Thermal transport in the Kitaev model

Joji Nasu

Department of Physics, Tokyo Institute of Technology

Collaborators: Yukitoshi Motome, Junki Yoshitake (UTokyo)

J. Nasu, J. Yoshitake, and Y. Motome, Phys. Rev. Lett. **119**, 127204 (2017).

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- Thermal transport w/o magnetic field
- Thermal transport w/ magnetic field
- Summary

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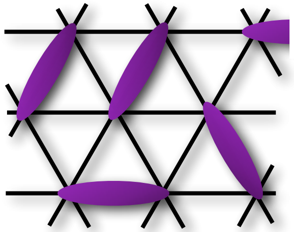
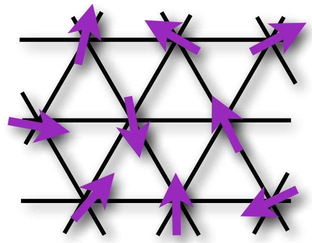
Quantum spin liquid (QSL)

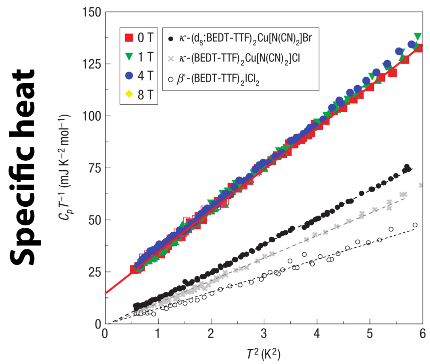




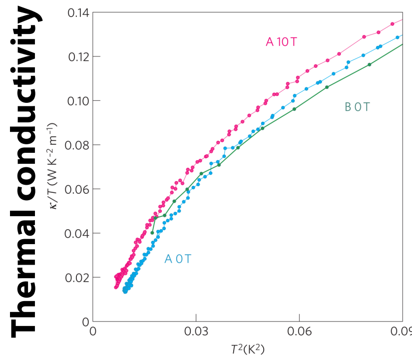
Quantum fluctuation disturbs orderings.

κ-(BEDT-TTF)$_2$Cu$_2$(CN)$_3$

S. Yamashita et al., Nat. Phys. **4**, 459 (2008).



M. Yamashita et al., Nat. Phys. **5**, 44 (2009).



Quantum spin liquid (QSL):

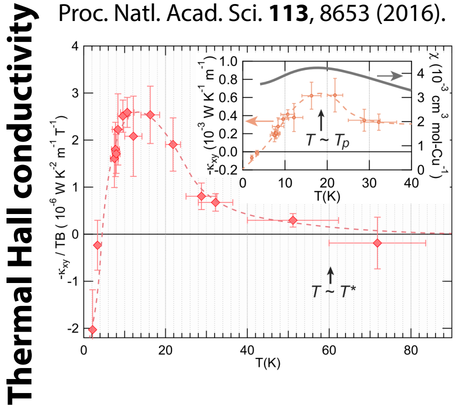
- No singularity in C_v or χ
- No apparent symmetry breakings down to low *T*
- ***Fractional*** excitations

Characterization of QSLs with ***emergent fermions***

- Low-*T* behavior of C_v (*T-linear*)
- **Dynamical response (*continuum*)**
- **Thermal transport**

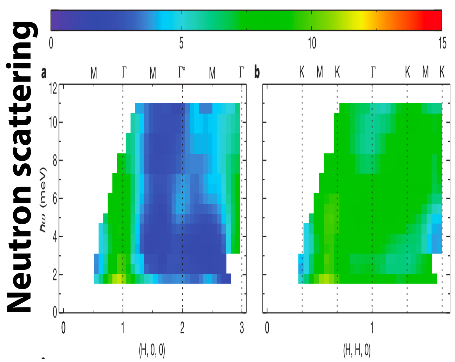
Kagomé volborthite

D. Watanabe *et al.*, Proc. Natl. Acad. Sci. **113**, 8653 (2016).



herbertsmithite

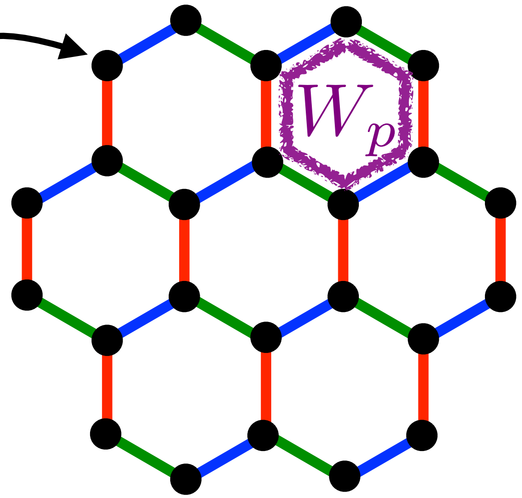
T.-H. Han et al., Nature **492**, 406 (2012).



Kitaev model

$$\mathcal{H} = -J_x \sum_{<ij>_x} S_i^x S_j^x - J_y \sum_{<ij>_y} S_i^y S_j^y - J_z \sum_{<ij>_z} S_i^z S_j^z$$

A. Kitaev, Annals of Physics **321**, 2 (2006).



☑ Bond-dependent interactions

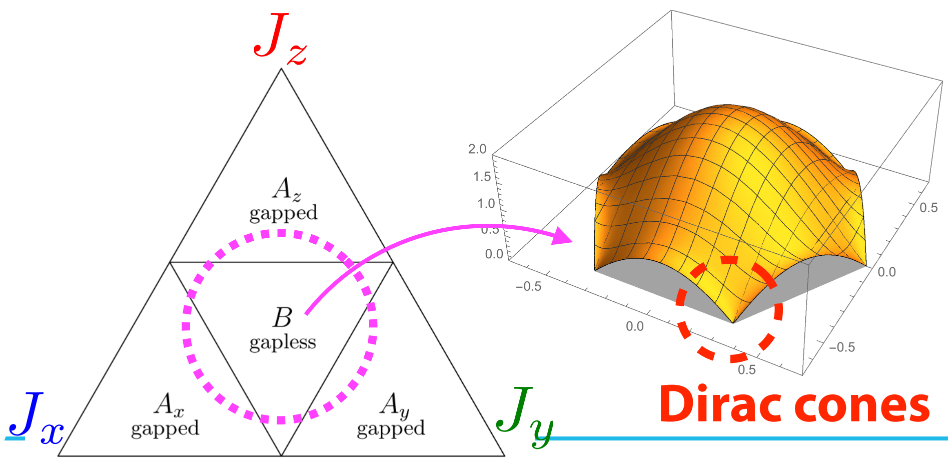
→ ***frustration***

☑ Z_2 flux (conserved quantity) W_p on each plaquette

→ ground state: ***quantum spin liquid***

(Only NN interactions are finite)

Assuming W_p=+1 → $\mathcal{H} = -\frac{iJ_\gamma}{4} \sum_{\langle ij \rangle_\gamma} c_i c_j$ $\{c_i\}$: Majorana fermions emerging from spins

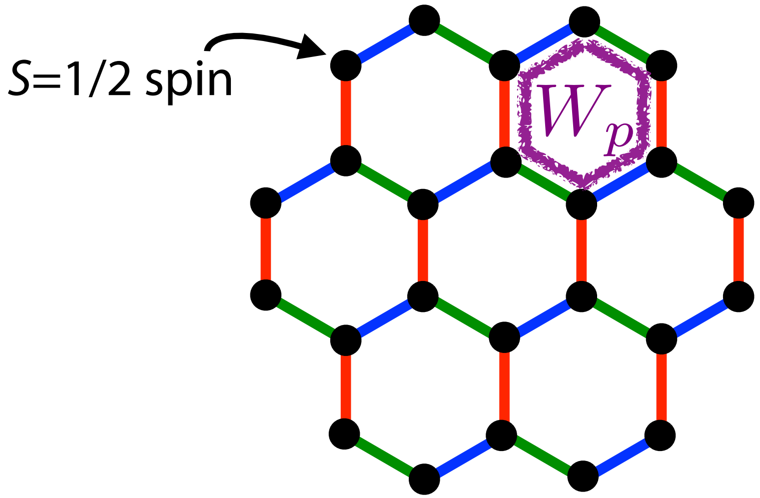


Free Majorana fermions on a honeycomb lattice; analogous to graphene

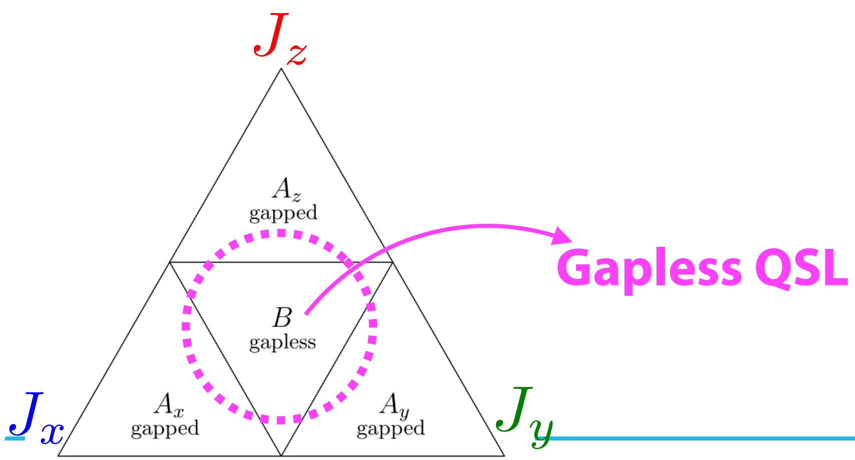
Kitaev model

$$\mathcal{H} = -J_x \sum_{<ij>_x} S_i^x S_j^x - J_y \sum_{<ij>_y} S_i^y S_j^y - J_z \sum_{<ij>_z} S_i^z S_j^z$$

A. Kitaev, Annals of Physics **321**, 2 (2006).



- ☑ Bond-dependent interactions
  → ***frustration***
- ☑ Z_2 flux (conserved quantity) W_p on each plaquette
  → ground state: ***quantum spin liquid***
  (Only NN interactions are finite)
- ☑ Fractional fermionic excitations
  → ***Emergent fermions may carry heat.***
- ☑ Majorana Chern insulator
  by applying magnetic field in gapless phase
  → ***Thermal Hall effect***

