Spin Liquid and Spin Hall Effect with Strong Spin-Orbit Coupling

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Novel Quantum States in Condensed Matter 2017

Yukawa Institute, Kyoto University, November 14, 2017

NSERC CRSNG

CIFAR
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Outline

I. Quantum Spin Liquid in Hydrogen-Intercalated Honeycomb Iridate, $H_3LiIr_2O_6$

II. Quantum Spin Liquid in α-$RuCl_3$

III. Large Intrinsic Spin Hall Effect in Iridate Semimetal, SrIrO3

“Kitaev Materials”
A short introduction

α-A_2IrO_3

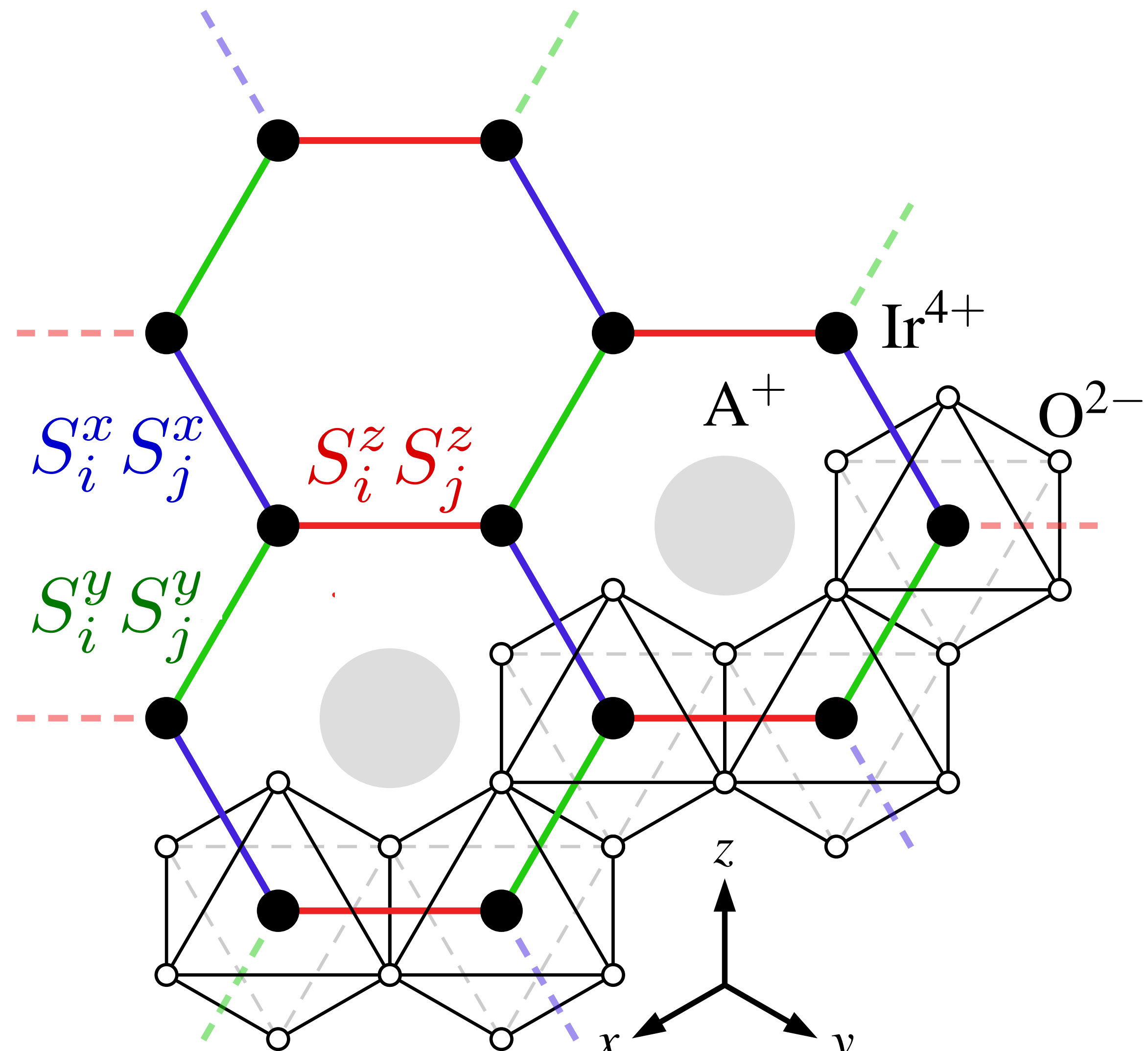
Kitaev Interaction ?

$$H = \sum_{\langle ij \rangle \in \gamma} -K S_i^\gamma S_j^\gamma$$

$$\gamma = x, y, z$$

G. Jackeli and G. Khaliullin, PRL 102, 256403 (2009)

J. Chaloupka, G. Jackeli and G. Khaliullin, PRL 105, 027204 (2010)



J_{eff}=1/2

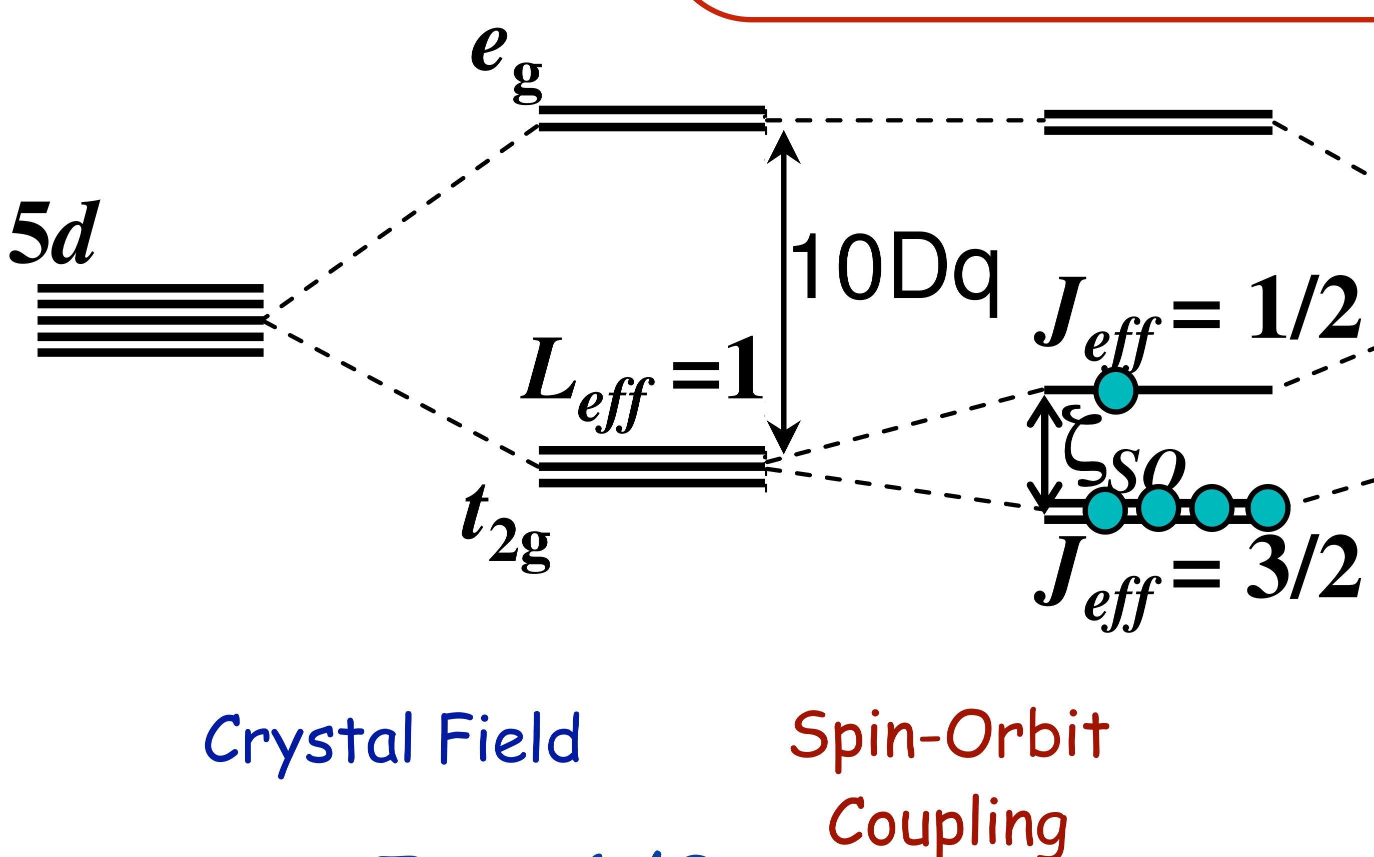
$$|\uparrow_j\rangle = \frac{1}{\sqrt{3}}(i|xz,\downarrow_s\rangle + |yz,\downarrow_s\rangle + |xy,\uparrow_s\rangle)$$

$$|\downarrow_j\rangle = -\frac{1}{\sqrt{3}}(i|xz,\uparrow_s\rangle - |yz,\uparrow_s\rangle + |xy,\downarrow_s\rangle)$$

Strong Spin-Orbit Coupling leads to Spin-Orbit entangled pseudo-spin basis (Kramers Doublet) α-A_2IrO_3 Kitaev Interaction ? A=Li, Na

α- $RuCl_3$

Clever way to lift orbital degeneracy !



Ir^{4+} = $5d^5$

$\lambda \sim 0.5$ eV

Ru^{3+} = $4d^5$

$\lambda \sim 0.15$ eV

J_{eff}=1/2

$$|\uparrow_j\rangle = \frac{1}{\sqrt{3}}(i|xz,\downarrow_s\rangle + |yz,\downarrow_s\rangle + |xy,\uparrow_s\rangle)$$
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Spin-Orbit entangled pseudo-spin basis (Kramers Doublet)

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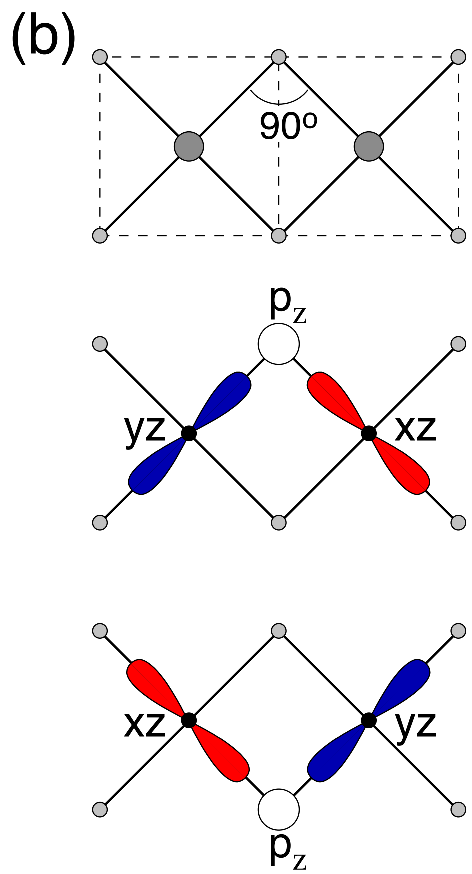


Edge-Sharing Oxygen Octahedra

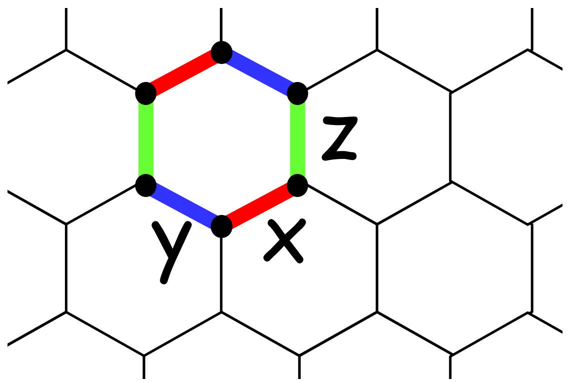
Including Hund's coupling and projecting to J_{eff}=1/2 manifold

J_{eff}=1/2

$$\boxed{\begin{aligned} |\uparrow_j\rangle &= \frac{1}{\sqrt{3}}(i|xz,\downarrow_s\rangle + |yz,\downarrow_s\rangle + |xy,\uparrow_s\rangle) \\ |\downarrow_j\rangle &= -\frac{1}{\sqrt{3}}(i|xz,\uparrow_s\rangle - |yz,\uparrow_s\rangle + |xy,\downarrow_s\rangle) \end{aligned}}$$

Strong Spin-Orbit Coupling leads to Spin-Orbit entangled pseudo-spin basis (Kramers Doublet)

Kitaev Model on Honeycomb Lattice: Exact Solution



$$\mathcal{H}_{\rm K} = -\sum_{\alpha-links} S_i^\alpha S_j^\alpha$$

A. Kitaev (2006)

$$S_i^\alpha = i b_i^\alpha c \qquad \{b_i^x, b_i^y, b_i^z, c\}$$

Four Majorana Fermions

$$\mathcal{H}_{\rm K} = \frac{i}{2} \sum_{\alpha-\text{links}} u_{ij}^\alpha c_i c_j \qquad (\text{where } \; u_{ij}^\alpha = i b_i^\alpha b_j^\alpha),$$

$\mathcal{W}_P = \prod_{\text{loop}} u_{ij}^\alpha$ commute with the Hamiltonian $\Longrightarrow$ $\mathcal{W}_P = \pm 1$

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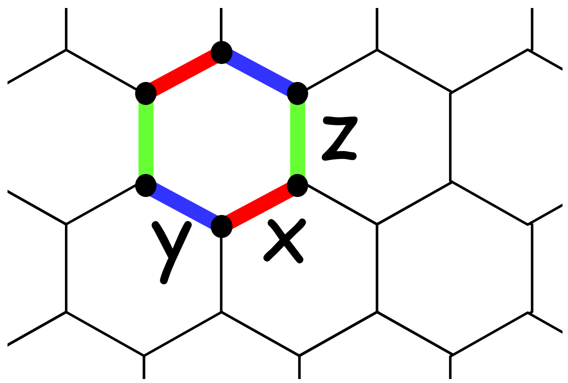

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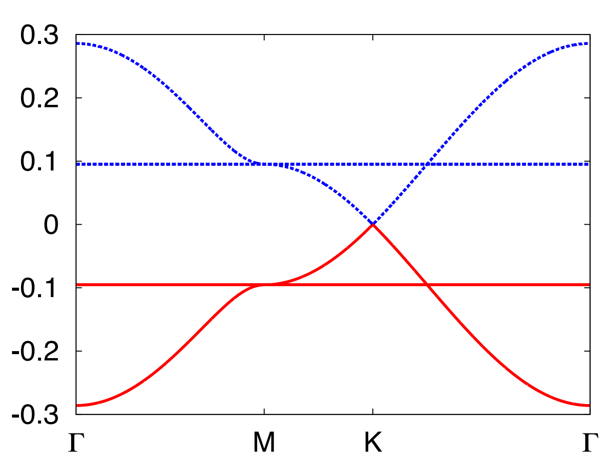
Ground state is in the zero-flux sector $u_{ij}^\alpha = +1 \; (\forall \langle ij \rangle)$



Majorana Fermions with
Dirac Dispersion

Realization of Kitaev Quantum Spin Liquid ?

2D

Honeycomb

α- Na_2IrO_3

α- Li_2IrO_3

α- $H_3LiIr_2O_6$

α- $RuCl_3$

β- Li_2IrO_3

3D Hyper-Honeycomb

γ- Li_2IrO_3

3D Stripy-Honeycomb

Realization of Kitaev Quantum Spin Liquid ?

2D Honeycomb

T_N

α- Na_2IrO_3	zig-zag, 14K
α- Li_2IrO_3	incomm. spiral, 15K
α- $H_3LiIr_2O_6$	no magnetic order (NMR)
α- $RuCl_3$	zig-zag, 7K

β- Li_2IrO_3 3D Hyper-Honeycomb	incomm. spiral, 38K
γ- Li_2IrO_3 3D Stripy-Honeycomb	incomm. spiral, 38K

Realization of Kitaev Quantum Spin Liquid ?

2D Honeycomb	T_N	suppressed magnetic order ?	
α- Na_2IrO_3	zig-zag, 14K		
α- Li_2IrO_3	incomm. spiral, 15K		
α- $H_3LiIr_2O_6$	no magnetic order (NMR)	Hydrogen intercalation	H. Takagi
α- $RuCl_3$	zig-zag, 7K	H_{in} > 8T	
		Banerjee, Nagler, Y.-J.Kim, Coldea, …	
β- Li_2IrO_3 (3D Hyper-Honeycomb)	incomm. spiral, 38K	P > 2.5 GPa	H. Takagi, D. Haskel
γ- Li_2IrO_3 (3D Stripy-Honeycomb)	incomm. spiral, 38K	P > 1.5 GPa	J. Analytis, D. Haskel

Three dimensional "Honeycomb" lattice

β- Li_2IrO_3

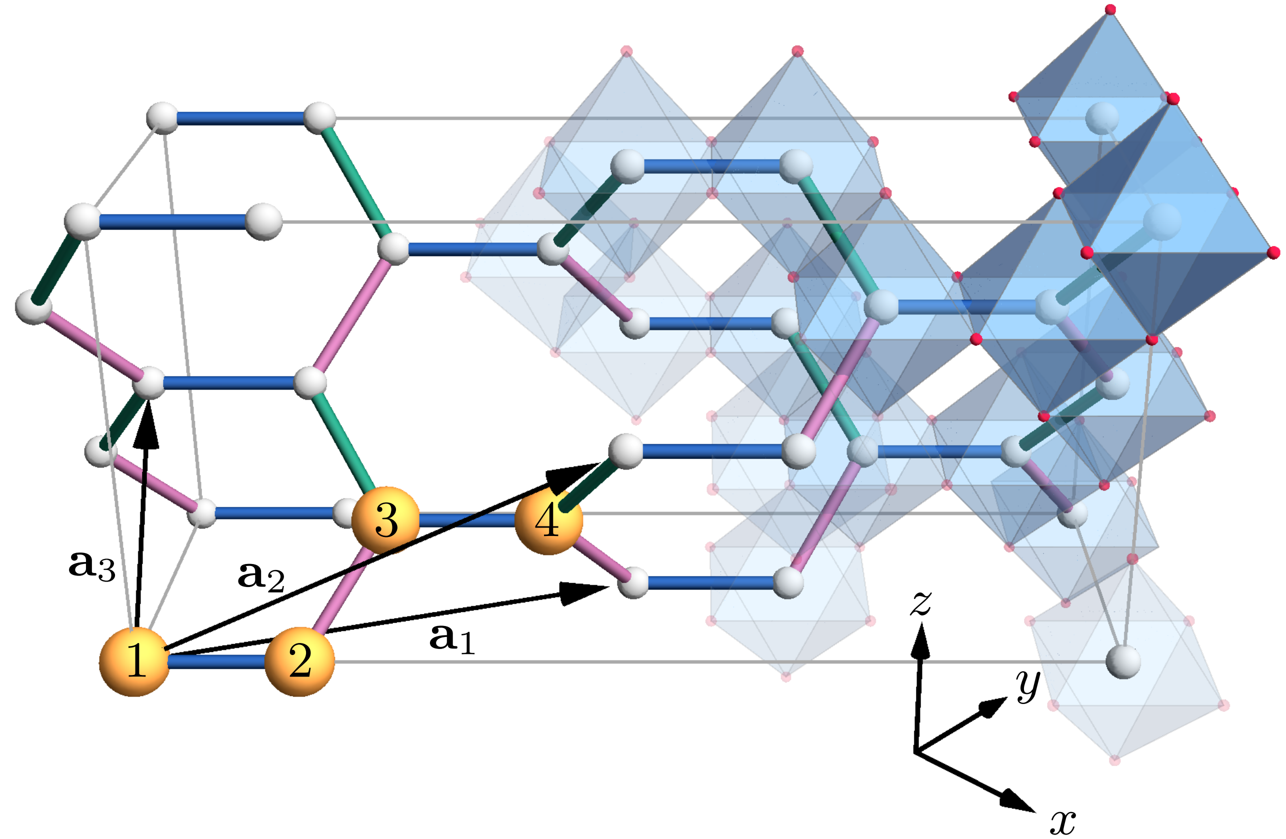
arXiv:1403.3296

H. Takagi (2013)

arXiv:1408.0246

P. Gegenwart

Hyper-Honeycomb



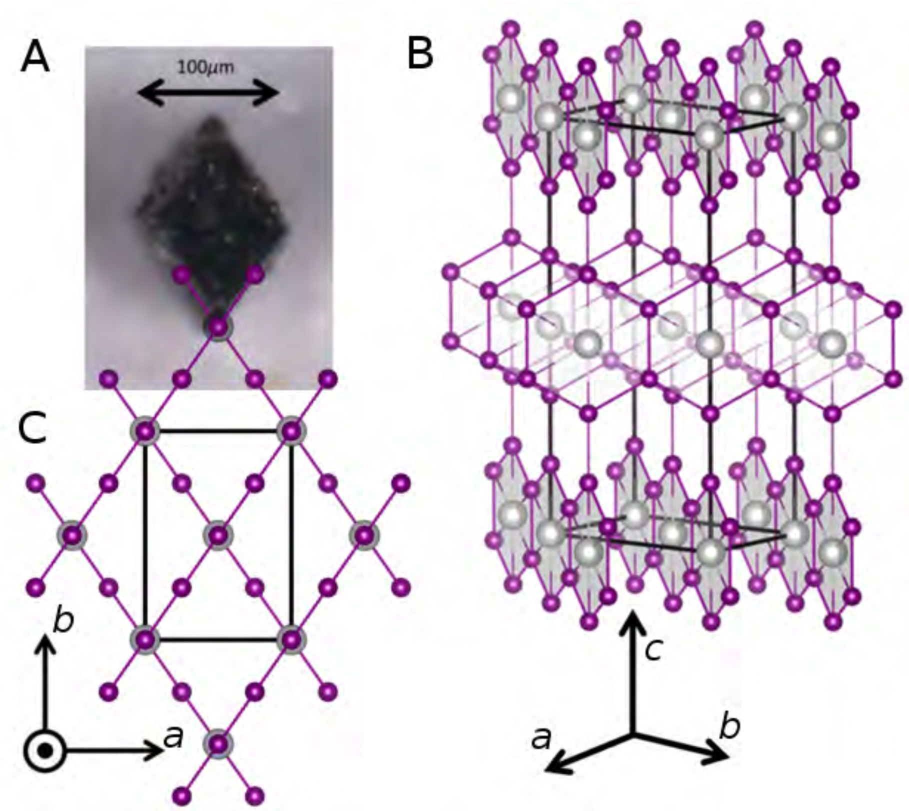
γ- Li_2IrO_3

arXiv:1402.3254

James Analytis

Radu Coldea

Stripy-Honeycomb



$$T_c = 38K$$

Strong Coupling Limit: Localized Pseudo-Spin Model

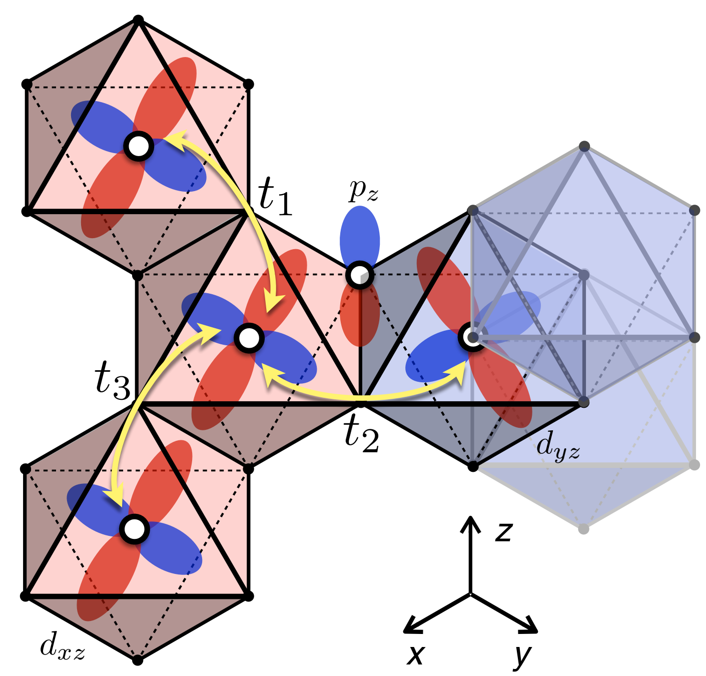
$$H = \sum_{\langle ij\rangle \in \alpha\beta(\gamma)} \left[J\vec{S}_i \cdot \vec{S}_j + K S_i^\gamma S_j^\gamma + \Gamma\left(S_i^\alpha S_j^\beta + S_i^\beta S_j^\alpha\right)\right]$$

e.g. In the limit of $U, J_H \gg \lambda \gg t$

$$J = \frac{4}{27}\left[\frac{6t_1(t_1+2t_3)}{U-3J_H} + \frac{2(t_1-t_3)^2}{U-J_H} + \frac{(2t_1+t_3)^2}{U+2J_H}\right]$$

$$K = \frac{8J_H}{9}\left[\frac{(t_1-t_3)^2-3t_2^2}{(U-3J_H)(U-J_H)}\right],$$

$$\Gamma = \frac{16J_H}{9}\left[\frac{t_2(t_1-t_3)}{(U-3J_H)(U-J_H)}\right].$$



$$t_1 = \frac{t_{dd\pi}+t_{dd\delta}}{2}, \quad t_2 = \frac{t_{pd\pi}^2}{\Delta_{pd}} + \frac{t_{dd\pi}-t_{dd\delta}}{2}, \quad t_3 = \frac{3t_{dd\sigma}+t_{dd\delta}}{4},$$

Strong Coupling Limit: Localized Pseudo-Spin Model

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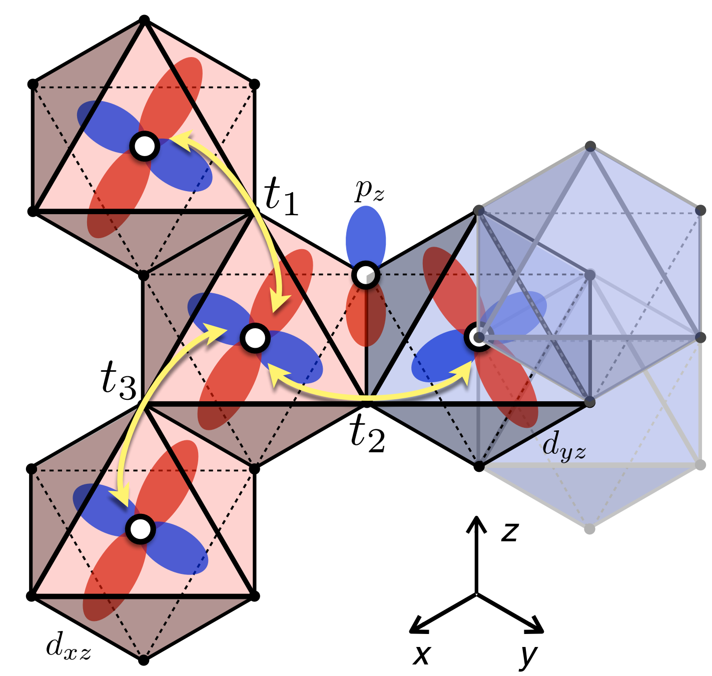


$$\boxed{t_1 = \frac{t_{dd\pi} + t_{dd\delta}}{2},} \quad t_2 = \frac{t_{pd\pi}^2}{\Delta_{pd}} + \boxed{\frac{t_{dd\pi} - t_{dd\delta}}{2},} \quad t_3 = \boxed{\frac{3t_{dd\sigma} + t_{dd\delta}}{4},}$$

Hydrogen-Intercalated Honeycomb Iridate

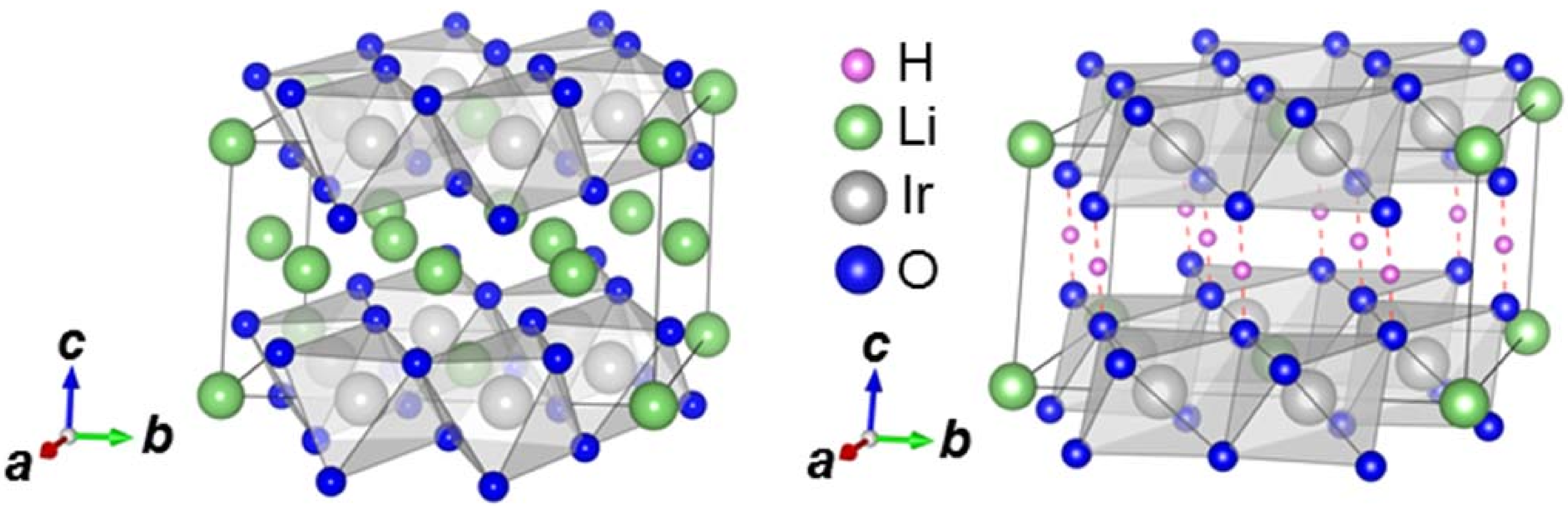
$H_3LiIr_2O_6$

Experiment: K. Kitagawa, T. Takayama, Y. Matsumoto, et al.
(H. Takagi's group at MPI-Stuttgart) (2017)

Theory: Kevin Slagle, Li Ern Chern, Wonjune Choi, YBK
arXiv:1710.01307

Spin-Orbital Entangled Quantum Liquid on Honeycomb Lattice

+K. Kitagawa[1], +T. Takayama[2], Y. Matsumoto[2], A. Kato[1], R. Takano[1], Y. Kishimoto[3], S. Bette[2], R. Dinnebier[2], G. Jackeli[2,4] and H. Takagi[1,2,4*]



α-Li_2IrO_3 $H_3LiIr_2O_6$

many stacking faults

$$a = 5.1633(2)\mathring{A} \qquad a = 5.3489(8)\mathring{A}$$

$$b = 8.9294(3)\mathring{A} \qquad b = 9.2431(14)\mathring{A}$$

$$c = 5.1219(2)\mathring{A} \qquad c = 4.8734(6)\mathring{A}$$

enlogated a/b

Reduced interlayer spacing

Spin-Orbital Entangled Quantum Liquid on Honeycomb Lattice

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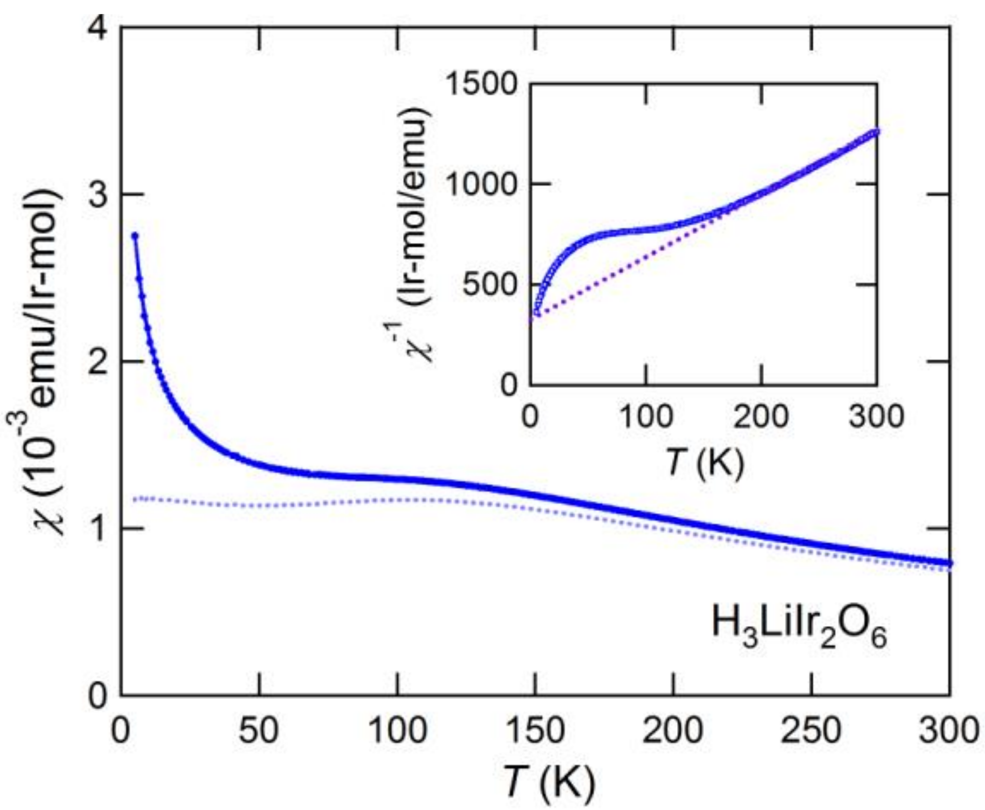

