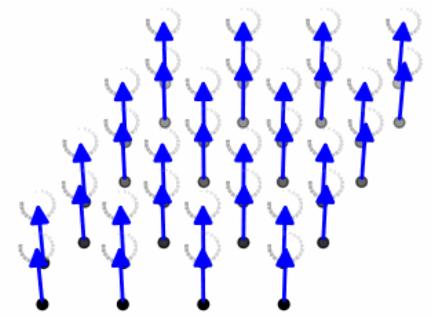
[1] G. Grissonnanche, Nature (London) 571, 376 (2019).
[2] M.-E. Boulanger, Nat. Commun. 11, 5325 (2020).
[3] G. Grissonnanche, Nat. Phys. 16, 1108 (2020).
[4] L. Chen, PNAS 119, (34) e2208016119 (2022).
[5] M.-E. Boulanger, PRB 105, 115101 (2022)

[6] X.Q. Sun, J.Y. Chen, S.A. Kivelson, PRB (2022)
[7] H. Guo, D.g. Joshi, S. Sachdev, PNAS (2022)
[8] L. Mangeolle, L. Balents, L. Savary, PRX (2022)
⋮

Magnon Thermal Hall Transport

Generically arises in systems that **break SU(2) symmetry**

e.g. Kitaev, Dzyaloshinskii-Moriya



NO-GO THEOREM *

Magnon Hall effect impossible on the **square lattice** for spin-rotationally symmetric systems

Katsura, Nagaosa, and Lee, *PRL* (2010)

*Assumptions:

Linear spin wave theory: non-interacting magnons and no scattering

Minimal chiral coupling: higher order exchange terms near the Mott transition

Requirements for observing **intrinsic thermal Hall** effect in **Mott insulators**?

CLAIM:

Need to break both **particle-hole** and **time-reversal** symmetry for finite thermal Hall

Symmetry argument

No thermal Hall when PHS and/or TRS

DQMC simulations

κ_{xy}/T on the order of ~0.01-0.1 $k_B^2/\hbar$

Possible Mechanism

Magnon-magnon scattering

A Symmetry Perspective

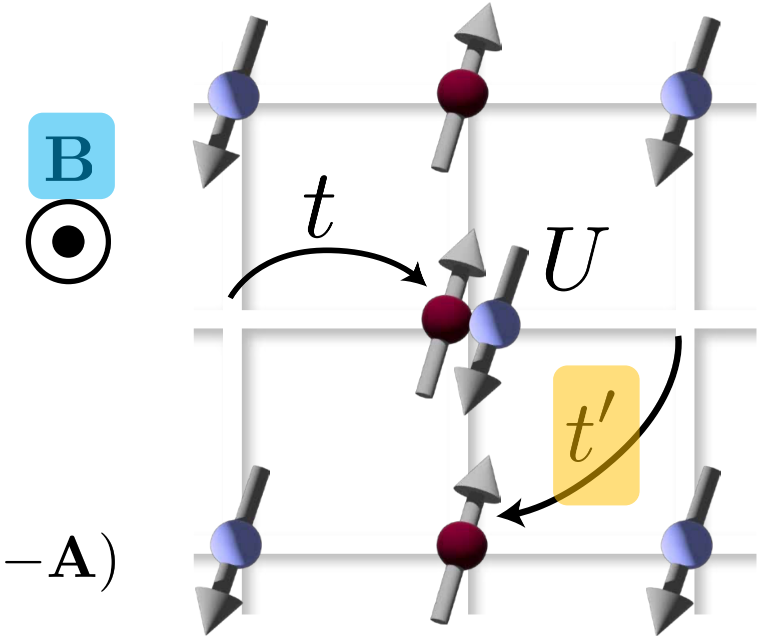
$$H = -\sum_{ij\sigma} t_{ij} \left\{ \exp\left[\mathrm{i}\varphi_{ij}\right] c^\dagger_{i\sigma} c_{j\sigma} + \mathrm{h.c.} \right\} - \mu \sum_{i\sigma} n_{i\sigma} + U \sum_i \left(n_{i\uparrow} - 1/2\right)\left(n_{i\downarrow} - 1/2\right)$$

breaks charge conjugation

$[\mathcal{H}, \mathcal{C}] \neq 0$

breaks time-reversal

$[\mathcal{H}, \mathcal{T}] \neq 0$



CONSTRAINT 1:

Onsager-Casimir relations $\kappa_{xy}(\mathbf{A}) = \kappa_{yx}(-\mathbf{A})$

CONSTRAINT 2:

Particle-hole symmetric Hamiltonian must have $\kappa_{xy}(\mathbf{A}) = \kappa_{xy}(-\mathbf{A})$

If both 1 and 2, then

$\kappa_{xy}(\mathbf{A}) = \kappa_{xy}(-\mathbf{A}) = 0$

If !(constraint 2)

$\kappa_{xy}(\mathbf{A}) \neq 0$

CLAIM:

Need to break both **particle-hole** and **time-reversal** symmetry for finite thermal Hall

Symmetry argument

No thermal Hall when PHS and/or TRS

DQMC simulations

κ_{xy}/T on the order of ~0.01-0.1 $k_B^2/\hbar$

Possible Mechanism

Magnon-magnon scattering

Determinantal Quantum Monte Carlo

Directly simulates the Hubbard model, **non-perturbative**

DQMC

Unequal-time correlators

$$\chi_{22,\alpha\beta}(\tau) = \frac{1}{V}\langle J_{Q,\alpha}(\tau) J_{Q,\beta}(0)\rangle$$

Analytic Continuation

Maximum entropy (MaxEnt) algorithm

$$\chi_{22,\alpha\beta}(\omega)$$

Proxies

$$\kappa_{xy}/T \approx R_{\mathrm{th},H}(i\omega_1)\kappa_{xx}^2 \frac{B}{T}$$

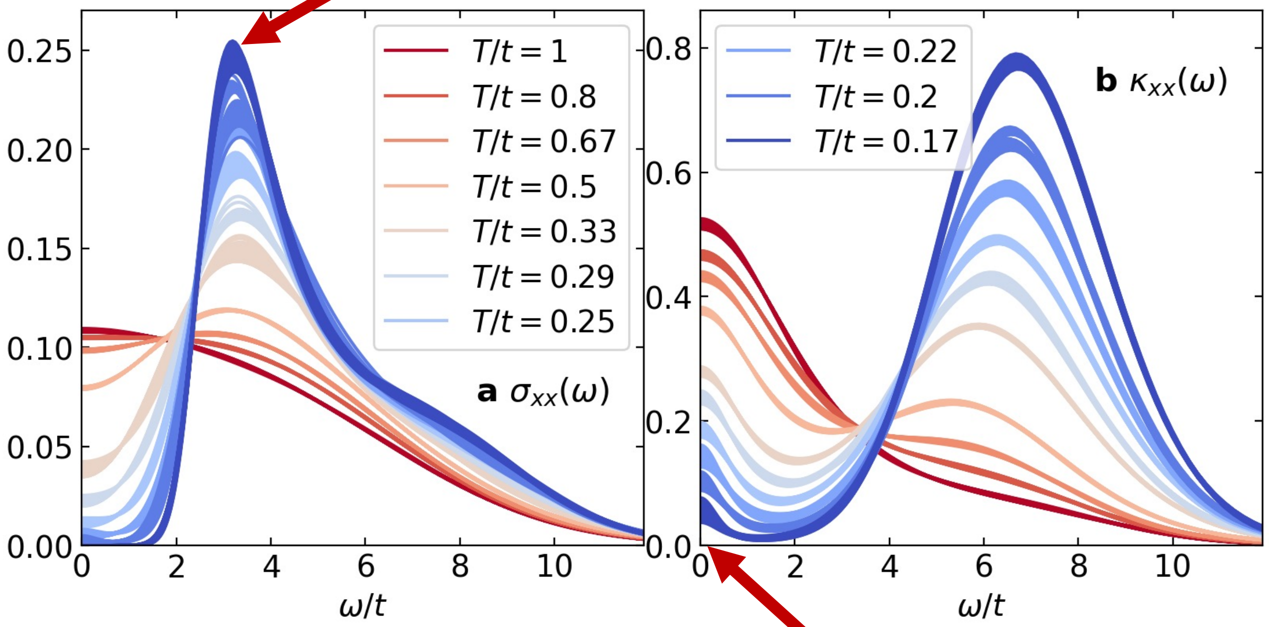
Transport Coefficients

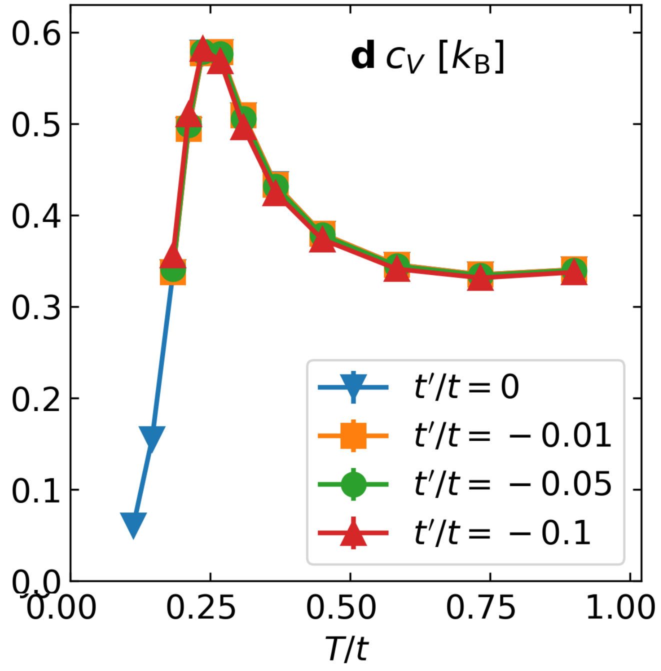
$$\kappa_{\alpha\beta}/T = \frac{1}{\hbar\omega V}\int_{-\infty}^{\infty} dt\, \theta(t) \left\langle \left[J^{\dagger}_{\mu,\alpha}(t), J_{\nu,\beta}(0) \right] \right\rangle_0 e^{i\omega t}$$