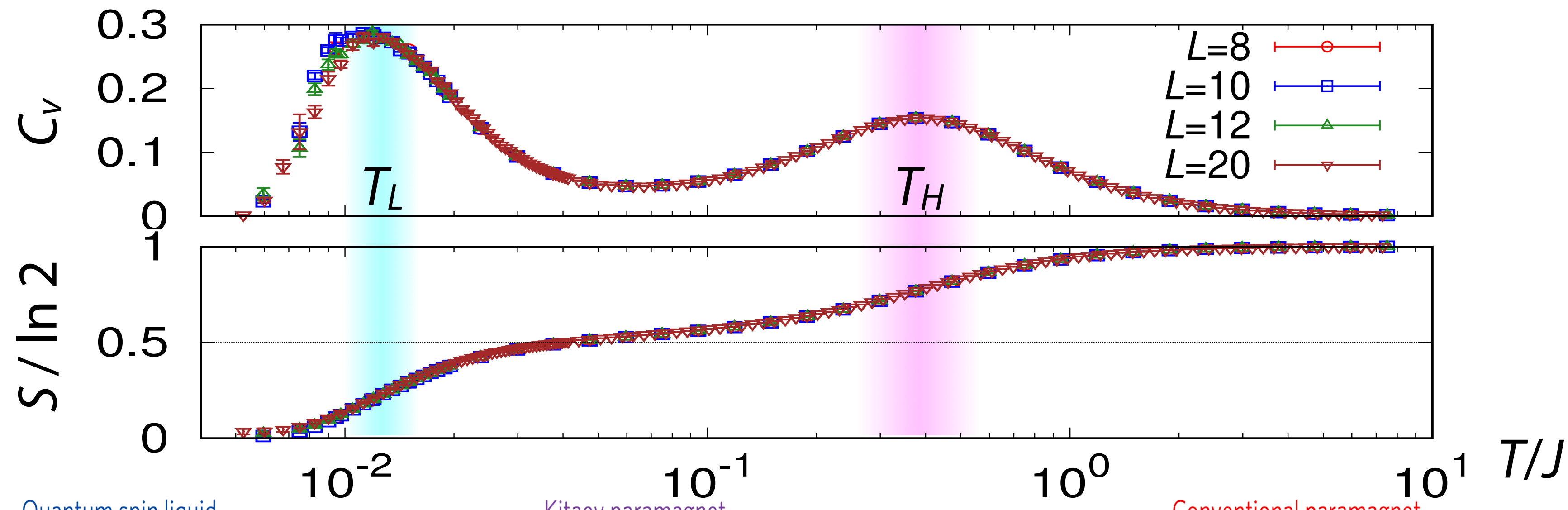


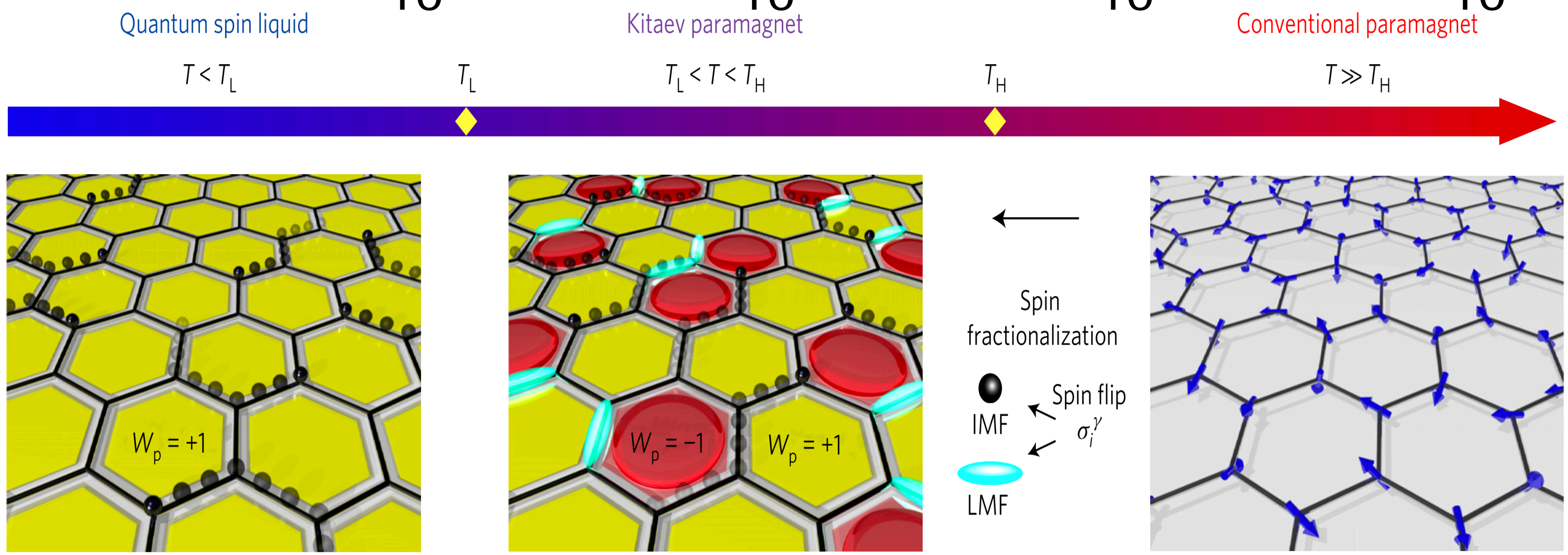
Kitaev spin liquid: fractionalization

Thermal fractionalization

JN, M. Udagawa, and Y. Motome, Phys. Rev. Lett. **113**, 197205 (2014).
JN, M. Udagawa, and Y. Motome, Phys. Rev. B **92**, 115122 (2015).

S_i → Itinerant Majorana fermions (IMF)
S_i → Localized Majorana fermions (LMF)

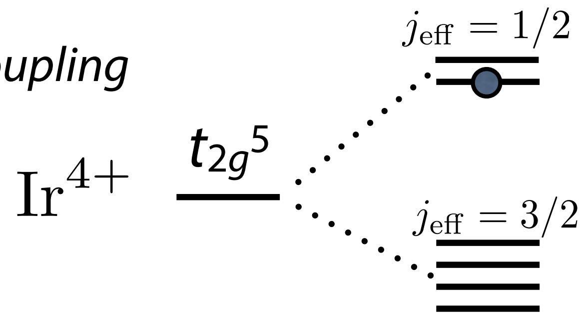


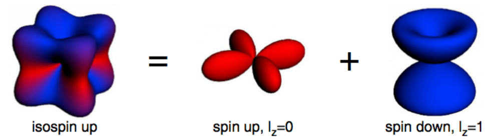


S.-H. Do et al., Nat. Phys. (2017).

Realization of Kitaev QSLs

Strong spin-orbit coupling





j_{eff}=1/2 localized spin

G. Jackeli and G. Khaliullin, Phys. Rev. Lett. **102**, 017205 (2009)

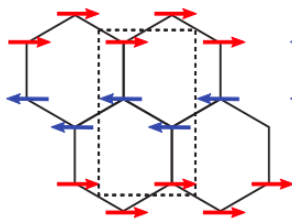
Kitaev-Heisenberg model

$$\mathcal{H} = -J_x \sum_{<ij>_x} S_i^x S_j^x - J_y \sum_{<ij>_y} S_i^y S_j^y - J_z \sum_{<ij>_z} S_i^z S_j^z + J_{\mathrm{H}} \sum_{<ij>} \boldsymbol{S}_i \cdot \boldsymbol{S}_j$$

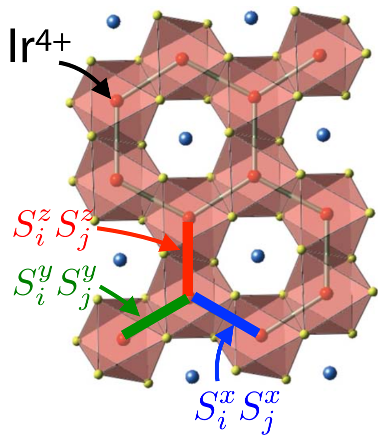
Magnetic order

☑ A_2IrO_3 (A=Li,Na) Ir^{4+} $5d^5$ T_c~10K

Y. Singh and P. Gegenwart, Phys. Rev. B **82**, 064412 (2010).
Y. Singh et. al., Phys. Rev. Lett. **108**, 127203 (2012).
R. Comin et. al., Phys. Rev. Lett. **109**, 266406 (2012).
S. K. Choi et. al., Phys. Rev. Lett. **108**, 127204 (2012).



zigzag



☑ α-$RuCl_3$ Ru^{3+} $4d^5$ T_c~10K

K. W. Plumb et al., Phys. Rev. B. **90**, 041112 (2014).
Y. Kubota et al., Phys. Rev. B **91**, 094422 (2015).
L. J. Sandilands et al., Phys. Rev. Lett. **114**, 147201 (2015).
J. A. Sears, M. Songvilay et al., Phys. Rev. B **91**, 144420 (2015).
M. Majumder et al., Phys. Rev. B **91**, 180401(R) (2015).

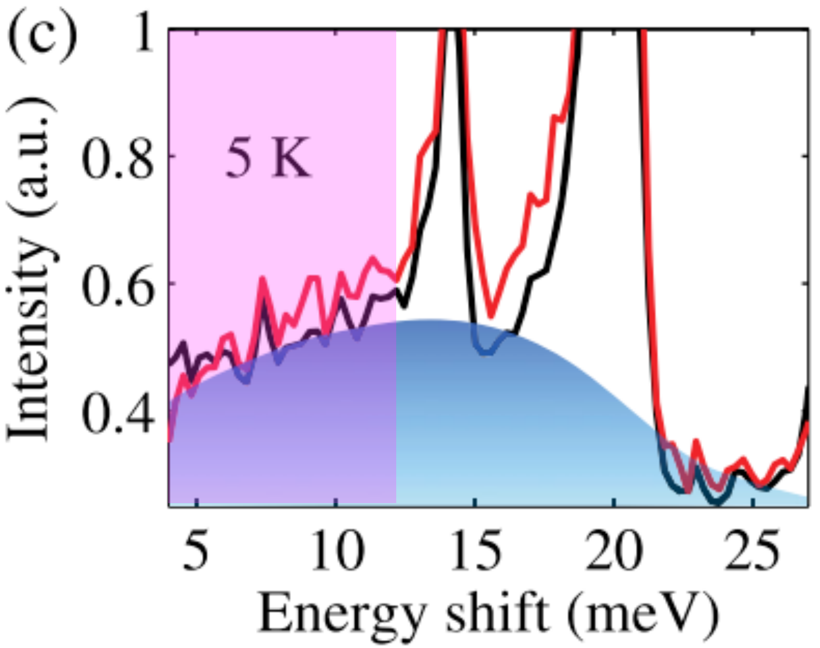
Kitaev term plays a dominant role.

Y. Yamaji et al., Phys. Rev. Lett. **113**, 107201 (2014).
K. Foyevtsova et al., Phys. Rev. B **88**, 035107 (2013).
A. Banerjee et al., Nat. Mater. **15**, 733 (2016).

