Thermal transport in Kitaev magnets

... fermions, fluxes, Heisenberg exchange, and (some) phonons

PRB **96**, 041115(R) (2017), PRB **96**, 205121 (2017),
PRB **99**, 075141 (2019), PRB **99**, 205129 (2019),
arXiv:1909.09360

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SFB 1143
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nano school for contacts in nanosystems

QUANOMET

QuantumFrontiers
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Outline

- Why thermal transport
- Models, Quantities, and Methods
- Thermal current dynamics
  - Kitaev ladder
  - Honeycomb Kitaev
  - Kitaev-Heisenberg ladder
- Phonons in the Kitaev QSL

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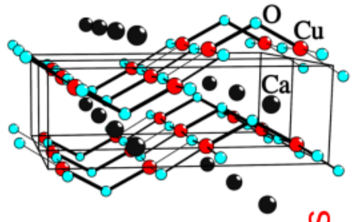
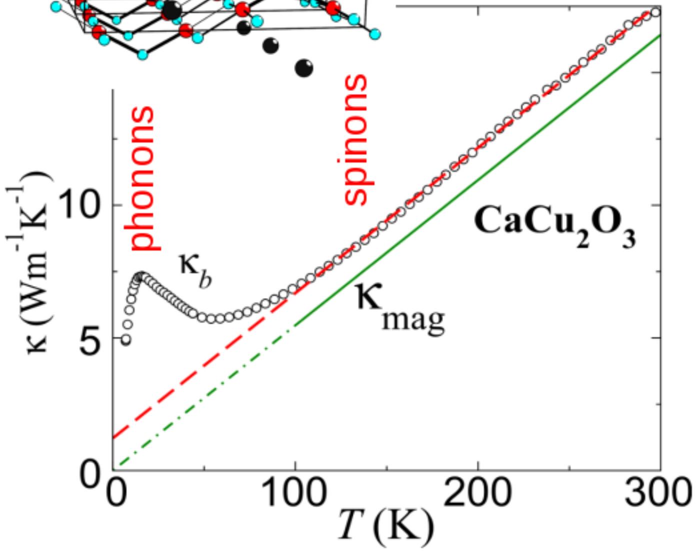
Bulk thermal transport in insulating quantum magnets ...



Hess, Büchner, WB, et al., PRL **98**, 027201 (2007)



- ... can corroborate exotic quasi particles

$$\kappa = \sum_k C_{V,k} \nabla_k \epsilon_k l_k$$

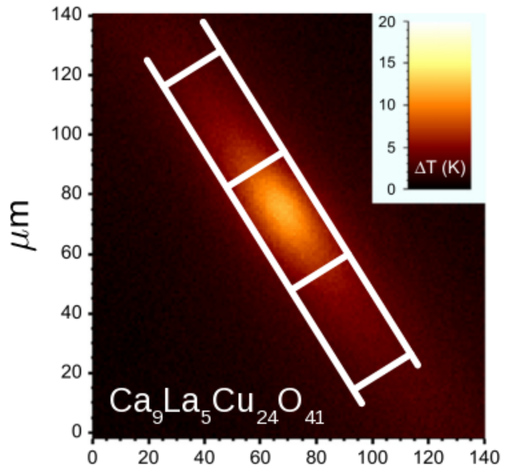
- triplons $Sr_{14}Cu_{24}O_{41}$ — Hess, Büchner, WB, et al., PRB **64**, 184305 (2001)
- monopoles $Ho_2Ti_2O_7$ — Toews, Zhang, Ross, et al., PRL **110**, 217209 (2013)
- ...

- ... can be measured dynamically

e.g. Flourescent Flash Method, t-domain $\gtrsim$ ms

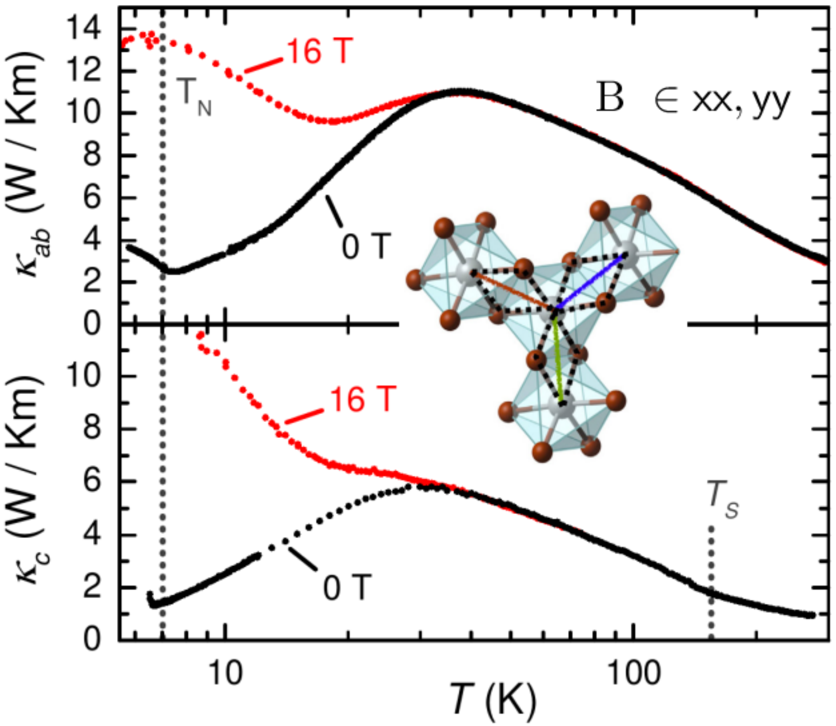
Otter, Loosdrecht, et al., JMMM **321**, 796 (2009)
Montagnese, et al., PRL **110**, 147206 (2013).

spinons $SrCuO_2$, triplons $Ca_9La_5Cu_{24}O_{41}$

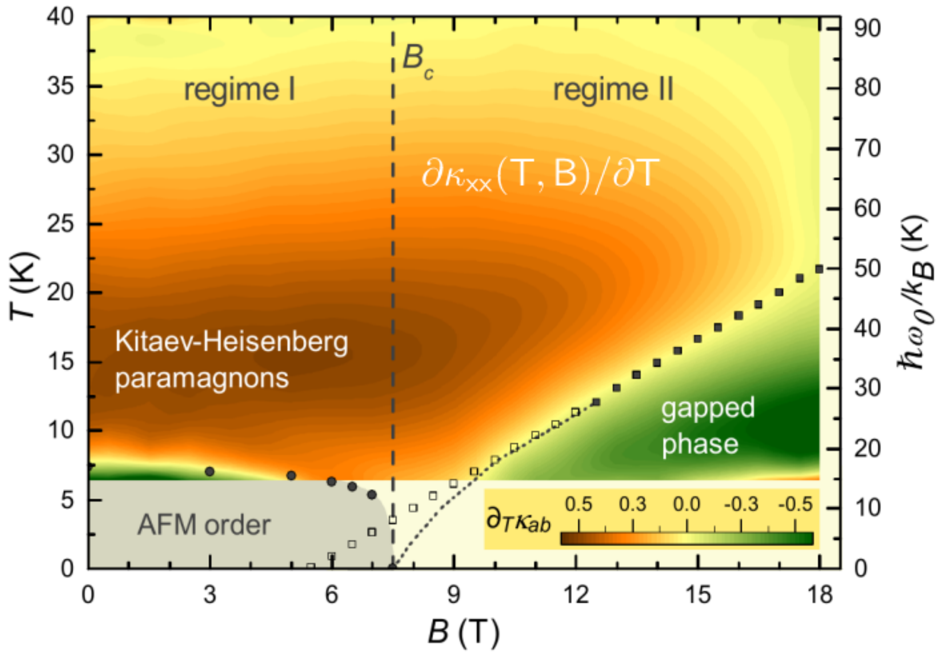


Longitudinal thermal conductivity κ_{xx} of α-$RuCl_3$

Hentrich, et al. PRL **120**, 117204 (2018)



- magnetic field dependence



Wolter, et al. PRB **96**, 041405(R) (17) C_V ✔

Wellm, et al., Phys. Rev. B **98**, 184408 (2018) ESR ✔

- $\kappa_{ab} \sim \kappa_c$: primarily phononic transport

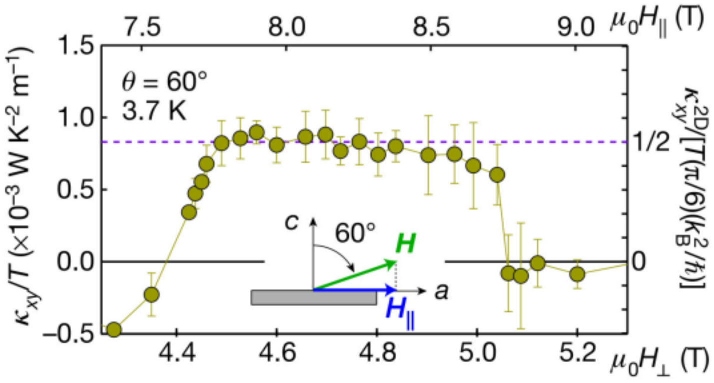
ab-only
Leahy, et al. PRL. **118**, 187203 (2017)
Hirobe, et al., PRB **95**, 241112 (2017)
Yu, et al. PRL **120**, 067202 (2018)

- dissipation by magnetic excitations: critical scattering at T_N, double peak in gapped phase, isothermals $\kappa_{ab}(B,T=\mathrm{const})$

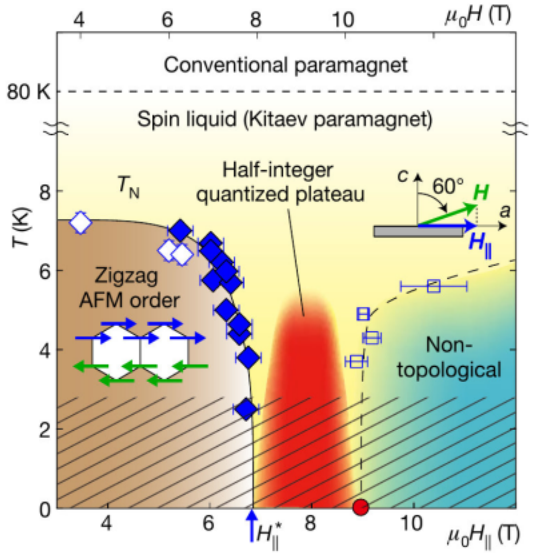
κ_{xy}: thermal Hall effect in α-$RuCl_3$