DQMC: Longitudinal Conductivities

Electrical conductivity gapped at low T

Crossover to magnon transport regime





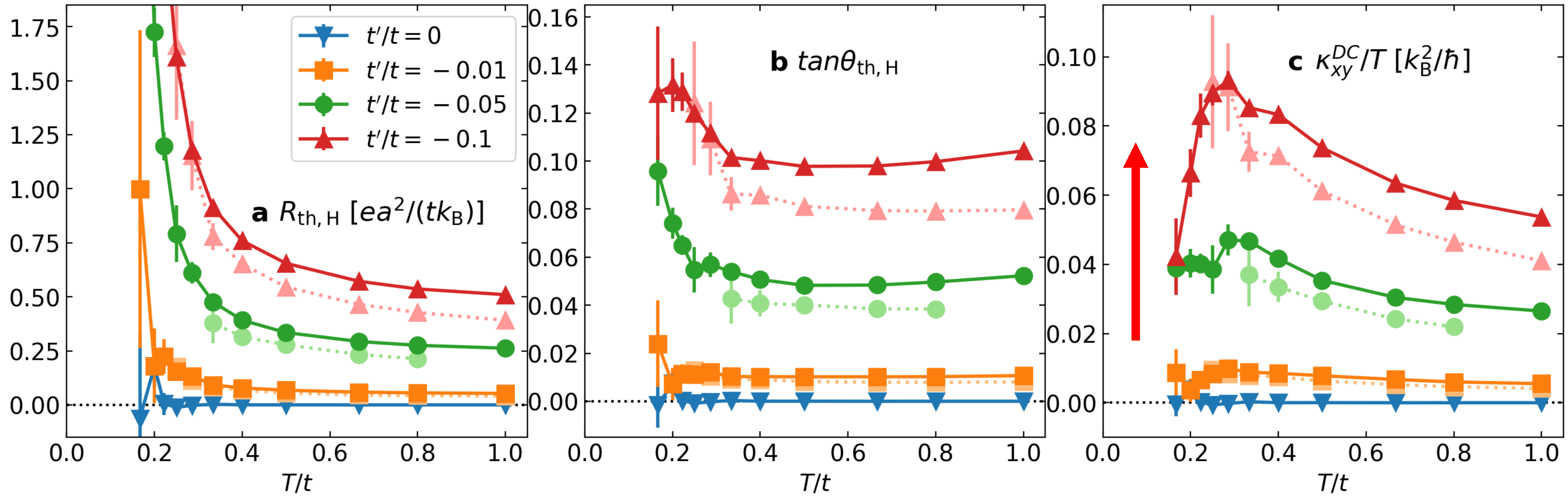
$t'/t = -0.1, B = 0.0625\Phi_0/a^2$

$8 \times 8, U = 6, T > t/6$

Finite DC heat conductivity

Electrical insulator, heat conductor

DQMC: Thermal Hall Conductivities



Proxy and analytical continuation methods **qualitatively agree**

Thermal conductivity **increases** with increasing t’

Low temperature (T<J) regime **violates no-go result!**

CLAIM:

Need to break both **particle-hole** and **time-reversal** symmetry for finite thermal Hall

Symmetry argument

No thermal Hall when PHS and/or TRS

DQMC simulations

κ_{xy}/T on the order of ~0.01-0.1 $k_B^2/\hbar$

Possible Mechanism

Magnon-magnon scattering

Wake me up before you no-go:
Magnon-magnon scattering

$$J_\chi = \frac{24t^2t'}{U^2}\sin(\pi B a^2/\Phi_0)$$

Strong coupling limit (U>>t)

$$H_{\text{eff}} = J_1 \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j + J_2 \sum_{\langle\langle ij \rangle\rangle} \vec{S}_i \cdot \vec{S}_j + J_\chi \sum_{\triangle_{ijk}} \vec{S}_i \cdot (\vec{S}_j \times \vec{S}_k)$$

Holstein-Primakoff Bosons + Bogoliubov Transformation

$$H^{(2)} = \sum_{\mathbf{k}} \varepsilon_{\mathbf{k}} (\alpha^\dagger_{\mathbf{k}} \alpha_{\mathbf{k}} + \beta^\dagger_{\mathbf{k}} \beta_{\mathbf{k}})$$

$$H^{(4)} = \sum_{\mathbf{k},\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3} \delta_{\mathbf{k}+\mathbf{k}_1+\mathbf{k}_2+\mathbf{k}_3} W^{\alpha\beta\gamma\delta}_{\mathbf{k},\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3} \psi^\alpha_{\mathbf{k}} \psi^\beta_{\mathbf{k}_1} \psi^\gamma_{\mathbf{k}_2} \psi^\delta_{\mathbf{k}_3}$$