Dynamical response

- Raman scattering in $RuCl_3$

L. J. Sandilands et al., Phys. Rev. Lett. **114**, 147201 (2015).

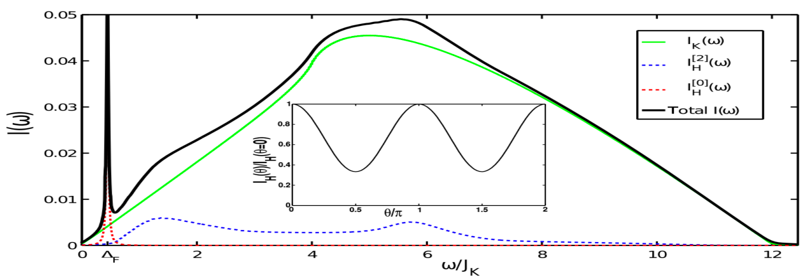


- Raman scattering in β-,γ-Li_2IrO_3

A. Glamazda et al., Nat. Commun. **7**, 12286 (2016).

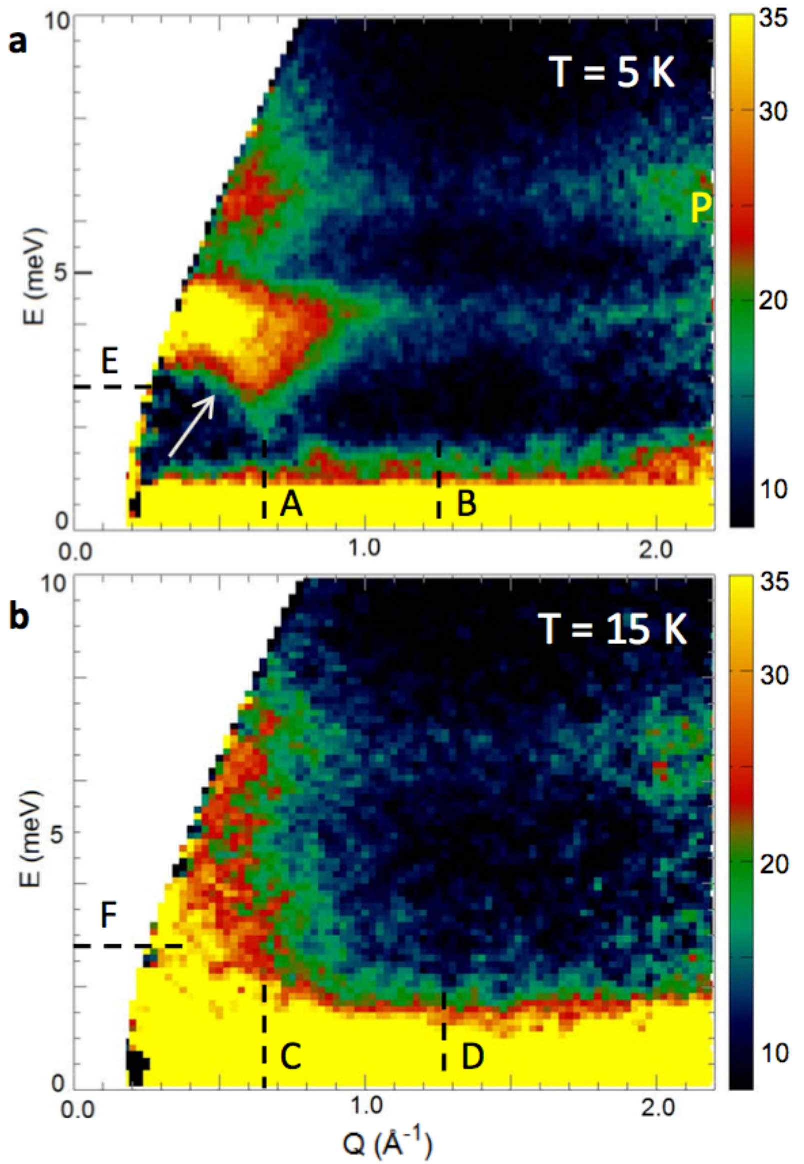
- Theory

J. Knolle et al., Phys. Rev. Lett. 113, 187201 (2014).



- Inelastic neutron scattering in $RuCl_3$

A. Banerjee et al., Nat. Mater., Nat. Mater. **15**, 733 (2016).



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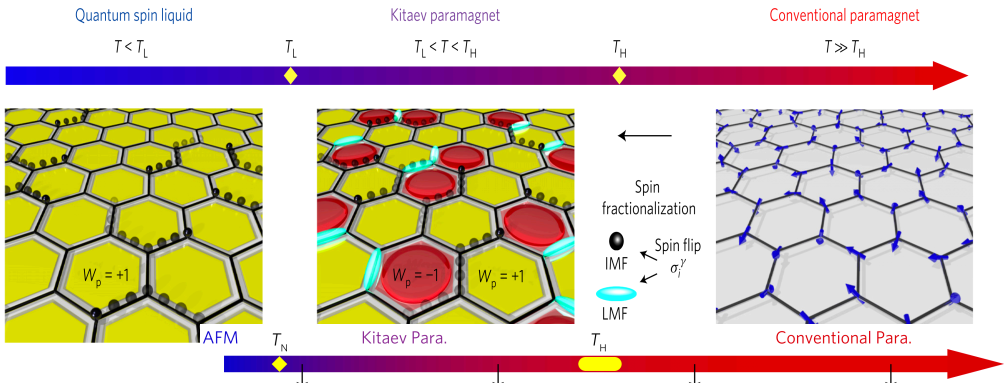
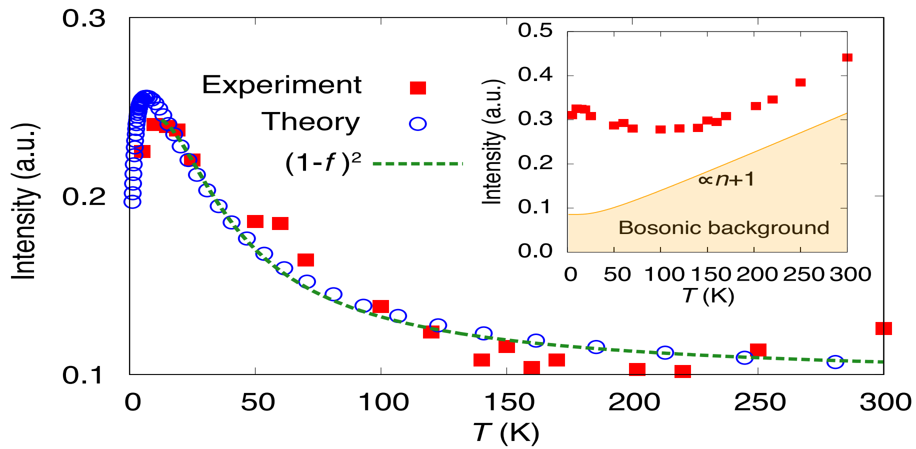
Comparison of experiment & theory



- Magnetic order occurs at ~10K in α-$RuCl_3$.

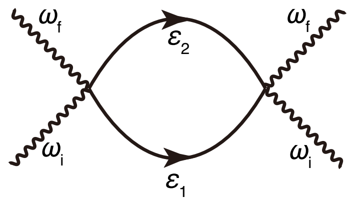
Raman scattering



- Good agreement between the present theory and experimental results

L. J. Sandilands et al., Phys. Rev. Lett. **114**, 147201 (2015).

JN, J. Knolle, D. L. Kovrizhin, Y. Motome, R. Moessner, Nat. Phys., 12, 912 (2016).



$\propto [1-f(\varepsilon_1)][1-f(\varepsilon_2)]$

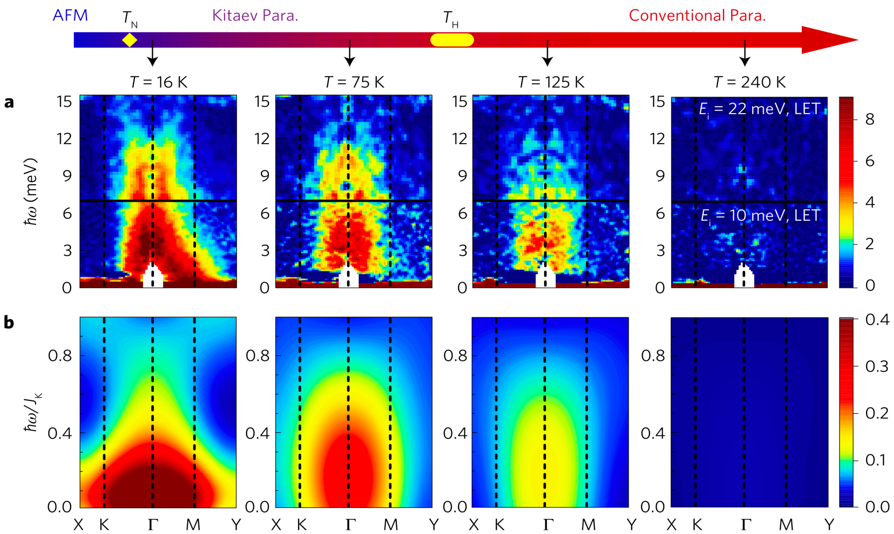
Two-fermion excitation

- Fermionic T dependence appears around 100K.

Dynamical spin correlation

Experiment

Theory



- High-energy features are consistent.

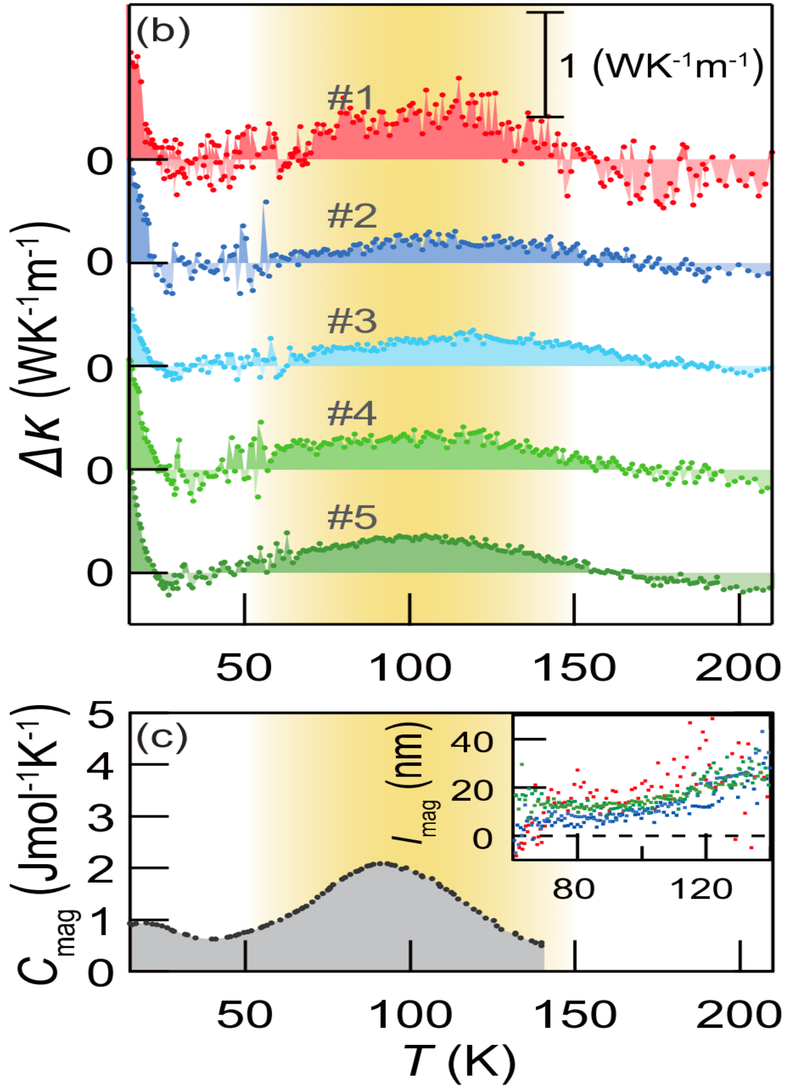
S.-H. Do et al., Nat. Phys. (2017).