- Majorana edge mode: κ_{xy}/T quantized

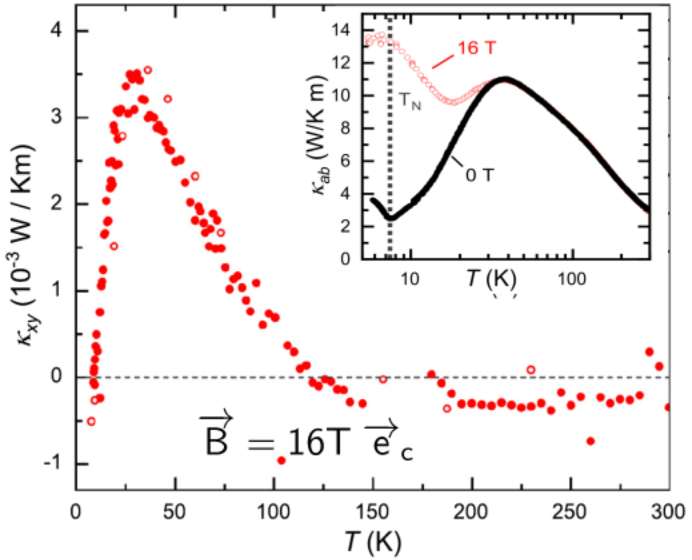
Kitaev, Ann. Phys. (N.Y.) **321**, 2 (06)



Kasahara, et al., Nature **559**, 227 (2018)

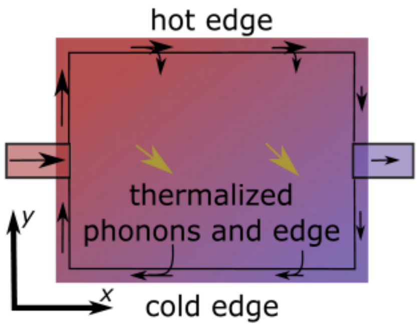


- Hall angle: ~10^{-4} = conventional



Hentrich, et al., PRB **99**, 085136 (2019)

- strong spin-phonon coupling required



Ye, et al., PRL **121**, 147201 (2018)

Vinkler-Aviv, Rosch, PRX **8**, 031032 (2018)

- What are signatures of magnetic bulk thermal transport in Kitaev spin systems**?**
- How do phonons dissipate in Kitaev spin systems**?**

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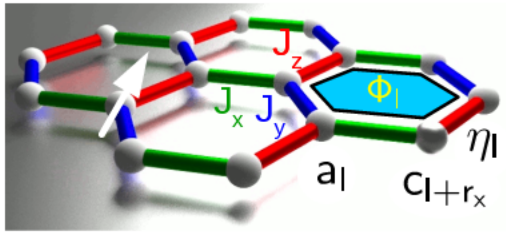
Models

(1) 2D Kitaev $H_K = \sum_{\mathbf{l},\alpha} J_\alpha S_{\mathbf{l}}^\alpha S_{\mathbf{l}+\mathbf{r}_\alpha}^\alpha = -\frac{i}{2}\sum_{\mathbf{l},\alpha} J_\alpha \eta_{\mathbf{l},\alpha}\, a_{\mathbf{l}} c_{\mathbf{l}+\mathbf{r}_\alpha} = \sum_{\{\eta\}}^{2^{N/2}} \sum_{\mu}^{N/2} \epsilon_\mu(\{\eta\})(2d_\mu^\dagger d_\mu - 1)$

$2^{N/2}$ spin liquids

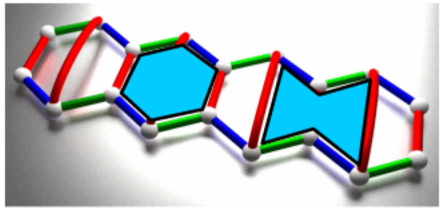


Majoranas $\{a_l, a_{l'}\} = \delta_{ll'}, \ldots$

Z_2 gauge fields $\eta_{\mathbf{l},z} = \eta_{\mathbf{l}} = \pm 1 \qquad \eta_{\mathbf{l},x(y)} = 1$

(2) Kitaev ladder

N/2 conserved fluxes $\Phi_l = \prod_j^6 \sigma_j^{\alpha_j} = \eta_l \eta_{l+xy}$



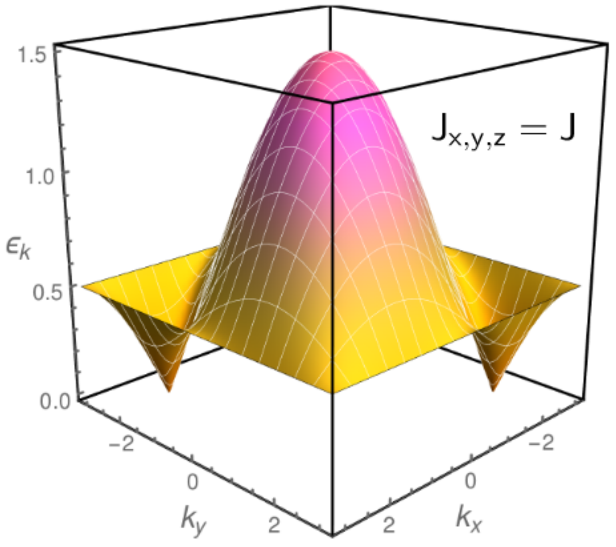
Majorana $(a_l, c_l) \rightarrow$ Dirac $f_\mu^{(\dagger)} \rightarrow$ Bogoliubov QP $d_\mu^{(\dagger)}$

Kitaev, Ann. Phys. (N.Y.) **321**, 2 (06), Feng, et al., PRL **98**, 087204 (07), Nussinov and Ortiz, PRB **79**, 214440 (09)

(3) Kitaev-Heisenberg ladder

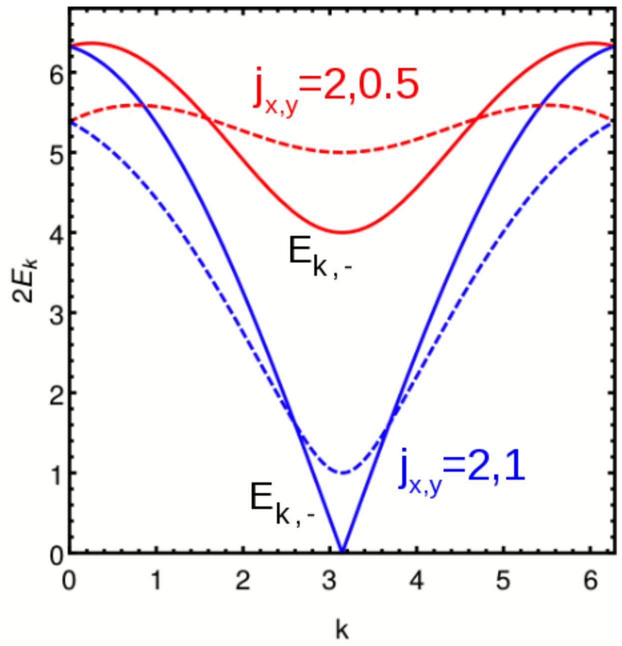
$$H_{KH} = H_K + \sum_{\langle l,m \rangle} J_{lm}\, \mathbf{S}_l \cdot \mathbf{S}_m$$

Ground state gauge sector & qp dispersion: honeycomb vs. ladder



- gauge field

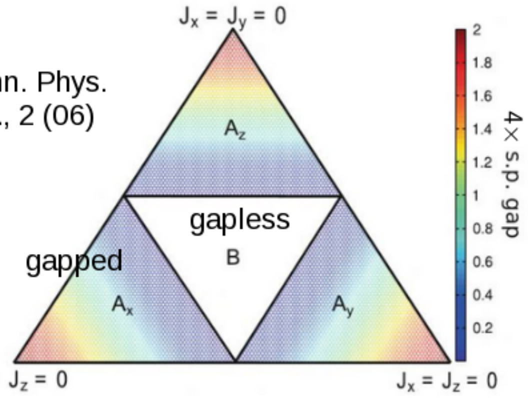
$\eta_l = 1$	$[\eta_1, \eta_2]_l =$ $[\pm 1, \mp 1]$ 2x deg. (all)

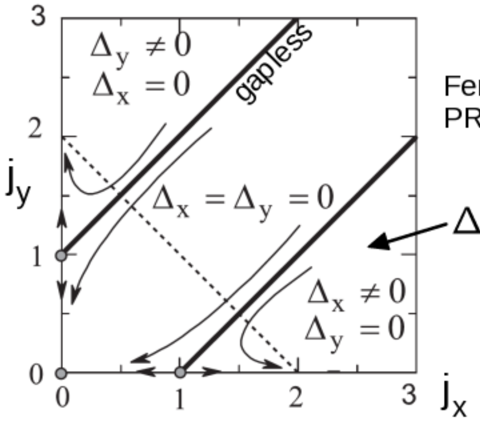


- qp dispersion

- phase diagram

Kitaev, Ann. Phys. (N.Y.) **321**, 2 (06)





Feng, et al. PRL **98** (2007)

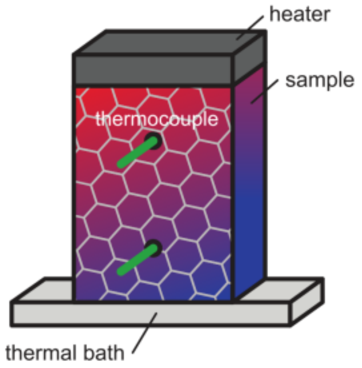
$\Delta_x = \langle \prod_l S_l^x \rangle$

SOP

Correlation functions (pure Kitaev)

(1) Thermal current $\mathcal{J}$: r-space continuity eqn.
with 'energy polarization' $\forall\{\eta_l\}$

$$\mathcal{J} = [\mathsf{H}, \sum_l l\, h_l] = \eta\text{−diagonal}, \quad \mathsf{H} = \sum_l h_l$$



dynamical current correlation function

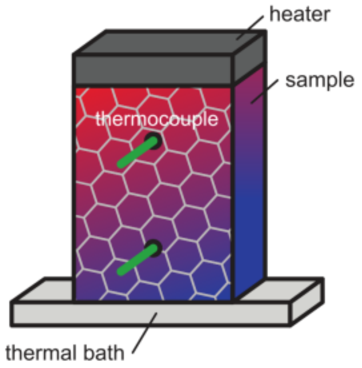
$$C(t) = \langle \mathcal{J}(t)\mathcal{J} \rangle = \frac{1}{Z} \mathrm{Tr}_{\{\eta\}} \mathrm{Tr}_{\{d\}} [e^{H/T} \mathcal{J}(t)\mathcal{J}]$$

gauge + fermion trace = Boltzmann Tr $2^{N/2}$ fermion conductivities

Correlation functions

(1) Thermal current $\mathcal{J}$: r-space continuity eqn. with 'energy polarization'

$$\mathcal{J} = [H, \sum_l l\, h_l] \qquad H = \sum_l h_l$$



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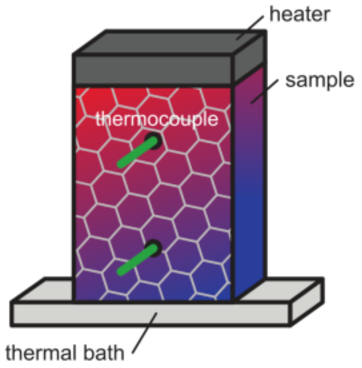


$$\mathcal{J} = [\mathsf{H}, \textstyle\sum_{\mathbf{l}} \mathbf{l}\, \mathsf{h}_{\mathbf{l}}] = \eta\text{−diagonal}, \quad \mathsf{H} = \sum_{\mathbf{l}} \mathsf{h}_{\mathbf{l}}$$