Purely real

$$\propto J_1/S, J_2/S$$

Purely imaginary

$$\propto iSJ_\chi$$

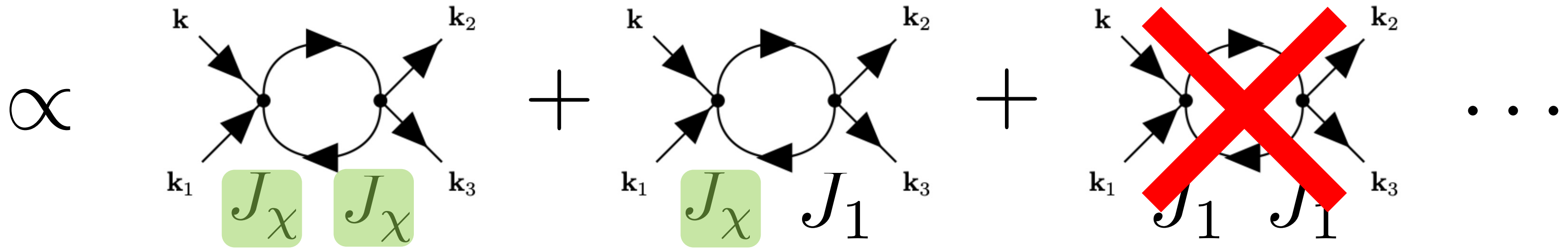
Wake me up before you no-go:
Magnon-magnon scattering

$$J_\chi = \frac{24t^2t'}{U^2}\sin(\pi B a^2/\Phi_0)$$

Boltzmann transport: $\kappa_{xy} \sim$ Rate of magnon mode collisions

Chatzichrysafis and Mook, arXiv:2407.00423 (2024)

Fermi's golden rule:



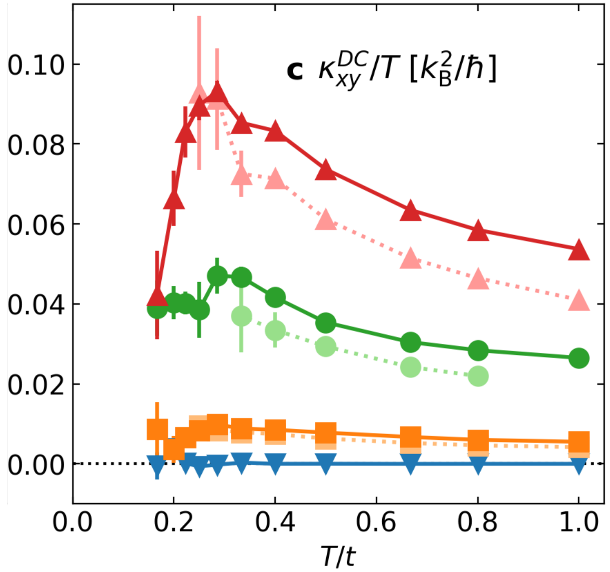
Only collisions mediated by J_χ contribute to off-diagonal scattering!

$$\kappa_{xy} \propto t' \sin(\pi B a^2/\Phi_0)$$

Summary

The *t-t'-U* Hubbard model on the square lattice exhibits a **nonzero thermal Hall effect** under an applied magnetic field.

One should not naively ignore potential magnon contributions based on the **no-go theorem.**



UNIVERSITY OF TORONTO
NSERC CRSNG
Stanford University
U.S. DEPARTMENT of ENERGY
NERSC

Symmetry argument

$$\mathcal{C}: \quad c_{i\sigma} \to (-1)^i c_{i\sigma}^\dagger, c_{i\sigma}^\dagger \to (-1)^i c_{i\sigma}$$
$$\mathcal{T}: \quad i \to -i$$

If t’ = 0:

$$H(\mathbf{A}) \quad \to \quad \mathcal{C}H(\mathbf{A})\mathcal{C}^{-1} = H(-\mathbf{A})$$
$$\mathbf{J}_Q(\mathbf{A}) \quad \to \quad \mathcal{C}\mathbf{J}_Q(\mathbf{A})\mathcal{C}^{-1} = \mathbf{J}_Q(-\mathbf{A})$$

$$\chi_{22,xy} = \frac{1}{V}\langle J_{Q,x}(\vec{A},\tau)J_{Q,y}(\vec{A})\rangle$$

$$\chi_{22,xy}(\mathbf{A}) = \chi_{22,xy}(-\mathbf{A})$$
$$\kappa_{xy}(\mathbf{A}) = \kappa_{xy}(-\mathbf{A})$$