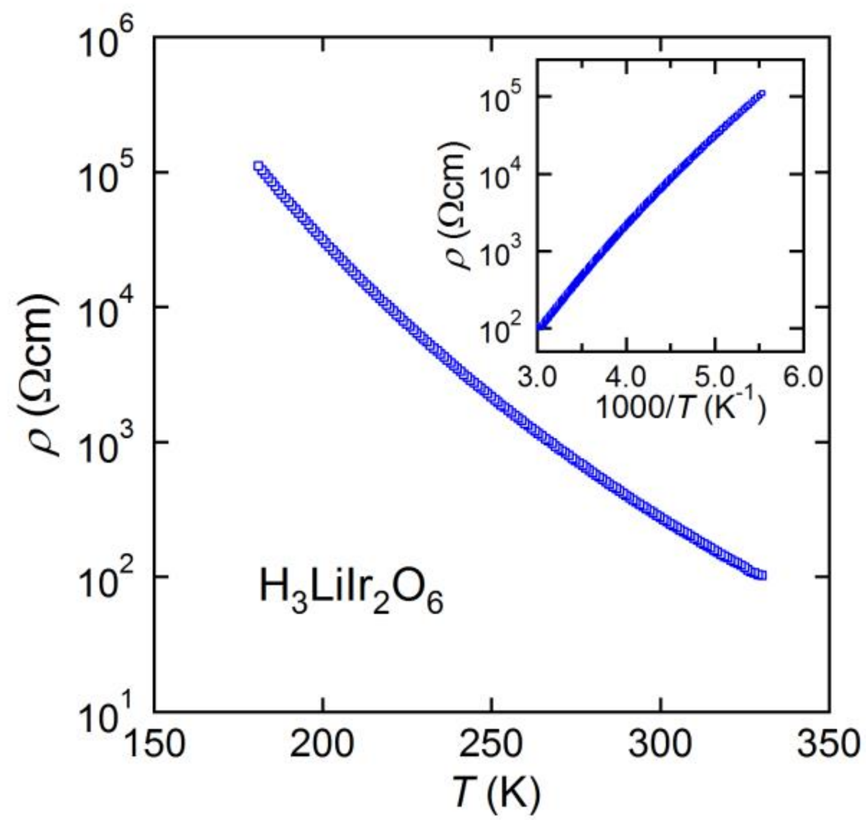

Curie-Weiss temperature

θ_{CW} = - 105 K

Transport Activation Energy

~ 0.1 eV

Spin-Orbital Entangled Quantum Liquid on Honeycomb Lattice

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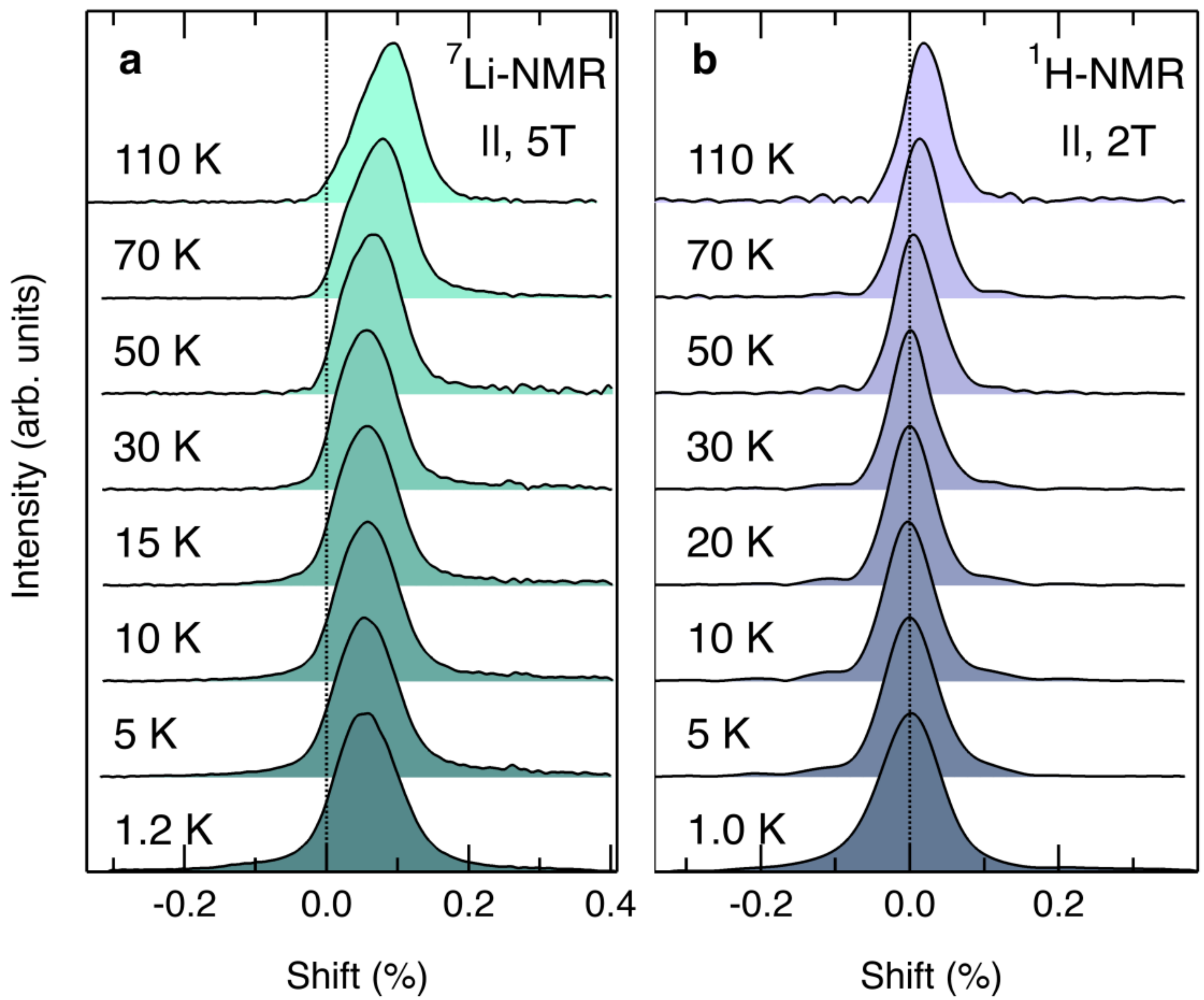
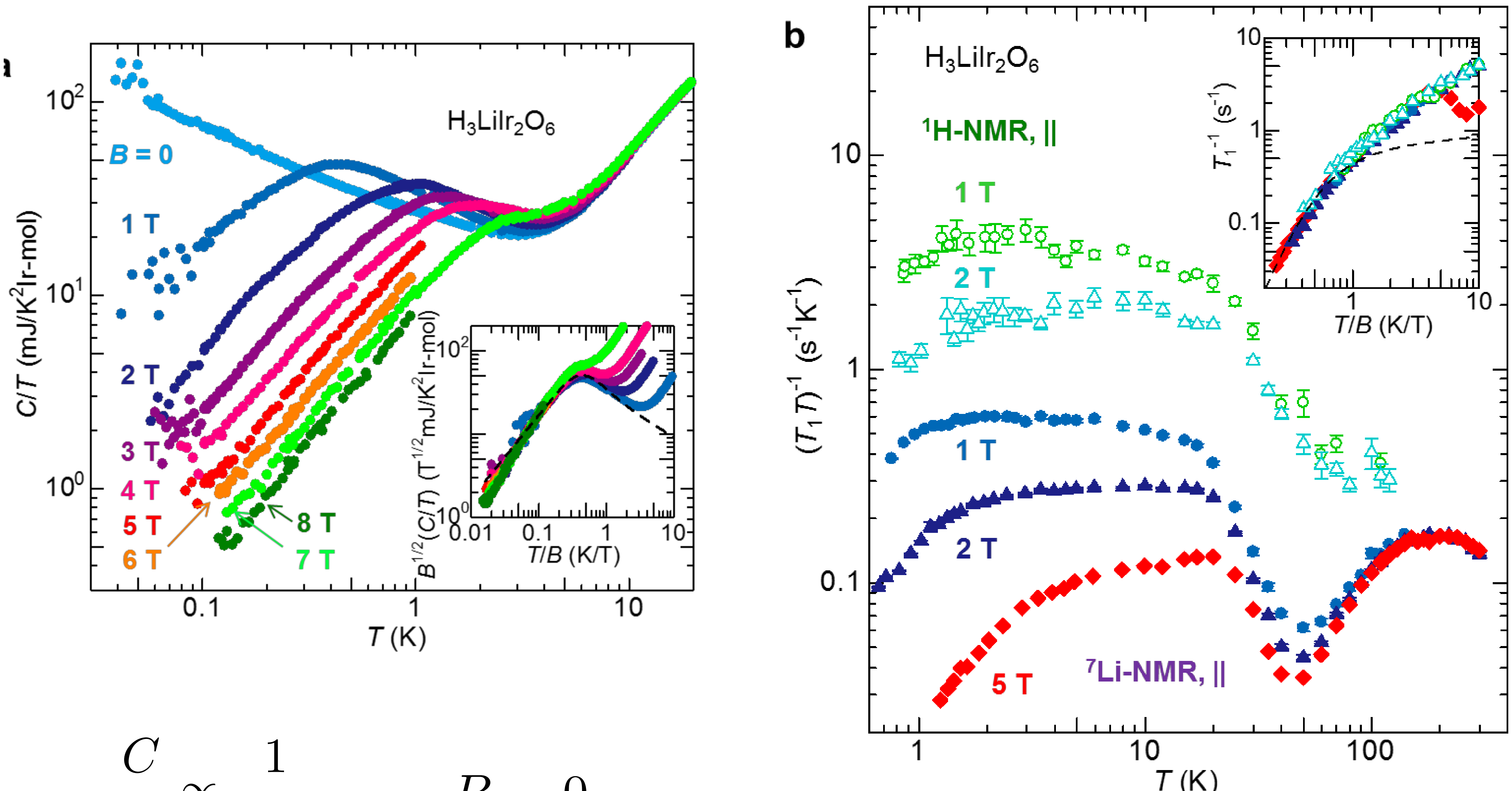


No broadening in Li^7 peak
- No magnetic order

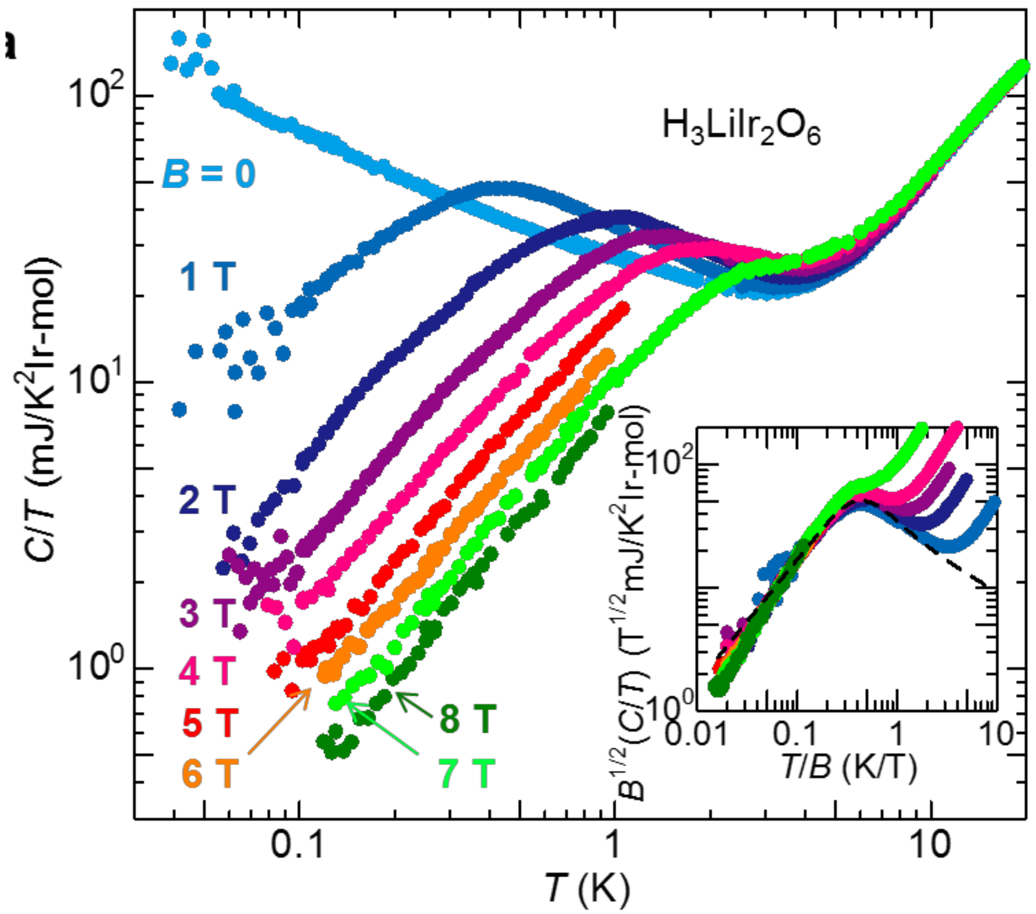
Only one peak for Li^7
- all the interlayer Li ions are replaced by H



$$\frac{C}{T} \propto \frac{1}{\sqrt{T}} \qquad B = 0$$

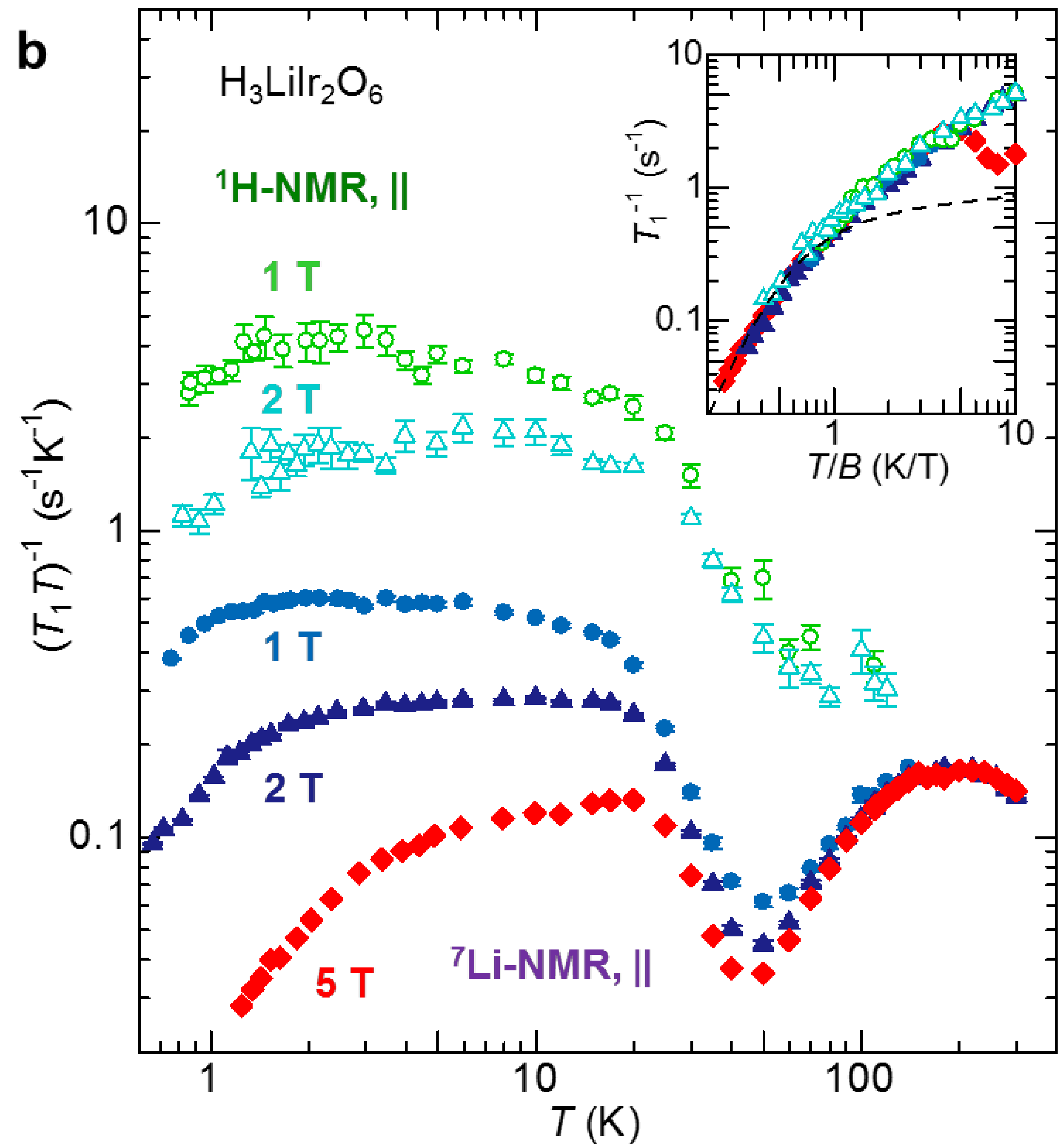
$$\frac{C}{T} \propto \frac{T}{B^{3/2}} \qquad B \neq 0$$

$$\frac{1}{T_1 T} \propto \left(\frac{C}{T}\right)^2$$



$$D(E) \propto \frac{1}{\sqrt{E}}$$

$$D(E) \propto \frac{E}{B^{3/2}}$$



$$\frac{1}{T_1 T} \propto \left(\frac{C}{T}\right)^2 \propto (N(0))^2$$

Density of States

Back of Envelope Estimation

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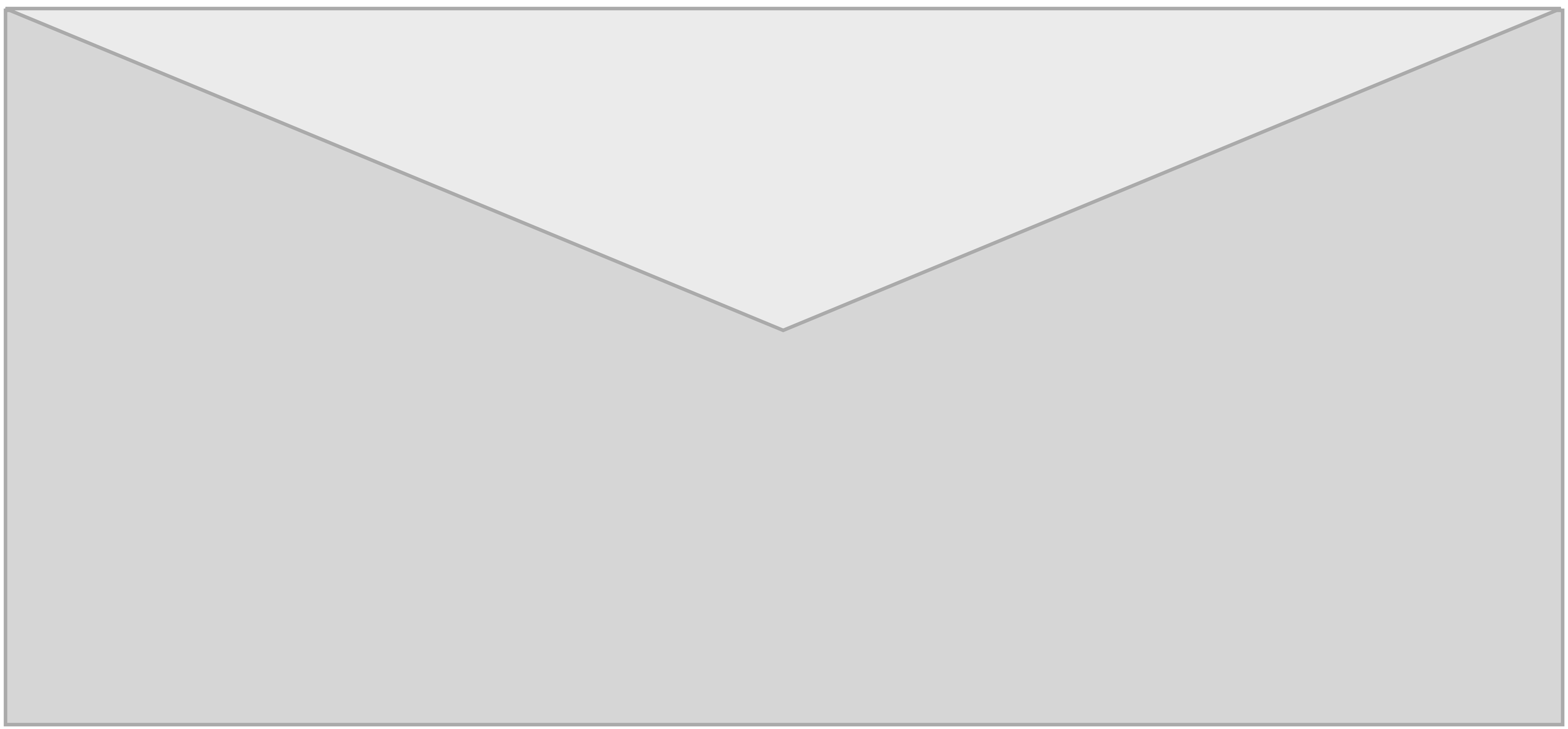
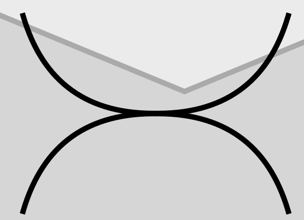
Back of Envelope Estimation



Density of States

Back of Envelope Estimation

$2D$ $\qquad \varepsilon = \alpha k^4$ band touching $\qquad D(\varepsilon) \propto \frac{1}{\sqrt{\varepsilon}}$

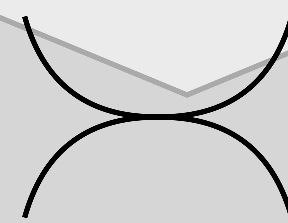


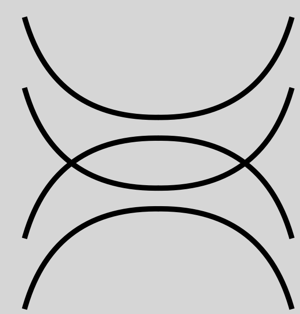
Density of States

Back of Envelope Estimation

$2D$ $\quad \varepsilon = \alpha k^4$ band touching $\quad D(\varepsilon) \propto \dfrac{1}{\sqrt{\varepsilon}}$

Zeeman energy $\quad \alpha k_0^4 \sim \mu_B B \quad k_0 \propto B^{1/4}$





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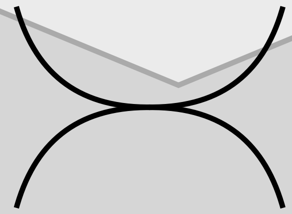
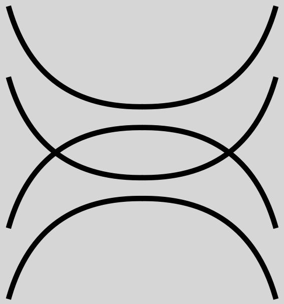




Dirac fermion $\quad \varepsilon \propto k_0^4 + 4k_0^3(k - k_0) + \mathcal{O}(k_0^2(k - k_0)^2)$

$$v \propto k_0^3 \propto B^{3/4} \qquad D(\varepsilon) \propto \frac{\varepsilon}{v^2} \propto \frac{\varepsilon}{B^{3/2}}$$

Clues for building a theoretical model

1) many stacking faults

different stacking patterns coexist

2) enlogated a/b parameters

direct overlap may be suppressed

Kitaev may dominate

3) Reduced interlayer spacing c

Interlayer interaction may be important

Theoretical Model

$$H = H_K + H_g + H_{\lambda'} \qquad N = 4$$

$$H_K = K \sum_{\ell=1}^{N} \sum_{\mu=x,y,z} \sum_{\langle i,j \rangle \in \mu} \sigma^{\mu}_{\ell,i} \sigma^{\mu}_{\ell,j}$$ Kitaev

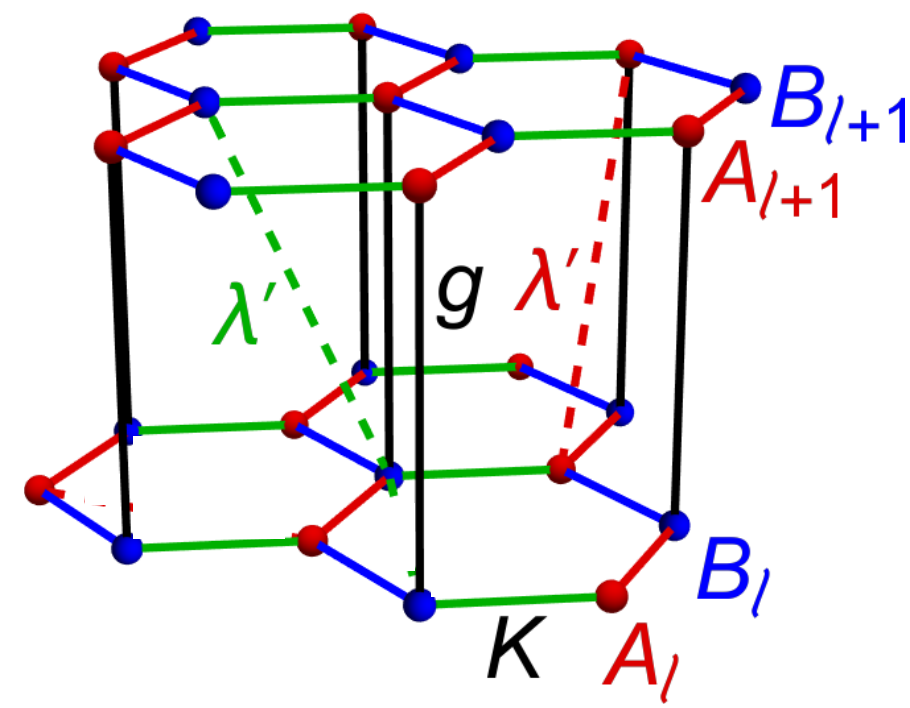
$$H_g = g \sum_{\ell=1}^{N-1} \sum_{\langle i,j \rangle}^{\mathrm{A\bar{B}}} \vec{\sigma}_{\ell+1,i} \cdot \vec{\sigma}_{\ell,j}$$ NN interlayer Heisenberg

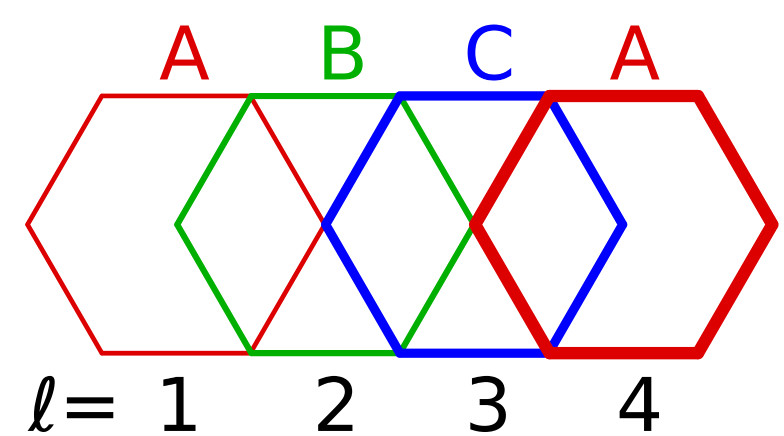
$$H_{\lambda'} = \lambda' \sum_{\ell=1,N-1} \left(\sum_{\langle\langle i,j \rangle\rangle}^{\mathrm{A\bar{A}}_x} \sigma^{x}_{\ell+1,i} \sigma^{x}_{\ell,j} + \sum_{\langle\langle i,j \rangle\rangle}^{\mathrm{B\bar{B}}_y} \sigma^{y}_{\ell+1,i} \sigma^{y}_{\ell,j} \right)$$

NNN interlayer bond-dependent Ising

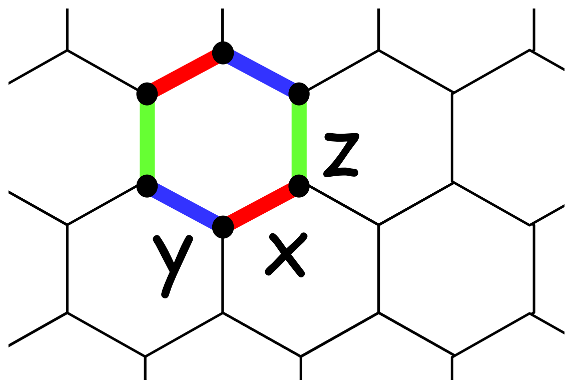
$$H_B = -\sum_{\ell,i,\mu} B_{\mu} \sigma^{\mu}_{\ell,i}$$ Zeeman

ABCA stacking





Kitaev Model: Exact Solution



$$\mathcal{H}_{\mathrm{K}} = -\sum_{\alpha-links} S_i^\alpha S_j^\alpha$$

$$S_i^\alpha = \frac{1}{2} i b_i^\alpha c_i \qquad \{b_i^x, b_i^y, b_i^z, c\}$$

Four Majorana Fermions

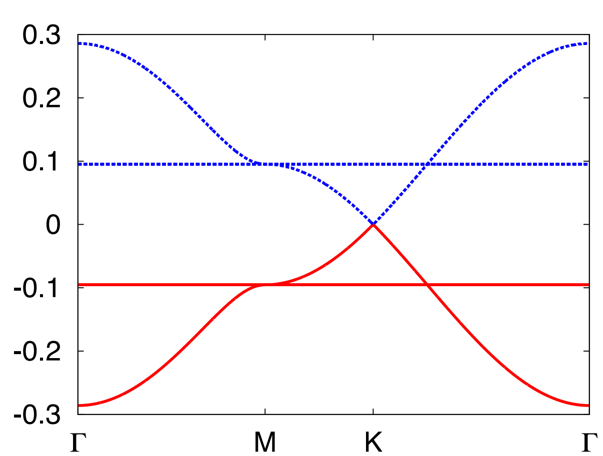
$$\mathcal{H}_K = -\frac{i}{4} \sum_{\alpha-links} u_{ij}^\alpha c_i c_j \qquad u_{ij}^\alpha = i b_i^\alpha b_j^\alpha$$