J. Yoshitake, JN, and Y. Motome, Phys. Rev. Lett. **117**, 157203 (2016)

J. Yoshitake, JN, Y. Kato, and Y. Motome, Phys. Rev. B **96**, 024438 (2017)

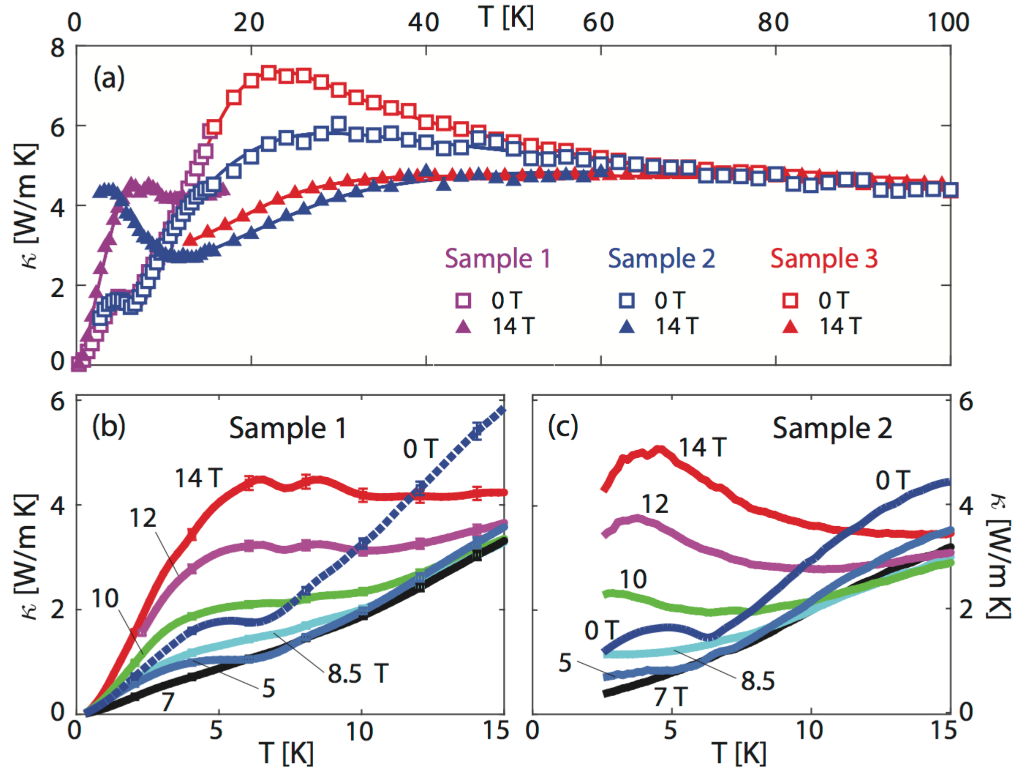
J. Yoshitake, JN, and Y. Motome, Phys. Rev. B **96**, 064433 (2017),

Thermal transport in α-$RuCl_3$



D. Hirobe, M. Sato, Y. Shiomi, H. Tanaka, and E. Saitoh, Phys. Rev. B **95**, 241112 (2017).

- Longitudinal thermal conductivity *κ* exhibits a peak at a peak in specific heat



I. A. Leahy et al., Phys. Rev. Lett. **118**, 187203 (2017).

- *κ* is enhanced in low-*T* whereas it is suppressed in intermediate-*T* by applying magnetic field.

- Another study for *κ* in $RuCl_3$

R. Hentrich et al., arXiv:1703.08623 (2017).

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Purpose

- Candidates of Kitaev materials → *Magnetic order at low T*

Two stances:

Cooperation effect of the Kitaev and Heisenberg interactions

What is the Kitaev QSL? How should it be observed?

Our starting point

Precursor of Kitaev QSL (***fractionalization***) above T_c (~10K)

- What occurs in the pure Kitaev limit at finite temperature?
  - Fractionalization of spins into Majorana fermions
  - Topological nature with magnetic field

Heat transport

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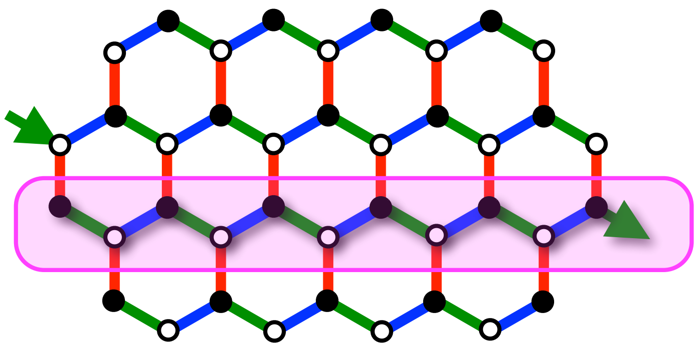
Jordan-Wigner transformation

$$\mathcal{H} = -J_x \sum_{<ij>_x} S_i^x S_j^x - J_y \sum_{<ij>_y} S_i^y S_j^y - J_z \sum_{<ij>_z} S_i^z S_j^z$$

Honeycomb lattice: a zigzag *xy* chain connected by *z*-bonds



Jordan-Wigner transformation

regarding the honeycomb lattice as *one open chain*

$$S_i^+ = (S_i^-)^\dagger = \prod_{i'=1}^{i-1}(1-2n_{i'})a_i^\dagger \qquad S_i^z = a_i^\dagger a_i - \frac{1}{2}$$

H.-D. Chen and J. Hu, Phys. Rev. B 76, 193101 (2007).
X. Y. Feng, G.-M. Zhang, and T. Xiang, Phys. Rev. Lett. 98, 087204 (2007).
H.-D. Chen and Z. Nussinov, J. Phys. A Math. Theor. 41, 075001 (2008).

Fermions: $a_i, \ a_i^\dagger$

Introducing *Majorana fermions*

$$c_i = a_i + a_i^\dagger$$
$$\bar{c}_i = (a_i - a_i^\dagger)/i$$

$$\mathcal{H} = \frac{iJ_x}{4}\sum_{\langle ij\rangle_x} c_i c_j - \frac{iJ_y}{4}\sum_{\langle ij\rangle_y} c_i c_j + \frac{J_z}{4}\sum_{\langle ij\rangle_z} \bar{c}_i\bar{c}_j c_i c_j$$

$$[\bar{c}_i\bar{c}_j, \mathcal{H}] = 0$$

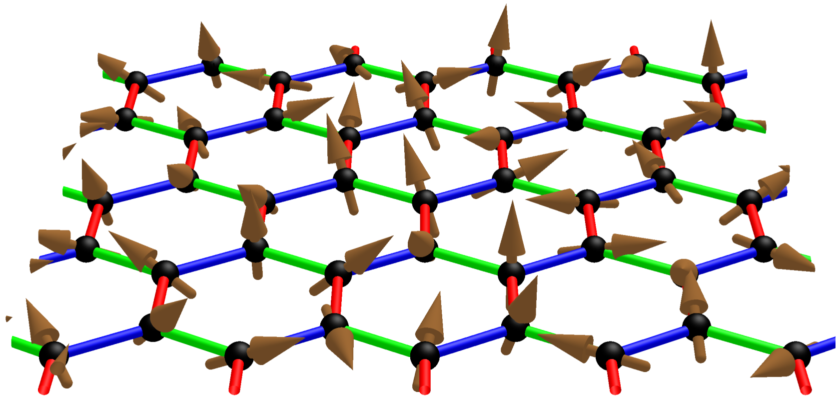
$\eta_r \equiv i\bar{c}_i\bar{c}_j$: ***local conserved quantity***

$$\mathcal{H} = \frac{iJ_x}{4}\sum_{\langle ij\rangle_x} c_i c_j - \frac{iJ_y}{4}\sum_{\langle ij\rangle_y} c_i c_j - \frac{iJ_z}{4}\sum_{\langle ij\rangle_z} \eta_r c_i c_j$$

Method

Quantum spin model

$$\mathcal{H} = -J_x \sum_{<ij>_x} S_i^x S_j^x - J_y \sum_{<ij>_y} S_i^y S_j^y - J_z \sum_{<ij>_z} S_i^z S_j^z$$



Jordan-Wigner transformation

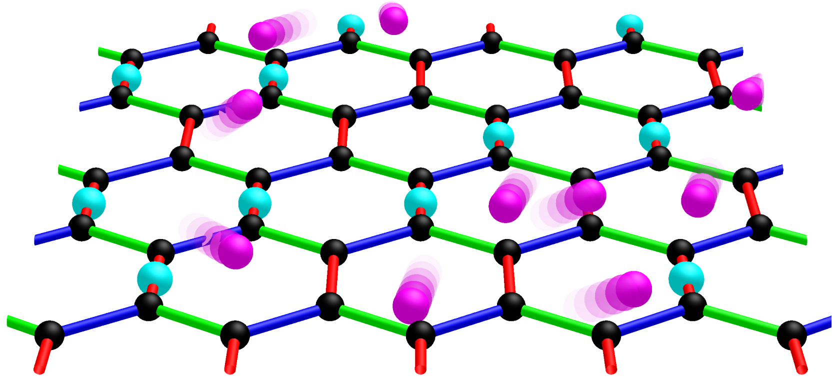
Itinerant fermion model

$$\mathcal{H} = \frac{iJ_x}{4} \sum_{\langle ij \rangle_x} c_i c_j - \frac{iJ_y}{4} \sum_{\langle ij \rangle_y} c_i c_j - \frac{iJ_z}{4} \sum_{\langle ij \rangle_z} \eta_r c_i c_j$$

S_i → c_i **: Itinerant Majorana**

S_i → $\bar{c}_i$ **: Localized Majorana**

$$\eta_r = i\bar{c}_i \bar{c}_j$$



Free Majorana fermion system with thermally fluctuating fluxes $W_p = \eta_r \eta_{r'}$