dynamical current correlation function

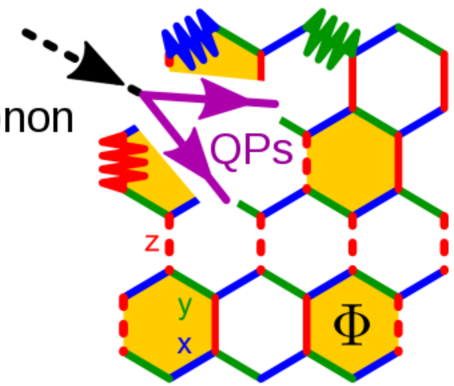
$$\mathsf{C}(\mathsf{t}) = \langle \mathcal{J}(\mathsf{t}) \mathcal{J} \rangle = \frac{1}{\mathsf{Z}} \mathrm{Tr}_{\{\eta\}} \mathrm{Tr}_{\{\mathsf{d}\}} [e^{\mathsf{H}/\mathsf{T}} \mathcal{J}(\mathsf{t}) \mathcal{J}]$$

gauge + fermion trace = Boltzmann Tr $2^{N/2}$ fermion conductivities

(2) Magnetoelastic spin-phonon coupling

$$\mathsf{H}_{\mathsf{MP}} = \textstyle\sum_{\mathbf{q}\mu} (\mathsf{b}_{\mathbf{q}\mu} + \mathsf{b}^{\dagger}_{-\mathbf{q}\mu}) \mathsf{V}_{\mathbf{q}\mu}$$

$$\mathsf{V}_{\mathbf{q}\mu} = \textstyle\sum_{\mathbf{l},\alpha} \mathsf{g}_{\mu,\mathbf{q}} e^{i\mathbf{q}\cdot\mathbf{l}} (e^{i\mathbf{q}\cdot\mathbf{r}_\alpha} - 1)\, \eta_{\mathbf{l},\alpha} \mathsf{a}_{\mathbf{l}} \mathsf{c}_{\mathbf{l}+\mathbf{r}_\alpha} = \eta\text{−diagonal}$$



phonon self-energy

$$\Sigma_{\mu\nu}(\mathbf{q}, \tau) = \langle \mathsf{T}_\tau [\mathsf{V}_{\mathbf{q},\mu}(\tau) \mathsf{V}^{\dagger}_{\mathbf{q},\nu}] \rangle_{\{\eta\}}$$ = Tr $2^{N/2}$ self-energies

Methods

PRB 96, 041115(R) (2017), PRB 96, 205121 (2017), PRB 99, 075141 (2019), PRB 99, 205129 (2019), arXiv:1909.09360

(1) Analytic evaluation in zero flux sector (ZFS) = BCS type-of analysis. For reference also at T≠0. ⚡ Gauge excitations. — Kitaev-only

(2) Exact diagonalization (ED): spin-basis ~24-32 sites — Heisenberg-Kitaev
fermion basis ~72-88 sites — Kitaev-only

Motome, Nasu, arXiv:1909.02234, ++

QMC

Methods

PRB 96, 041115(R) (2017), PRB 96, 205121 (2017),
PRB 99, 075141 (2019), PRB 99, 205129 (2019),
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For reference also at $T \neq 0$. ↯ Gauge excitations.

(2) Exact diagonalization (ED): spin-basis ~24-32 sites — Heisenberg-Kitaev
fermion basis ~72-88 sites — Kitaev-only

(3) Average gauge configuration approximation (AGC) — Kitaev-only

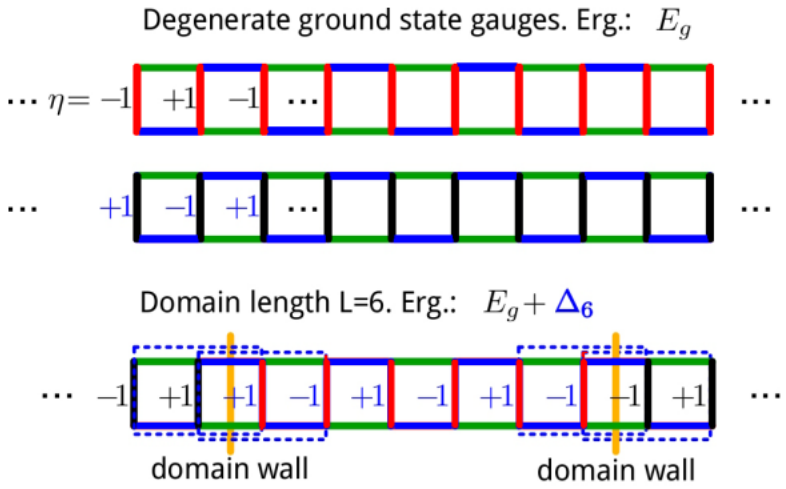
Motome, Nasu, arXiv:1909.02234,
++

poor man's
evasion of
QMC

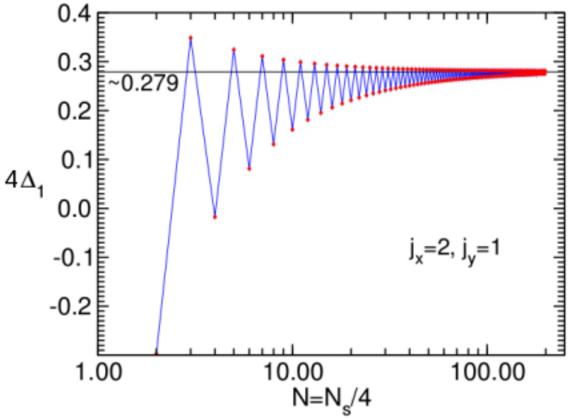
Average gauge configuration approximation: quasi 1D

PRB **96**, 041115(R)(2017)

$$C(t) = \frac{1}{Z}\, \mathrm{Tr}_{\{\eta\}}\, \mathrm{Tr}_{\{a\}} \left[e^{\beta H(\eta, a)} J(t) J \right]$$



- trace only 'mean' gauge configs.
  - $T \ll J_{x,y,z}$: effect. gauge Hamiltonian from fermionic ground states
  - any gauge config. = sequence of black-red ground state domains
  - erg. of gauge domain L=1: gap Δ_1

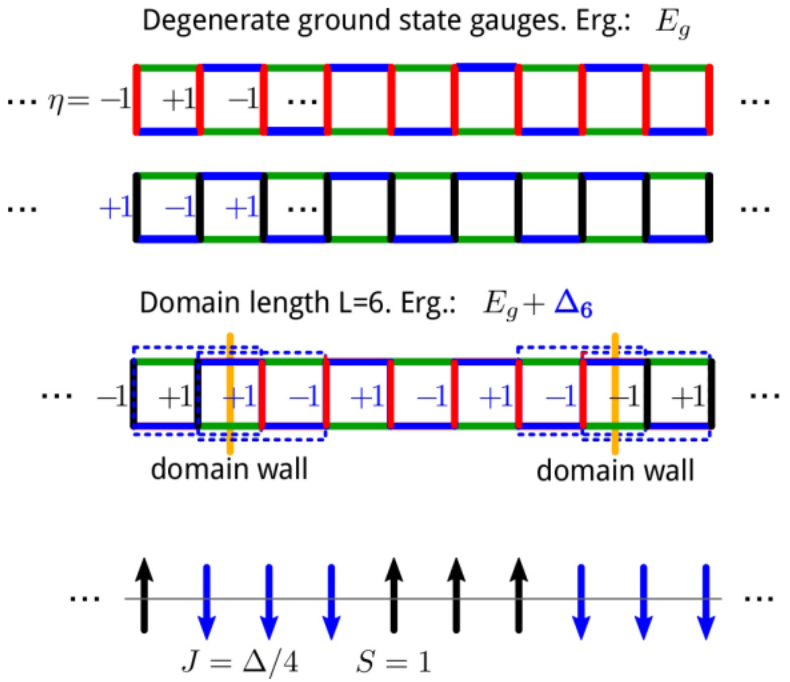


Average gauge configuration approximation: quasi 1D

PRB **96**, 041115(R)(2017)

$$C(t) = \frac{1}{Z}\,\mathrm{Tr}_{\{\eta\}}\,\mathrm{Tr}_{\{a\}}\left[e^{\beta H(\eta,a)} J(t) J\right]$$

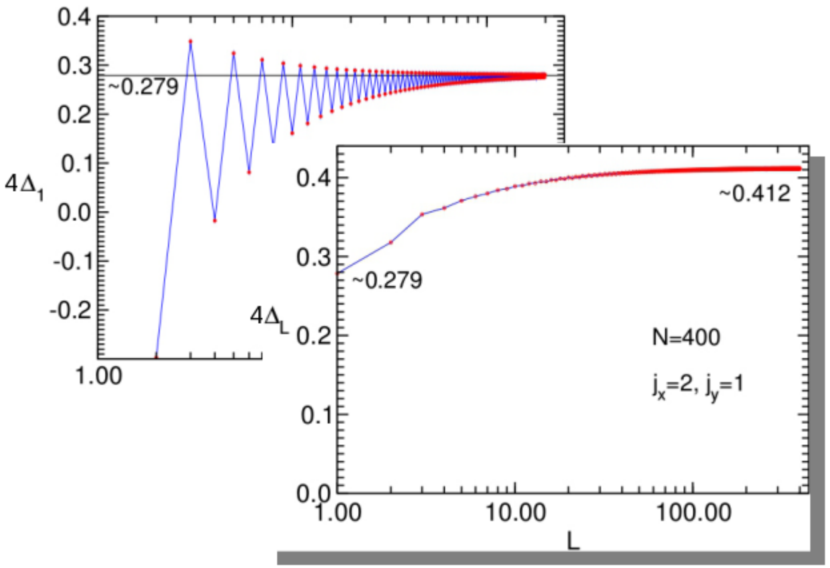
$$\approx \left\langle \left\langle J(t) J \right\rangle_{\mathrm{thermal}\ d(\eta)} \right\rangle_{\mathrm{disorder}\ n(T)}$$



- eff. H_{gauge} pseudo-S=1 1D Ising model $J=\Delta/4$

domain wall density $n(T)|_{exact} = \frac{1}{e^{\Delta/2T}+1}$

- trace only 'mean' gauge configs.
  - $T \ll J_{x,y,z}$: effect. gauge Hamiltonian from fermionic ground states
  - any gauge config. = sequence of black-red ground state domains
  - erg. of gauge domain L=1: gap Δ_1
  - domain walls are deconfined: erg. of $L \rightarrow \infty$, Δ_∞=const~$O(\Delta_1)$
  - No gauge LRO