$\mathcal{W}_P = \prod_{\text{loop}} u_{ij}^\alpha$ commute with the Hamiltonian $\Longrightarrow \mathcal{W}_P = \pm 1$

$$W_p = 2^6 S_1^x S_2^y S_3^z S_4^x S_5^y S_6^z$$

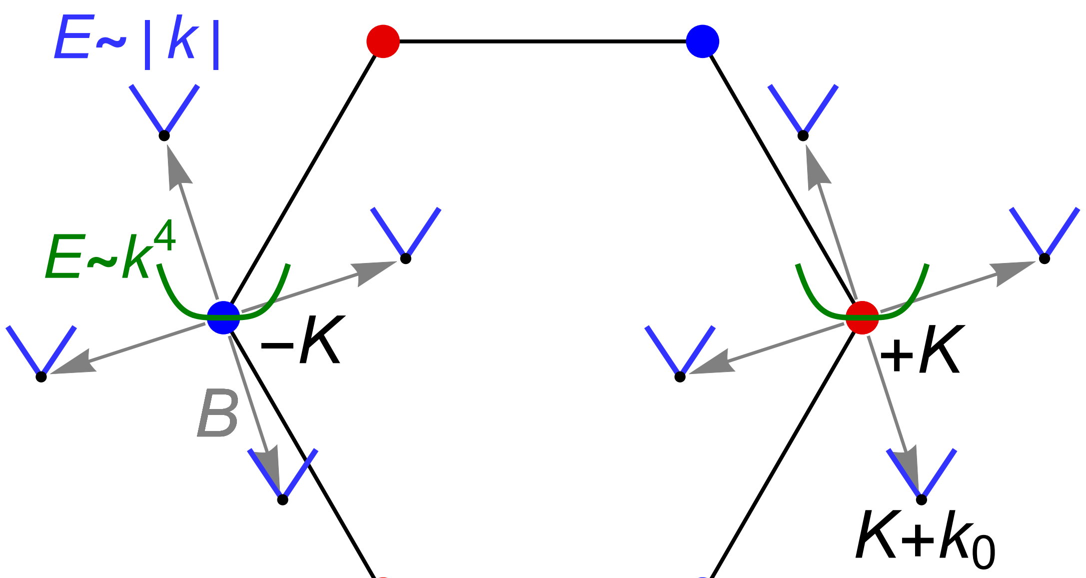
Ground state is in the zero-flux sector $u_{ij}^\alpha = +1 \; (\forall \langle ij \rangle)$

$$W_p = +1$$



Majorana Fermions with Dirac Dispersion

Mean-Field Theory



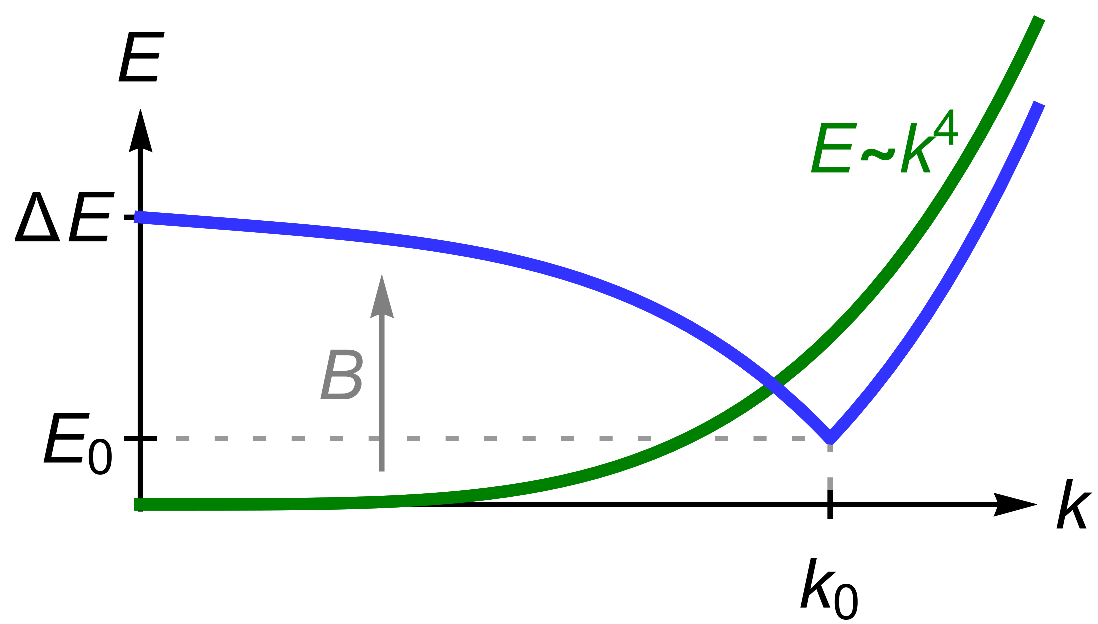
$$E \propto k^4 \qquad B = 0$$

Majorna mode resides mostly on the top and bottom layers

split into 8 Majorana cones

$$k_0 \propto B^{1/4} \qquad v \propto B^{3/4}$$

$$B \neq 0$$



In reality, there is a small excitation gap

$$E_0 \propto B^3$$

Theoretical Model

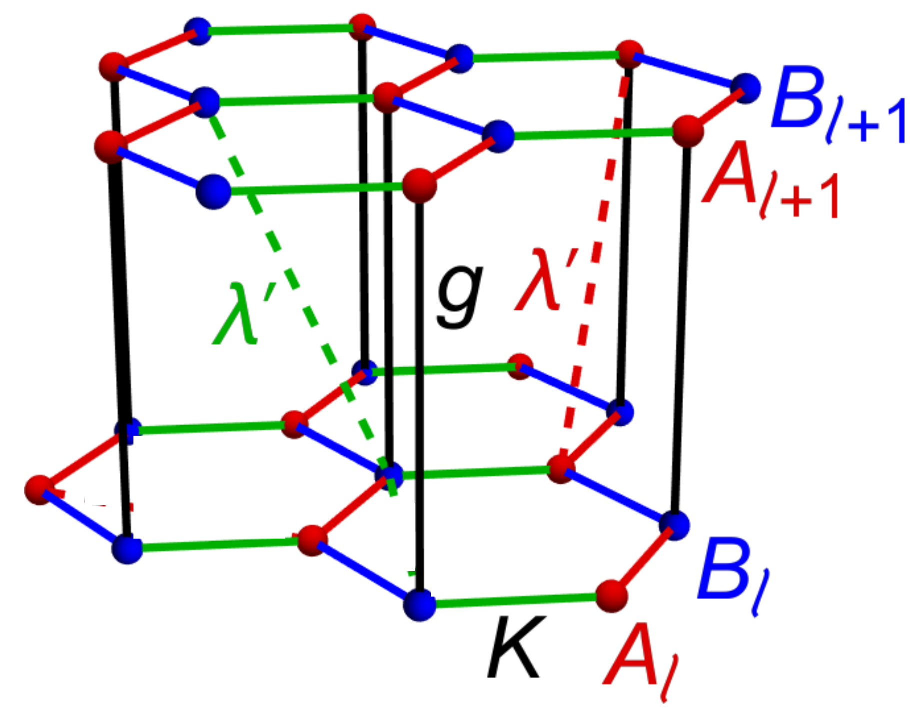
$$H = H_K + H_g \qquad N = 4$$

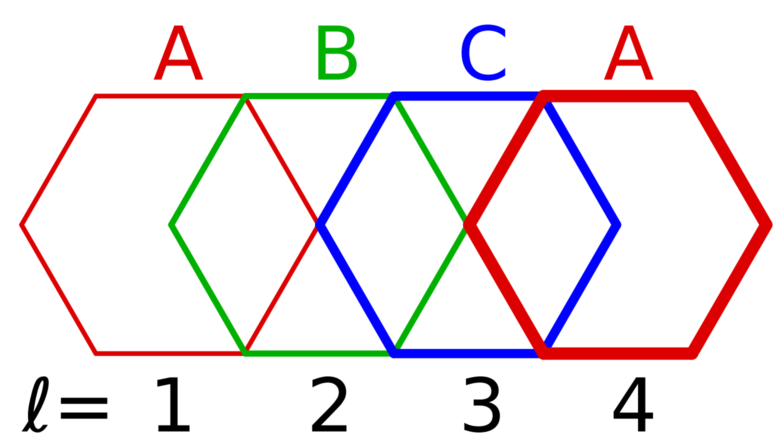
$$H_K = K \sum_{\ell=1}^{N} \sum_{\mu=x,y,z} \sum_{\langle i,j\rangle \in \mu} \sigma^{\mu}_{\ell,i} \sigma^{\mu}_{\ell,j}$$ Kitaev

$$H_g = g \sum_{\ell=1}^{N-1} \sum_{\langle i,j \rangle}^{\mathrm{A}\bar{\mathrm{B}}} \vec{\sigma}_{\ell+1,i} \cdot \vec{\sigma}_{\ell,j}$$ NN interlayer Heisenberg

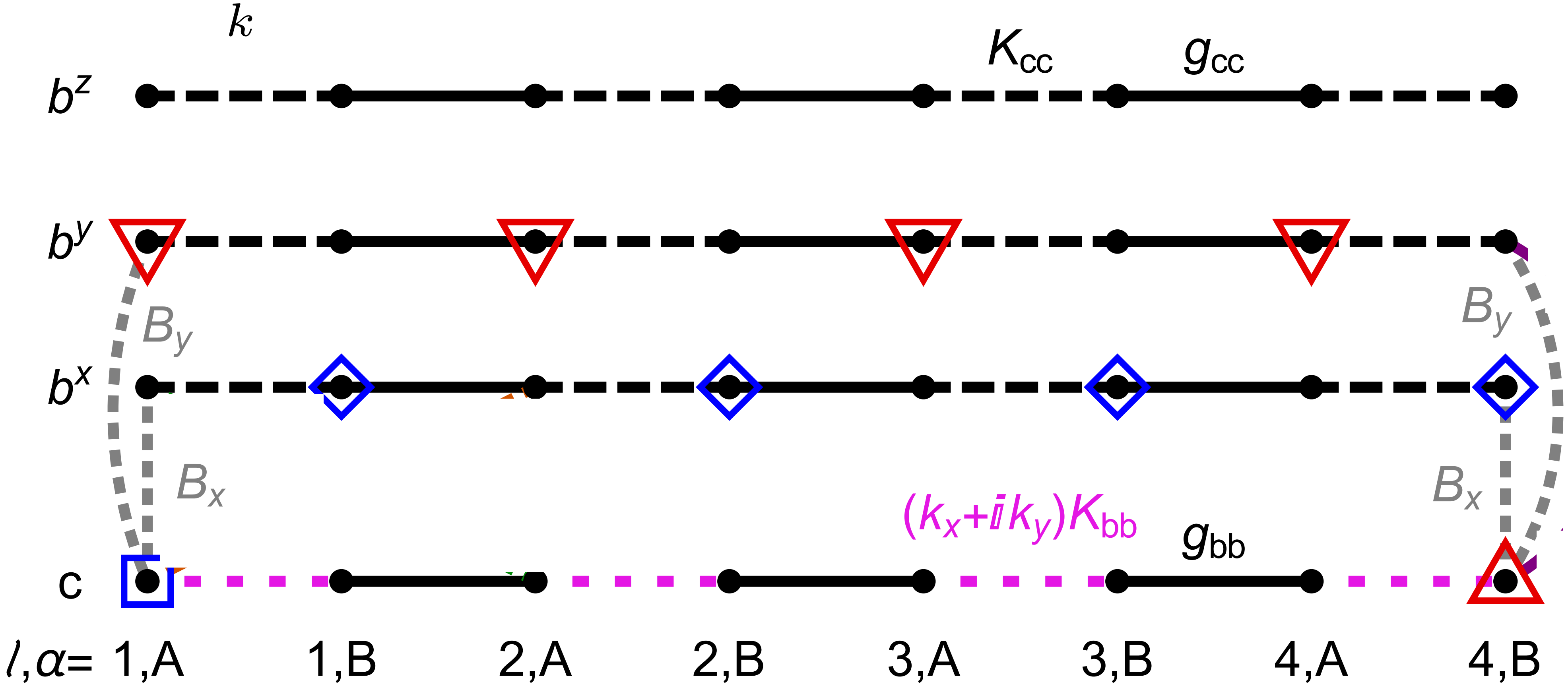
$$H_B = -\sum_{\ell,i,\mu} B_\mu \sigma^{\mu}_{\ell,i}$$ Zeeman

ABCA stacking





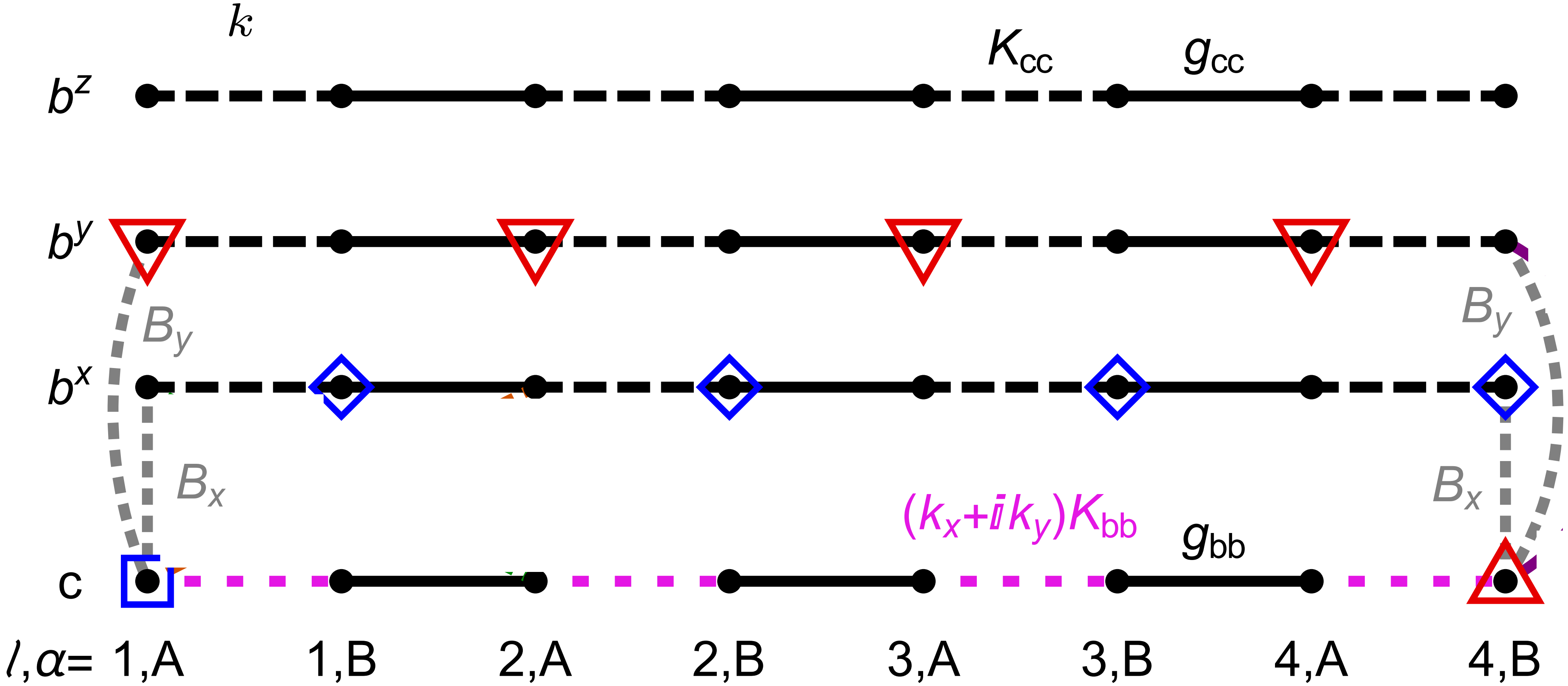
$$H^{\mathrm{MF}} = \sum_k H_k^{\mathrm{MF}} \qquad S_i^\alpha = \frac{1}{2} i b_i^\alpha c_i \qquad \{b_i^x, b_i^y, b_i^z, c\}$$



$$K_{\mathrm{bb}} \equiv K\langle \mathrm{i}\, b_{\ell i}^\mu b_{\ell j}^\mu \rangle \qquad g_{cc} = g\langle \mathrm{i}\ c_{\ell+1,i} c_{\ell j}\rangle$$

$$K_{\mathrm{cc}} \equiv K\langle \mathrm{i}\, c_{\ell i} c_{\ell j} \rangle \qquad g_{bb} = g\langle \mathrm{i}\ b_{\ell+1,i}^\mu b_{\ell j}^\mu\rangle$$

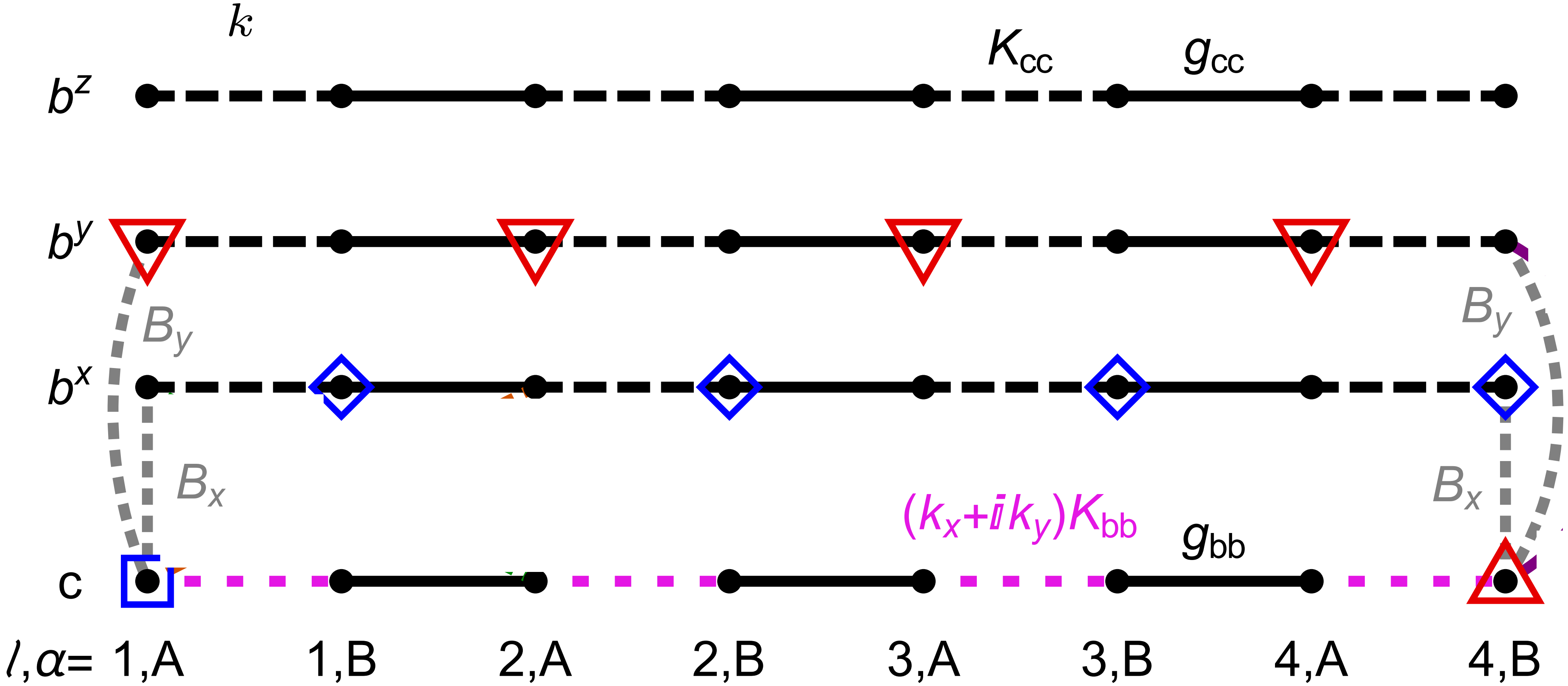
$$H^{\mathrm{MF}} = \sum_k H_k^{\mathrm{MF}} \qquad S_i^\alpha = \frac{1}{2} i b_i^\alpha c_i \qquad \{b_i^x, b_i^y, b_i^z, c\}$$



Boundary modes coupled via $(k_x + ik_y)K_{bb}$

$$E \propto |k|^4$$

$$H^{\mathrm{MF}} = \sum_k H_k^{\mathrm{MF}} \qquad S_i^\alpha = \frac{1}{2} i b_i^\alpha c_i \qquad \{b_i^x, b_i^y, b_i^z, c\}$$



Boundary modes coupled via $(k_x + ik_y)K_{bb}$

$$E \propto |k|^4$$

$$k_0^4 \propto B^2$$

$$k_0 \propto B^{1/2} \qquad v \propto B^{3/2} \qquad D(E) \propto \frac{E}{B^3}$$

wrong scaling !

Theoretical Model

$$H = H_K + H_g + H_{\lambda'} \qquad N = 4$$

$$H_K = K \sum_{\ell=1}^{N} \sum_{\mu=x,y,z} \sum_{\langle i,j \rangle \in \mu} \sigma^{\mu}_{\ell,i} \sigma^{\mu}_{\ell,j}$$ Kitaev

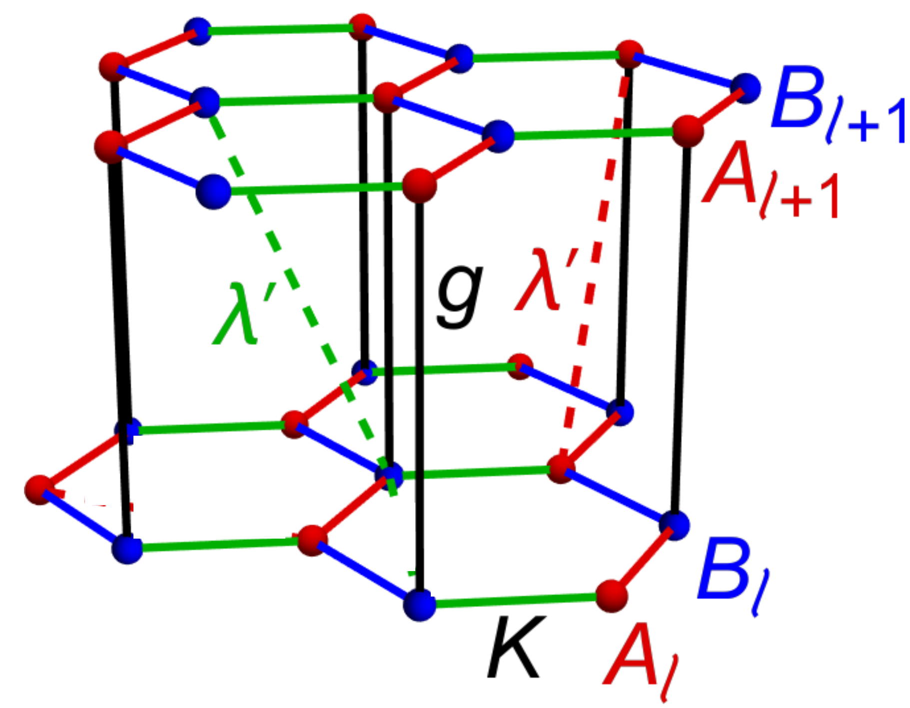
$$H_g = g \sum_{\ell=1}^{N-1} \sum_{\langle i,j \rangle}^{\mathrm{A\bar{B}}} \vec{\sigma}_{\ell+1,i} \cdot \vec{\sigma}_{\ell,j}$$ NN interlayer Heisenberg

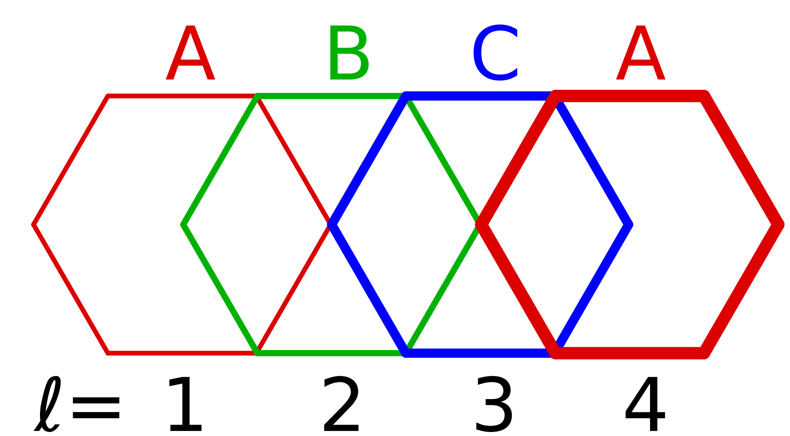
$$H_{\lambda'} = \lambda' \sum_{\ell=1,N-1} \left(\sum_{\langle\langle i,j \rangle\rangle}^{\mathrm{A\bar{A}}_x} \sigma^{x}_{\ell+1,i} \sigma^{x}_{\ell,j} + \sum_{\langle\langle i,j \rangle\rangle}^{\mathrm{B\bar{B}}_y} \sigma^{y}_{\ell+1,i} \sigma^{y}_{\ell,j} \right)$$

NNN interlayer bond-dependent Ising

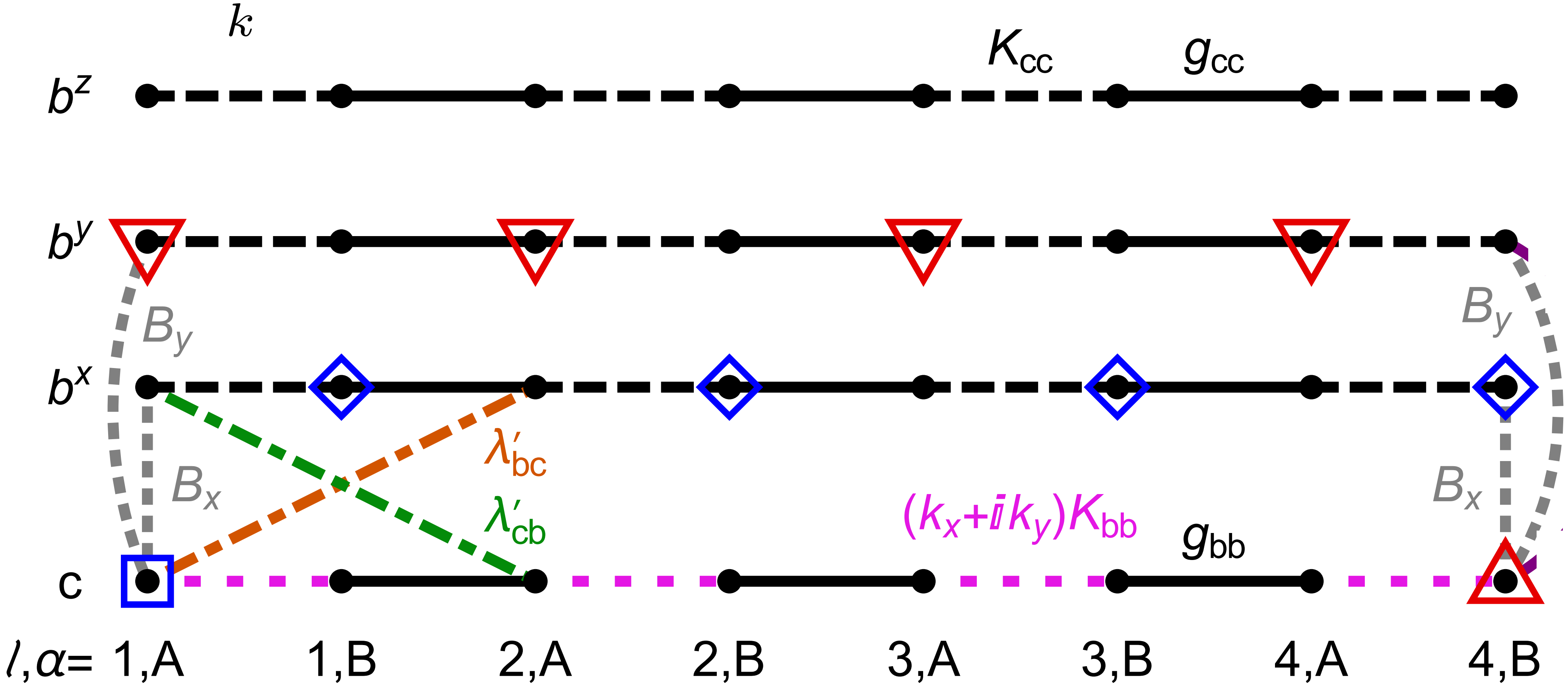
$$H_B = -\sum_{\ell,i,\mu} B_{\mu} \sigma^{\mu}_{\ell,i}$$ Zeeman

ABCA stacking





$$H^{\mathrm{MF}} = \sum_k H_k^{\mathrm{MF}} \qquad S_i^\alpha = \frac{1}{2} i b_i^\alpha c_i \qquad \{b_i^x, b_i^y, b_i^z, c\}$$



Boundary modes coupled via $(k_x + ik_y)K_{bb}$

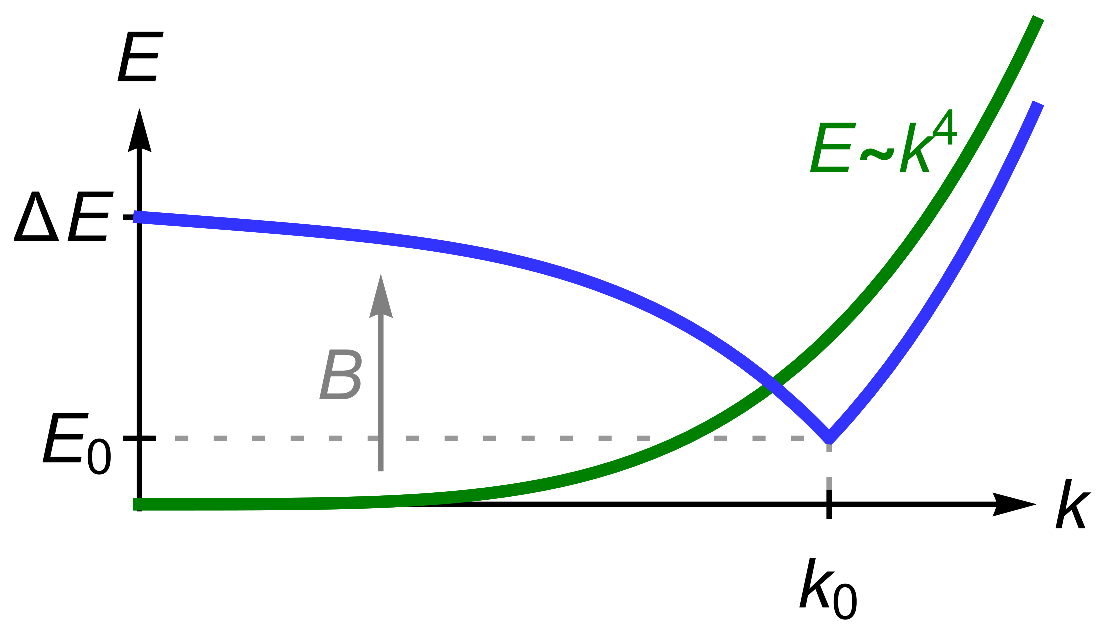
$$E \propto |k|^4$$

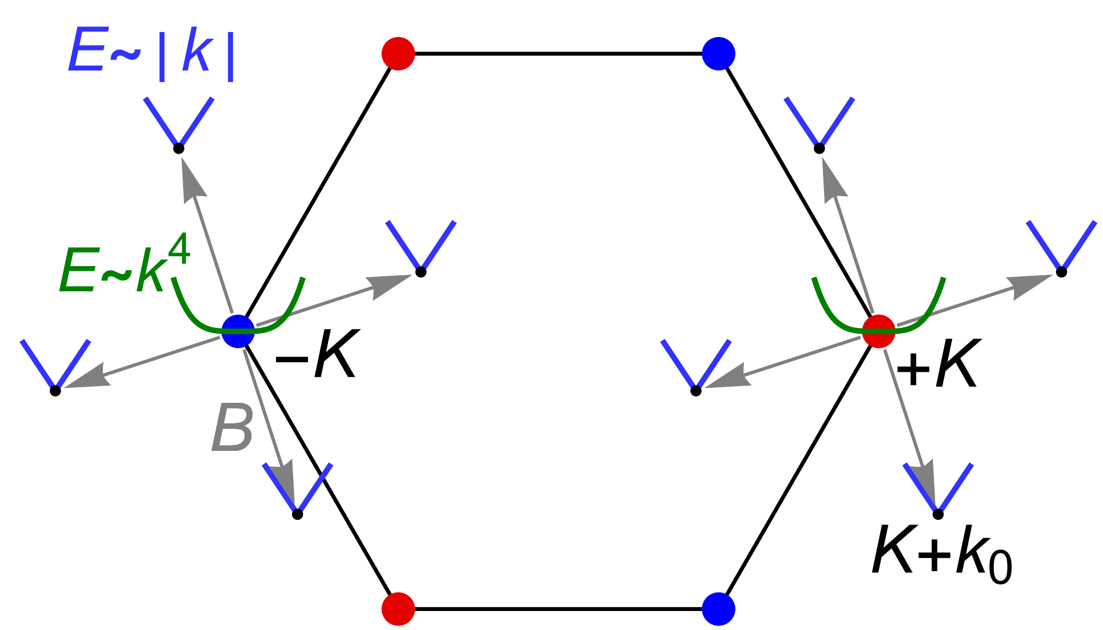
$$k_0^4 \propto B$$

$$k_0 \propto B^{1/4} \qquad v \propto B^{3/4} \qquad D(E) \propto \frac{E}{B^{3/2}}$$

In reality, there is an excitation gap due to

$$H' \propto B^3 \sum_{ijk} S_i^\alpha S_j^\beta S_k^\gamma \qquad \text{Kitaev}$$





Gap may not be seen for small magnetic fields

Almost linear dispersion

split into 8 Majorana cones

$$k_0 \propto B^{1/4} \qquad v \propto B^{3/4}$$

$$B \neq 0$$

ABCA would be a small fraction of possible stacking patterns

This spin liquid state would make up a small fraction of the total magnetic entropy

Why four layers ?   Other choices are possible

ABCAC $E \sim k^4$ $E \sim k$

ABCACB $E \sim k^4$ $E \sim k^2$

But the coherence should be maintained at least for four layers

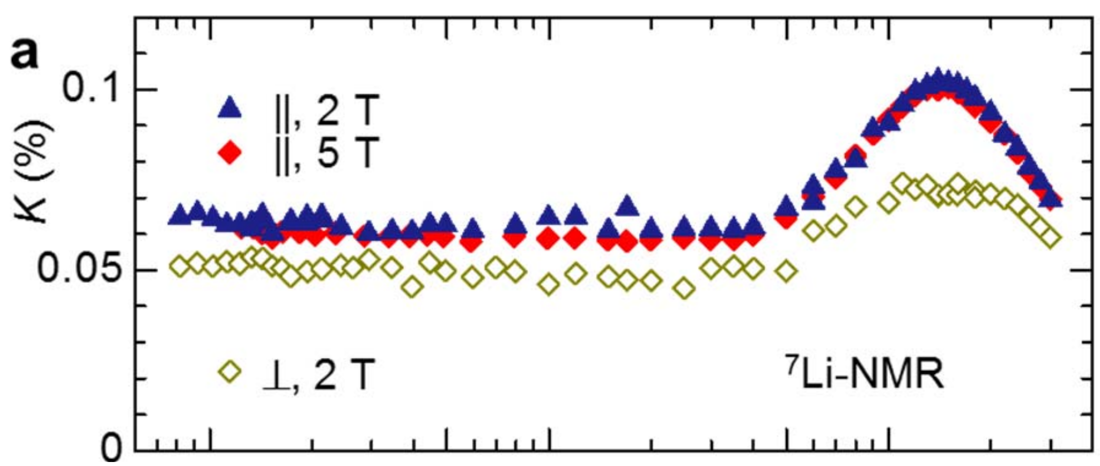
This is consistent with

1) The singular entropy is only about 5% percent of the total magnetic entropy

2) The singular part of the magnetic entropy is related to the bulk susceptibility via

$$(\partial S/\partial B)_T = (\partial M/\partial T)_B$$

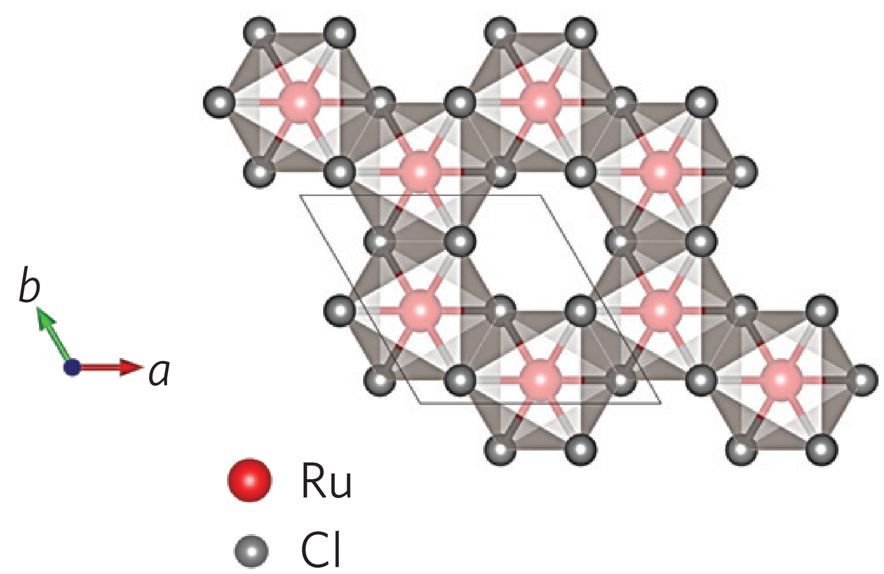
3) The Knight shift is not dominated by this "spin" contribution (spin-orbit) [Knight shift insensitive to the "impurity" contribution]