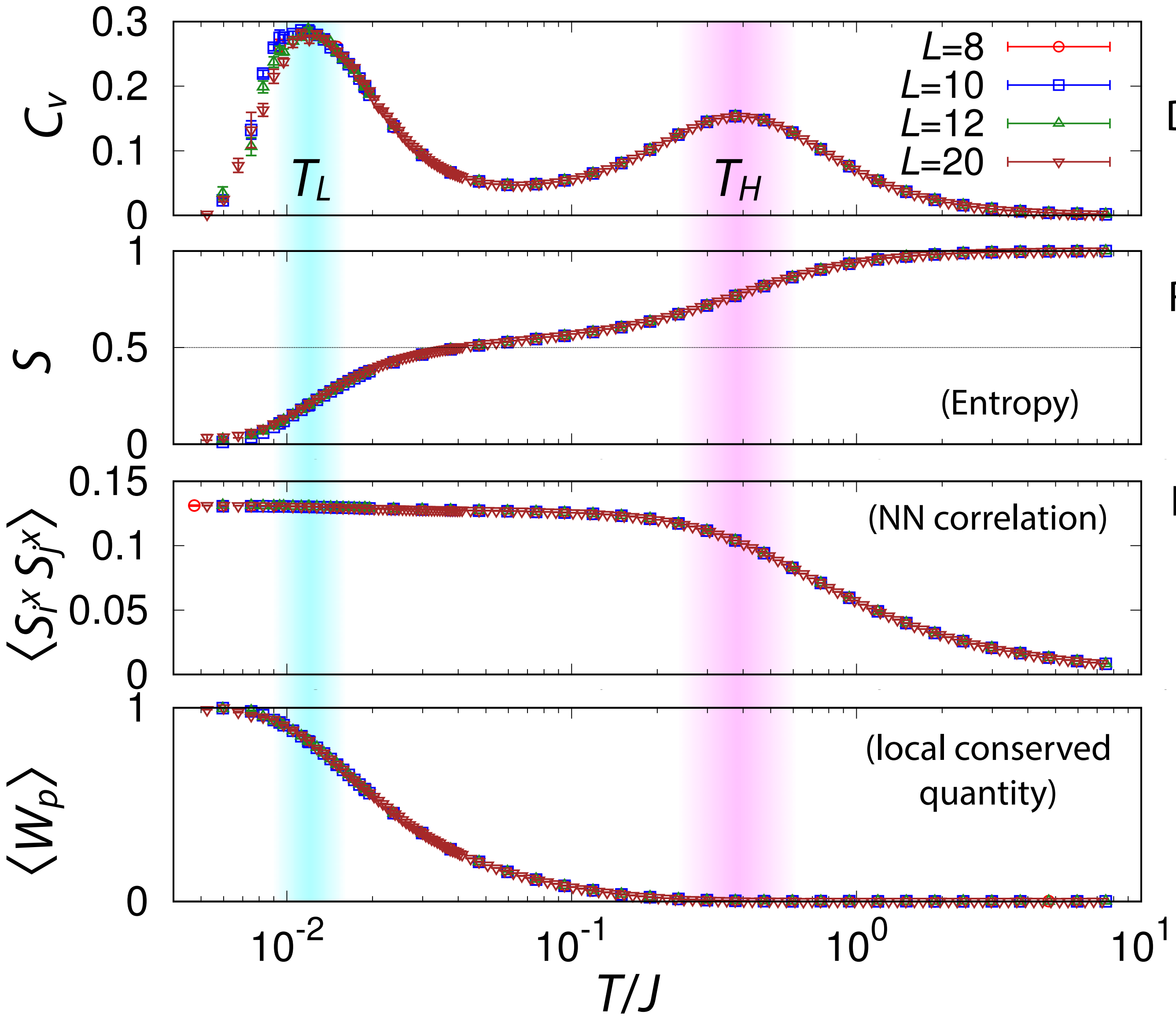
- Sign problem-free "*Quantum*" Monte Carlo simulations

  Quantum nature of S=1/2 spins is fully taken into account!

- Simulations are *classical* and done for flipping Ising valuables η_r.

$$J_x = J_y = J_z = J$$

Specific heat and entropy



Double peak structure

Release of a half of entropy at each crossover

NN x bond $S_i^x S_j^x = -\frac{i}{4} c_i c_j$

c_i : **itinerant Majorana (matter Majorana)**

Local conserved quantity

$$W_p = \prod_{r \in p} \eta_r \qquad \eta_r = i\bar{c}_i \bar{c}_j$$

$\bar{c}_i$: **localized Majorana (flux Majorana)**

S_i → c_i : **itinerant Majorana** ⟷ **Entropy release at T^{**}** ⟷ **development of spin correlation**

S_i → $\bar{c}_i$: **localized Majorana** ⟷ **Entropy release at T^{*}** ⟷ **coherent develop of W_p**

Contents

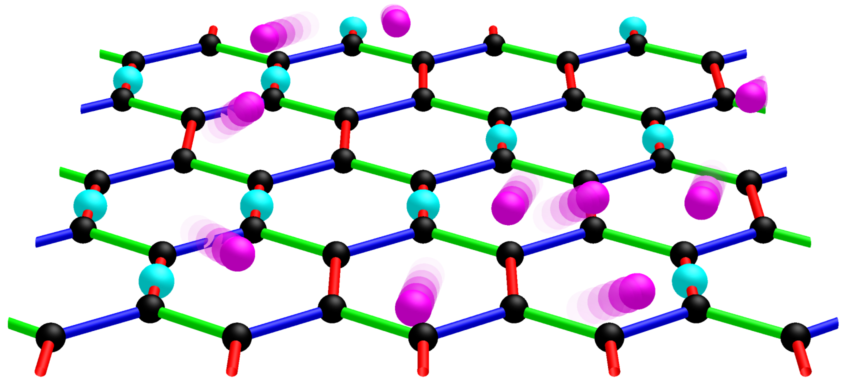
Thermal conductivity

Itinerant fermion model

$$\mathcal{H} = \frac{iJ_x}{4}\sum_{\langle ij\rangle_x} c_i c_j - \frac{iJ_y}{4}\sum_{\langle ij\rangle_y} c_i c_j - \frac{iJ_z}{4}\sum_{\langle ij\rangle_z} \eta_r c_i c_j$$

S_i → c_i : **Itinerant Majorana**, $\bar{c}_i$: **Localized Majorana**

$$\eta_r = i\bar{c}_i\bar{c}_j$$



- **Itinerant Majoranas** carry thermal current: $J_Q^\gamma = -\kappa^{\gamma\gamma'}\partial_{\gamma'}T$

Energy polarization: $\boldsymbol{P}_E = -\sum_{\langle ij\rangle_\gamma} \frac{\boldsymbol{r}_i + \boldsymbol{r}_j}{2} J_\gamma S_i^\gamma S_j^\gamma$

Energy current: $\boldsymbol{J}_E = i[\mathcal{H}, \boldsymbol{P}_E]$ which is written by **itinerant Majoranas**

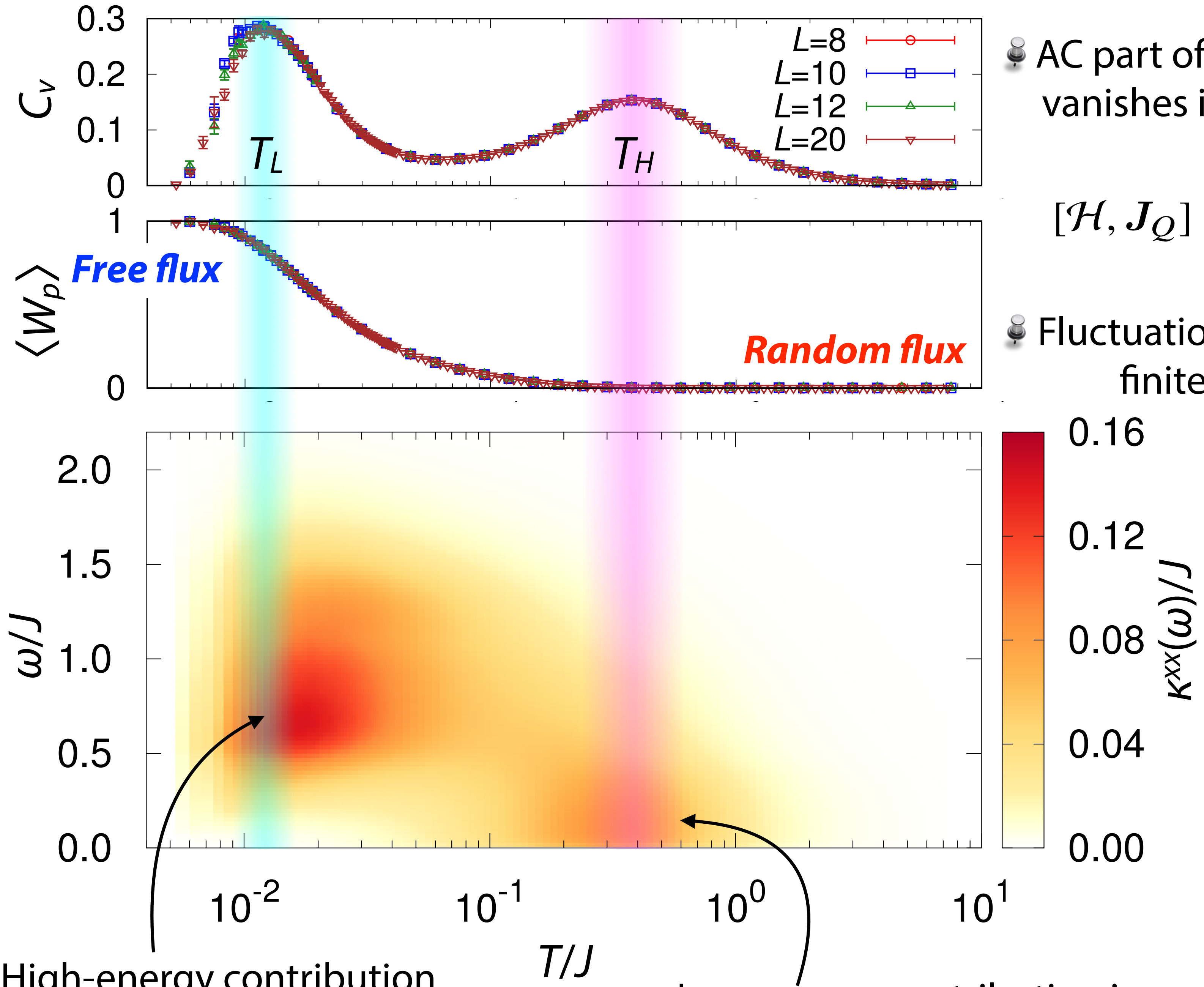
Thermal current: $\boldsymbol{J}_Q = \boldsymbol{J}_E$ (zero chemical potential for Majorana fermions)

Kubo formula + "gravitomagnetic energy magnetization"

K. Nomura, S. Ryu, A. Furusaki, and N. Nagaosa, Phys. Rev. Lett. **108**, 26802 (2012), H. Sumiyoshi and S. Fujimoto, JPSJ **82**, 023602 (2013).