Average gauge configuration approximation: honeycomb

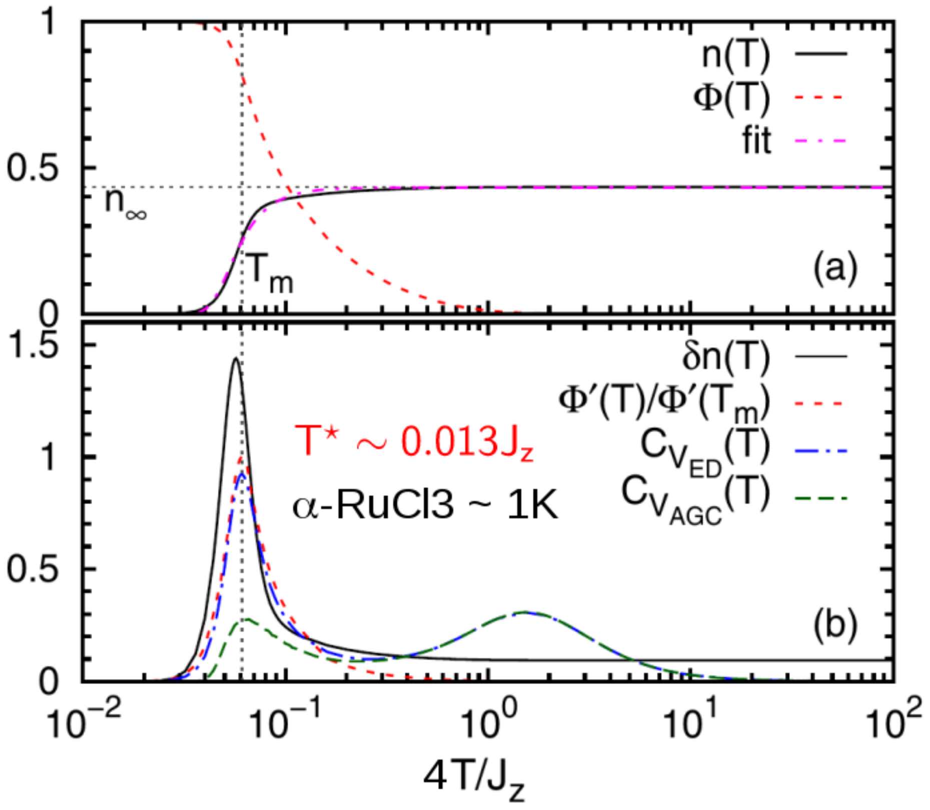
- no simple 1-to-1 mapping gauge $\leftrightarrow$ flux: only use fully disordered Z_2-field for $T > T^\star$
- Fix $T^\star$ from ED-thermodynamics:

spec. heat $\quad C_V(T)$

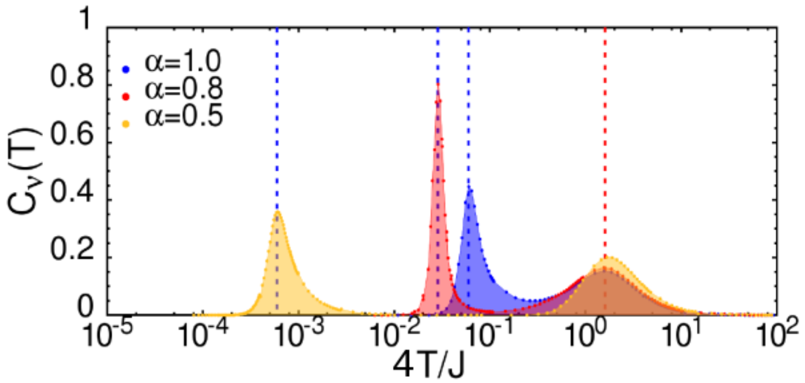
excit. gauges $\quad n(T) = \frac{1}{ZN} \mathrm{Tr}_\eta Z_{d(\eta)} n_\eta$

flux dens. $\quad \Phi(T) = \frac{1}{ZN} \sum_{\{\eta_\mathbf{r}\}} Z_{d(\eta)} \sum_\mathbf{r} \Phi_\mathbf{r}$

$$\Phi_\mathbf{r} = \eta_\mathbf{r} \eta_{\mathbf{r}+\mathbf{e}_x-\mathbf{e}_y}$$



- anisotropy reduces $T^\star$ (cf. toric code)



PRB **96**, 205121 (2017),
99, 075141 (2019),
99, 205129 (2019),
arXiv:1909.09360

consistent with QMC

Nasu, Yoshitake, Motome
PRL **119**, 127204 (2017);
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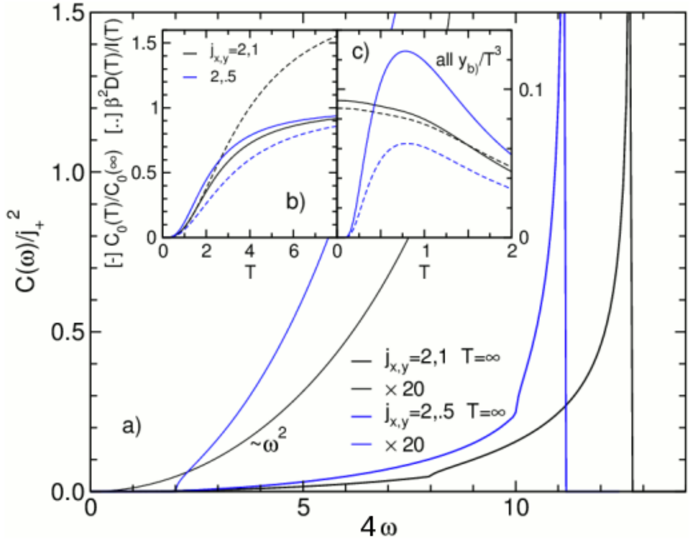
Zero flux sector

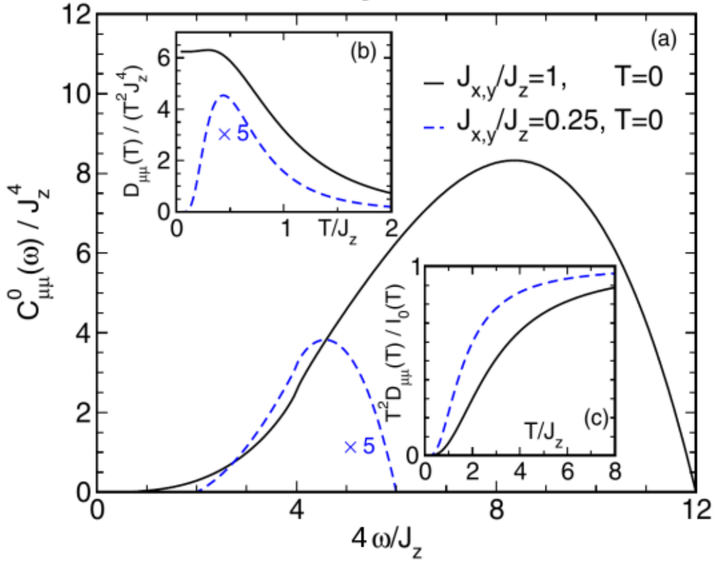
- ~nodal superconductor $C(\omega) = 4\pi T^2 D(T)\delta(\omega) \quad + \quad \sum_{k,\mu} M_\pm(k,\mu,T)\delta(\omega \mp 2E_{k,\mu})$

  qp fermion Drude weight $\sim(1-f)f$ pair breaking $\sim(1-f)^2$

ladder



honeycomb



- D(T) ~ T in gapless case
  ~ $e^{T/\Delta}$ " gapped "

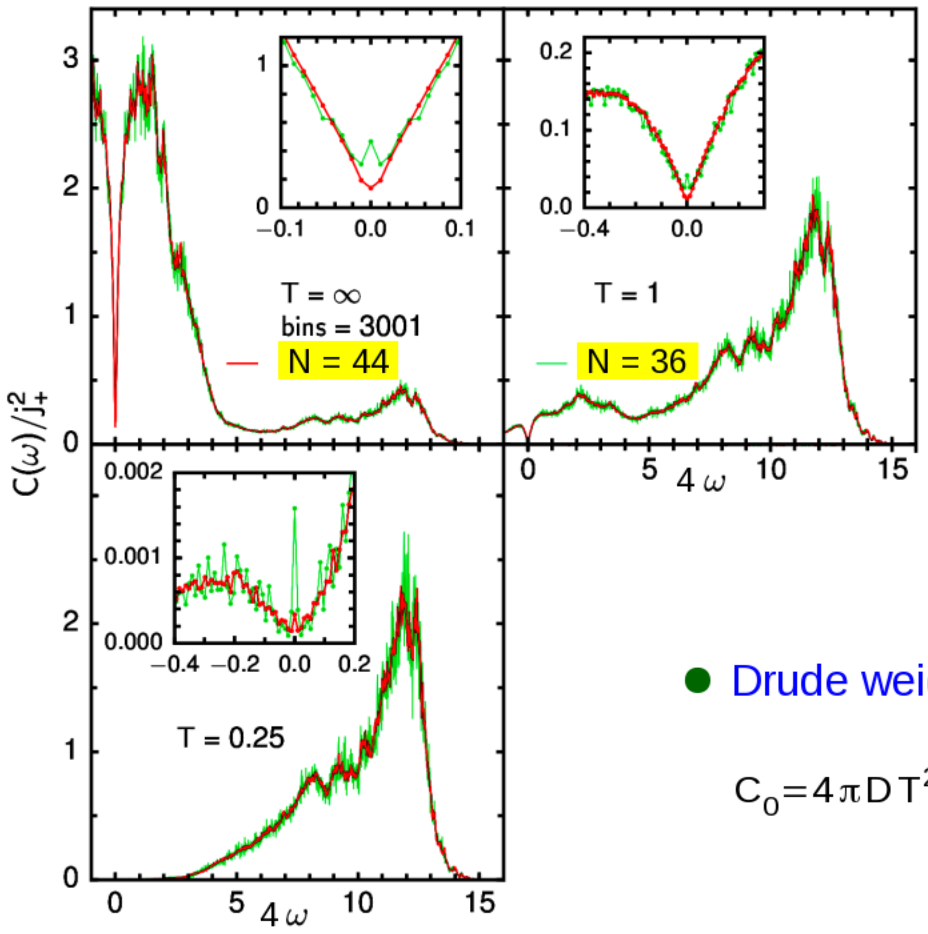
- D(T) ~ T^2 in gapless case
  ~ $e^{T/\Delta}$ " gapped "

- $\beta^2 D(T)$ is substantial fraction of $I(T) = \int_{0^+}^{\infty} C(\omega)\, d\omega$

Ballistic heat conductors

Ladder: all-gauge-sector-summation ED

- sum $2^{N/2}$ corr. functs. $C(t) = \mathrm{Tr}_{\{a\}} [e^{\beta H(\eta,a)} J(t) J]\Big|_{\{\eta\}} / Z$ of N/2 fermions ↔ N spins



- Low-ω hump + mobility gap
- DC of C(ω) ~0 at any T for N→∞
- Drude-δ(ω) ~0 at any T for N→∞
- Finite-ω resonances
- Ground state C(ω) for T→0

- Drude weight vs. N

$$C_0 = 4\pi D T^2 = \frac{1}{2Z} \sum_{E_l = E_m} e^{-E_l/T} \langle l|J|m\rangle\langle m|J|l\rangle$$