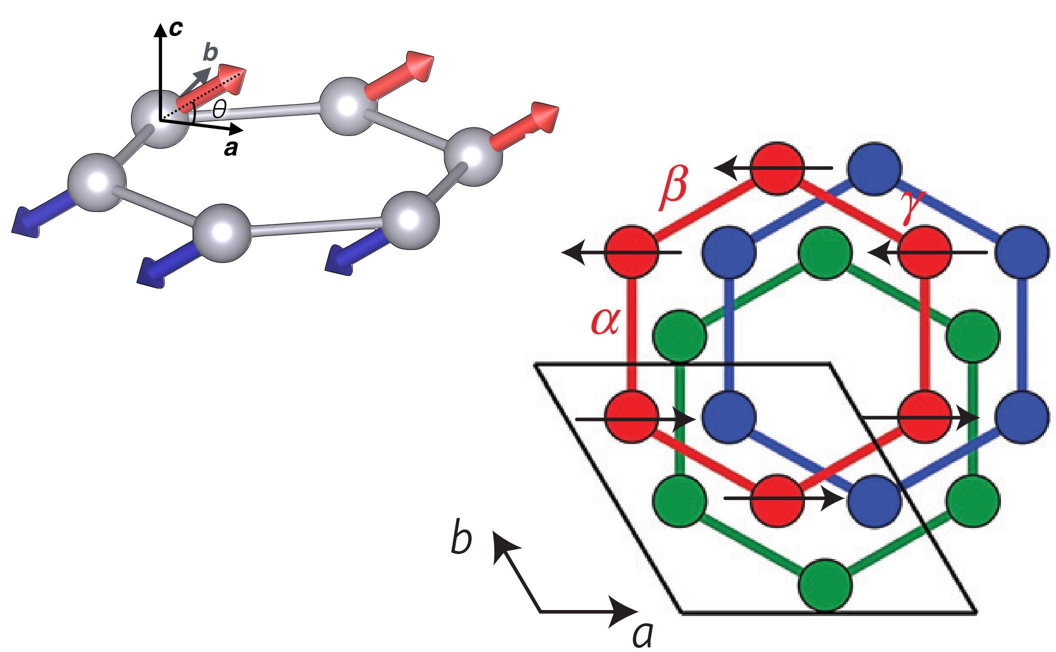


α-$RuCl_3$
Two-dimensional
Honeycomb lattice

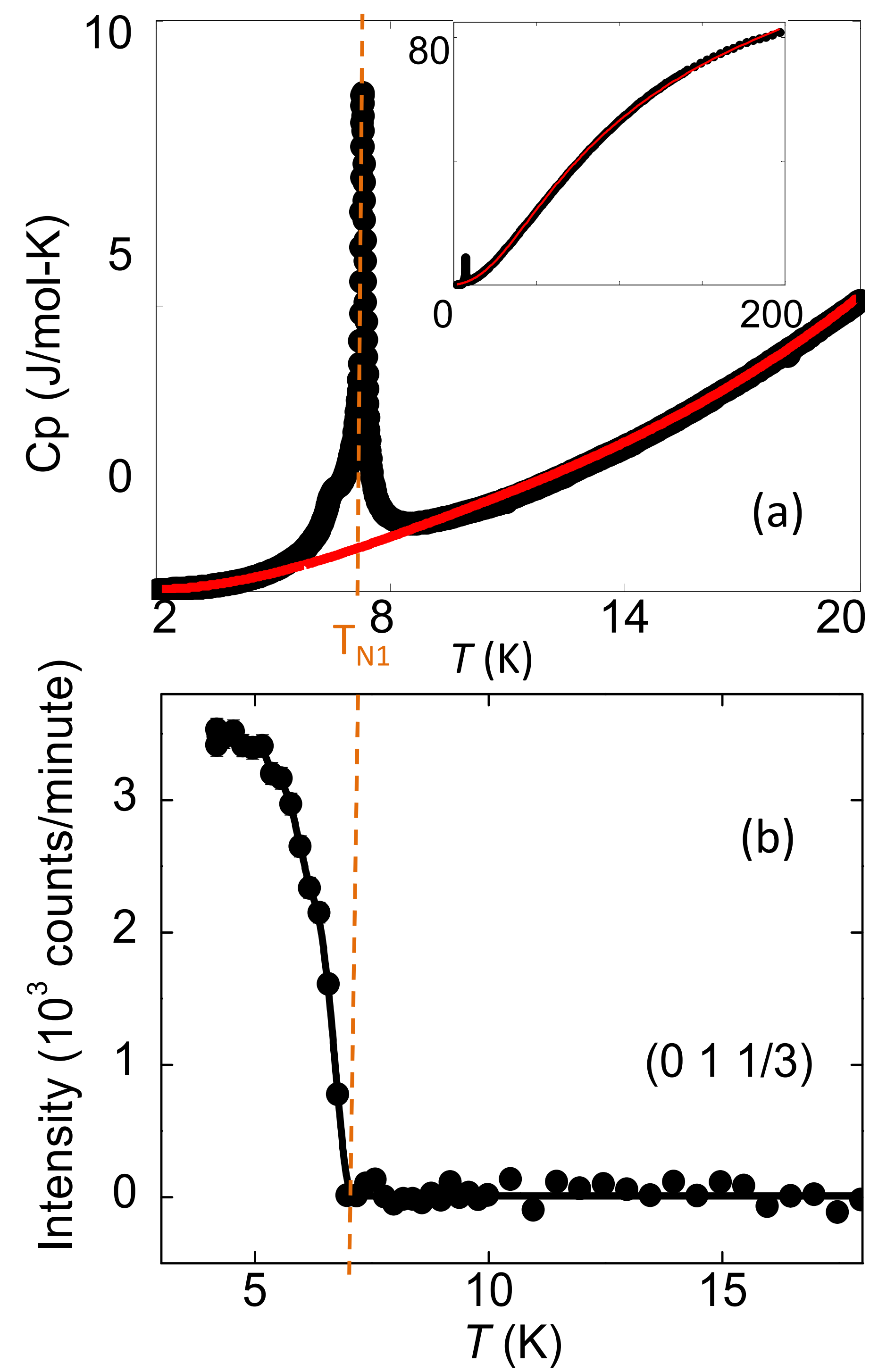
Matthias Gohlke, Gideon Wachtel, Youhei Yamaji,
Frank Pollmann, YBK, arXiv:1706.09908

α- $RuCl_3$ (S. Nagler, Y. J. Kim, R. Coldea)





Zig-Zag Order



nature materials

ARTICLES

PUBLISHED ONLINE: 4 APRIL 2016 | DOI: 10.1038/NMAT4604

Proximate Kitaev quantum spin liquid behaviour in a honeycomb magnet

A. Banerjee[1*], C. A. Bridges[2], J.-Q. Yan[3,4], A. A. Aczel[1], L. Li[5], M. B. Stone[1], G. E. Granroth[1,6], M. D. Lumsden[1], Y. Yiu[5], J. Knolle[7], S. Bhattacharjee[8,9], D. L. Kovrizhin[7], R. Moessner[8], D. A. Tennant[10], D. G. Mandrus[3,4] and S. E. Nagler[1,11*]

PRL **114,** 147201 (2015) PHYSICAL REVIEW LETTERS week ending 10 APRIL 2015

Scattering Continuum and Possible Fractionalized Excitations in α-$RuCl_3$

Luke J. Sandilands, Yao Tian, Kemp W. Plumb, and Young-June Kim
Department of Physics, University of Toronto, 60 St. George St., Toronto, Ontario M5S 1A7, Canada

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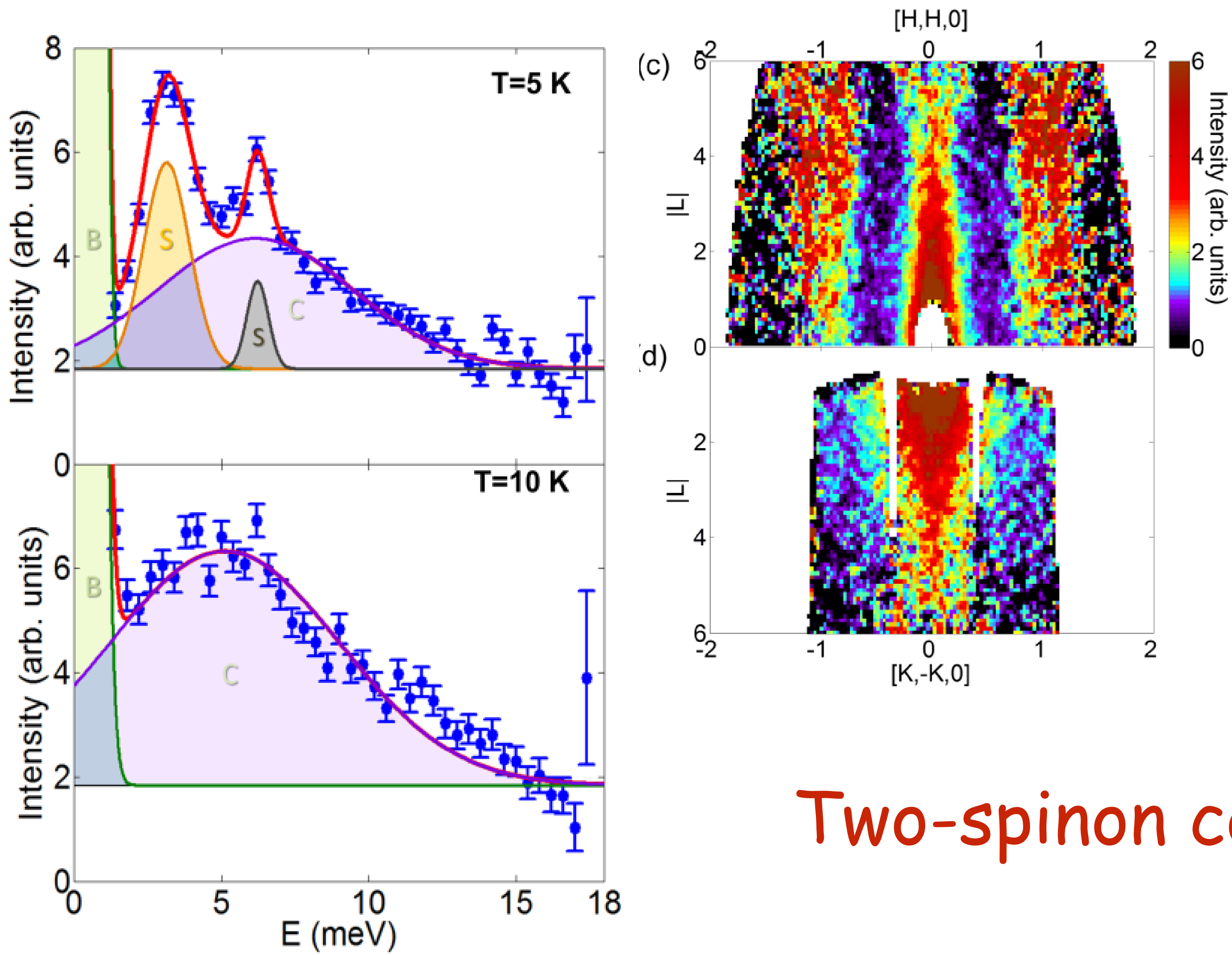
Department of Physics, Boston College, 140 Commonwealth Avenue, Chestnut Hill, Massachusetts 02467, USA

(Received 12 October 2014; published 6 April 2015)

arXiv:1609.00103

Neutron tomography of magnetic Majorana fermions in a proximate quantum spin liquid

Authors: Arnab Banerjee[1]*, Jiaqiang Yan[2], Johannes Knolle[3], Craig A. Bridges[4], Matthew B. Stone[1], Mark D. Lumsden[1], David G. Mandrus[2], David A. Tennant[5,6], Roderich Moessner[7], Stephen E. Nagler[1]*.



Continuum of excitations seen below and above the ordering temperature

Two-spinon continuum ?

Two-particle continuum in Quantum Spin Liquid

Neutron Scattering -- Spin-1 excitations

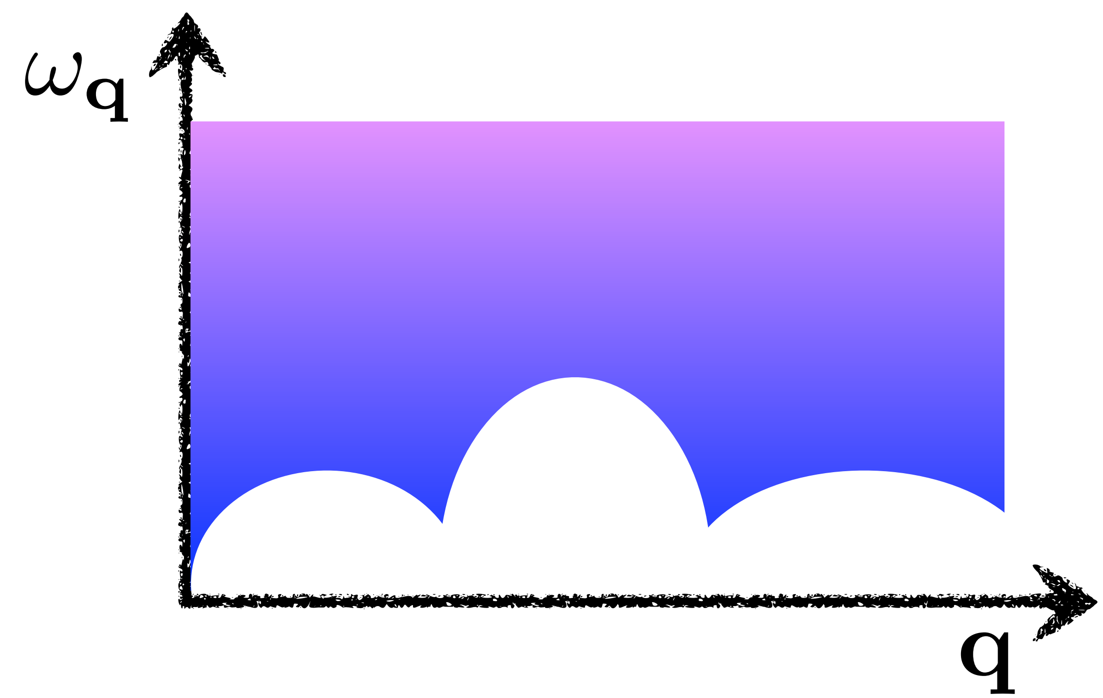
Spinon-Antispinon pair excitations

Well-defined dispersion -->

Threshold energy for pair excitations

$$\omega_{\mathbf{q}} \sim \min \left[\varepsilon_{\frac{\mathbf{q}}{2}+\frac{\mathbf{p}}{2}} + \varepsilon_{\frac{\mathbf{q}}{2}-\frac{\mathbf{p}}{2}} \right]$$

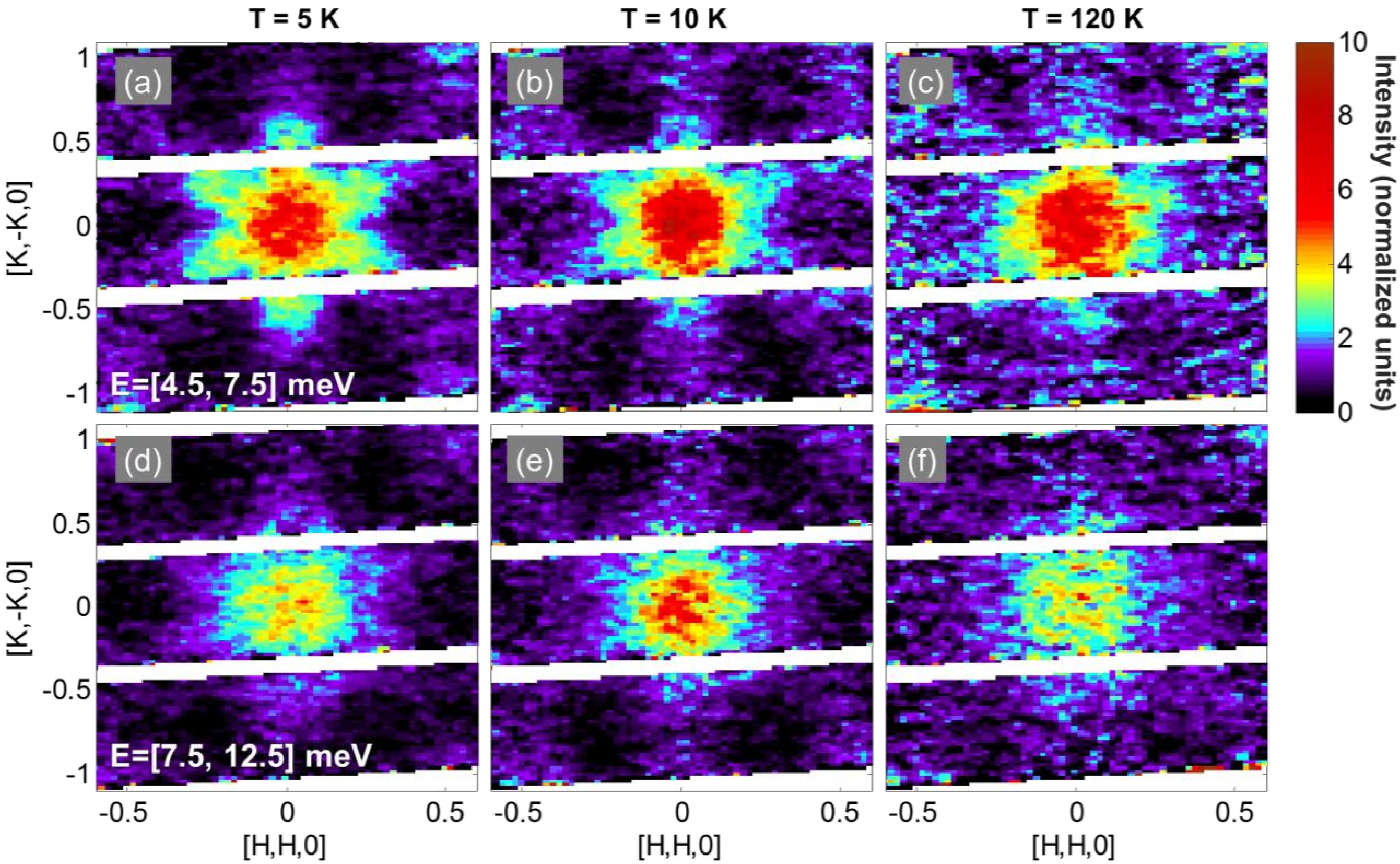
for all possible $\mathbf{p}$



c.f. Kitaev Model: Mind the flux gap ! (J. Knolle, R. Moessner)

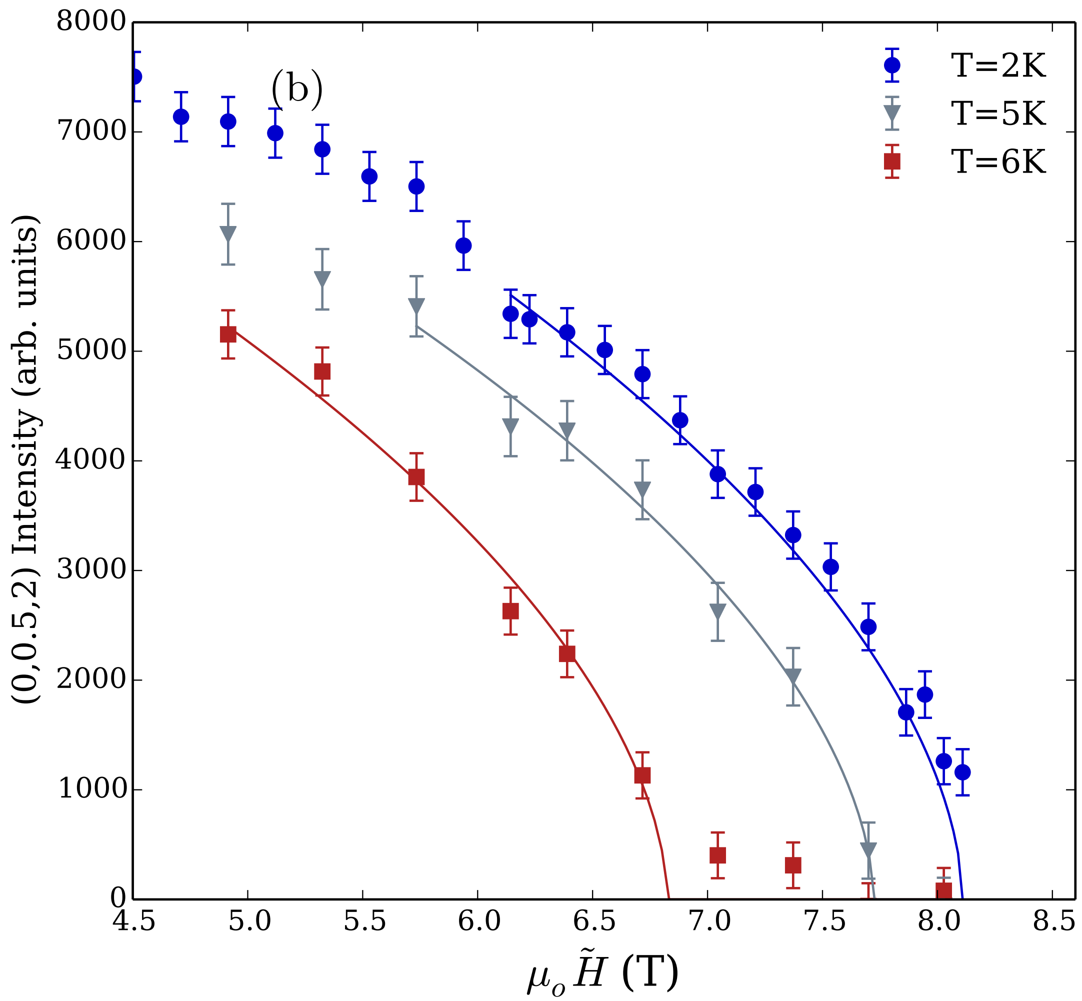
"Star-shape" intensity at low energy

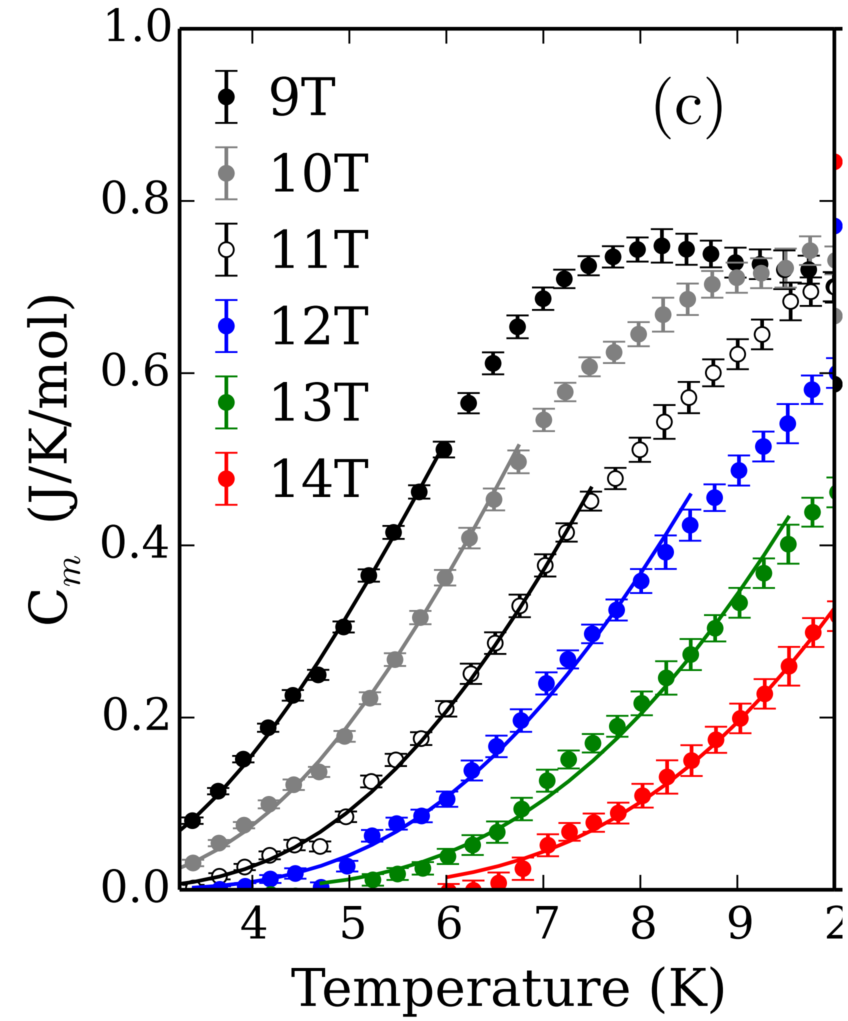
Pure Kitaev model does not have this feature



arXiv:1609.00103

Field-induced Paramagnet: Spin Liquid ?



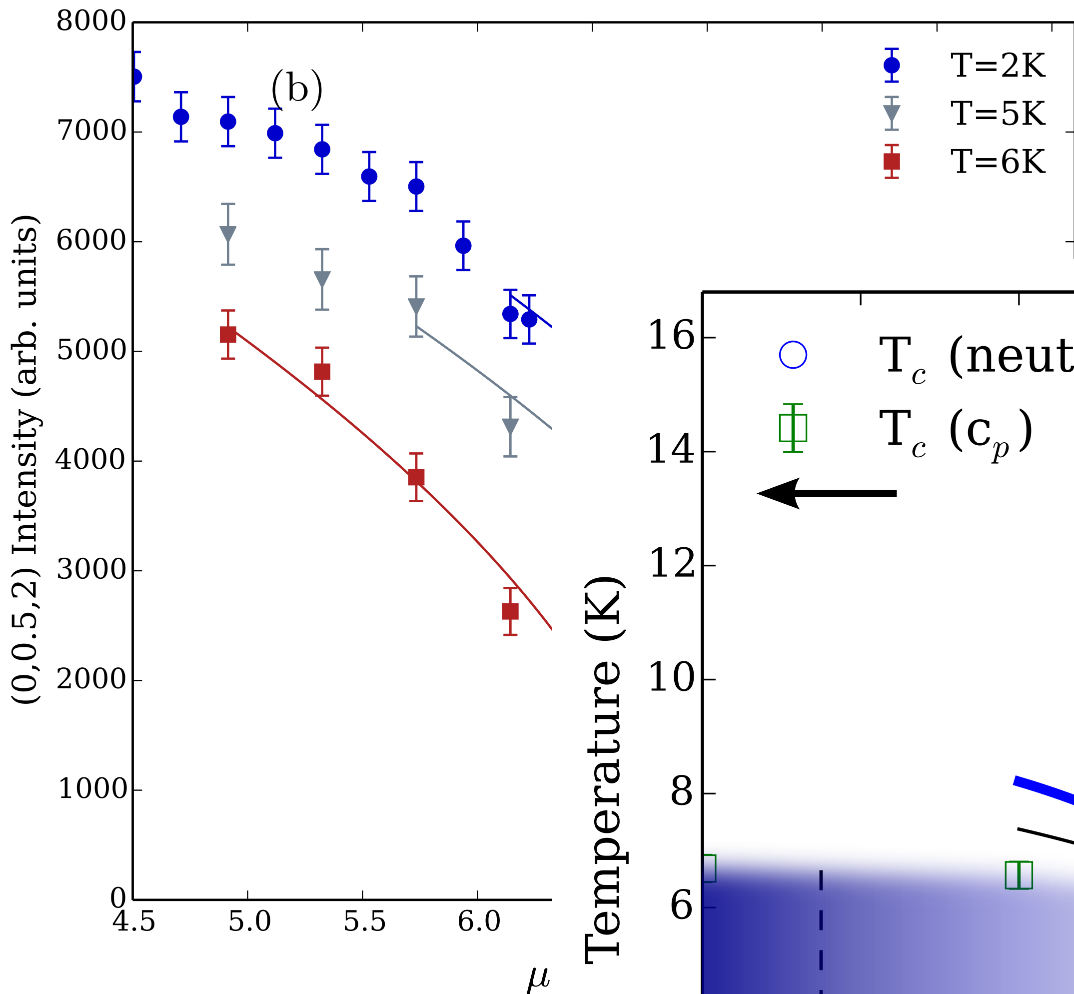


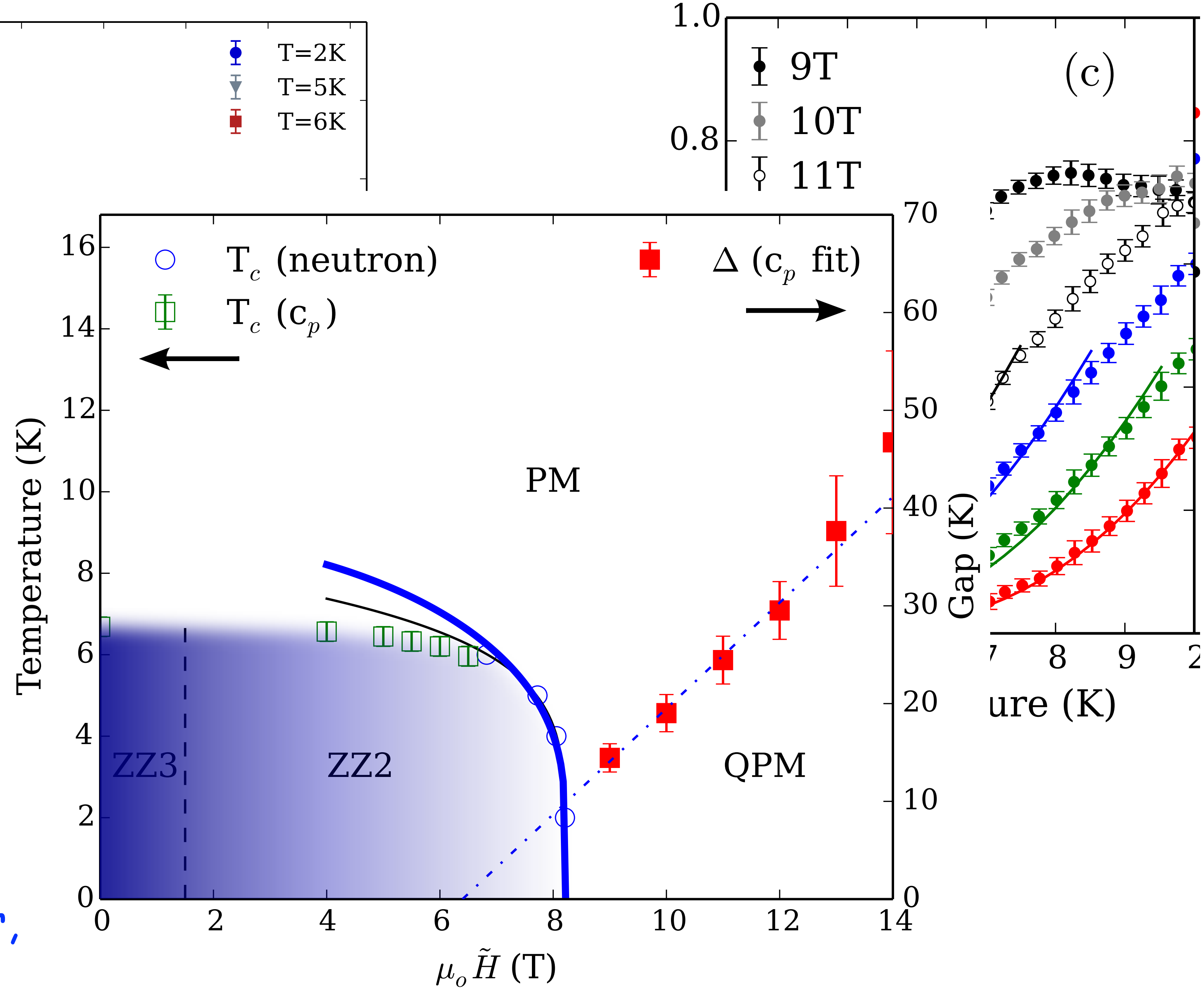
many related works

A.Banerjee, S. Nagler,
R.Coldea, Y.-J.Kim, …

Y.-J.Kim arXiv:1703.08431

Field-induced Paramagnet: Spin Liquid ?





many related works

A.Banerjee, S. Nagler, R.Coldea, Y.-J.Kim, ...