- Isotropic case $J_x = J_y = J_z = J$ → $\kappa^{xx} = \kappa^{yy}$

AC thermal conductivity



- AC part of thermal conductivity vanishes in the ***free-flux case***. $W_p = +1$

$[\mathcal{H}, J_Q] = 0$ with $W_p = +1$

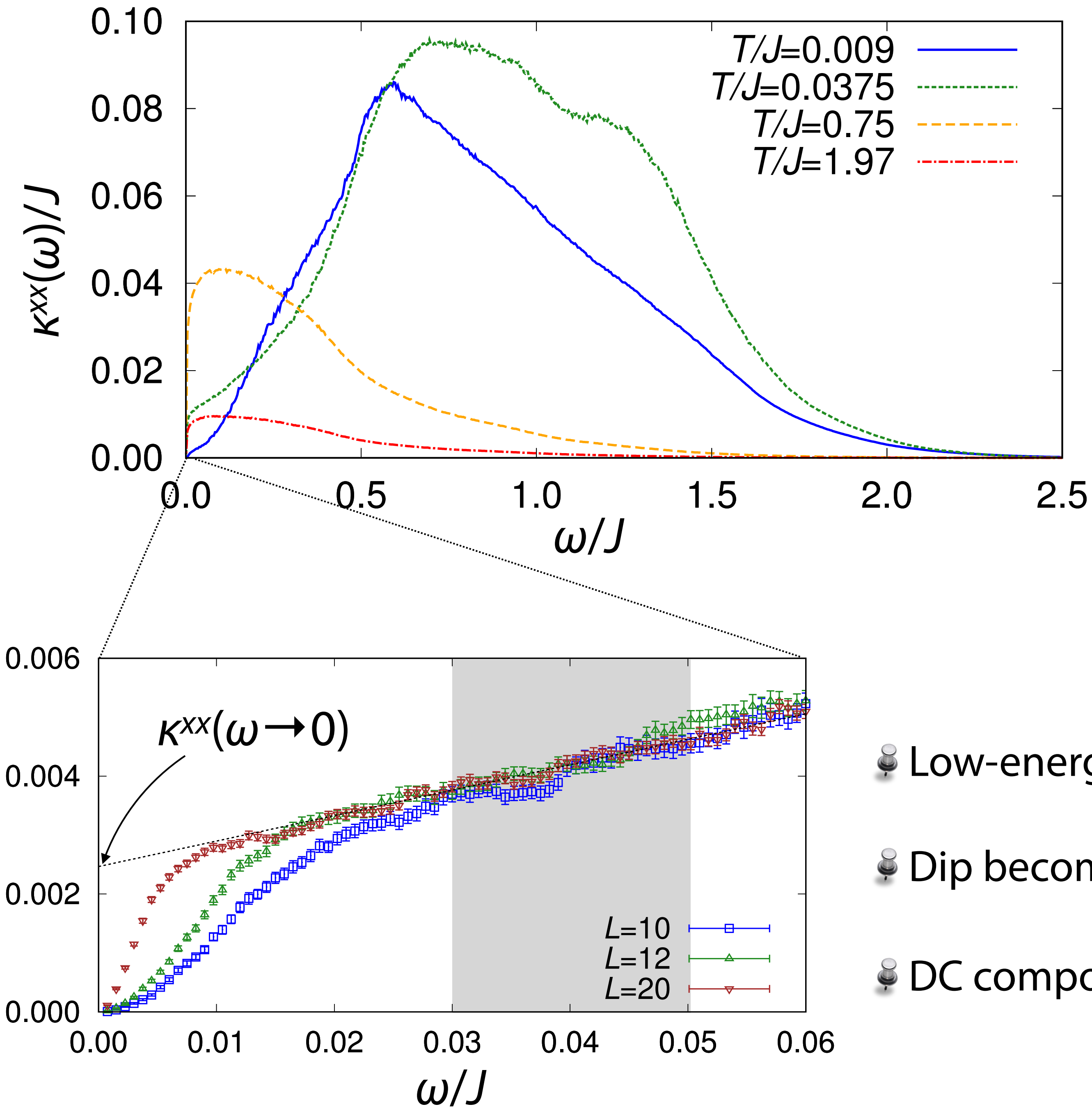
- Fluctuation of fluxes yields finite value of $\kappa^{xx}(\omega)$.

Finite-ω contribution detects ***flux fluctuations***.

High-energy contribution develops around T_L

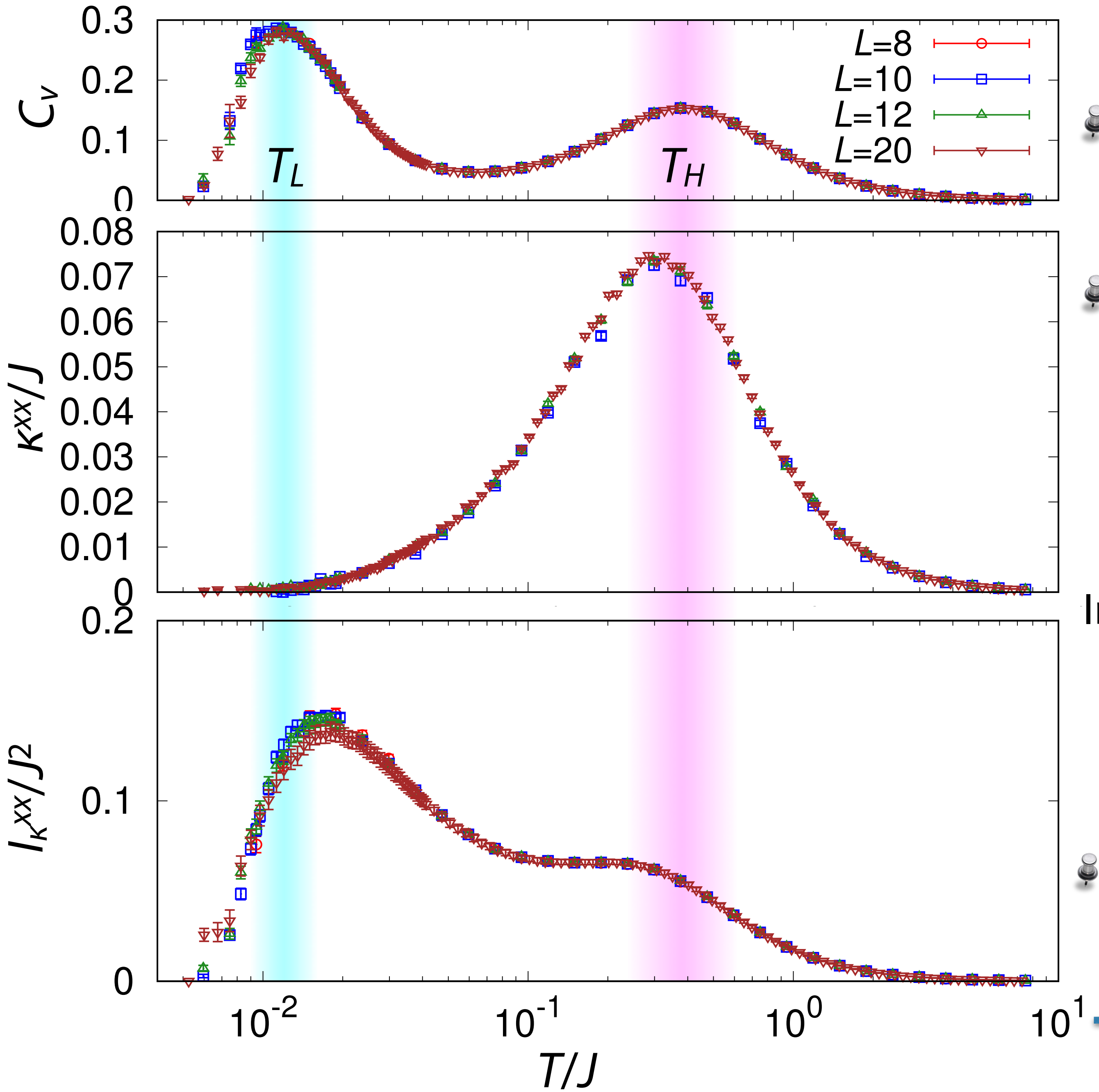
Low-energy contribution increases around T_H

AC thermal conductivity



- AC part of thermal conductivity vanishes in the ***free-flux case***.
  $W_p = +1$
  $[\mathcal{H}, \boldsymbol{J}_Q] = 0$ with $W_p = +1$
- AC component grows with increasing *T*.
- The peak shifts to low-*T* side and decreases.
- Low-energy part shows size dependence.
- Dip becomes smaller with increase of size.
- DC component is obtained by the extrapolation.

Thermal conductivity



- DC component is obtained by extrapolation.
- κ^{xx} takes a peak around T_H.

➡ Transport is governed by itinerant Majoranas.

Integrated AC thermal conductivity:

$$I_\kappa^{xx} = \int_0^\infty \kappa^{xx}(\omega)d\omega$$

- Fluctuation of fluxes yields finite value of I_κ^{xx} .

➡ I_κ^{xx} detects ***flux fluctuations***.

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Introduction of magnetic field

$$\mathcal{H}_{\rm K} = -J_x \sum_{<ij>_x} S_i^x S_j^x - J_y \sum_{<ij>_y} S_i^y S_j^y - J_z \sum_{<ij>_z} S_i^z S_j^z$$

A. Kitaev, Annals of Physics **321**, 2 (2006).

Magnetic field for the direction ***perpendicular*** to the honeycomb plane

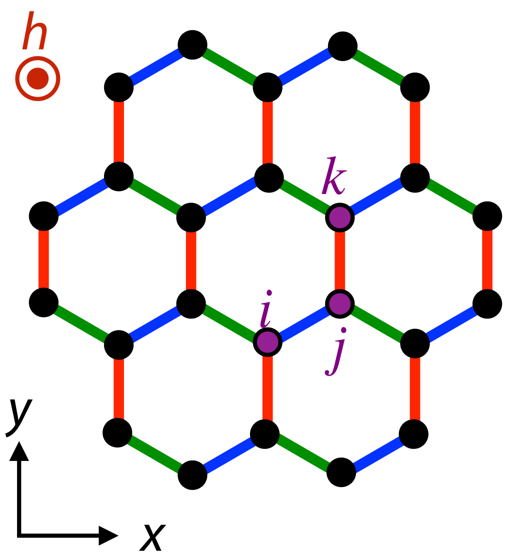
$$\mathcal{H}_h = -h \sum_i \left(S_i^x + S_i^y + S_i^z \right)$$

$$\rightarrow \quad \mathcal{H}_h^{\rm eff} = -\tilde{h} \sum_{(ijk)} S_i^x S_j^y S_k^z$$:*low-energy* effective model