Ladder: all-gauge-sector-summation ED

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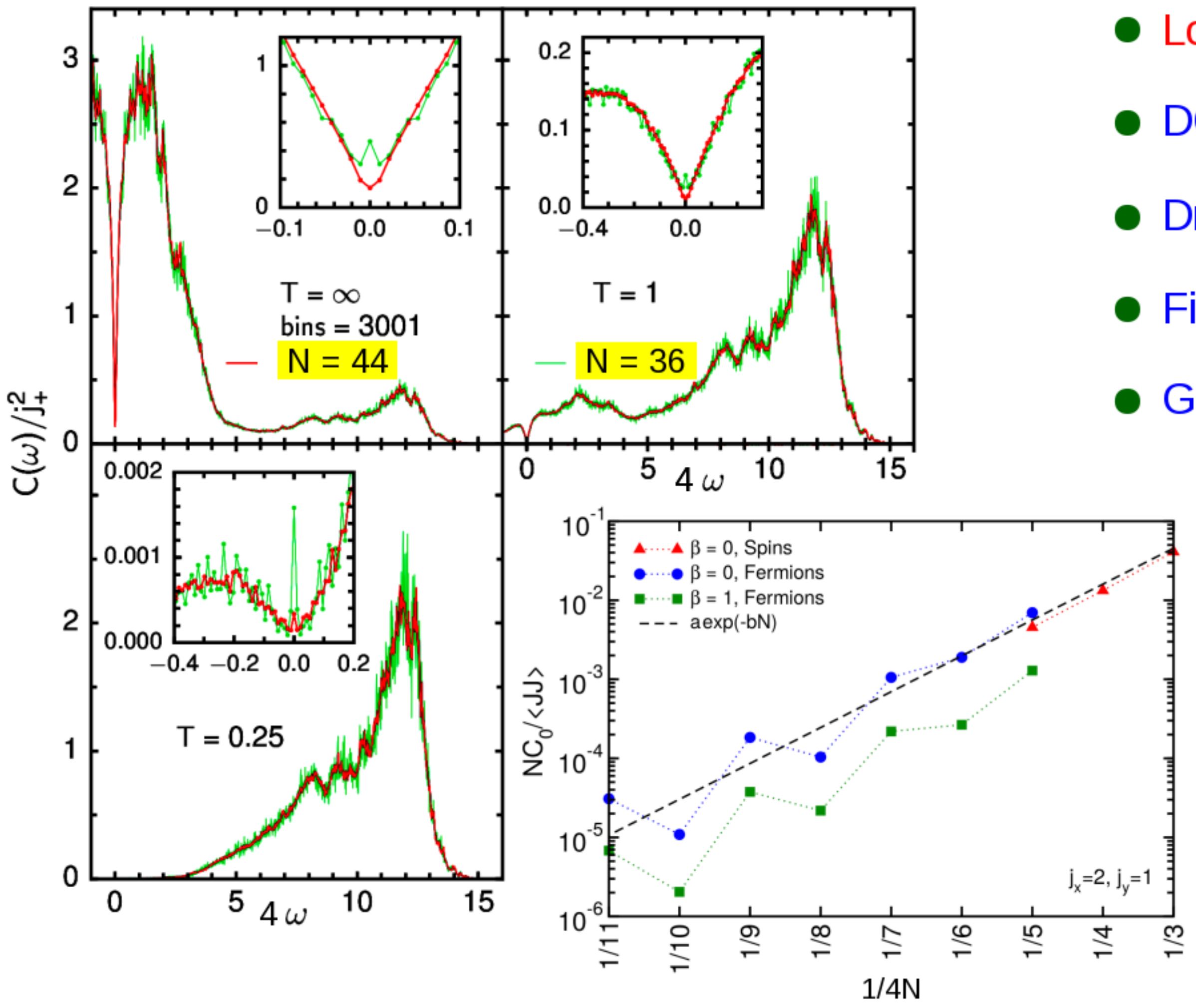


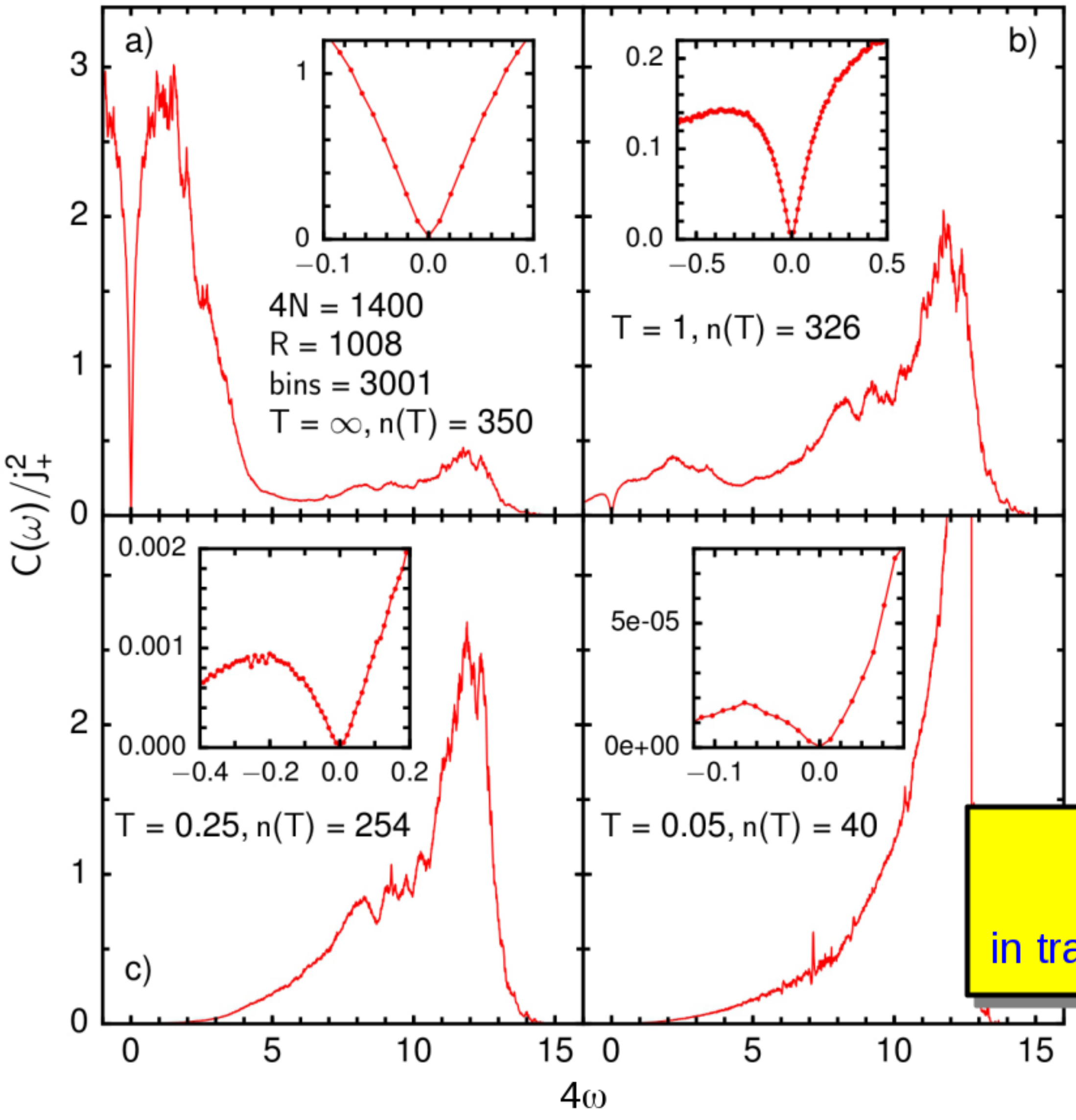
- Low-ω hump + mobility gap
- DC of C(ω) ~0 at any T for N→∞
- Drude-δ(ω) ~0 at any T for N→∞
- Finite-ω resonances
- Ground state C(ω) for T→0

- Drude-δ(ω) scales to zero exponentially with N

Heat insulator

translationally invariant spin system

Ladder: average gauge configuration approximation



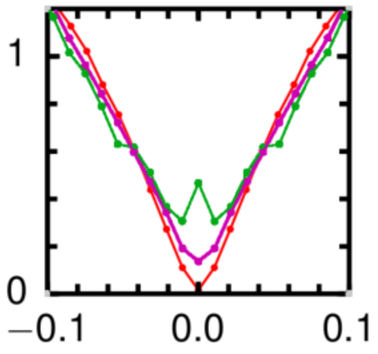
- Large systems N~O(10³)
- Clear mobility gap
- No Drude-δ(ω) at any T
  D-weight shifted to finite ω
- Zero DC limit of C(ω) at any T
- Some finite-ω structure due to matter-(single/many)-gauge resonances
- T→0: ground state C(ω) resurfaces

Localization of heat due to T-induced emergent disorder in translationally invariant spin system

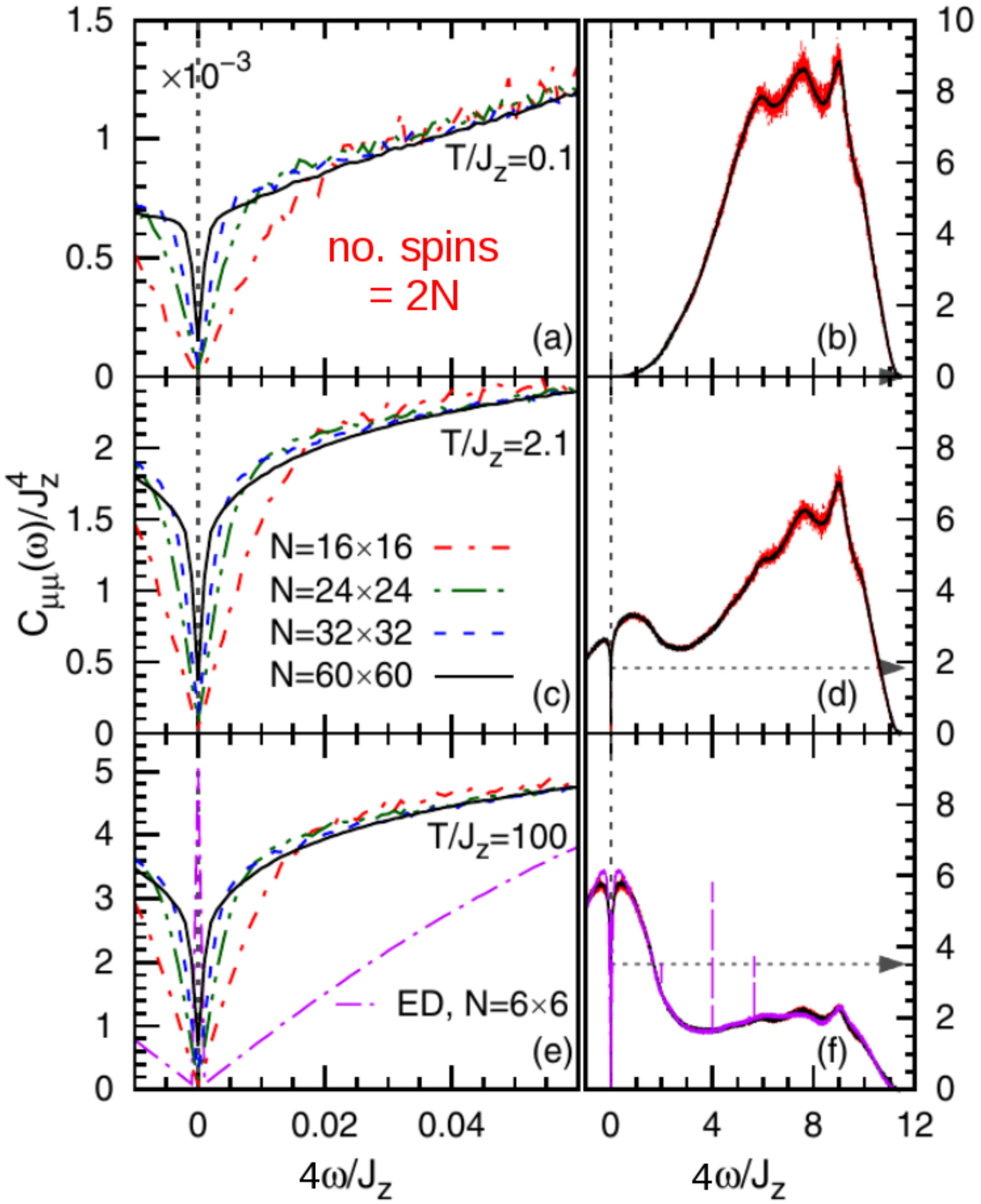
Honeycomb: average gauge configuartion approximation