Y.-J.Kim arXiv:1703.08431

Dominant exchange interactions

$$H = \sum_{\langle\langle\langle ij \rangle\rangle\rangle} J_3^{ij} \vec{S}_i \cdot \vec{S}_j + \sum_{\langle ij \rangle,\gamma} K^\gamma S_i^\gamma S_j^\gamma + \sum_{\langle ij \rangle,\gamma} \sum_{\alpha,\beta\neq\gamma} \Gamma^\gamma [S_i^\alpha S_j^\beta + S_i^\beta S_j^\alpha]$$

TABLE IV. Complete magnetic interactions in meV for the $C2/m$ structure of α-$RuCl_3$ from Ref. 14 obtained by exact diagonalization on six-site bridge and hexagon clusters employing $U = 3.0$, $J_H = 0.6$, $\lambda = 0.15$ eV, and full crystal field terms Δ_n. The largest terms are bolded. Site labels for $\mathbf{D}_{ij}$ refer to Fig. 1(a).

Bond	J_n	K_n	ξ_n	Γ_n	Γ'_n	ζ_n
X_1, Y_1	-1.4	**-7.5**	+0.2	**+5.9**	-0.8	+0.2
Z_1	-2.2	**-5.0**	–	**+8.0**	-1.0	–
X_2, Y_2	-0.1	-0.6	+0.1	+0.6	+0.6	+0.1
Z_2	+0.1	-0.9	–	+0.6	+0.3	–
X_3,Y_3	**+3.0**	-0.1	0.0	-0.1	-0.1	-0.1
Z_3	**+2.4**	+0.3	–	-0.1	-0.1	–

Bond	Sites (i, j)	$\mathbf{D}_{ij}$
X_2	(1, 3) , (4, 6)	(-0.3, -0.5, -0.5)
Y_2	(5, 1) , (2, 4)	(-0.5, -0.3, -0.5)
Z_2	(6, 2) , (3, 5)	(-0.4, -0.4, -0.1)

Nearest-Neighbour K < 0

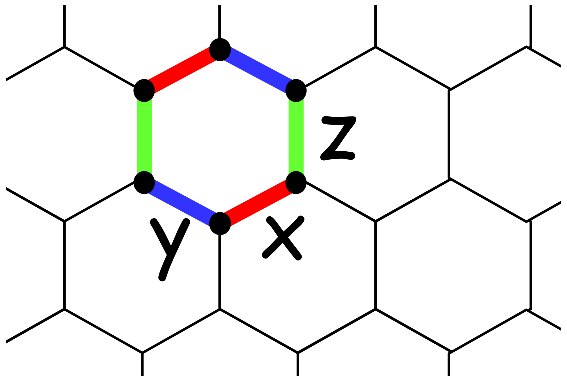
Nearest-Neighbour Γ > 0

|K| ~ |Γ|

Third-Neighbour J_3 > 0

Winter, Li, Jeschke, Valenti (2016)

Minimal Model



$$H_0 = \sum_{\gamma \in x,y,z} H^\gamma$$

K and Γ limits
highly frustrated

N. Perkins

$$H^z = \sum_{\langle ij \rangle \in z-bond} [K^z S_i^z S_j^z + \Gamma^z (S_i^x S_j^y + S_i^y S_j^x)]$$

etc.

$$\boxed{\begin{aligned} K^z &= -(1+2a)\cos\phi \\ K^x = K^y &= -(1-a)\cos\phi \end{aligned}}$$

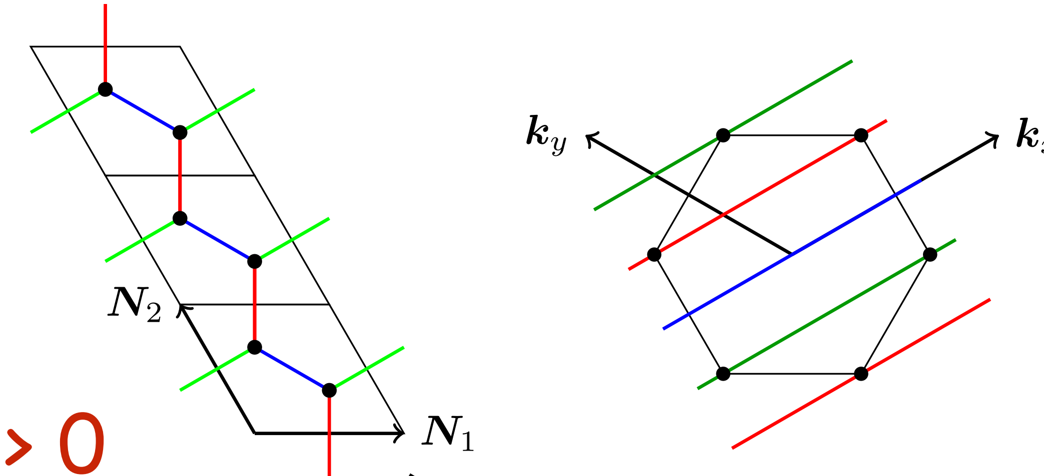
$$\boxed{\Gamma = \Gamma^x = \Gamma^y = \Gamma^z = \sin\phi}$$

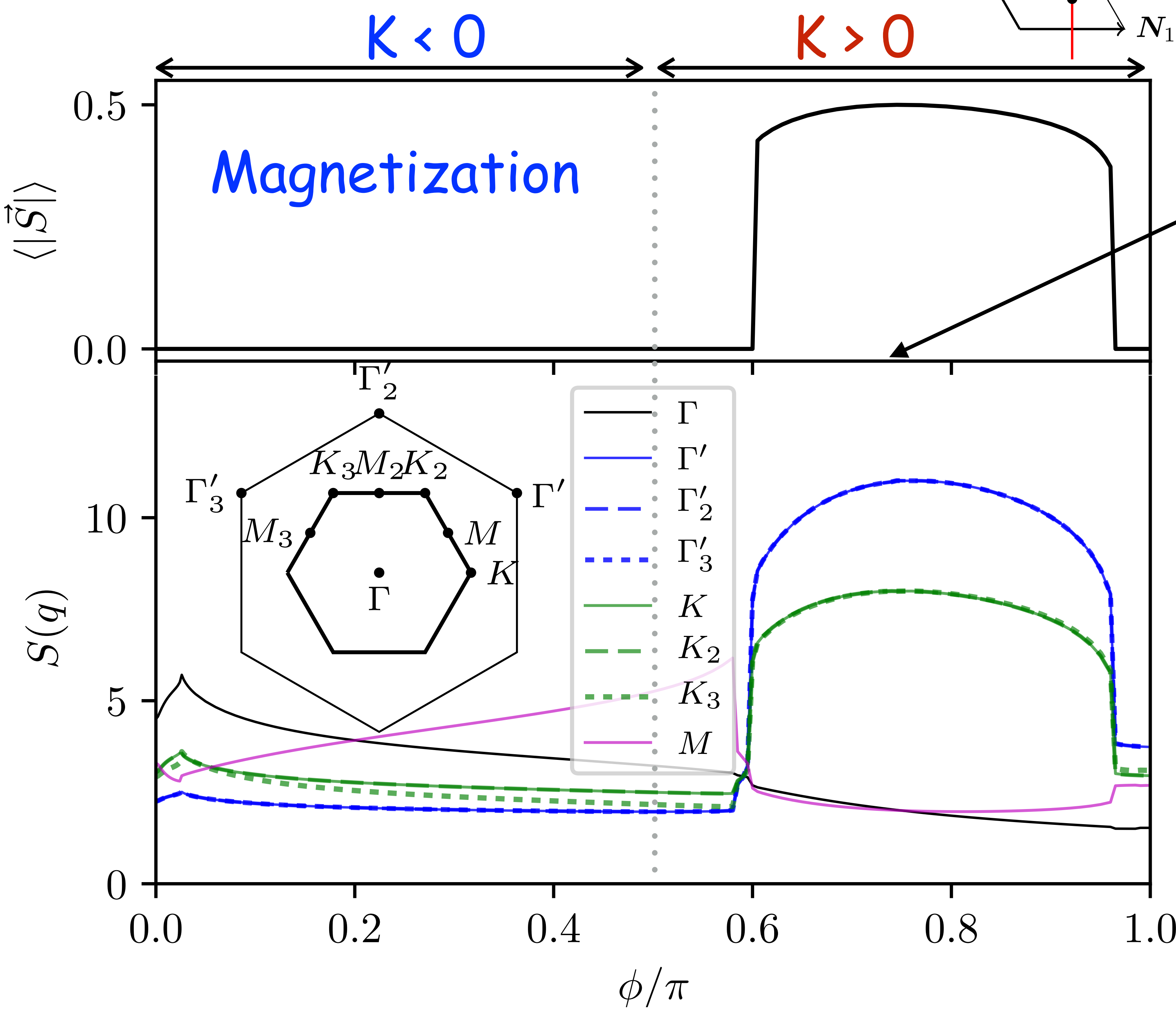
$$\phi = 0 \quad \xleftrightarrow[K<0]{} \quad \phi = \pi/2 \quad \xleftrightarrow[K>0]{} \quad \phi = \pi$$

Ferro-Kitaev   pure-Γ   AF-Kitaev

iDMRG (Matthias Golke)

a = 0





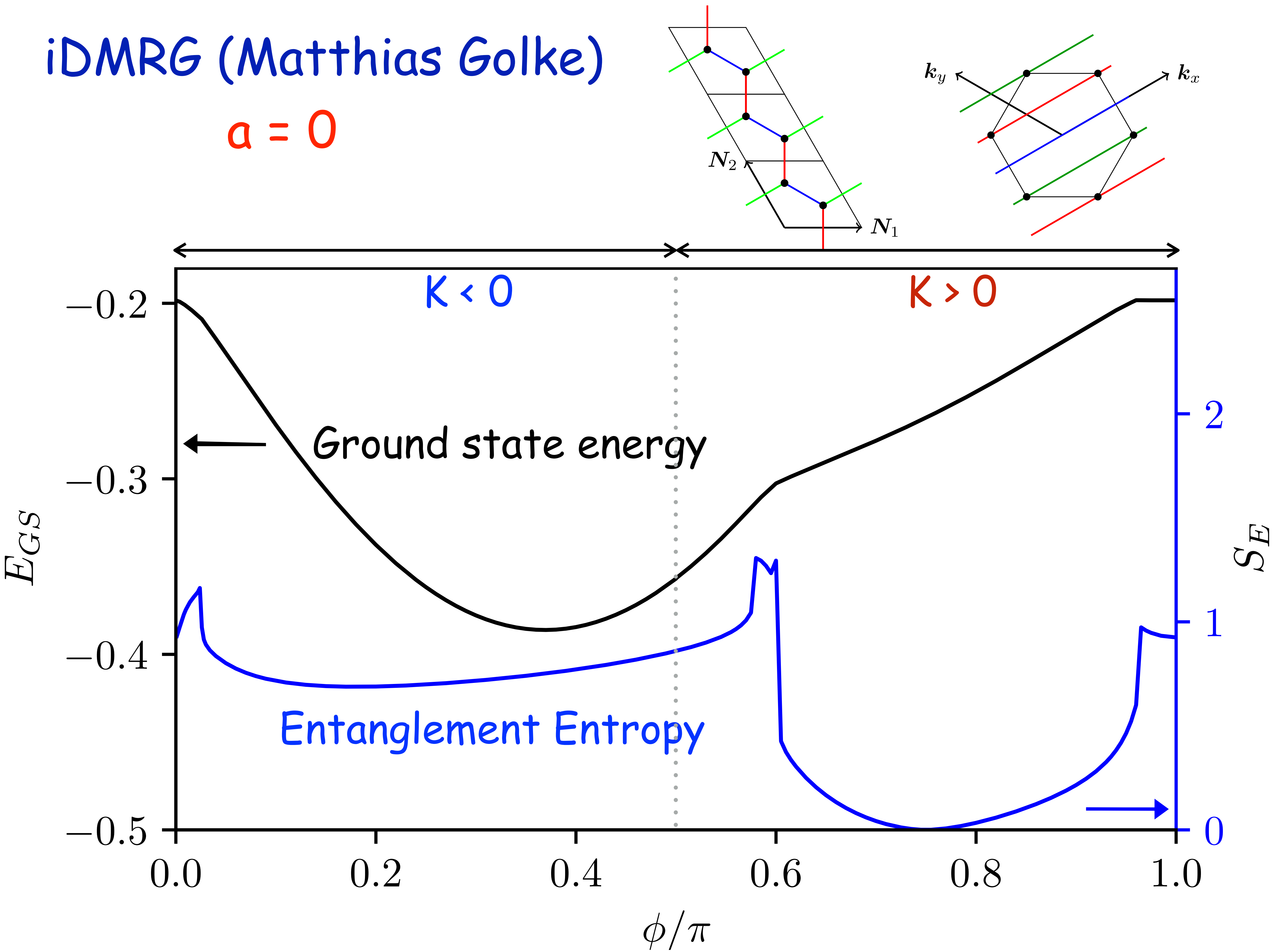
Hidden SU(2) product state "Vortex" order

$\phi = 0.75\pi$

Equal-time Spin Structure Factor

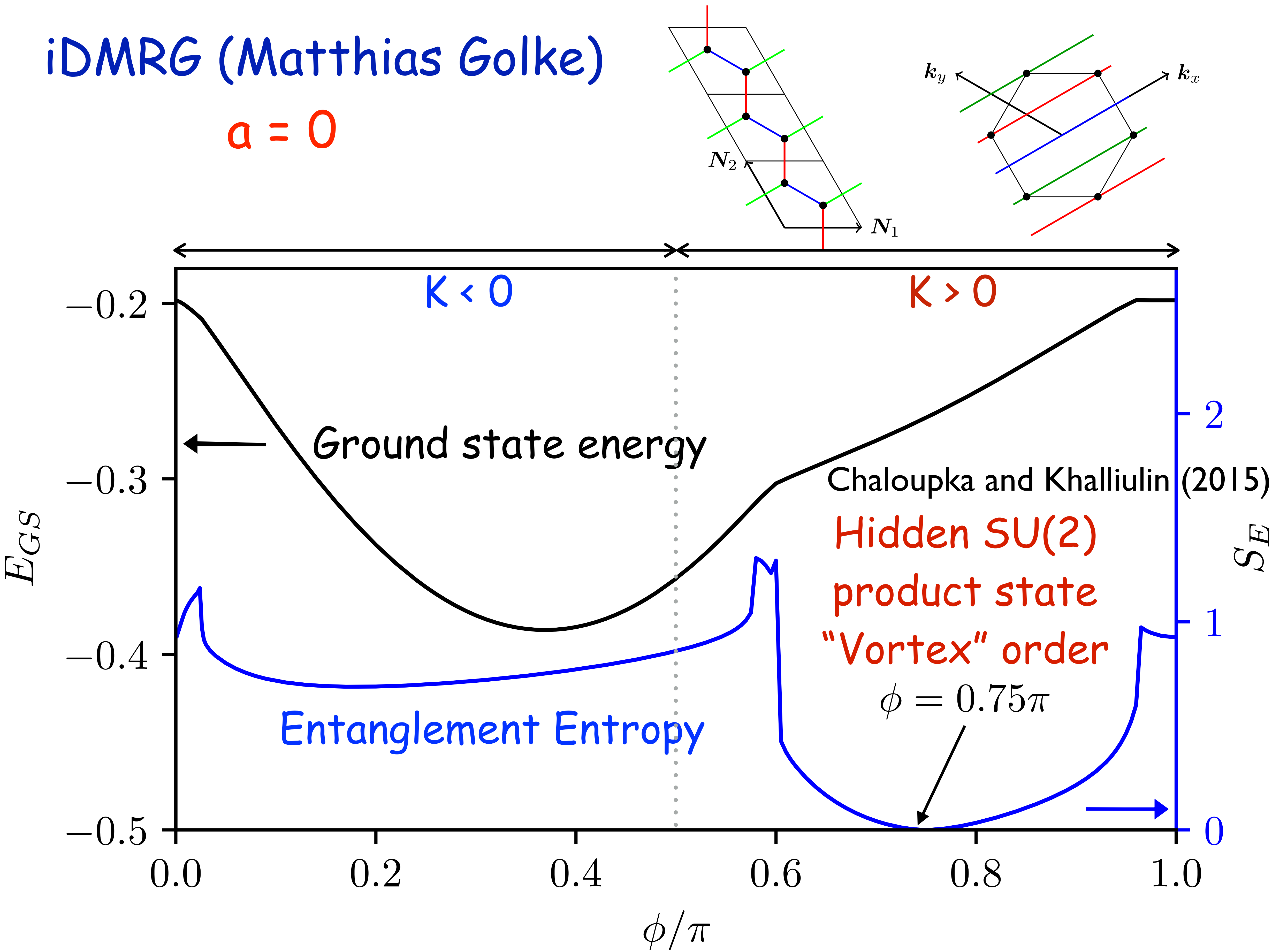
iDMRG (Matthias Golke)

a = 0



iDMRG (Matthias Golke)

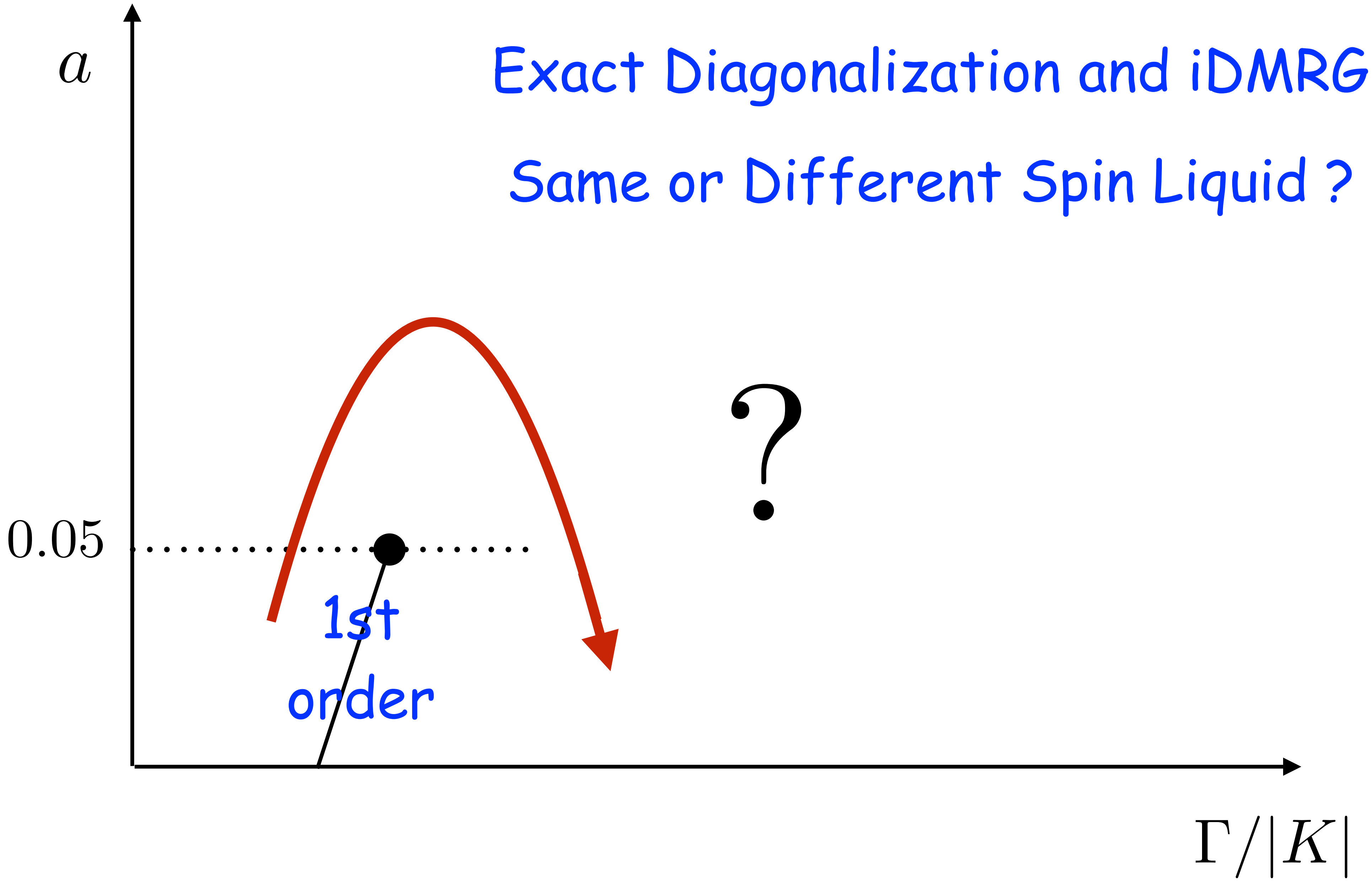
a = 0



Schematic Phase Diagram

Exact Diagonalization and iDMRG

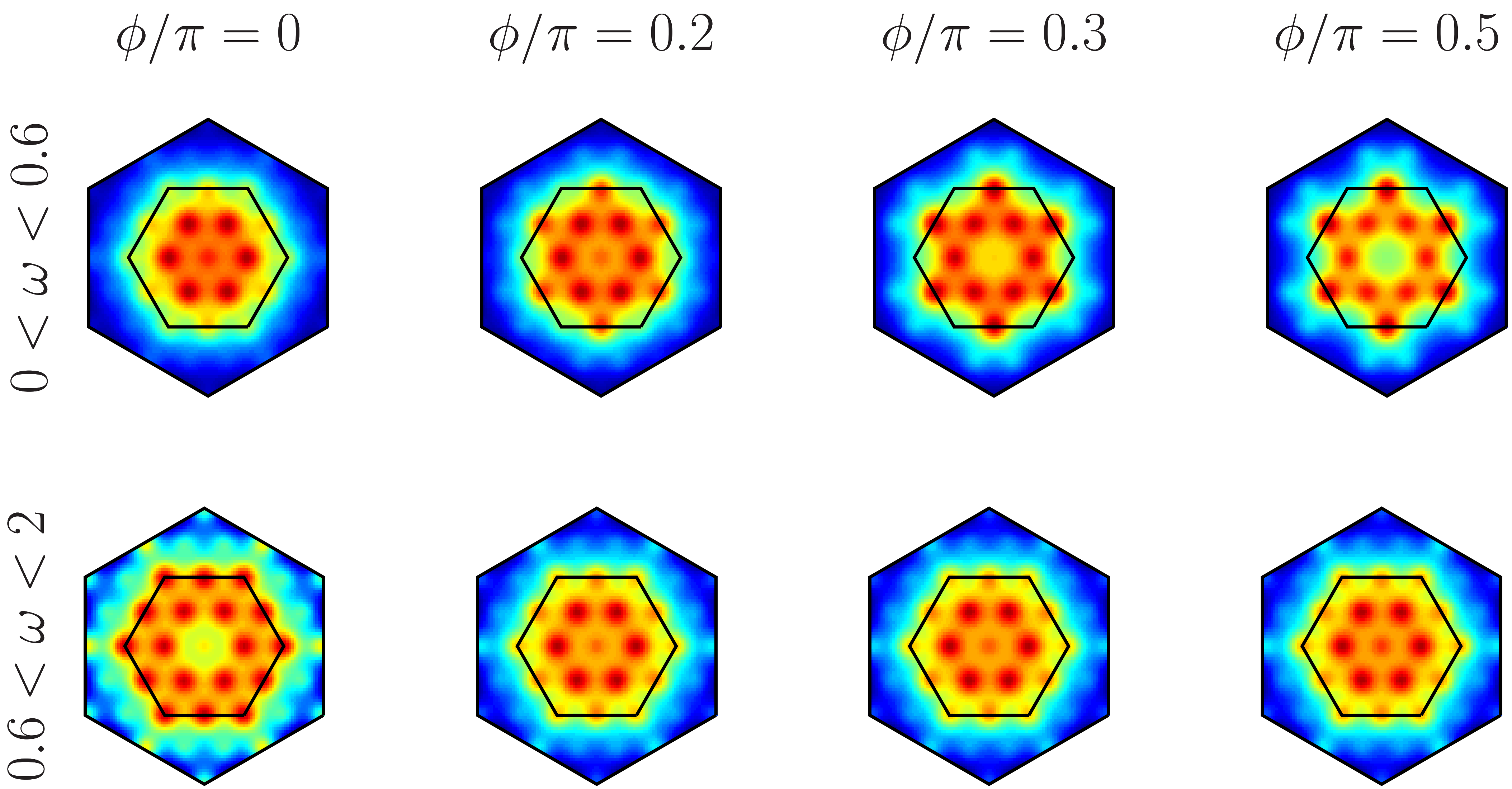
Same or Different Spin Liquid ?



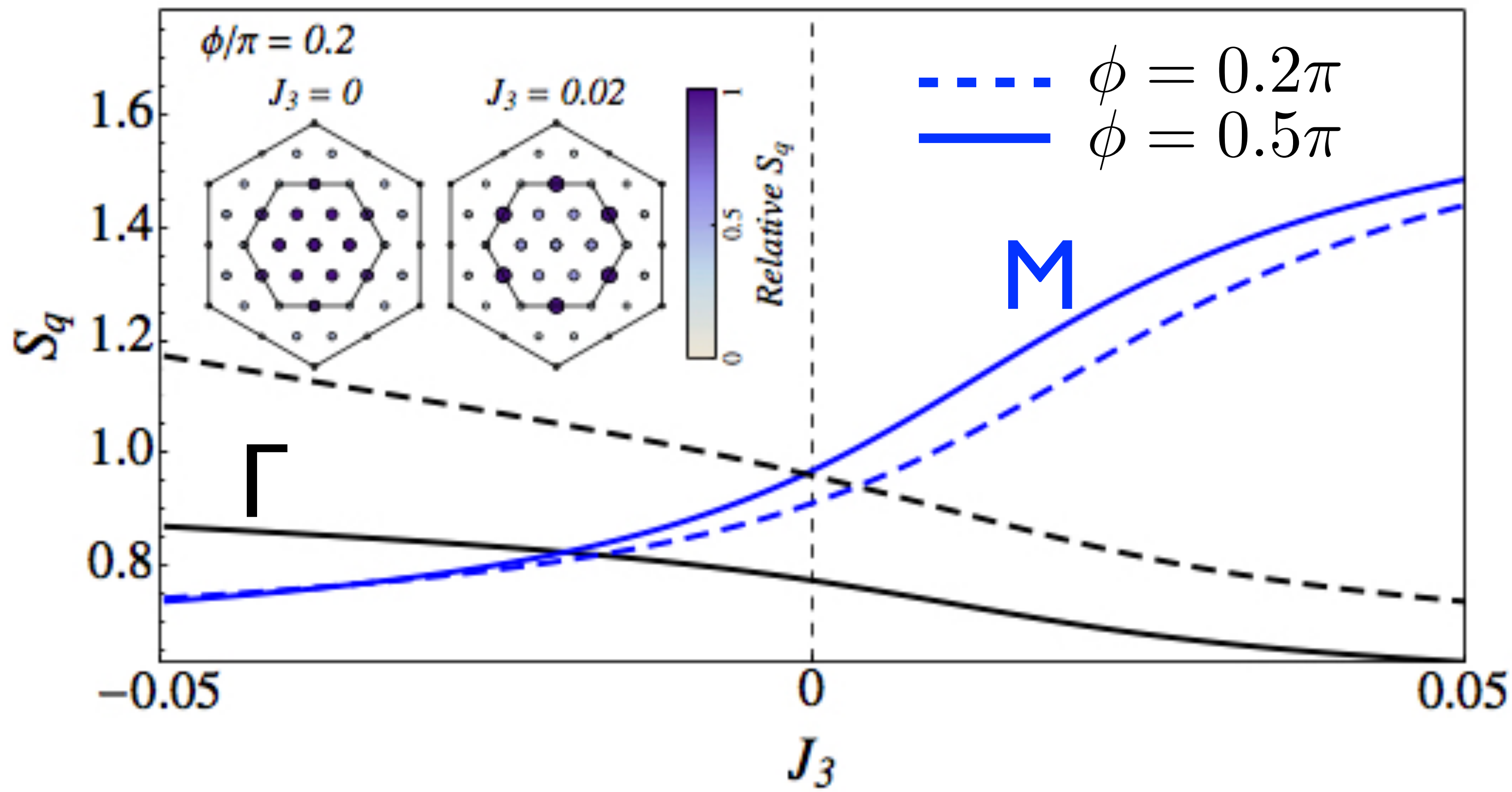
A. Catuneanu, Y. Yamaji, G. Wachtel, H.-Y. Kee, YBK, (2017)

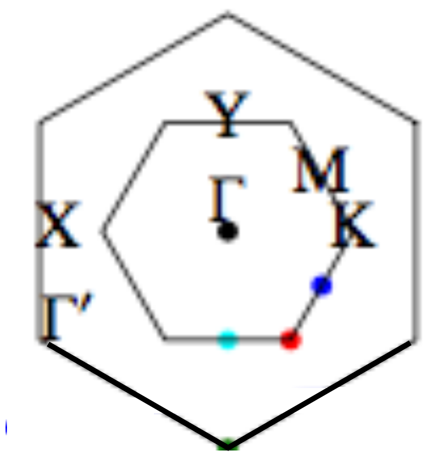
Dynamical Structure Factor (Yamaji, 24-site)

energy-integrated over two windows (just like the experiment)



Enhancement of the zig-zag order (M) upon addition of small J_3





Consistent with previous computations

Winter, Li, Jeschke, Valenti (2016)

Transfer Matrix Spectrum

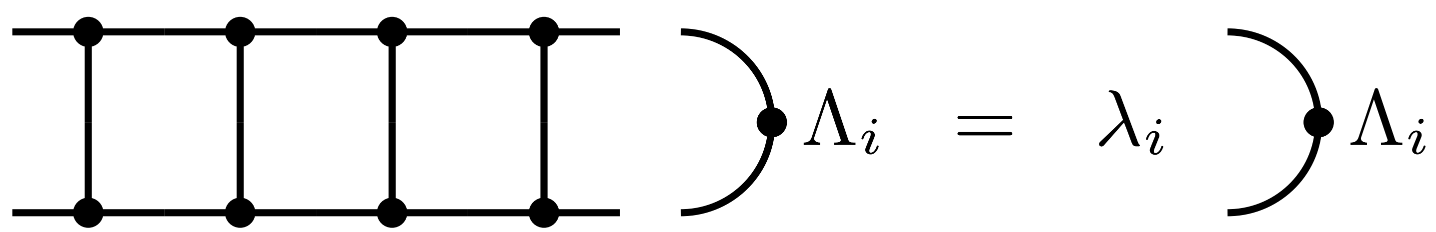
V. Zauner, F.Verstraete et. al (2014)

Correspondence between the complex eigenvalues and the lower boundaries of multi-particle excitation spectrum of the ground state

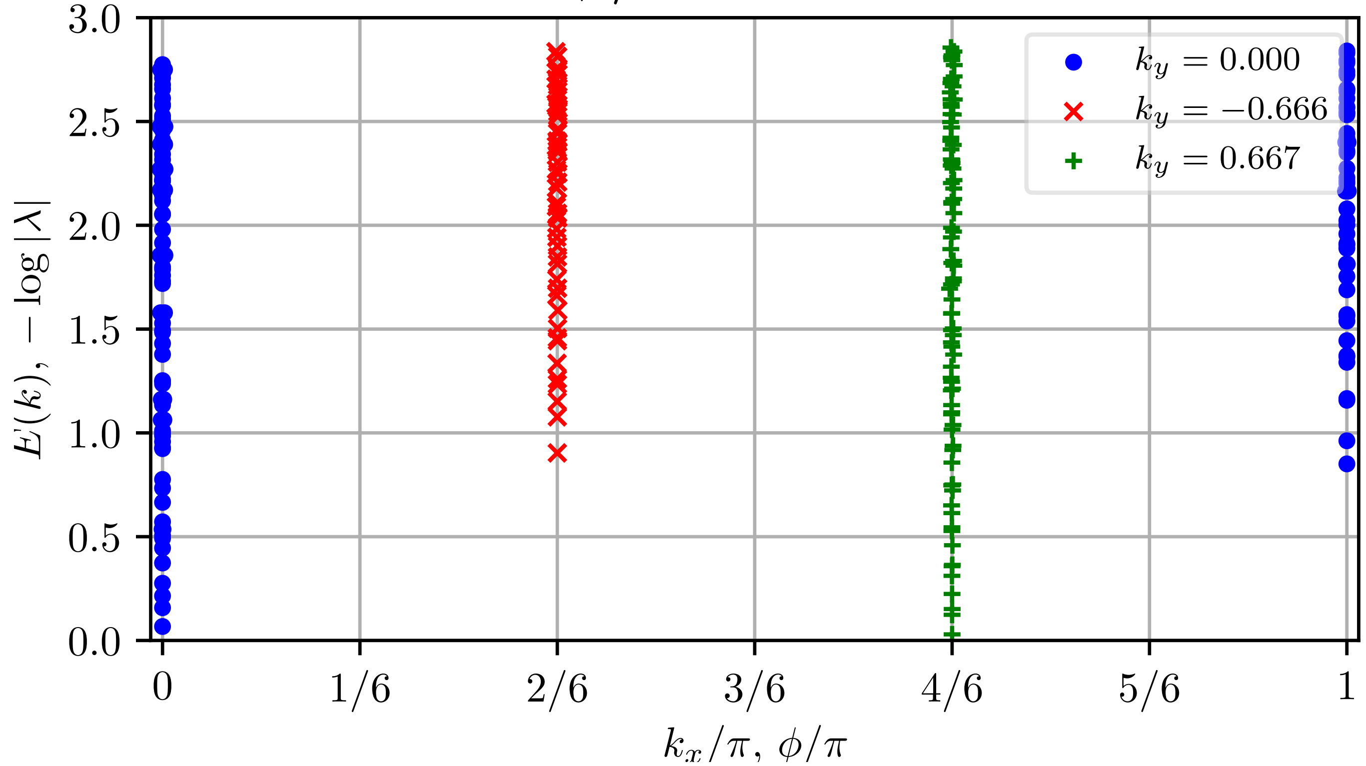
$$E_{\text{lowest}} \sim \xi^{-1}$$

$$\lambda_i = e^{-\epsilon_i + i\eta_i} \quad \Longleftrightarrow \quad \begin{aligned} E_i &\sim \epsilon_i = -\ln|\lambda_i| \\ k_i &\sim \eta_i = \arg\lambda_i \end{aligned}$$