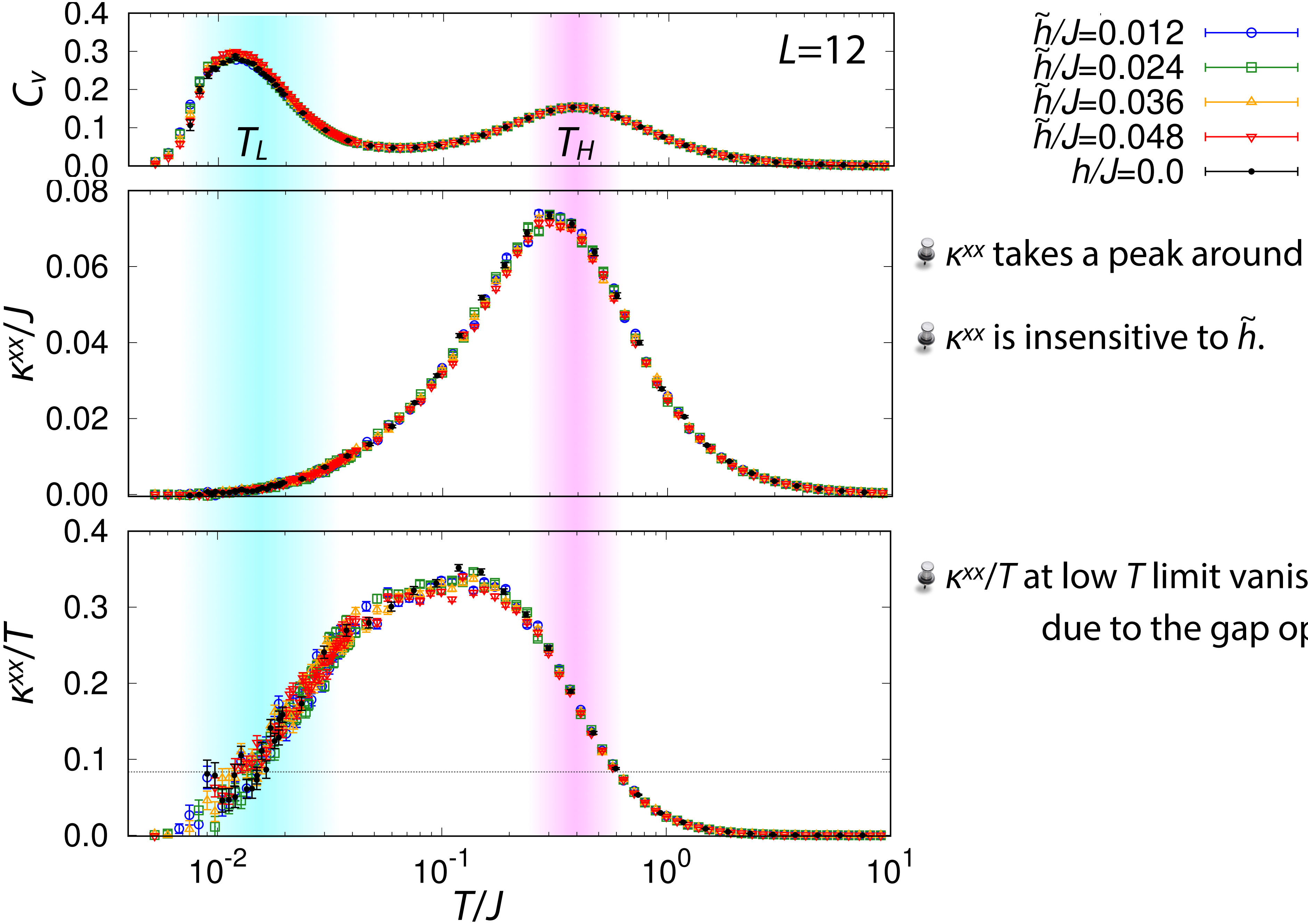
Model Hamiltonian: $\mathcal{H} = \mathcal{H}_{\rm K} + \mathcal{H}_h^{\rm eff}$

- Effective magnetic field: $\tilde{h} = \lambda h^3 \sim \frac{h^3}{\Delta^2}$ with $\Delta / J \sim 0.1$
- Majorana Chern insulator by applying the Magnetic field

  → *Chiral edge mode*

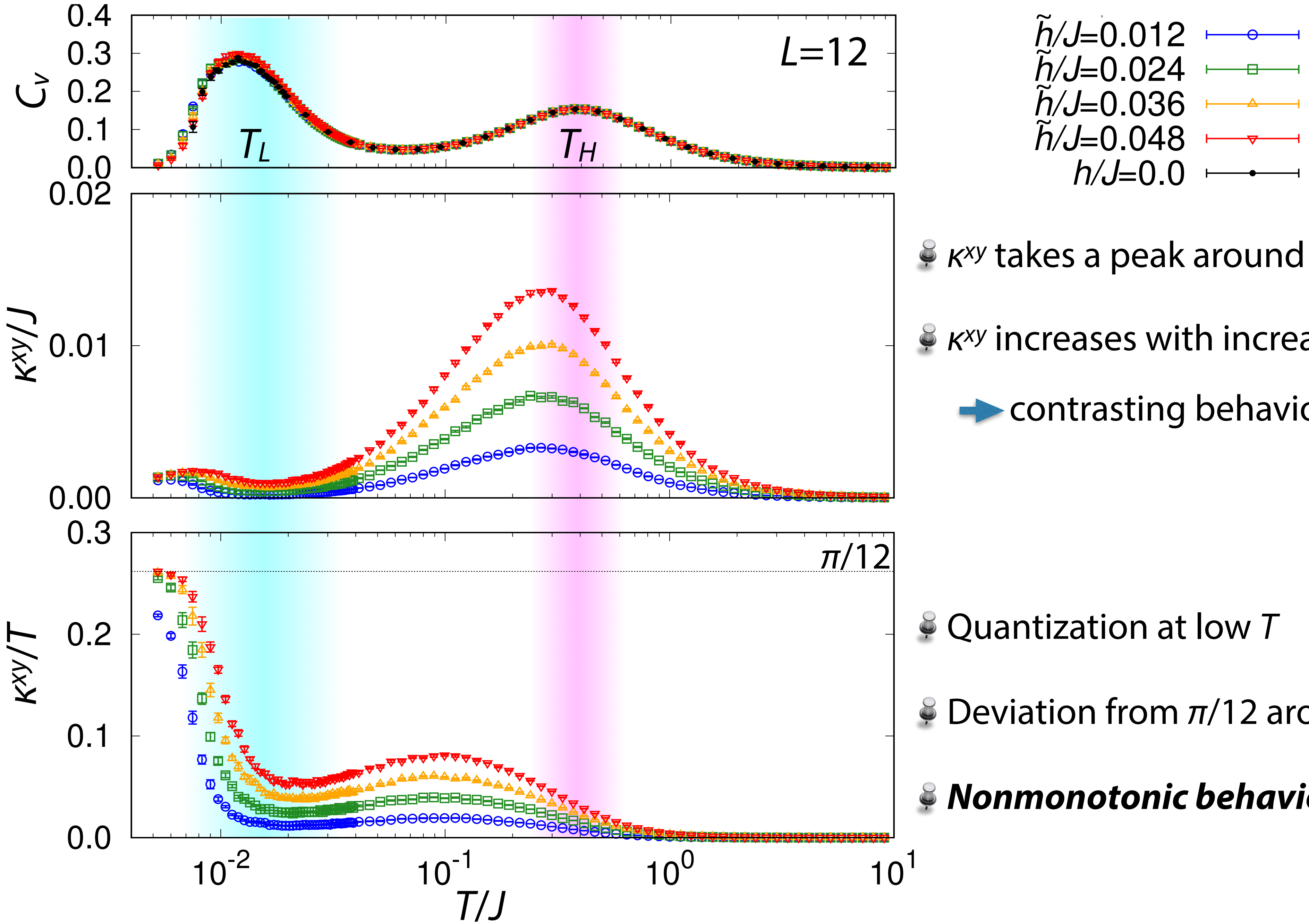


Longitudinal thermal conductivity



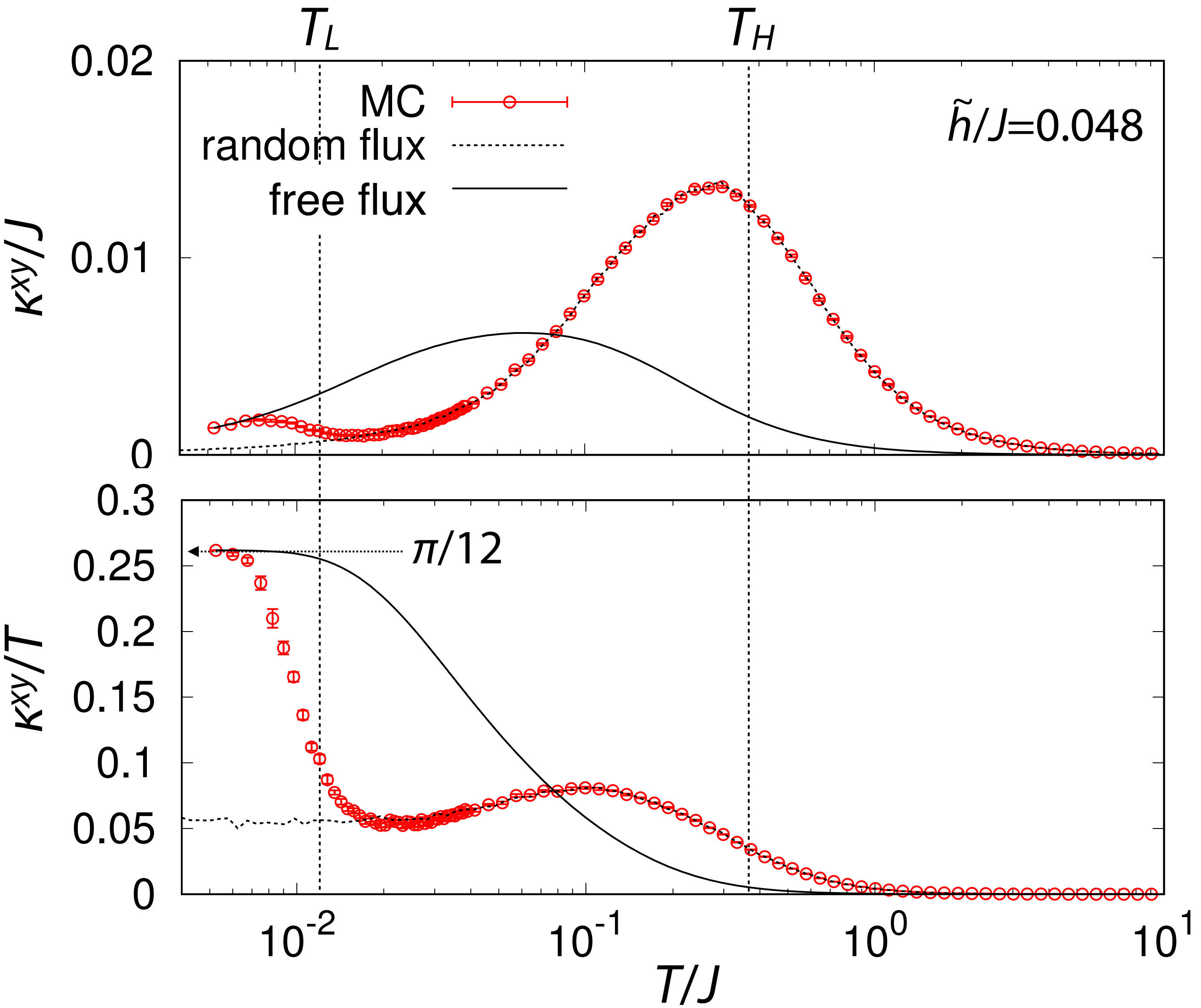
- κ^{xx} takes a peak around T_H.
- κ^{xx} is insensitive to $\tilde{h}$.
- κ^{xx}/T at low T limit vanishes due to the gap opening.