- AGC: pseudogap closes N→∞

- scaling of gap for Kitaev ladder



N = 1400, 44, 36



Honeycomb: average gauge configuartion approximation

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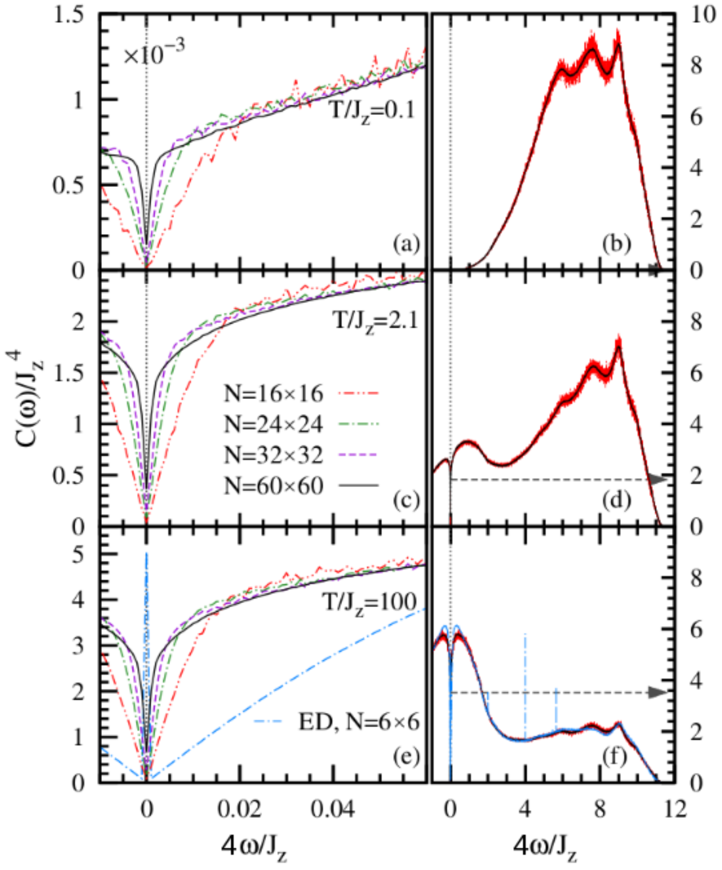
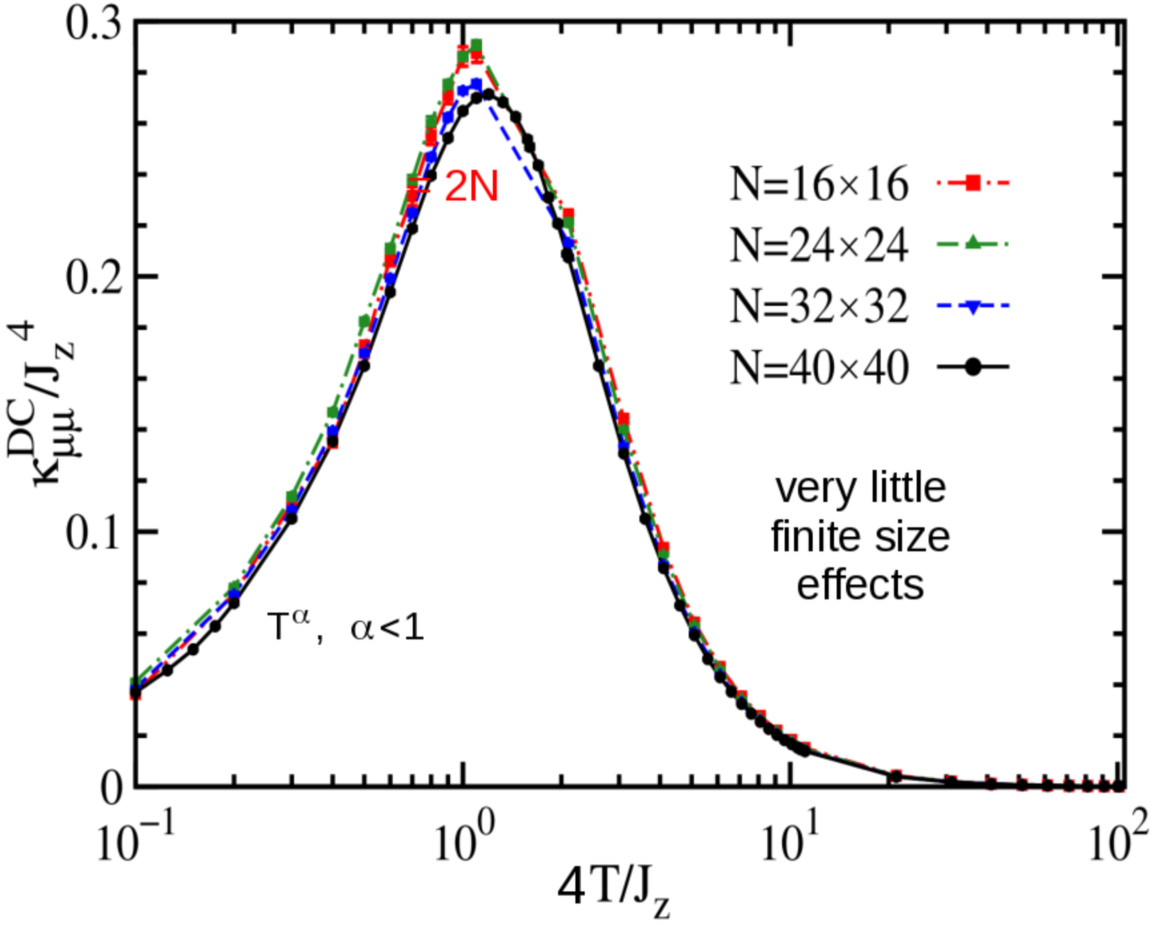
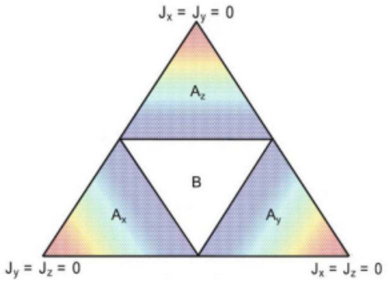