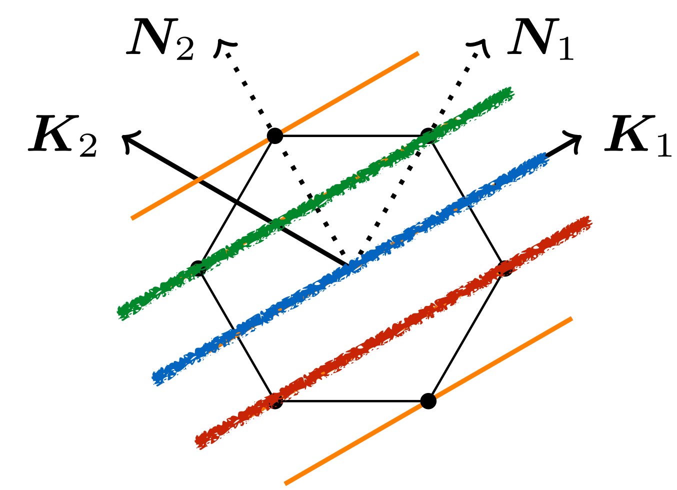
$\mathcal{T}$:



$\phi/\pi = 0$

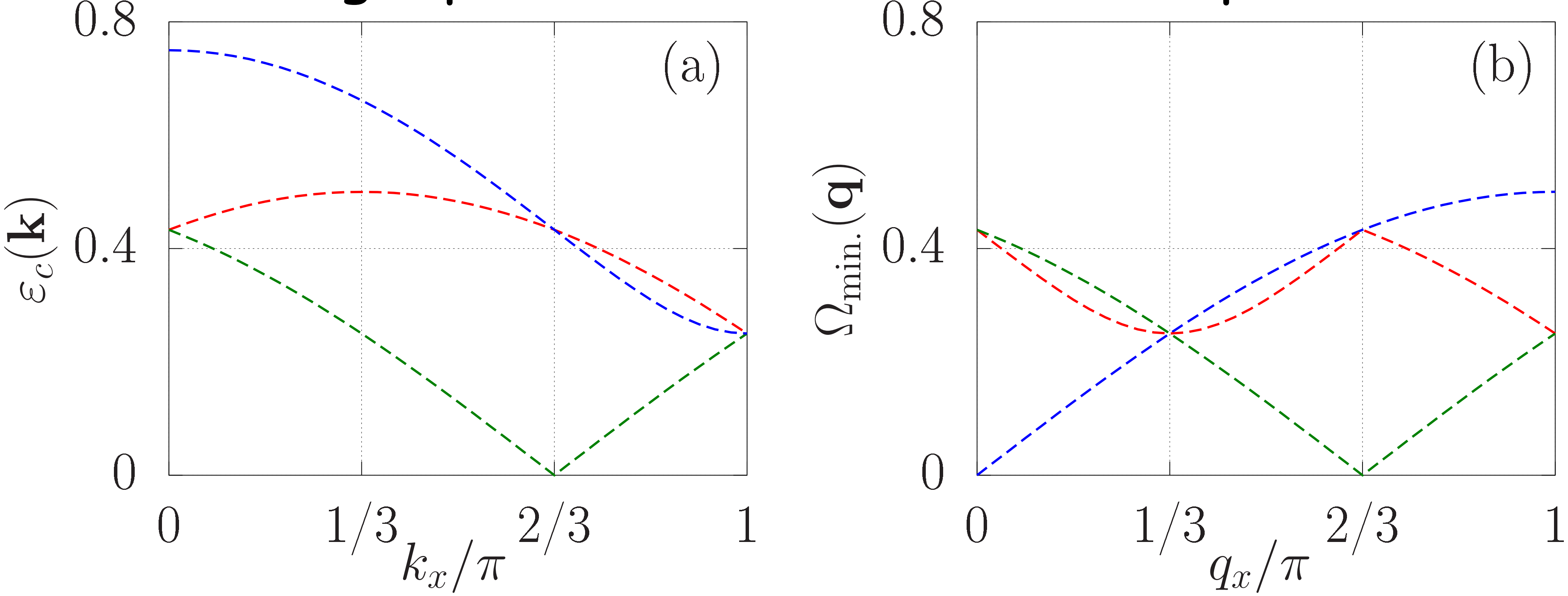


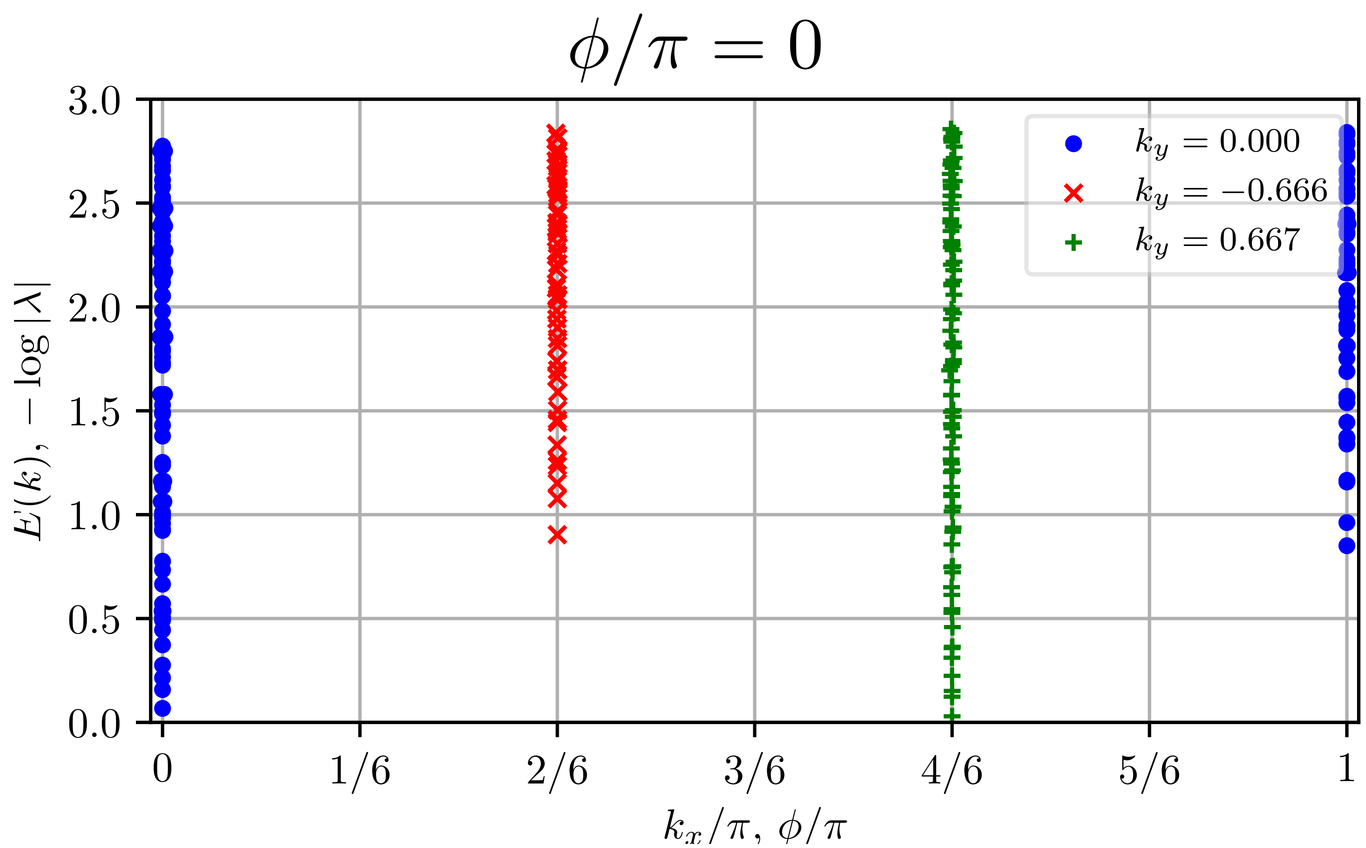
$K_x = K_y = K_z = 1$

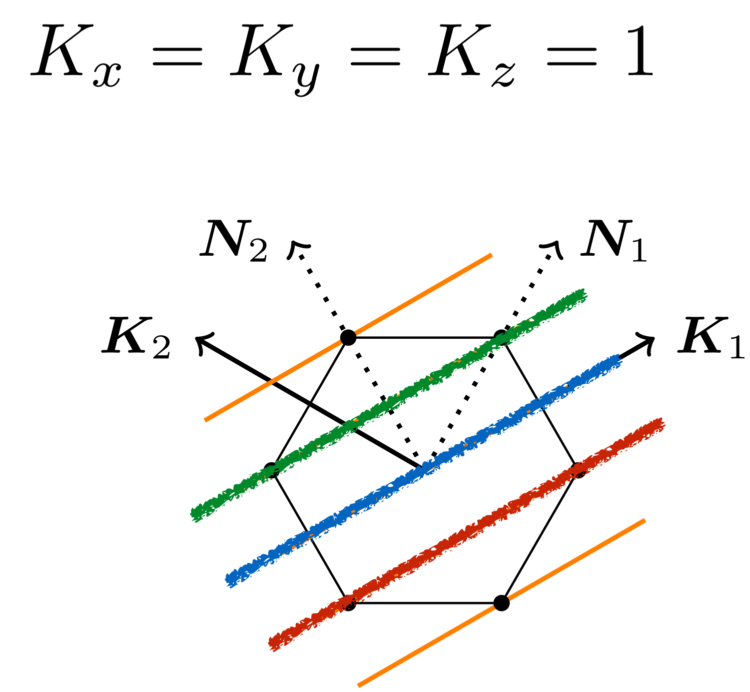


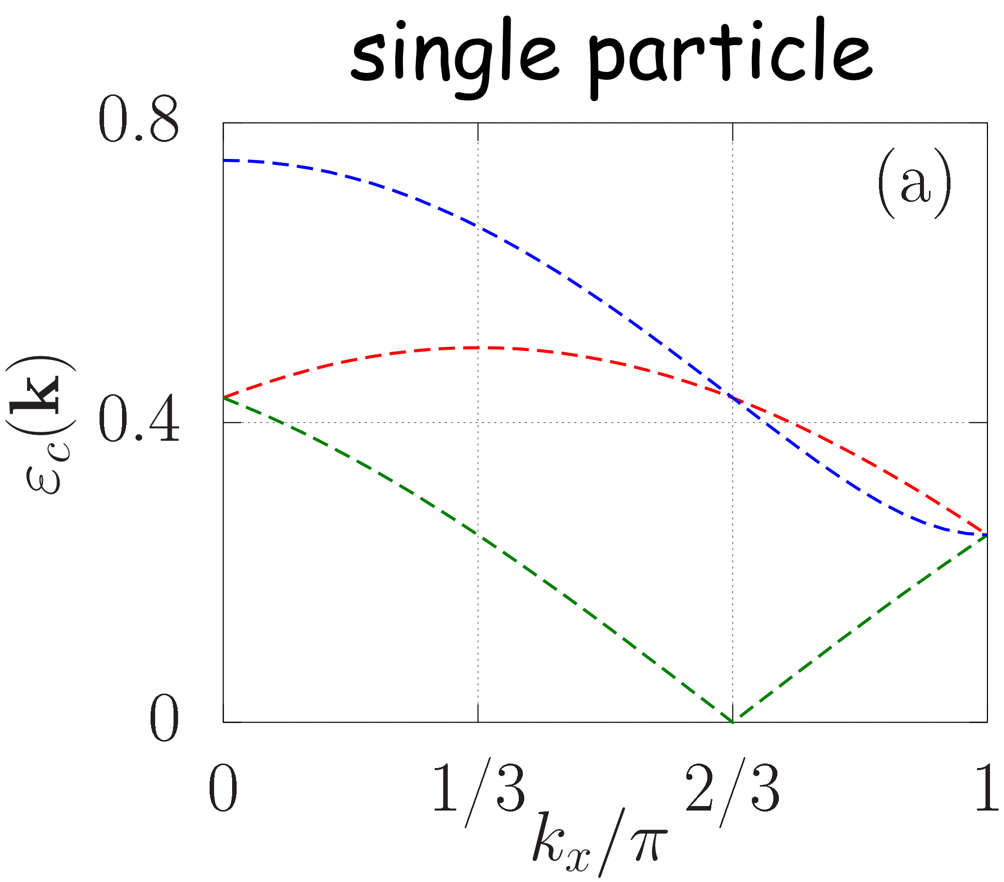
single particle

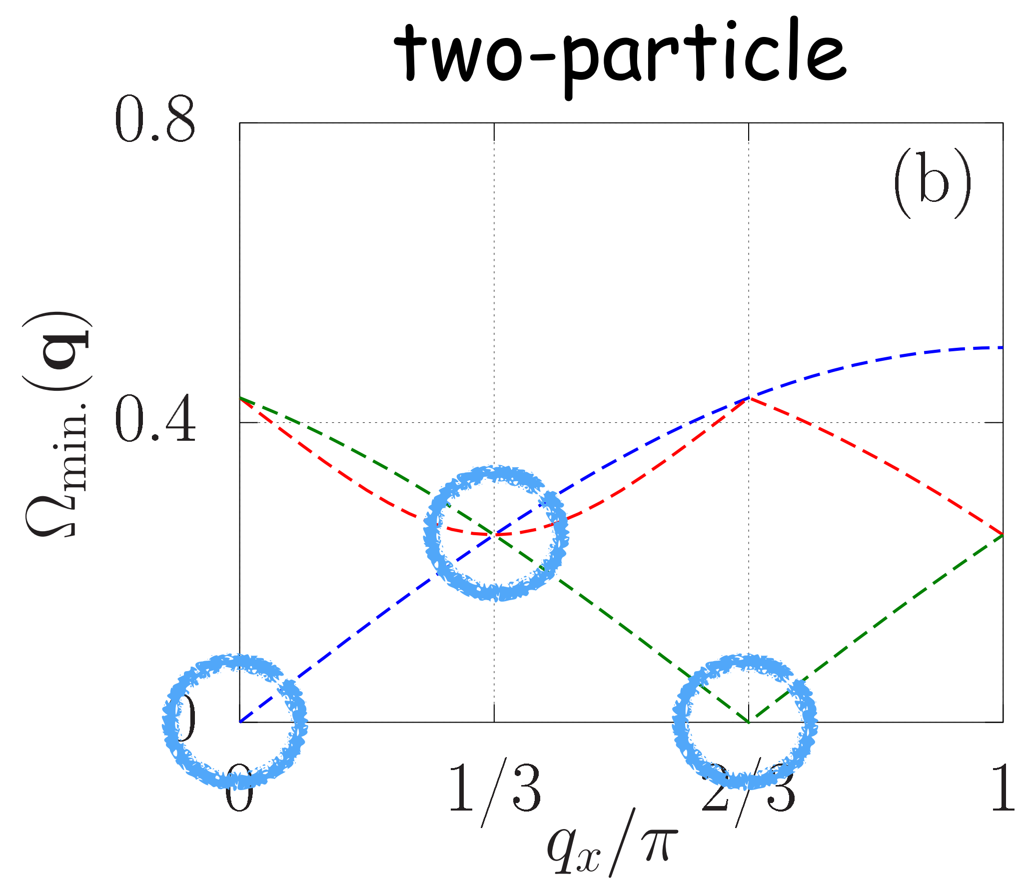
two-particle




$\phi/\pi = 0$
$k_y = 0.000$
$k_y = -0.666$
$k_y = 0.667$
$E(k), -\log|\lambda|$
$k_x/\pi,\ \phi/\pi$
0.0
0.5
1.0
1.5
2.0
2.5
3.0
0
1/6
2/6
3/6
4/6
5/6
1


$K_x = K_y = K_z = 1$
$\boldsymbol{N}_2$
$\boldsymbol{N}_1$
$\boldsymbol{K}_2$
$\boldsymbol{K}_1$

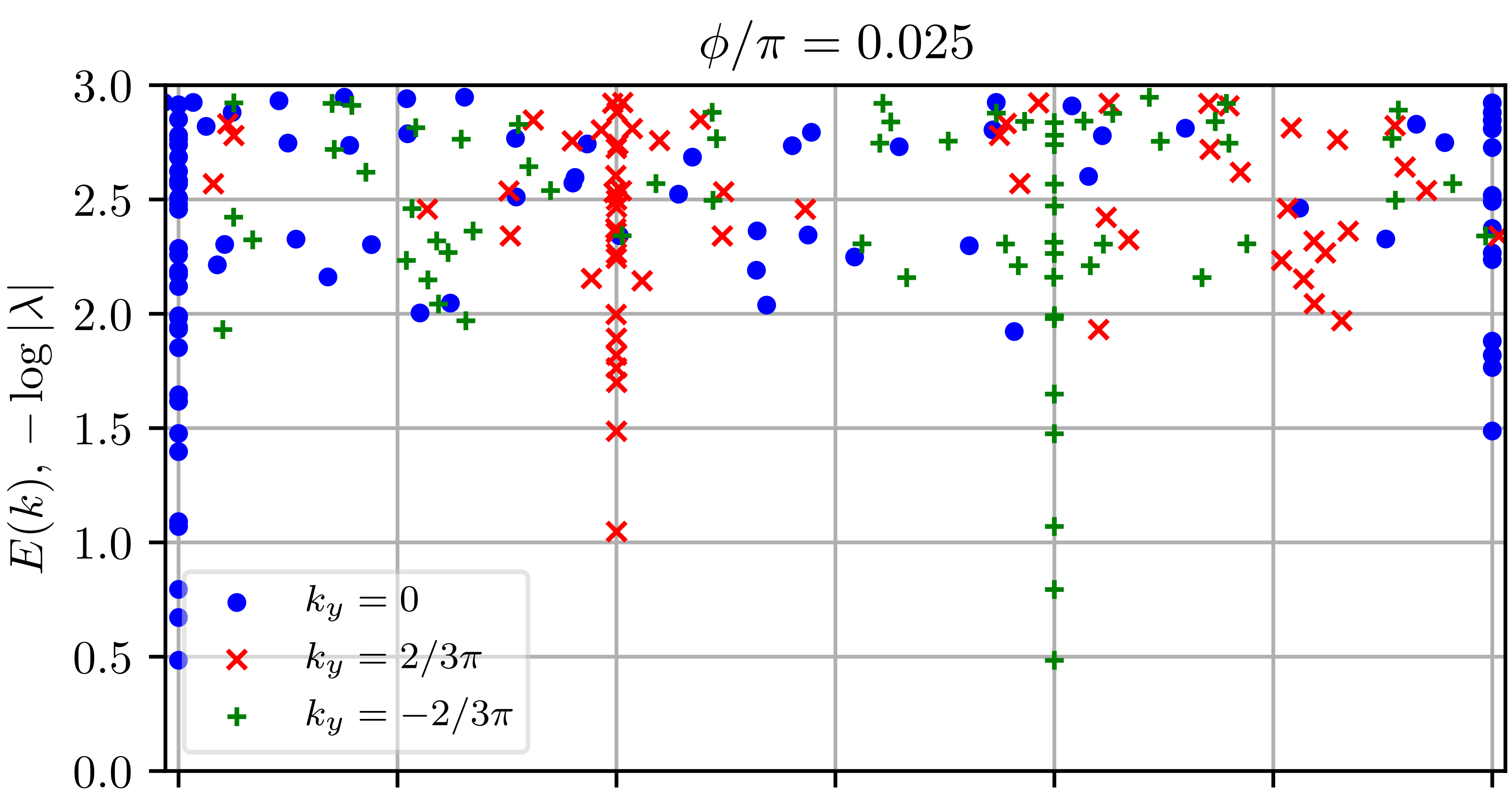

single particle
(a)
$\varepsilon_c(\mathbf{k})$
k_x/π
0
0.4
0.8
0
1/3
2/3
1

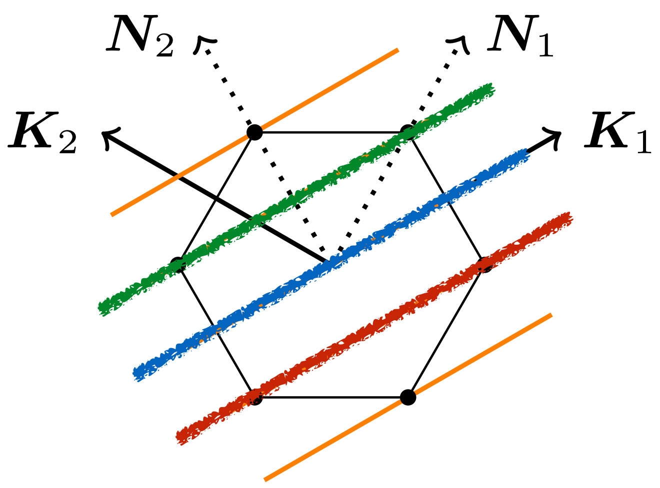

two-particle
(b)
$\Omega_{\mathrm{min.}}(\mathbf{q})$
q_x/π
0
0.4
0.8
0
1/3
2/3
1

Transfer Matrix Spectrum

V. Zauner, F.Verstraete et. al (2014)

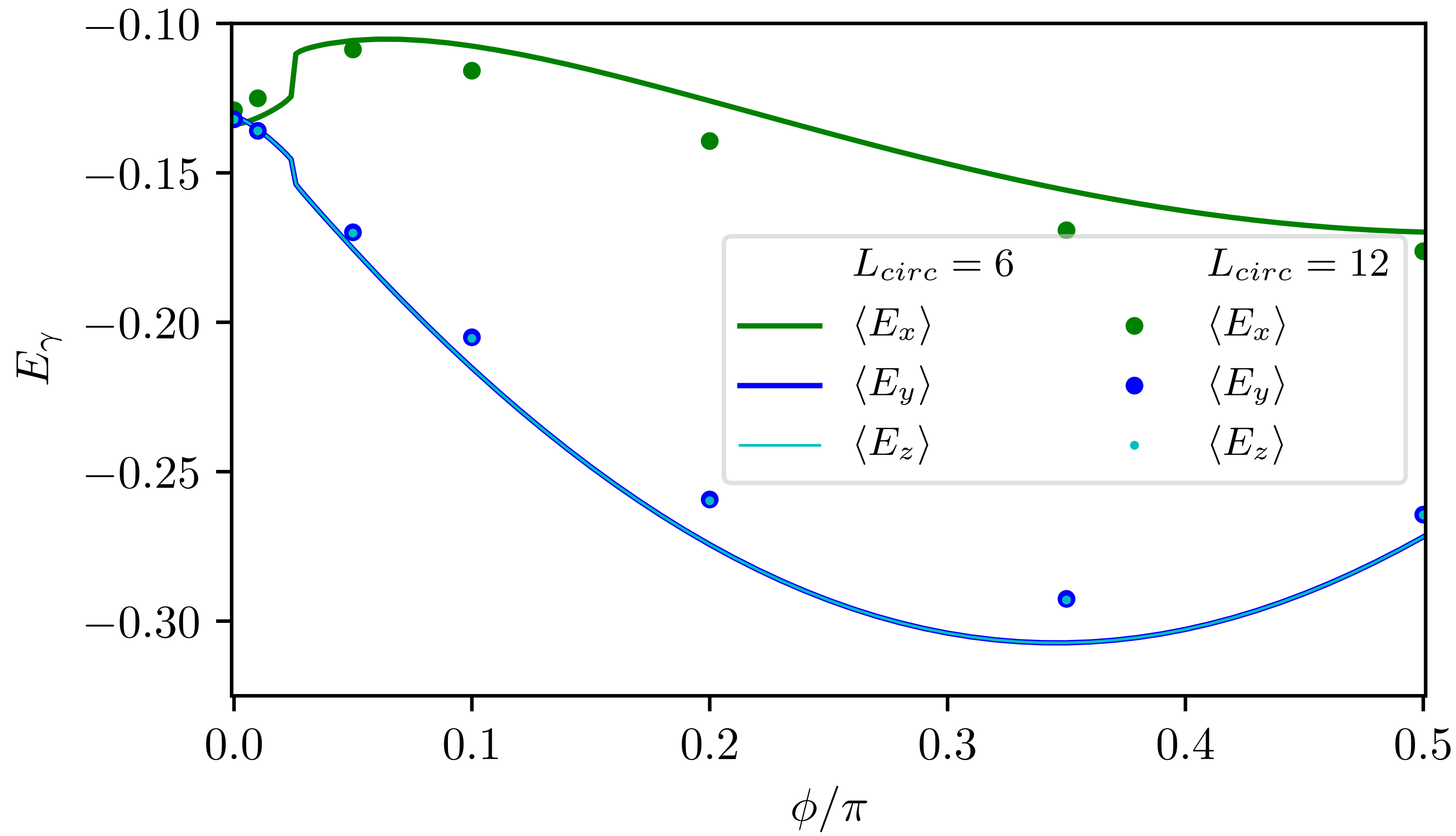
Correspondence between the complex eigenvalues and the lower boundaries of multi-particle excitation spectrum of the ground state





Transfer Matrix Spectrum

need to be a bit more careful here …



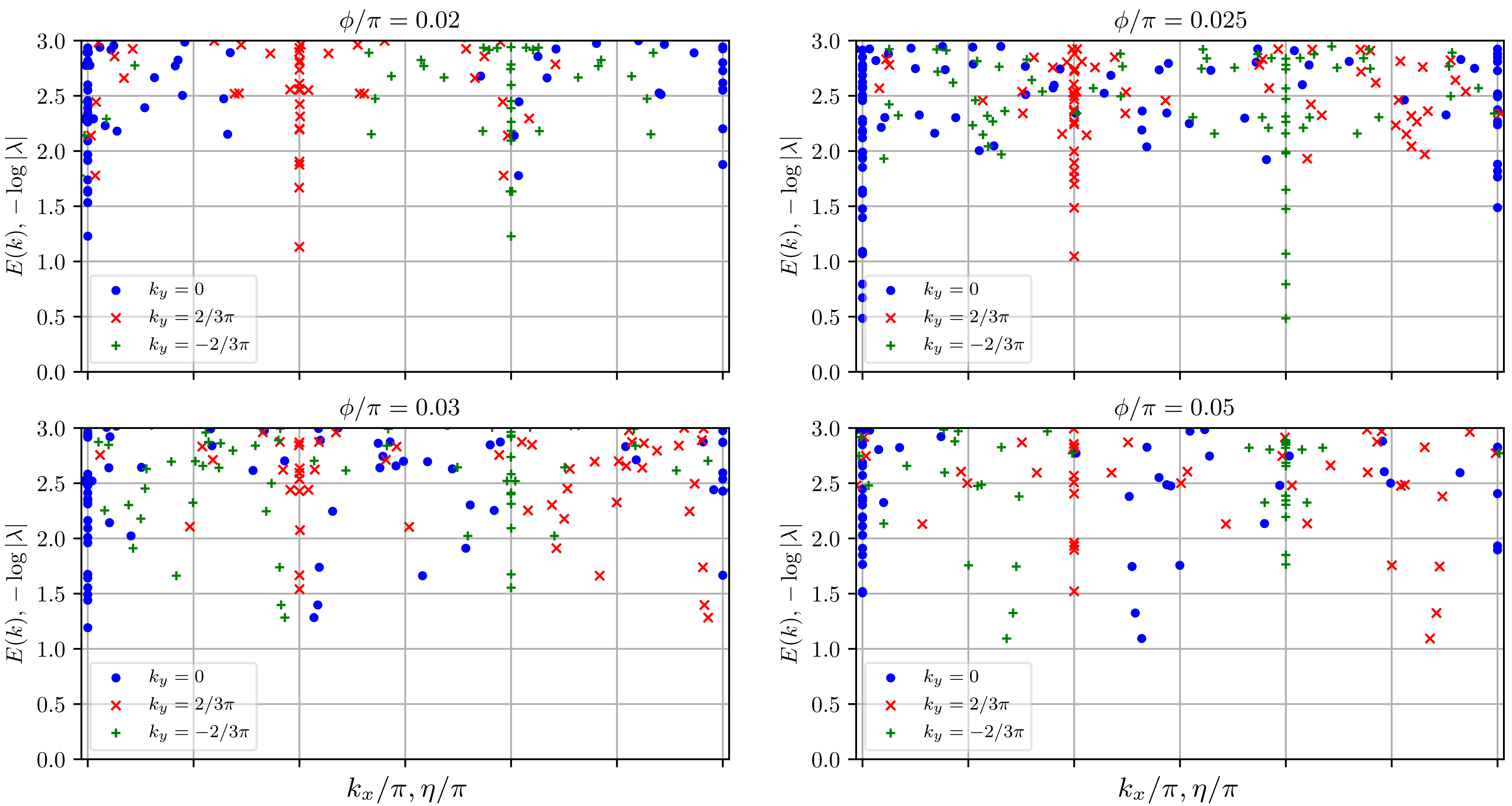
Anisotropy due to cylinder geometry

Locations of dispersion minima would move around

(we take an advantage of this)

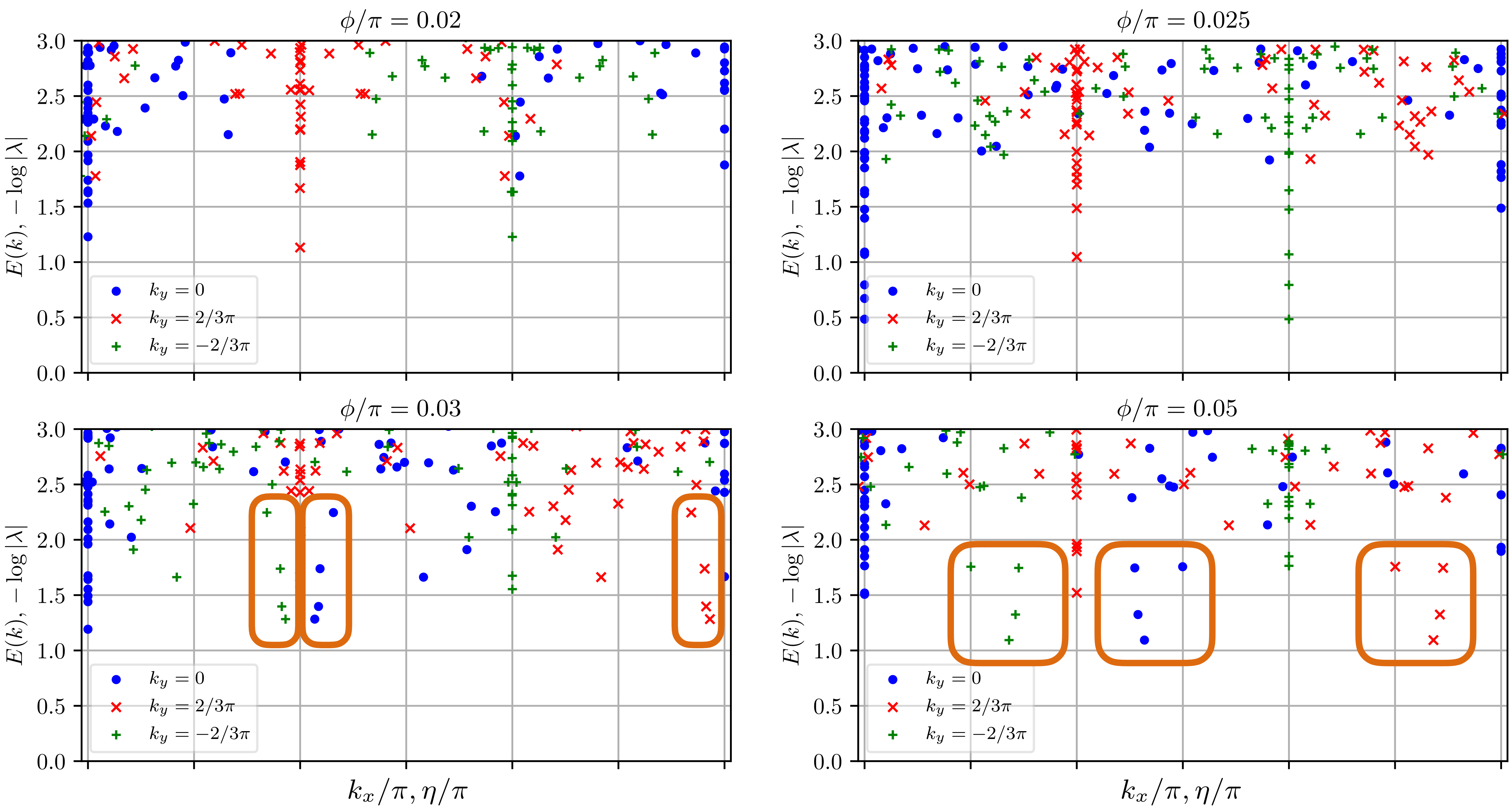
Evolution of Two-Particle Spectra

Coherent (gapped) 2D excitations !