Transverse thermal conductivity

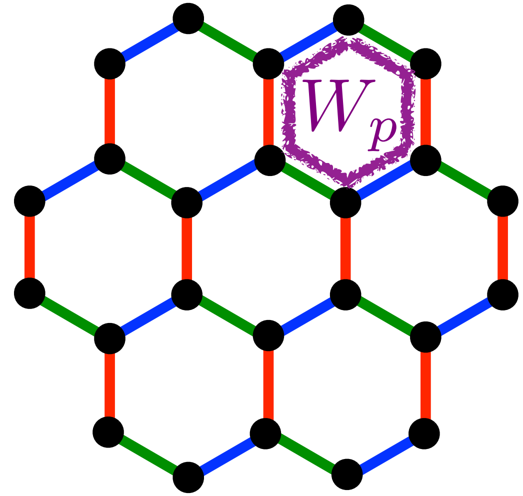


- κ^{xy} takes a peak around T_H.
- κ^{xy} increases with increasing $\tilde{h}$.
  - → contrasting behavior to κ^{xx}
- Quantization at low T
- Deviation from $\pi/12$ around T_L
- ***Nonmonotonic behavior***

Effect of flux excitation



$W_p = \pm 1$: Z_2 flux



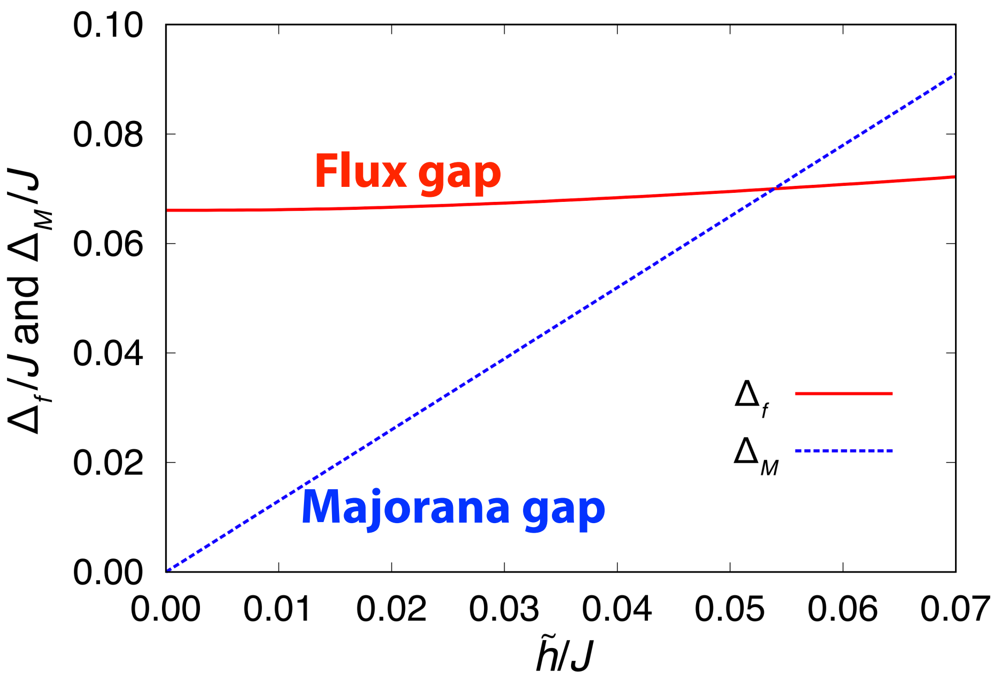
$W_p \equiv +1$: ground state (free flux)

$W_p = -1$: flux excitation

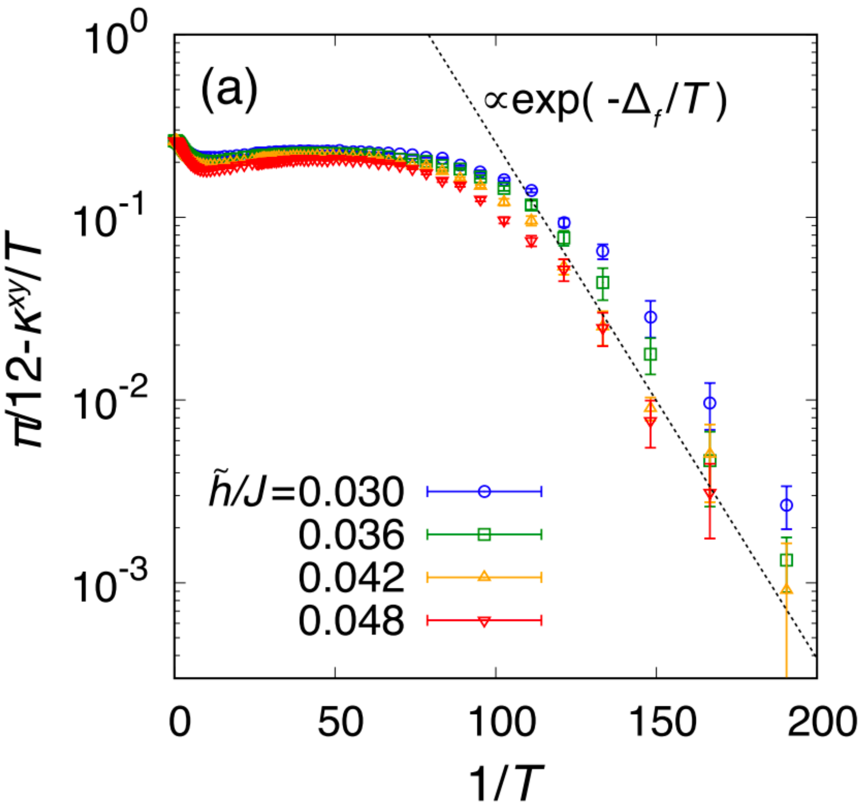
- MC result deviates from zero-flux one around low-T crossover.
- High-T peak is well accounted for by random flux excitation.

Deviation from Plateau

Magnetic field dependence of gaps

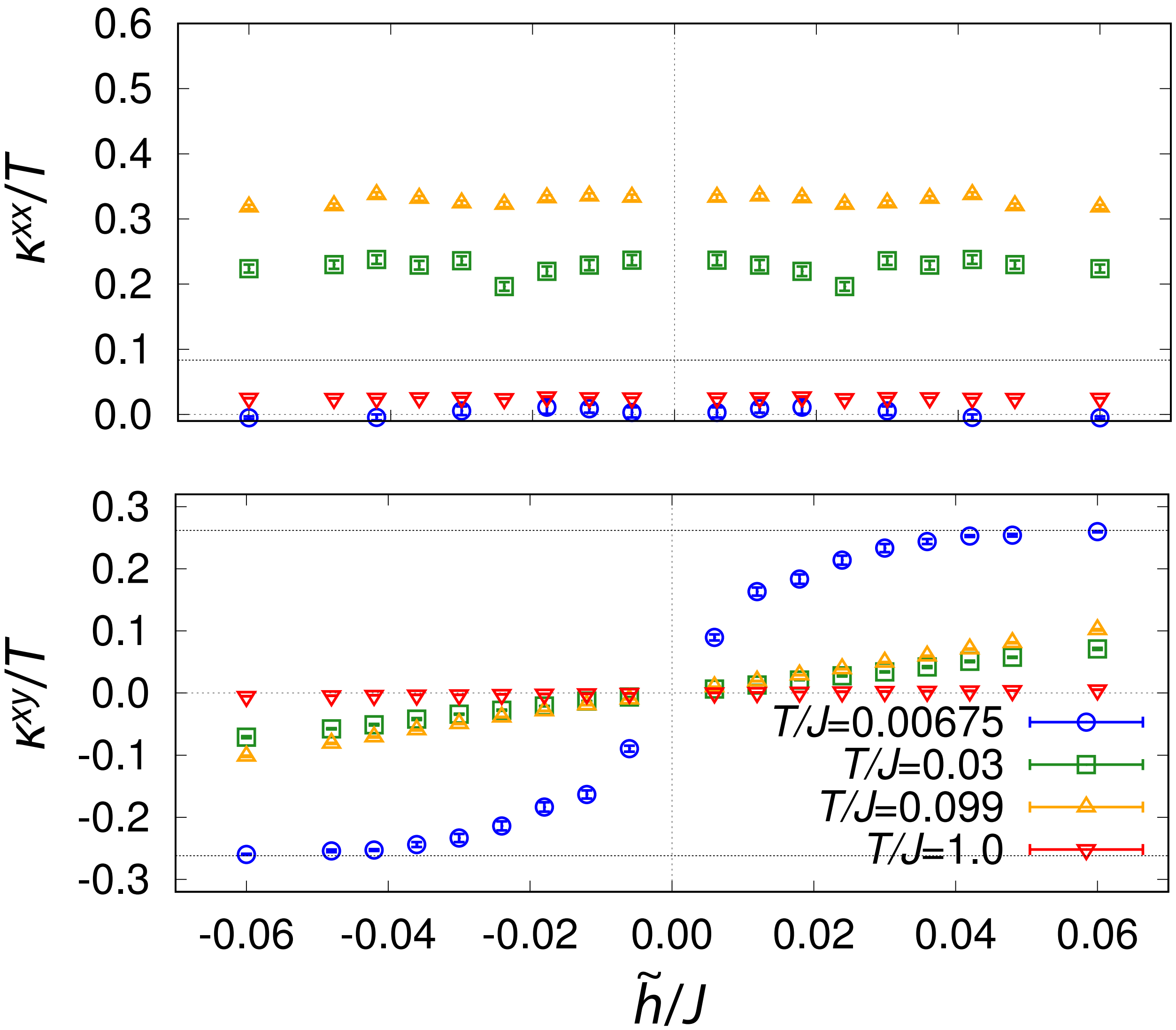


Arrhenius plot for κ^{xy}/T



- Flux gap is almost independent of $\tilde{h}$.
- Majorana gap linearly depend on $\tilde{h}$.
- Deviation of κ^{xy}/T from the quantized value is determined by the **flux gap**.

Magnetic field dependence



Longitudinal component

- Almost zero at low T
- almost unchanged by $\tilde{h}$

Transverse component

- Enhancement by $\tilde{h}$
- *Linear* dependence for $\tilde{h}$ at finite T

➡ **κ^{xy} is proportional to h^3.**

$$\tilde{h} \sim \frac{h^3}{\Delta^2}$$

Contrasting magnetic-field dependence between κ^{xx} and κ^{xy}.

Contents

- Introduction
- Method
- Thermal transport w/o magnetic field
- Thermal transport w/ magnetic field
- Summary

Summary

- **Kitaev model on a honeycomb lattice**
  - "Quantum" Monte Carlo simulation in Majorana representation
  - Magnetic field is introduced as an effective model.
- **Without magnetic field**
  - Longitudinal thermal conductivity exhibits a peak at high-T crossover attributed to the ***itinerant Majorana fermions***
  - Dynamical component detects ***flux fluctuation***.
- **With magnetic field**
  - Thermal Hall conductivity is proportional to h^3.
  - Peculiar T dependence of κ^{xy}/T due to the ***flux excitations***.