- Matter-fermion dissipative thermal DC transport



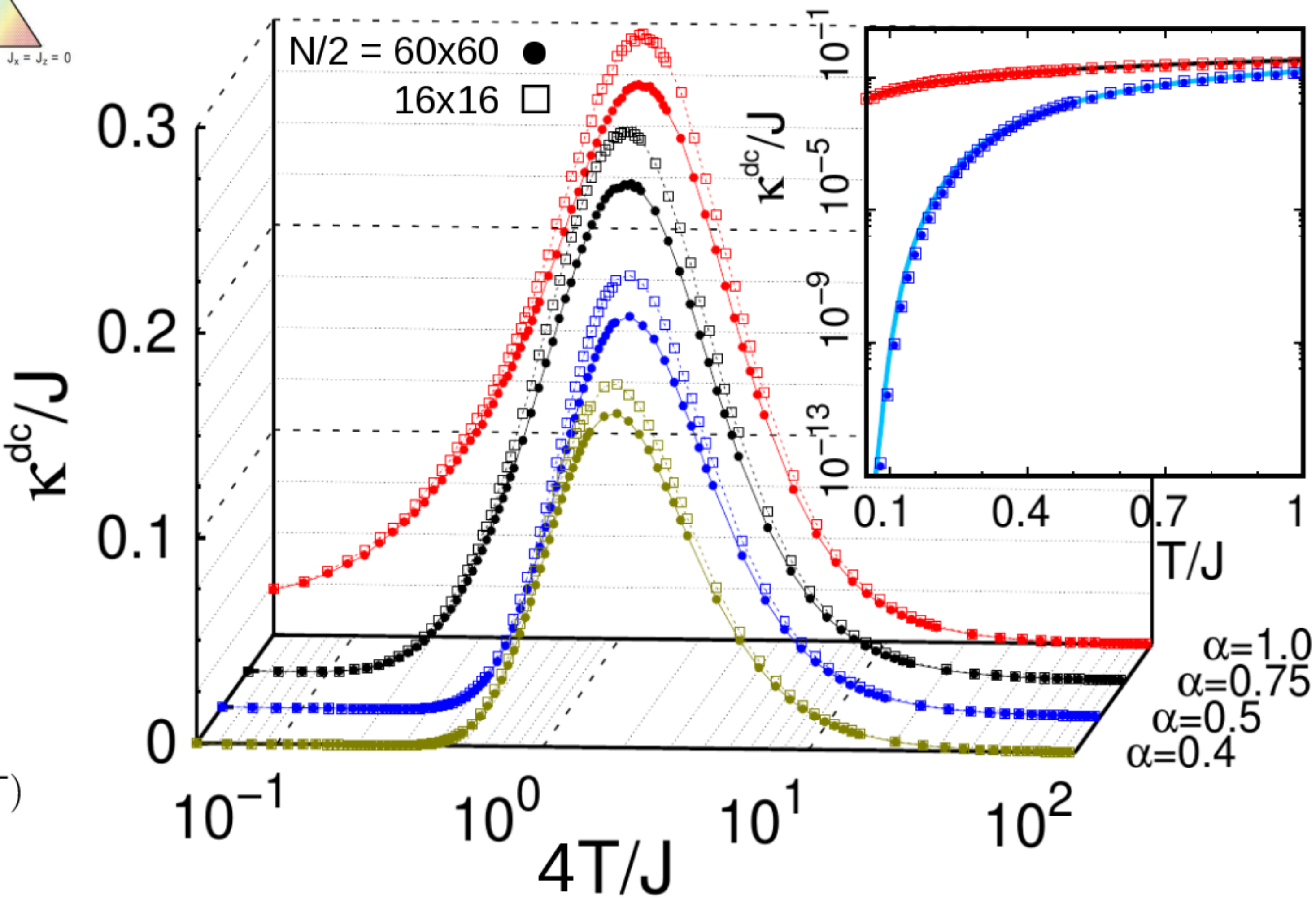
- Dimensionality matters

Anisotropy



$J_x = J_y = \alpha$

$J_z = 3 - 2\alpha$



B-phase

$\sim T^{\gamma},\ \gamma<1$

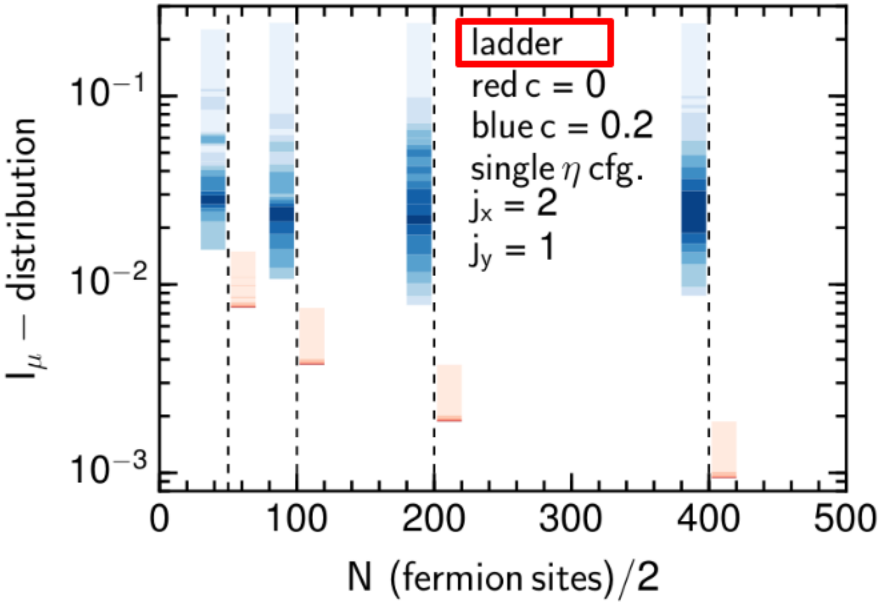
A-phase

$\sim \exp(-\Delta/T)$

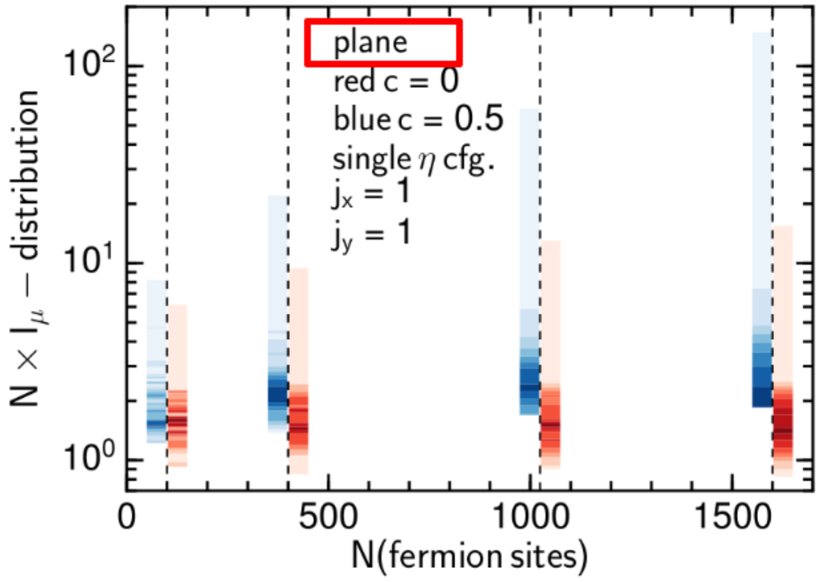
Why the difference

- inverse participation ratio $I_\mu = \sum_i |\psi_\mu(i)|^4$

$$\lim_{N\to\infty} I_\mu = \begin{cases} 1/N & \to \text{extended} \\ \text{const.} & \to \text{localized} \end{cases}$$



localized

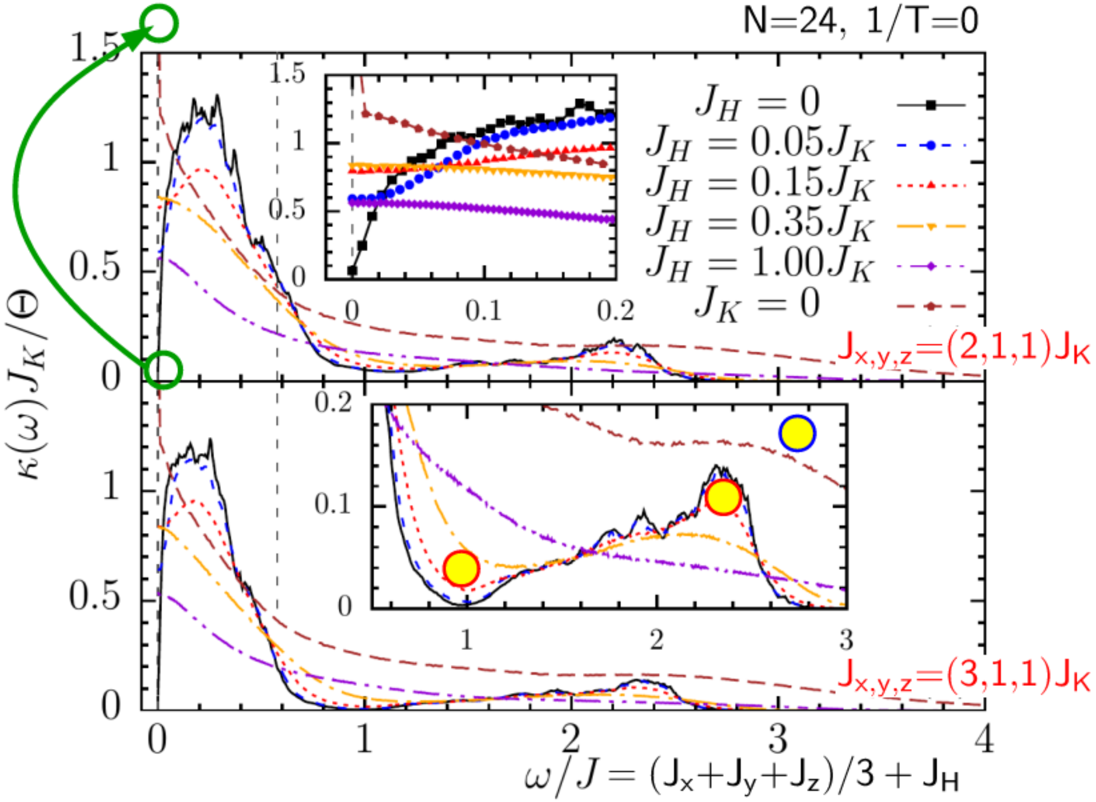


extended

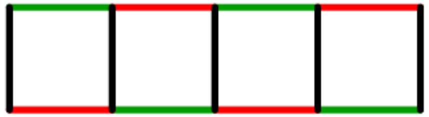
Kitaev-Heisenberg Ladder

PRB **99**, 205129 (2019)

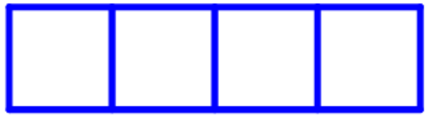
- ED & Quantum typicality



Kitaev: Z_2 spin-liquid
dirac fermion
heat insulator



$$H = \sum_{\langle l,m\rangle} (J_\alpha S_l^\alpha S_m^\alpha + J_H \mathbf{S}_l \cdot \mathbf{S}_m)$$



Heisenberg: ~VBC system
dissipative triplon
heat conductor

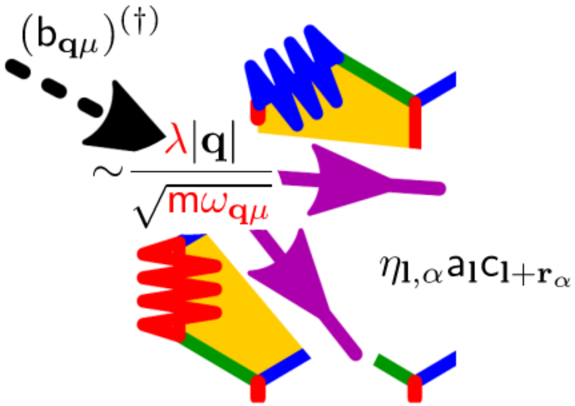
- $C(\omega=0)$ inc. vs. J_H/J_K, heat localization lost ⇔ flux mobility: insulator-conductor crossover
- dip & 2-fermion peak up to $J_K/J_h \sim 0.5$
- series expansions J_H^{leg}/J_H^{rung}: at $J_K=0$ weak 2-triplon continuum

Outline

- Why thermal transport
- Models, Quantities, and Methods
- Thermal current dynamics
  - Kitaev ladder
  - Honeycomb Kitaev
  - Kitaev-Heisenberg ladder
- Phonons in the Kitaev QSL

Phonon self-energy: Zero flux sector

arXiv:1909.09360

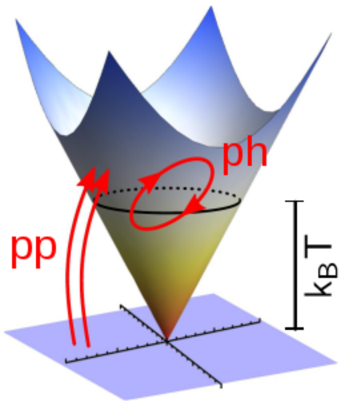


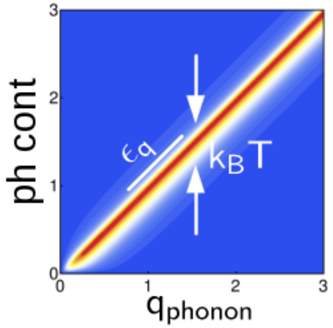
λ, "m" open issues

single spin procs.?

$$\Sigma_{\mu\nu}(\mathbf{q}, z) = \Sigma^{ph}_{\mu\nu}(\mathbf{q}, z) + \Sigma^{pp}_{\mu\nu}(\mathbf{q}, z)$$

$$\Sigma^{\times}_{\mu\nu}(\mathbf{q}, z) = \sum_{\mathbf{k}} A^{\times}_{k,q,\mu} A^{\times\star}_{k,q,\nu}\, \Pi^{\times}(\mathbf{q}, z, \mathbf{k}, T)$$