Evolution of Two-Particle Spectra

Coherent (gapped) 2D excitations !



$$E(k_x, k_y) = E(k_x + 2\pi/3, k_y - 2\pi/3)$$

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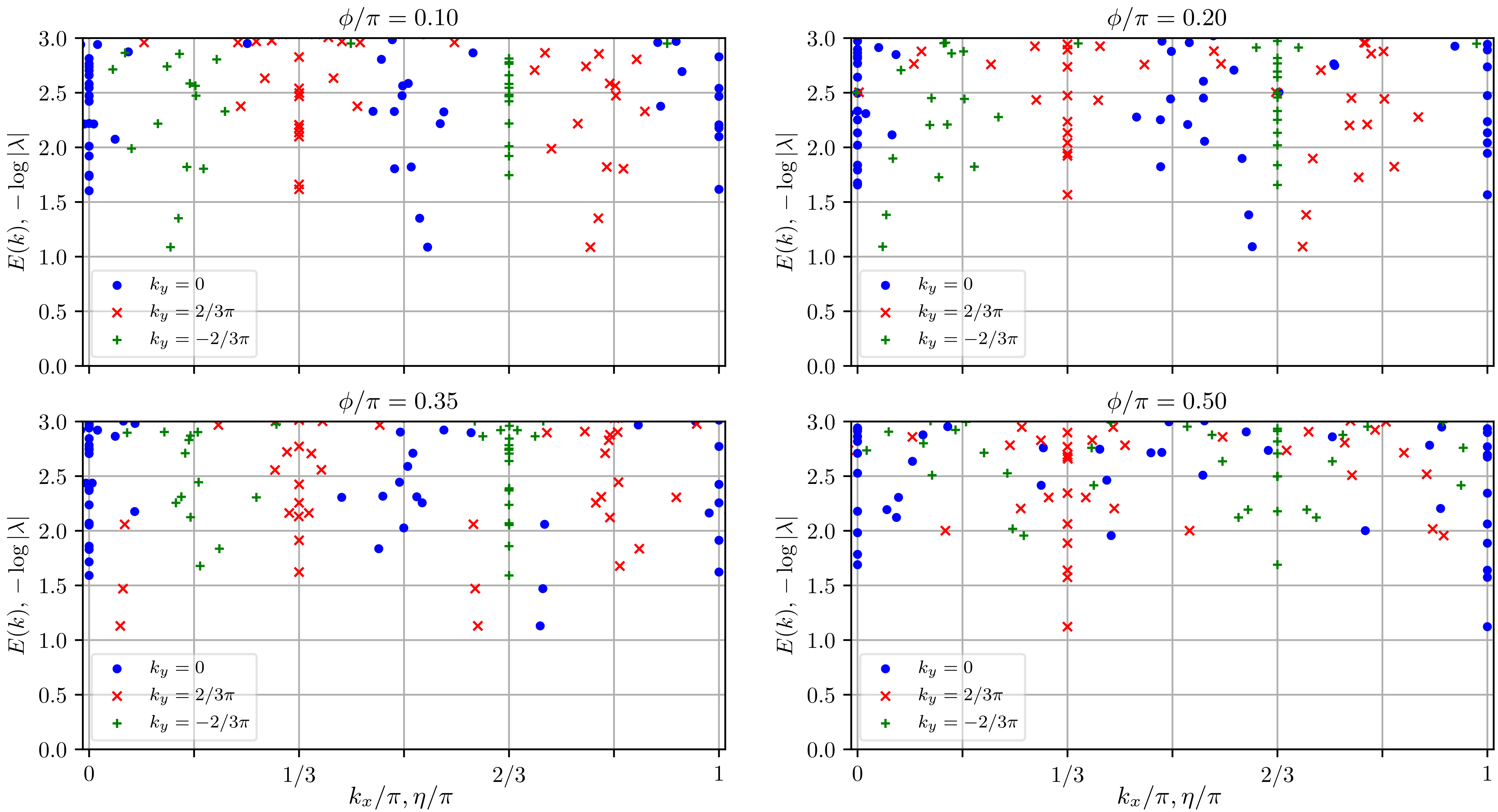
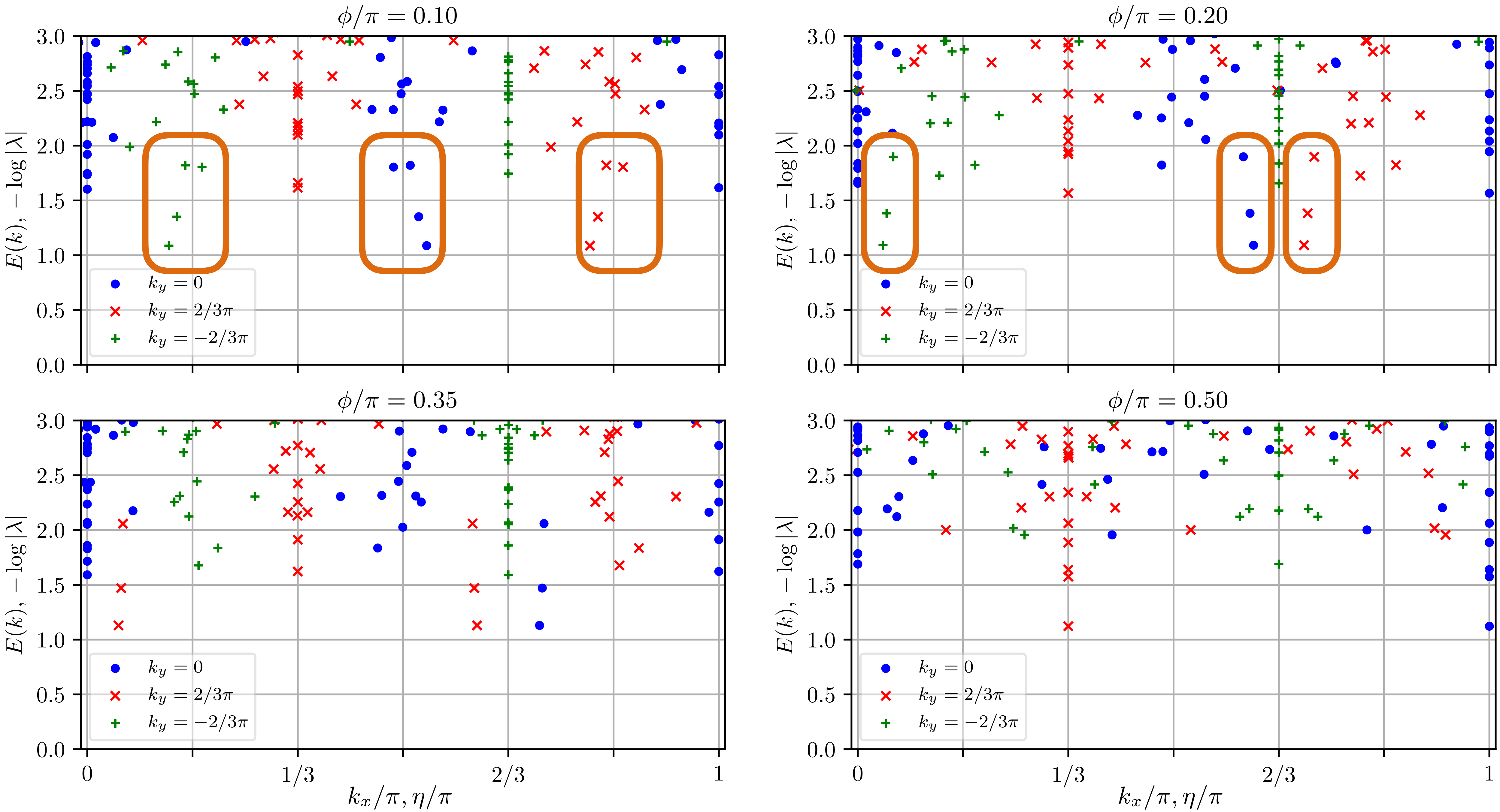


Evolution of Two-Particle Spectra

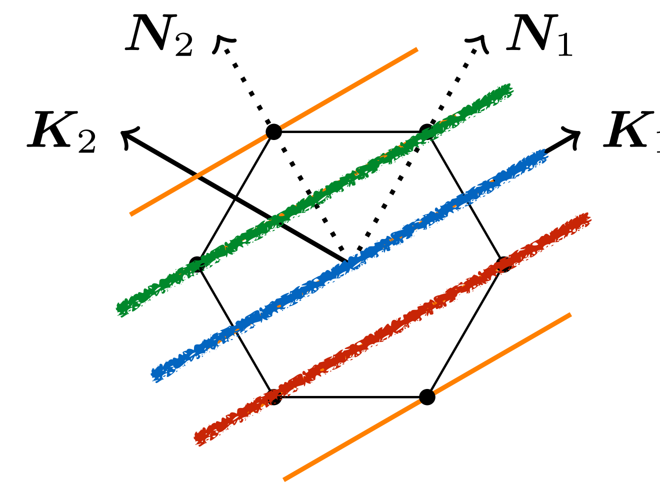
Coherent (gapped) 2D excitations !



$$E(k_x, k_y) = E(k_x + 2\pi/3, k_y - 2\pi/3)$$

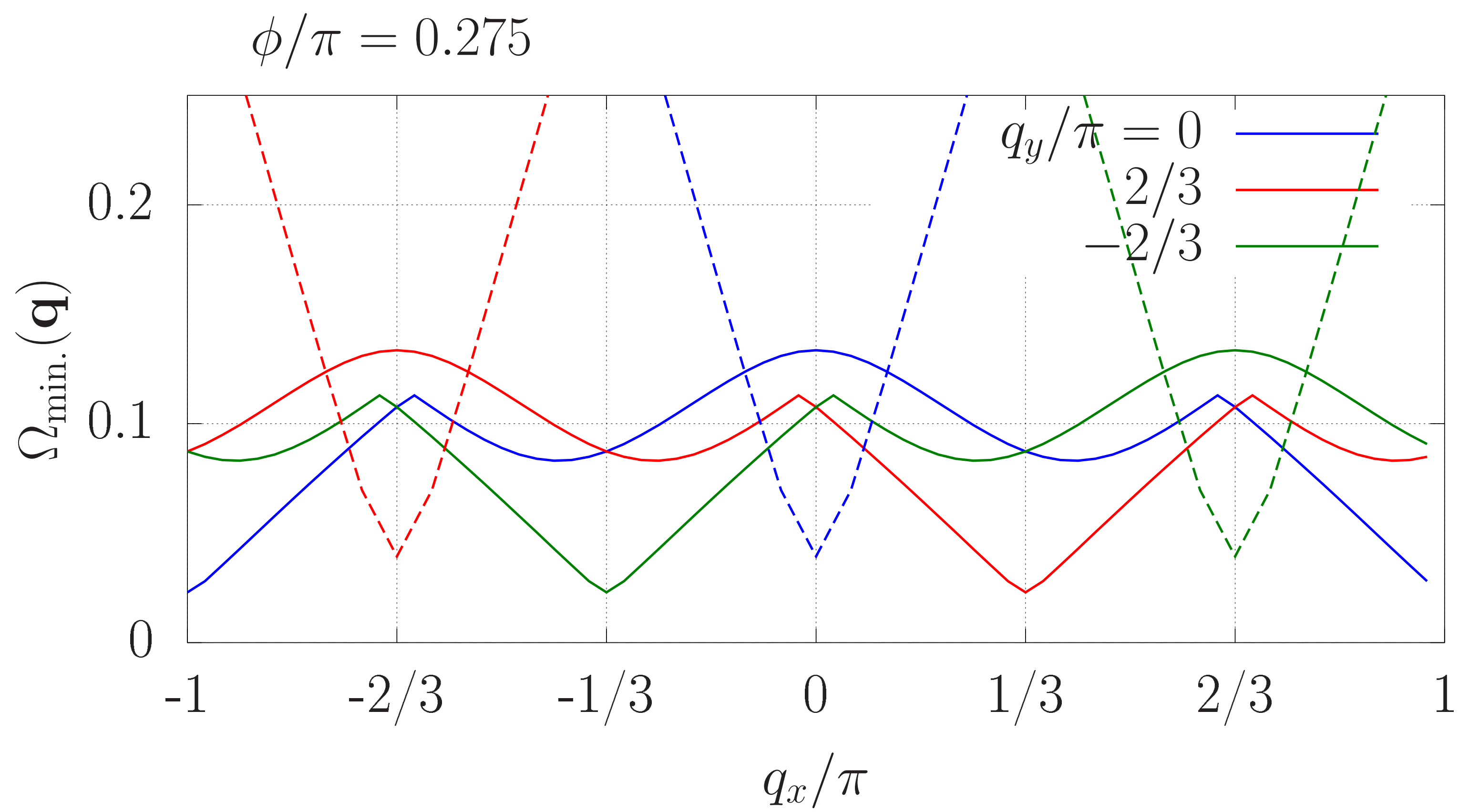
Mean-field theory on Cylinder

$$S_i^\alpha = \frac{1}{2} i b_i^\alpha c_i$$



two-particle spectrum

$$\Omega_{\text{min.}}(\mathbf{q}) = \min_{\mathbf{k}} \left(|\varepsilon_{b,c}(\mathbf{q}-\mathbf{k})| + |\varepsilon_c(\mathbf{k})| \right)$$



$b+c$ (solid)

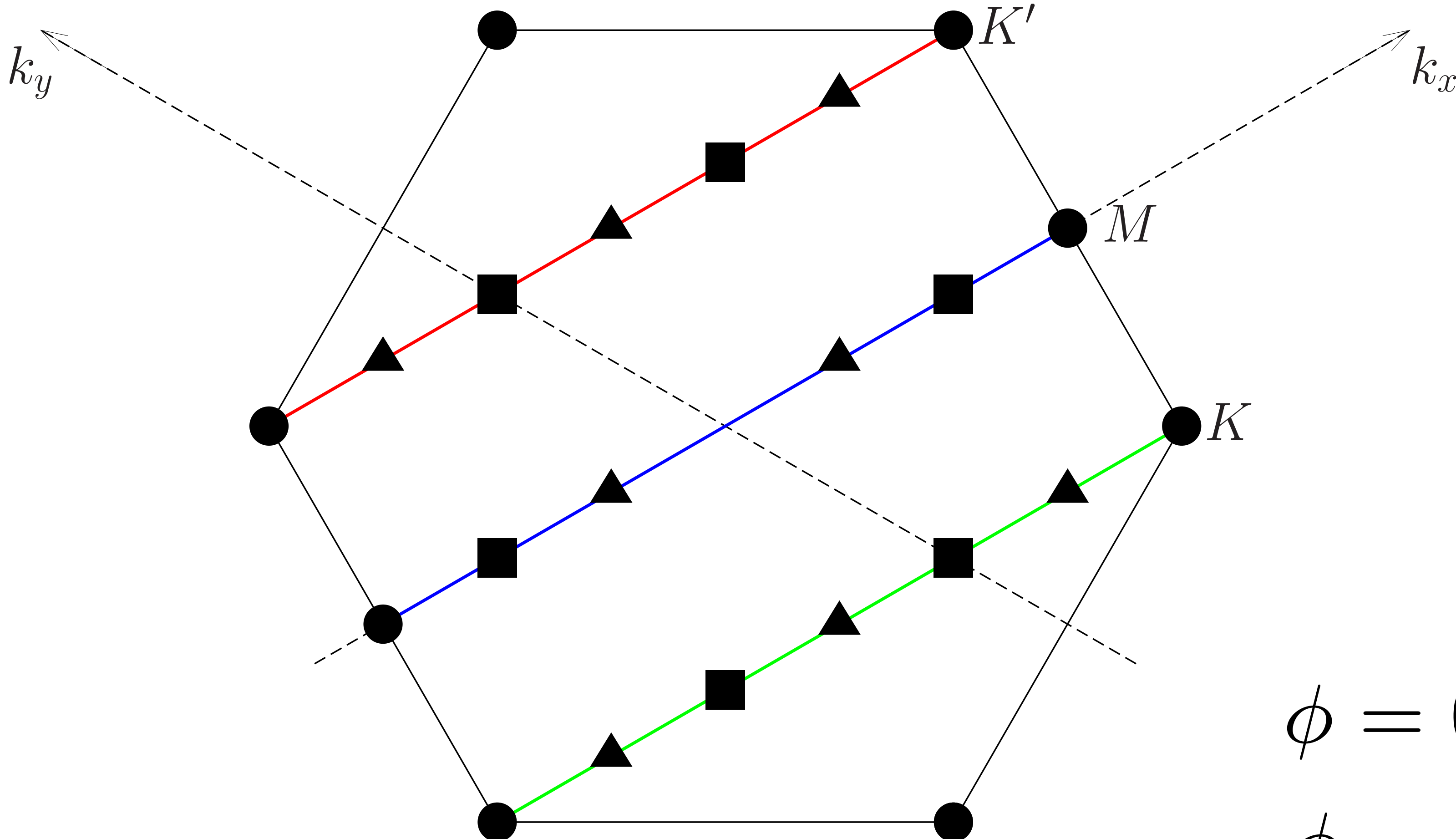
$c+c$ (dashed)

$$\varepsilon_b(\mathbf{k}) = \varepsilon_b(\mathbf{k}\pm\mathbf{K})$$

$$\Omega_{b+c}(\mathbf{q}\pm\mathbf{K},\mathbf{k}) = \Omega_{b+c}(\mathbf{q},\mathbf{k})$$

Same symmetry as in the Majorana MFT

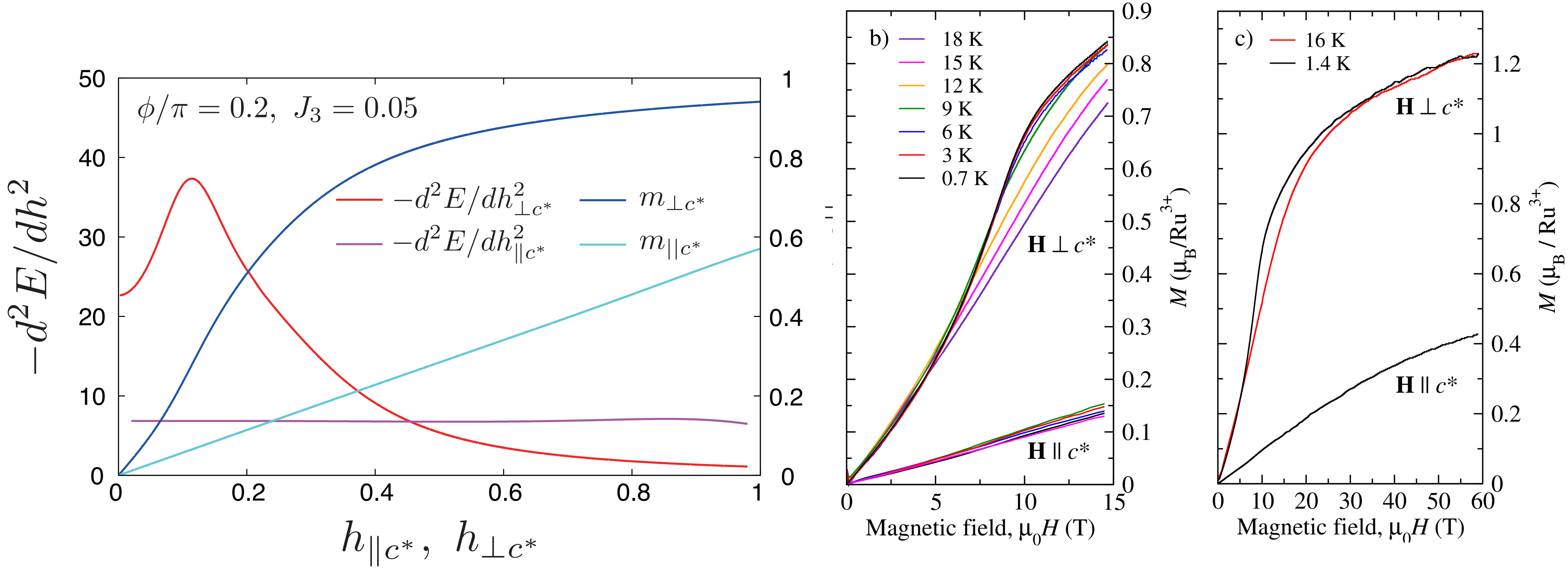
Evolution of two-particle excitation minima



$\phi = 0.03\pi$ (▲)

$\phi = 0.2\pi$ (■)

Effect of Magnetic Field



Coldea, Valenti (2015)

For the in-plane field, the transition occurs at about 1/10 of the exchange energy scale

Conclusion

K-Γ model gives quantum spin liquid phases in an extended region of phase diagram when K < 0

There are coherent 2D excitations while there is no magnetic order for K < 0, Γ > 0

Transfer matrix spectra can be interpreted as lower boundary of two-spinon excitations

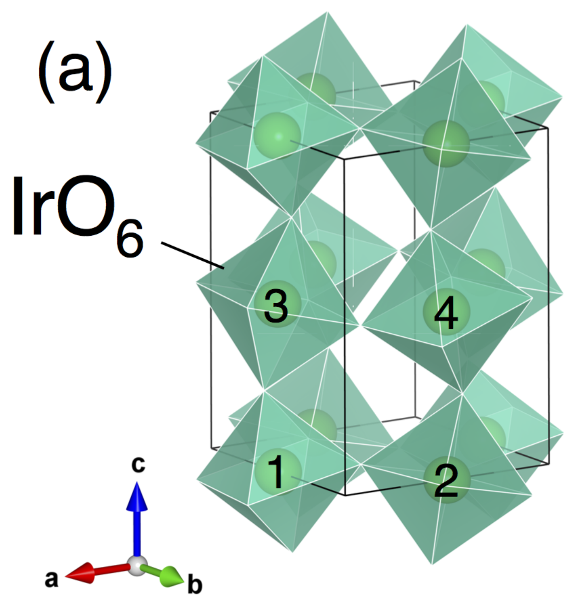
The "phase transition" is a result of the change in anisotropy of the bond energy:
Meta-nematic transition ?
Survives in 2D limit or not ?

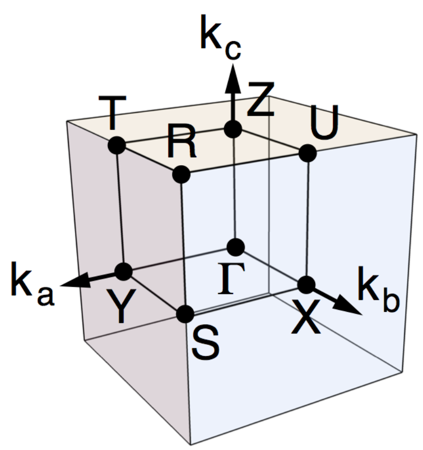
Other perturbations such as J_3 give the Zig-Zag order

Large Intrinsic Spin Hall Effect in Iridate Semimetal $SrIrO_3$

A. S. Patri, K. Hwang, H.-W. Lee, YBK, arXiv:1711.00861

Orthorhombic Perovskite $SrIrO_3$





U=$(0, \pi,\pi)$ X=$(0,\pi,0)$
R=(π,π,π) Y=$(\pi,0,0)$
Z=$(0,0,\pi)$

Non-symmorphic Space Group

$$Pbnm$$

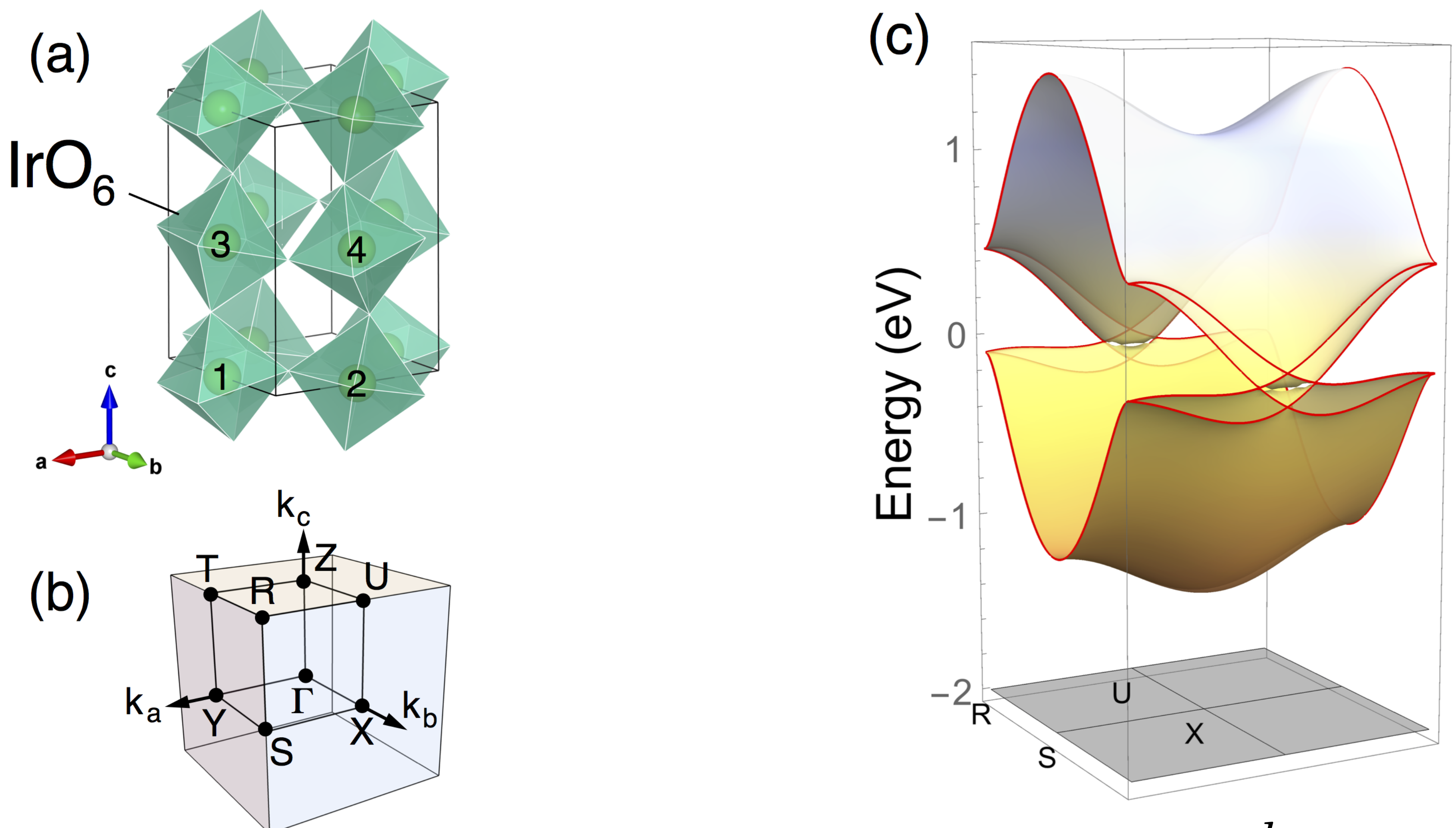
Symmetry	$\mathbf{R}'$
n-glide (G_n)	$a+\frac{1}{2},\ -b+\frac{1}{2},\ c+\frac{1}{2}$
b-glide (G_b)	$-a+\frac{1}{2},\ b+\frac{1}{2},\ c$
Mirror (m)	$a,\ b,\ -c+\frac{1}{2}$
Inversion ($\bar{I}$)	$-a,\ -b,\ -c$
a-screw (S_a)	$a+\frac{1}{2},\ -b+\frac{1}{2},\ -c$
b-screw (S_b)	$-a+\frac{1}{2},\ b+\frac{1}{2},\ -c+\frac{1}{2}$
c-screw (S_c)	$-a,\ -b,\ c+\frac{1}{2}$

$$\mathbf{R}=a\hat{a}+b\hat{b}+c\hat{c} \to \mathbf{R}'=a'\hat{a}+b'\hat{b}+c'\hat{c}$$

$$(k_a, k_b, k_c)$$
$$=(\mathbf{k}\cdot\mathbf{a}, \mathbf{k}\cdot\mathbf{b}, \mathbf{k}\cdot\mathbf{c})$$

$\{\mathbf{a}, \mathbf{b}, \mathbf{c}\}$
orthorhombic lattice vectors

Orthorhombic Perovskite $SrIrO_3$



$k_b = \pi$ plane (R-U-X-S)

U$=(0,\ \pi,\pi)$ X$=(0,\pi,0)$

R$=(\pi,\pi,\pi)$ Y$=(\pi,0,0)$

Z$=(0,0,\pi)$

$$(k_a, k_b, k_c)$$

$$=(\mathbf{k}\cdot\mathbf{a}, \mathbf{k}\cdot\mathbf{b}, \mathbf{k}\cdot\mathbf{c})$$

$\{\mathbf{a}, \mathbf{b}, \mathbf{c}\}$

orthorhombic lattice vectors

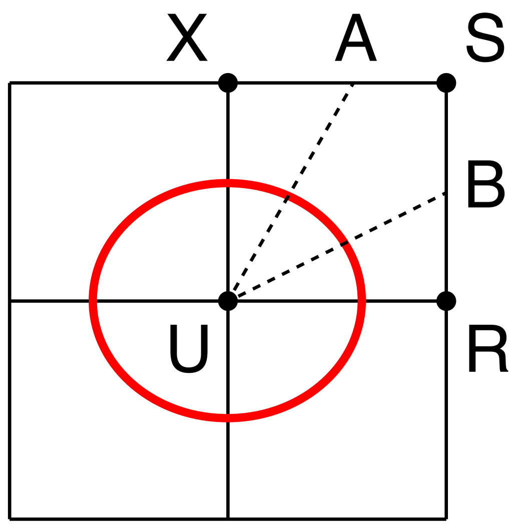
Nodal line semimetal

Elements of the little group of $H_{\mathbf{k}}$

	$\mathbf{k}$	G_n	G_b	S_a
$k_b = \pi$ plane	(k_a, π, k_c)	✓		
U point	$(0, \pi, \pi)$	✓	✓	✓
RS line	(π, π, k_c)	✓	✓	
SX line	$(k_a, \pi, 0)$	✓		✓

$\Theta = \mathcal{T} \times I$

$$
\begin{aligned}
&(\mathrm{U}) \quad [G_n, G_b] = [G_n, S_a] = \{G_b, S_a\} = 0,\\
&(\mathrm{RS}) \quad \{G_n, G_b\} = 0,\\
&(\mathrm{SX}) \quad \{G_n, S_a\} = 0.
\end{aligned}
$$



$k_b = \pi$ plane

Nodal line semimetal

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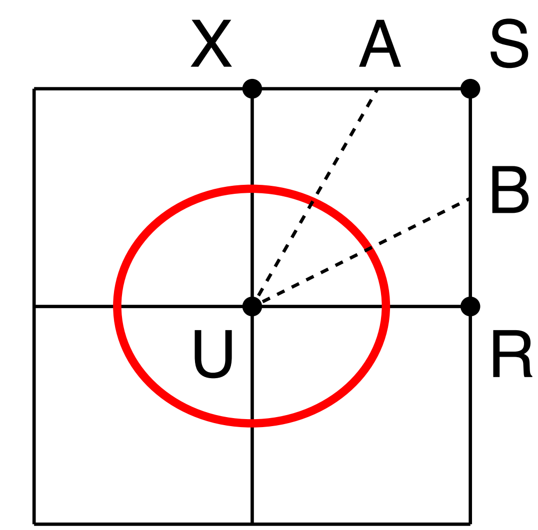
SX line	$(k_a, \pi, 0)$	✓		✓



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&(\mathrm{SX}) \quad \{G_n, S_a\} = 0.
\end{aligned}
$$