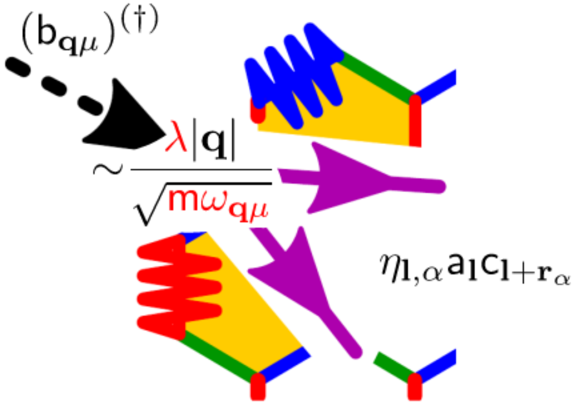




- $T < T^\star$: no. fermions small
- pp channel dominant

Phonon self-energy: Zero flux sector

arXiv:1909.09360



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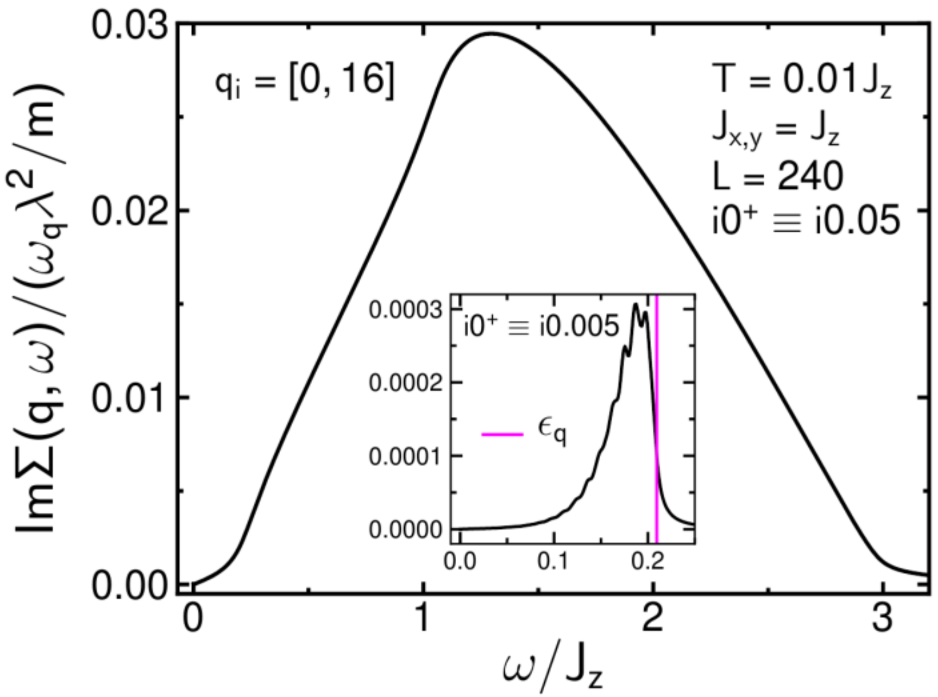
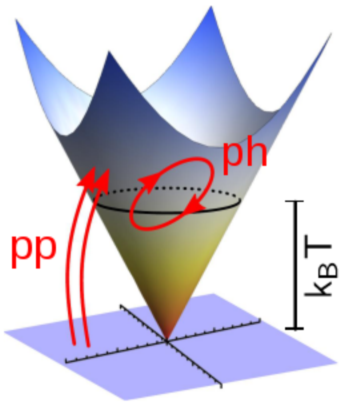
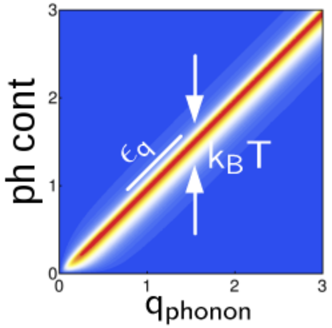


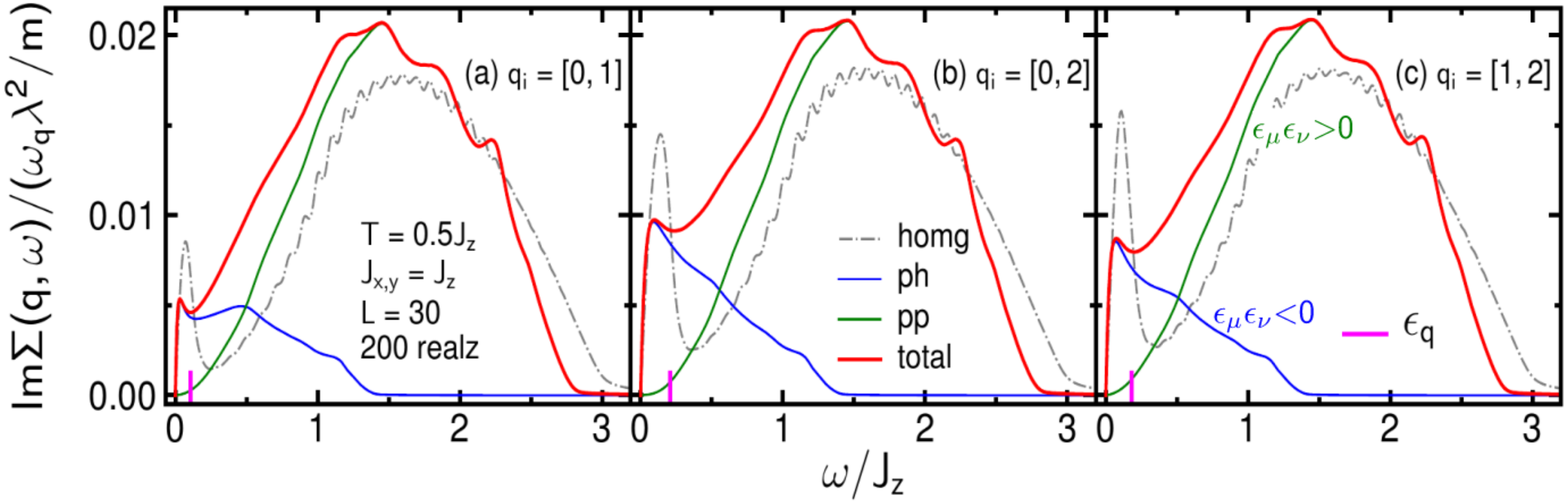




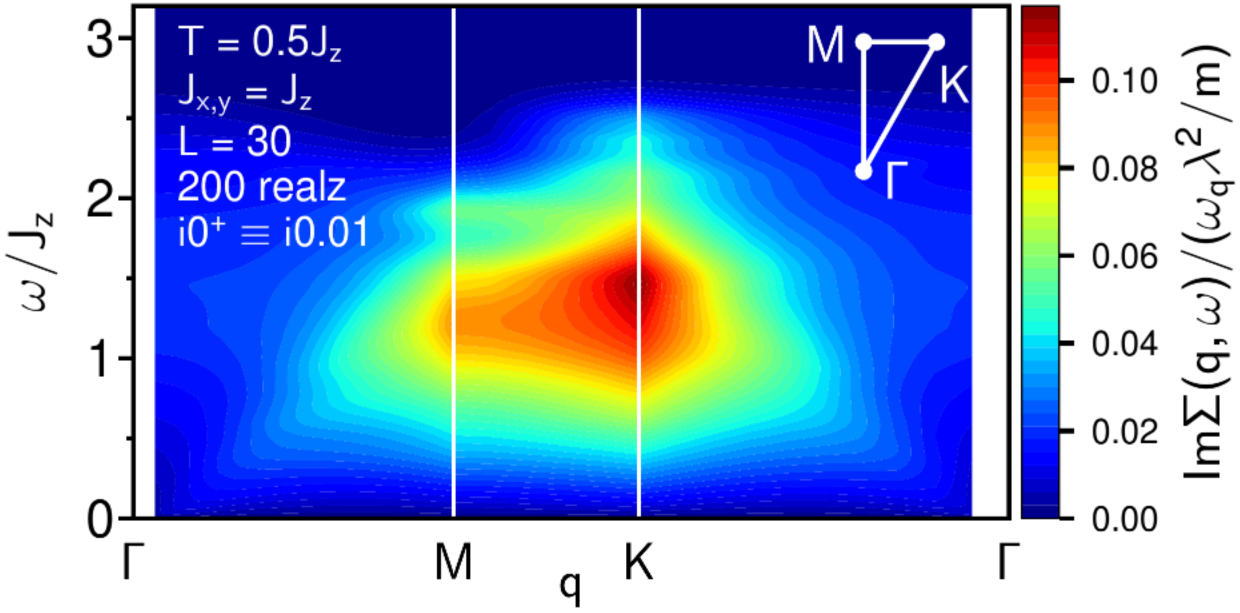
- $T < T^\star$: no. fermions small
- pp channel dominant

Phonon self-energy: average gauge configuration approach

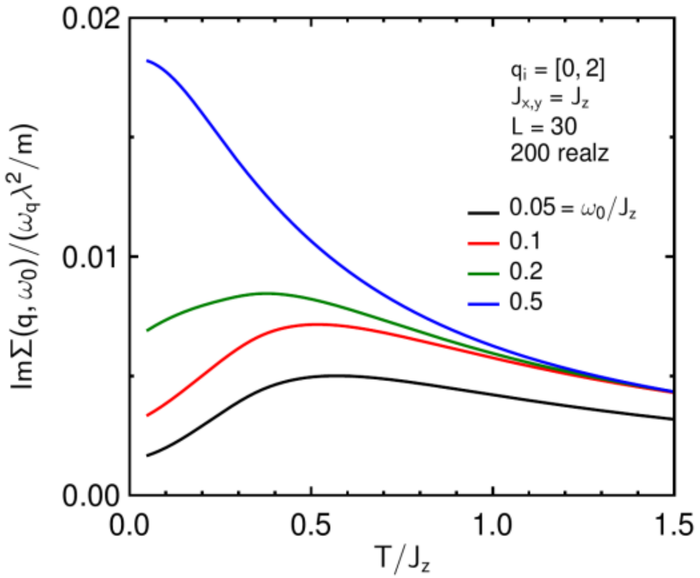
- Small q-regime $T > T^\star$



- Homogenous gauge: ph-continuum remains dispersive, weight inc. with T, shape remains narrow
- With flux excitations: ph-continuum spreads over ~O(J), ~non-dispersive, shape modulated
- pp-continuum less sensitive
- Similar to thermal conductivity



- $T > T^\star$ phonon-damping vs. momentum on BZ-path
  - featureless
  - broad
  - ph remnants



- phonon-damping vs. T
  - depends on details of $\omega_{\mathbf{q}\mu}$. RIP
  - undressing for T>J
  - higher order terms?
  - α-$RuCl_3$??

Conclusion

- Fractionalization has a profound impact on heat transport in Kitaev-Heisenberg models
  - static gauge fluxes serve as an emergent thermally activated disorder
  - in quasi 1D ladder case localization of heat results in pure Kitaev case
  - Heisenberg-Xchg induces insulator ↔ conductor crossover in ladder
  - 2D Kitaev magnet exhibits dissipative Majorana matter heat transport
  - phonons may dissipate within the Majorana continua
- Consistent scenario obtained from three complementary approaches: complete gauge trace, average gauge state, and ED of spin model