$\{G_b, S_a\} = 0 \qquad |a_+\rangle \overset{G_b}{\leftrightarrow} |a_-\rangle$

$\{G_n, S_a\} = 0 \quad |n_+\rangle \overset{S_a}{\leftrightarrow} |n_-\rangle$

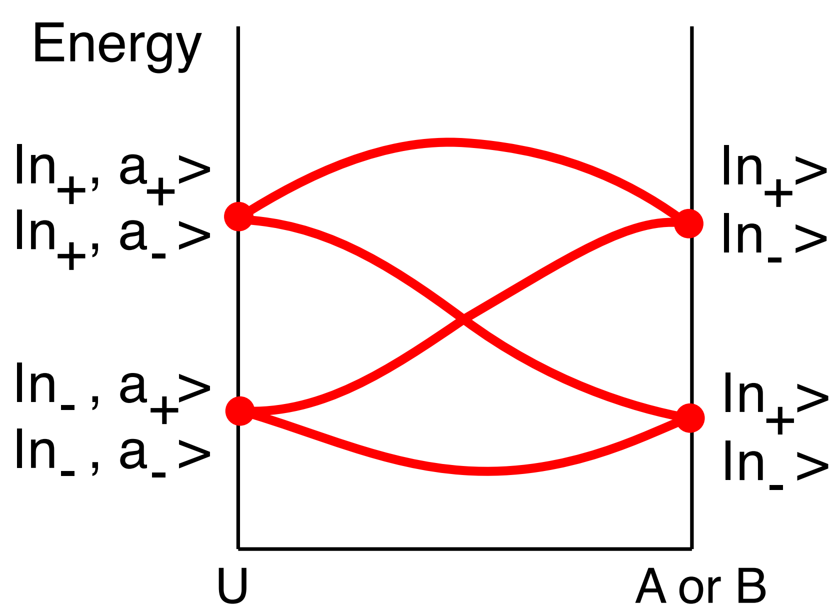
SX line

$|n_+, a_+\rangle \quad |n_+, a_-\rangle$

$\Theta|n_+, a_+\rangle \quad \Theta|n_+, a_-\rangle$

$|n_-, a_+\rangle \quad |n_-, a_-\rangle$

$\Theta|n_-, a_+\rangle \quad \Theta|n_-, a_-\rangle$



$|n_+\rangle, \quad |n_-\rangle$

$\Theta|n_+\rangle, \quad \Theta|n_-\rangle$

Intrinsic Spin Hall Conductivity

$$\sigma^{\rho}_{\mu\nu} = \frac{2e\hbar}{V} \sum_{\mathbf{k}} \sum_{\epsilon_{n\mathbf{k}}<\epsilon_F<\epsilon_{m\mathbf{k}}} \mathrm{Im}\left[\frac{\langle m\mathbf{k}|\mathcal{J}^{\rho}_{\mu}|n\mathbf{k}\rangle\langle n\mathbf{k}|J_{\nu}|m\mathbf{k}\rangle}{(\epsilon_{m\mathbf{k}} - \epsilon_{n\mathbf{k}})^2}\right]$$

$$\sigma^{\rho}_{\mu\nu} \; = \; \textstyle\sum_{n,\mathbf{k}} [\Omega^{\rho}_{\mu\nu}]_{n\mathbf{k}} \;\; f_{n\mathbf{k}}$$

$$\langle \mathcal{J}^{\rho}_{\mu} \rangle \; = \; \sigma^{\rho}_{\mu\nu} E^{\nu}$$

$$\mathcal{J}^{\rho}_{\mu} = \; \tfrac{1}{4}\{\sigma^{\rho}, J_{\mu}\}$$

spin current

$$J_{\nu} = \; \textstyle\sum_{\mathbf{k}} \psi^{\dagger}_{\mathbf{k}} \frac{\partial H_{\mathbf{k}}}{\partial k_{\nu}} \psi_{\mathbf{k}}$$

charge current

Intrinsic Spin Hall Conductivity

Pseudo-cubic $\{\mathbf{x}, \mathbf{y}, \mathbf{z}\}$	Orthorhombic $\{\mathbf{a}, \mathbf{b}, \mathbf{c}\}$
$[100]_c$	$[1\text{-}10]_o$
$[010]_c$	$[110]_o$
$[001]_c$	$[001]_o$

$$\sigma^{\rho}_{\mu\nu} = \sum_{n,\mathbf{k}} [\Omega^{\rho}_{\mu\nu}]_{n\mathbf{k}} \; f_{n\mathbf{k}}$$

$$\langle \mathcal{J}^{\rho}_{\mu} \rangle = \sigma^{\rho}_{\mu\nu} E^{\nu}$$

$$\mathcal{J}^{\rho}_{\mu} = \frac{1}{4}\{\sigma^{\rho}, J_{\mu}\}$$

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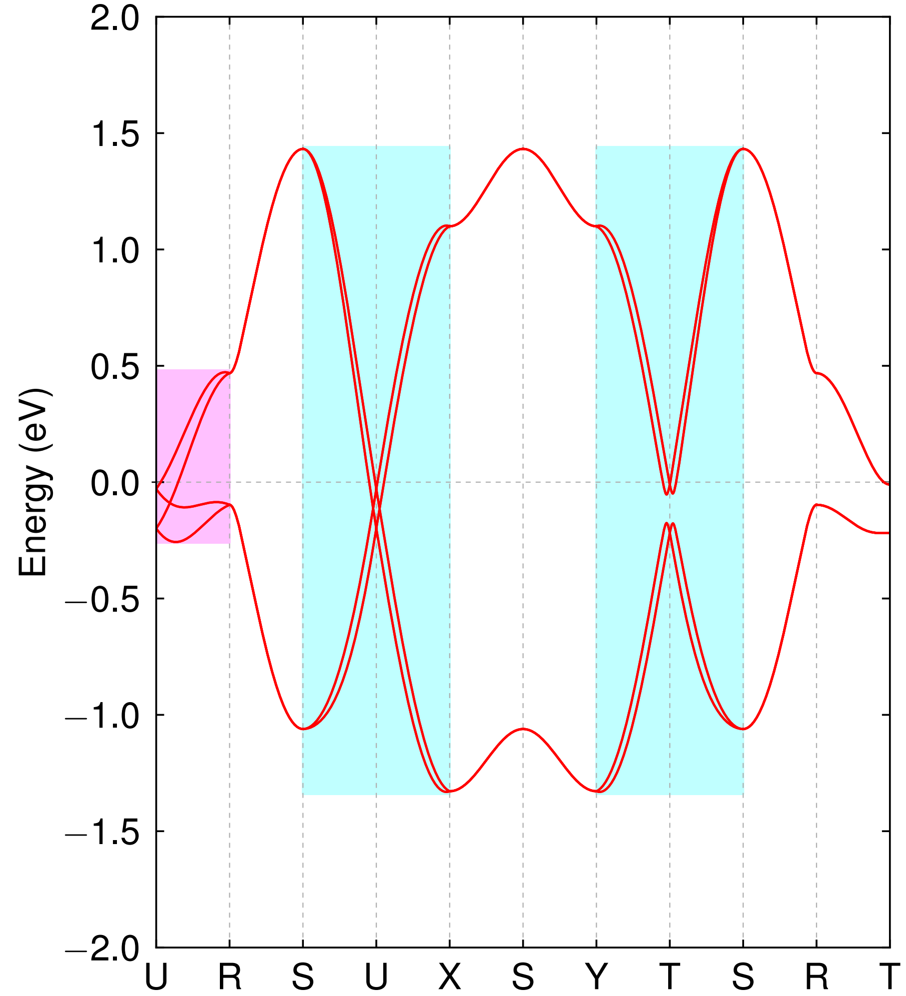
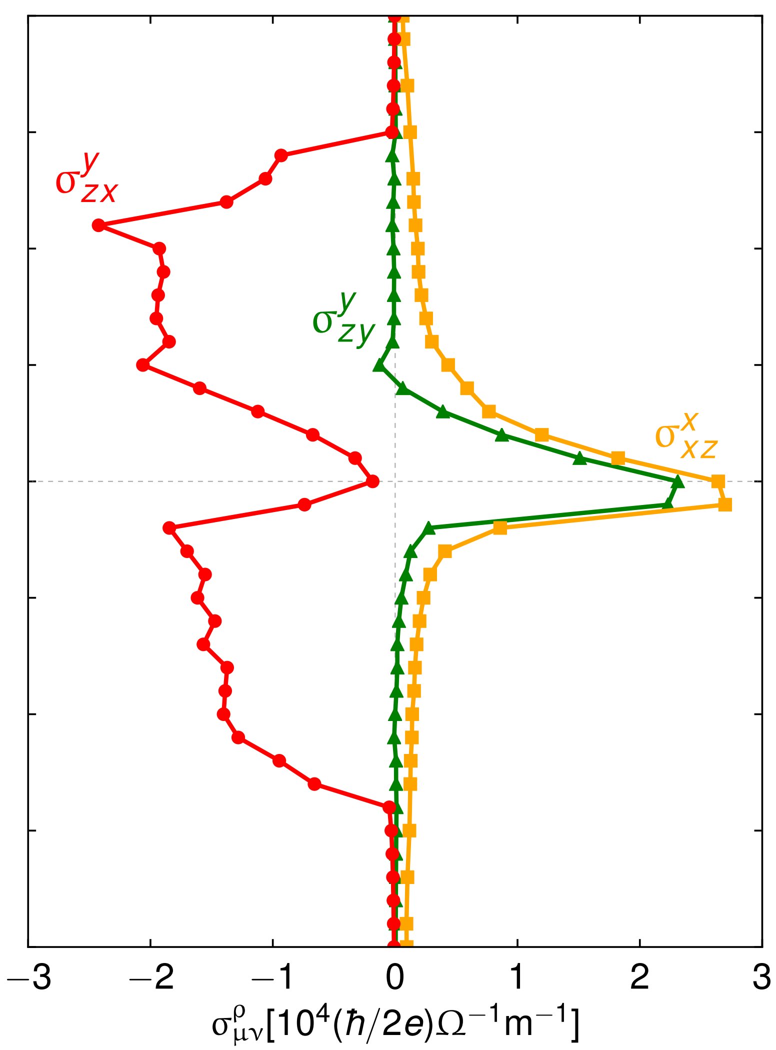
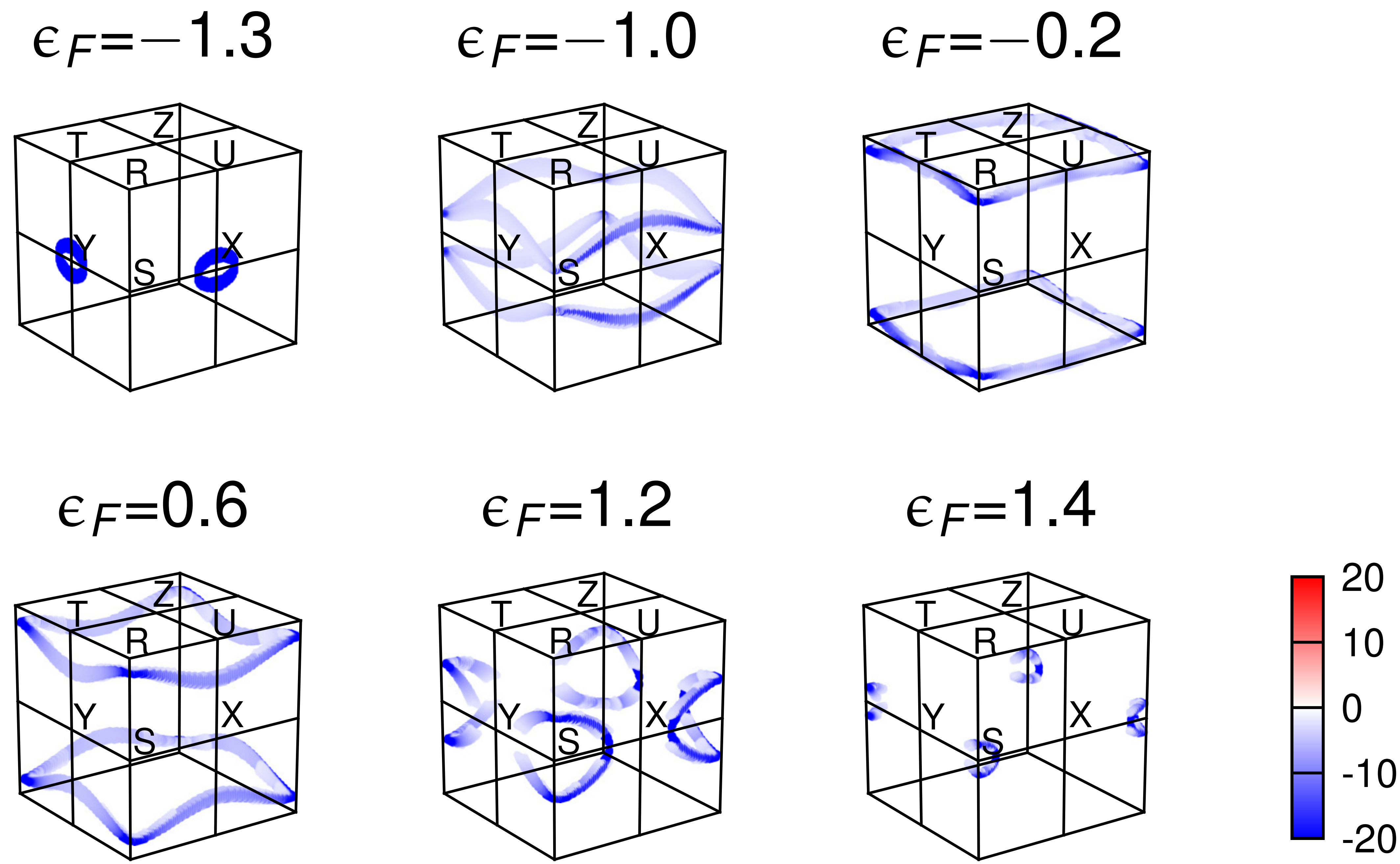
charge current





$\Omega^{y}_{zx}(\mathbf{k})$ as a function of the Fermi level ϵ_F

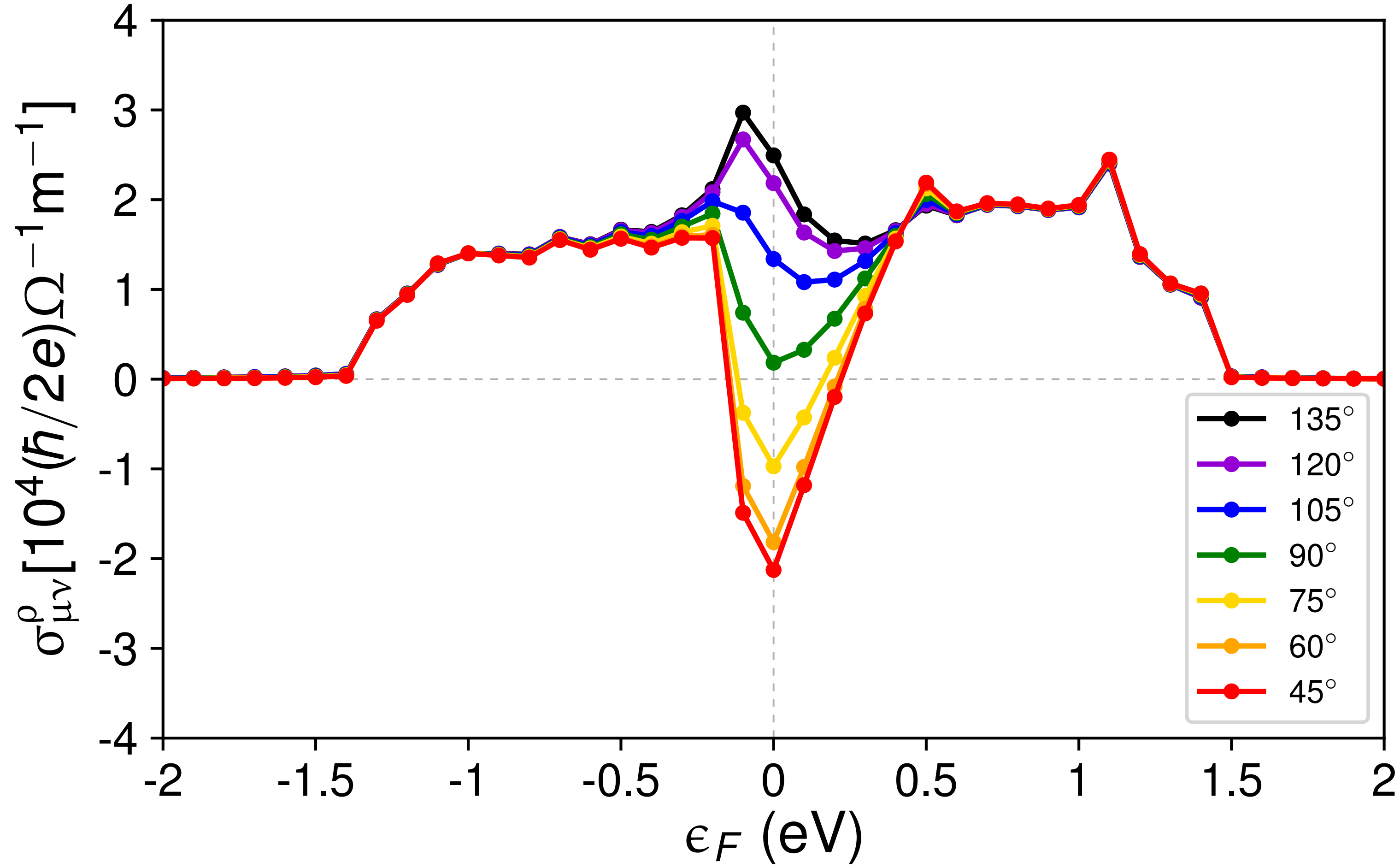


Direction Dependence

Here, the field direction (ν) is changed within the xy plane by the angle θ from the x axis with keeping the three directions $\{\rho, \mu, \nu\}$ orthogonal.

$$\begin{array}{lcc} \nu & \| & \hat{x}\ \cos\theta + \hat{y}\ \sin\theta \\ \mu & \| & \hat{z}, \\ \rho & \| & \hat{x}\ \sin\theta - \hat{y}\ \cos\theta \end{array}$$

$$\sigma^{\rho}_{\mu\nu} = -\sigma^{y}_{zx} - \sigma^{y}_{zy}\ \sin 2\theta$$

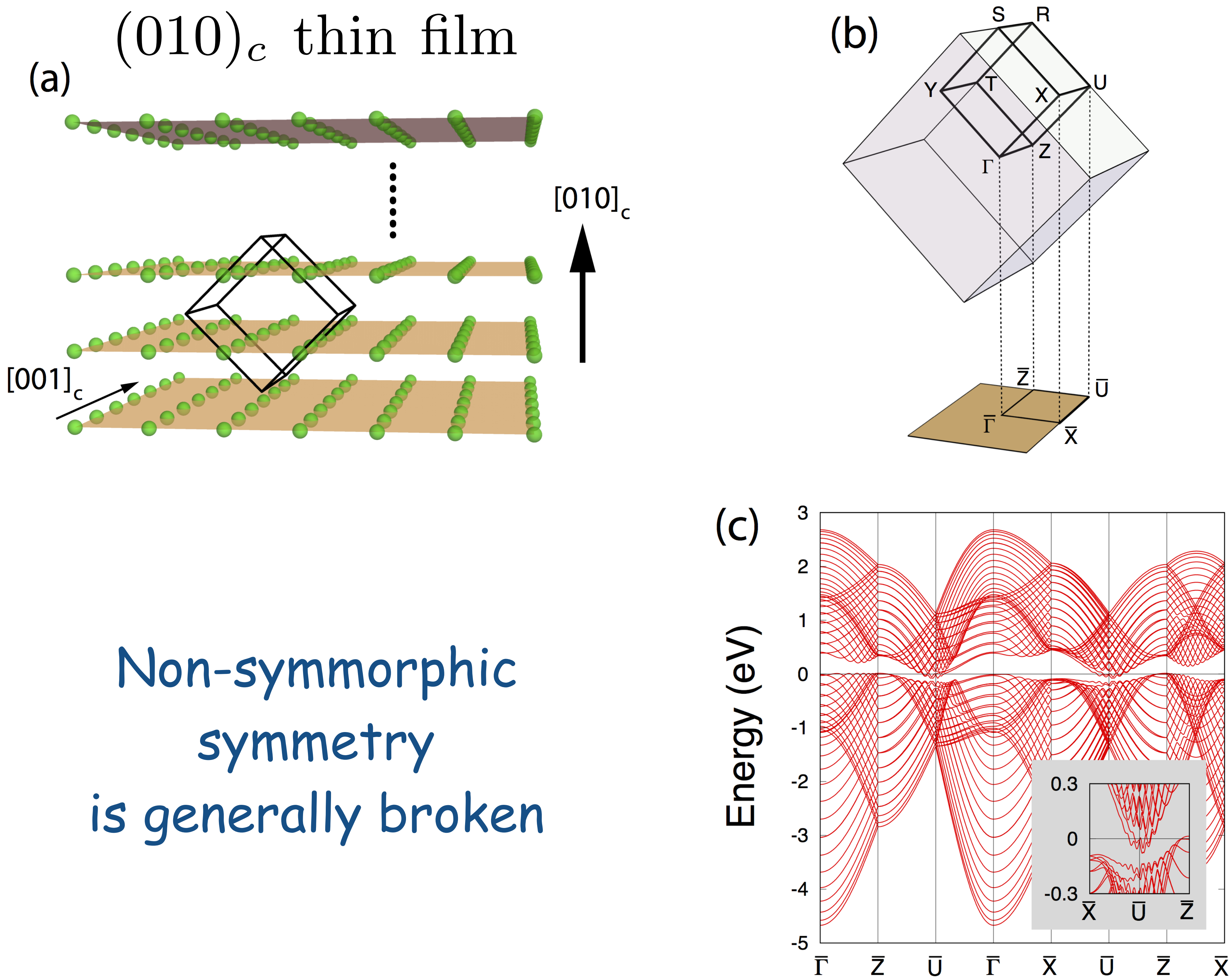


Robust to perturbations (bulk)

Spin Hall conductivity remains very large even when the non-symmorphic symmetry is broken such that the nodal line is gently gapped out.

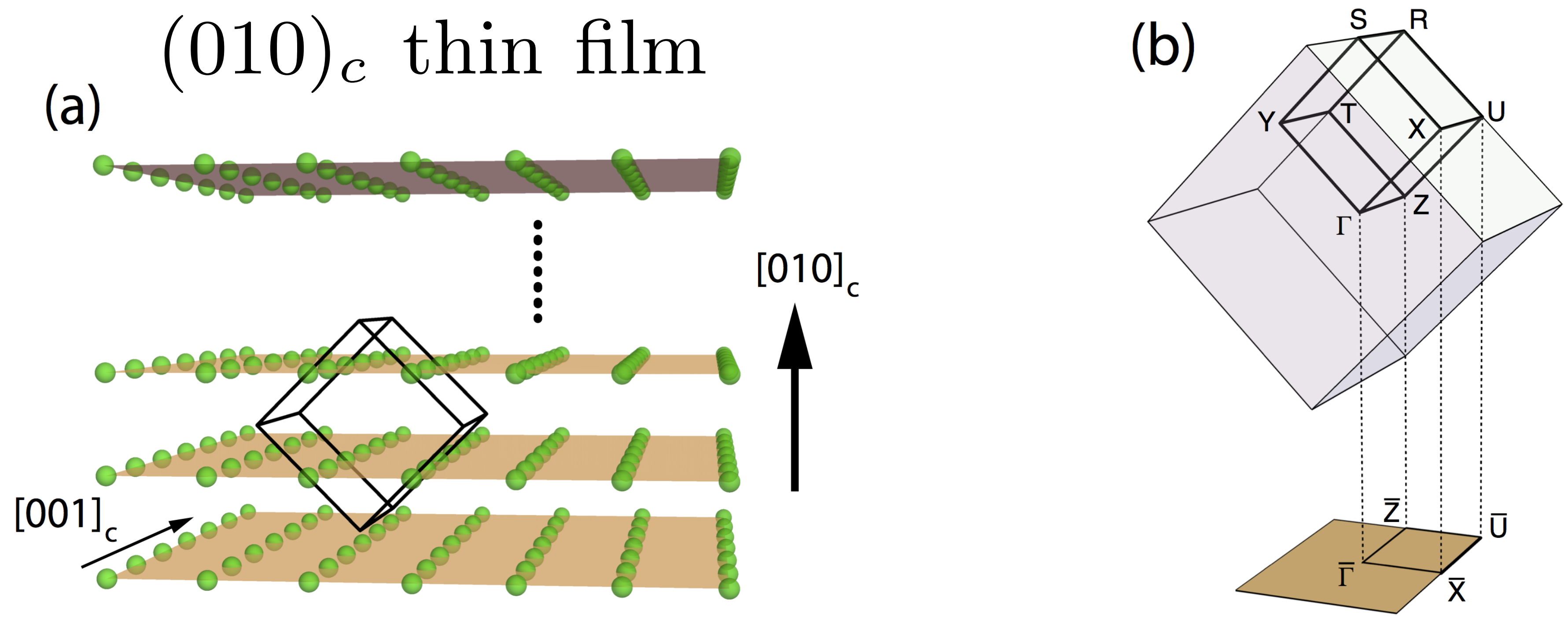
Nodal line itself does not contribute much to the spin Hall conductivity. However, the nearly degenerate energy level structures are robust and provide large contributions

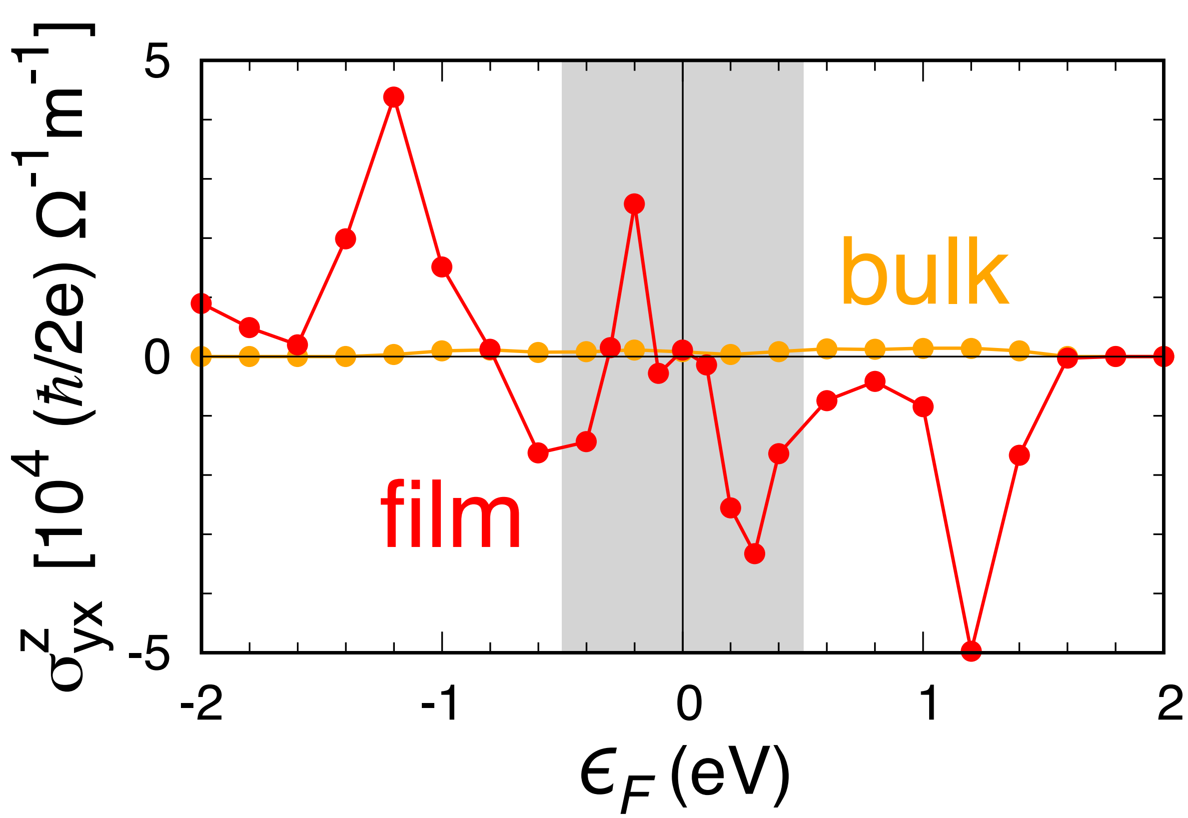
Intrinsic Spin Hall Conductivity in Films



Non-symmorphic symmetry is generally broken

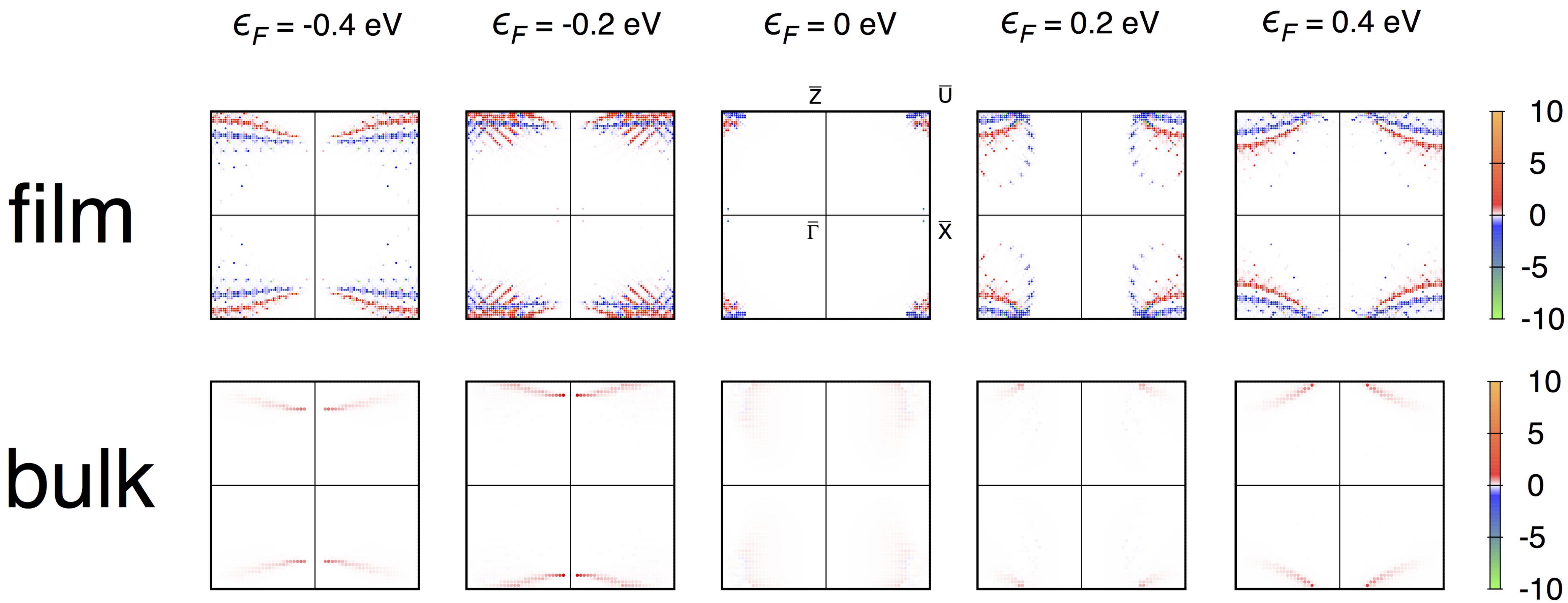
Intrinsic Spin Hall Conductivity in Films

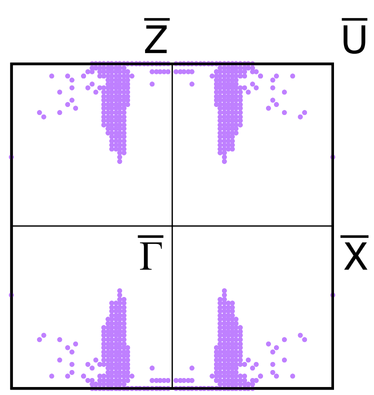




Large enhancement of the spin Hall conductivity

$$\Omega^z_{yx}(\mathbf{k})$$

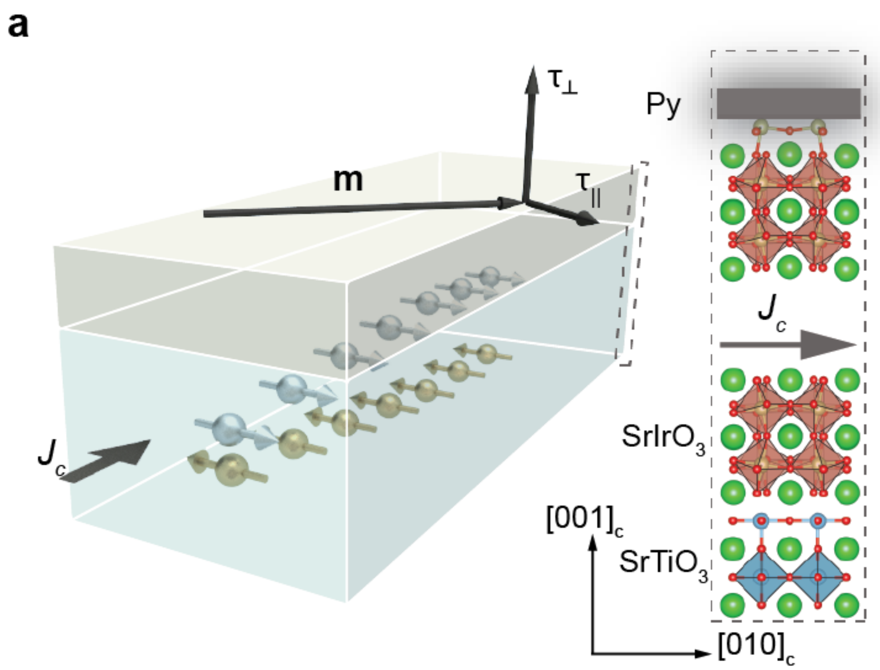




Large contributions from "modified" bulk states, not from the surface states

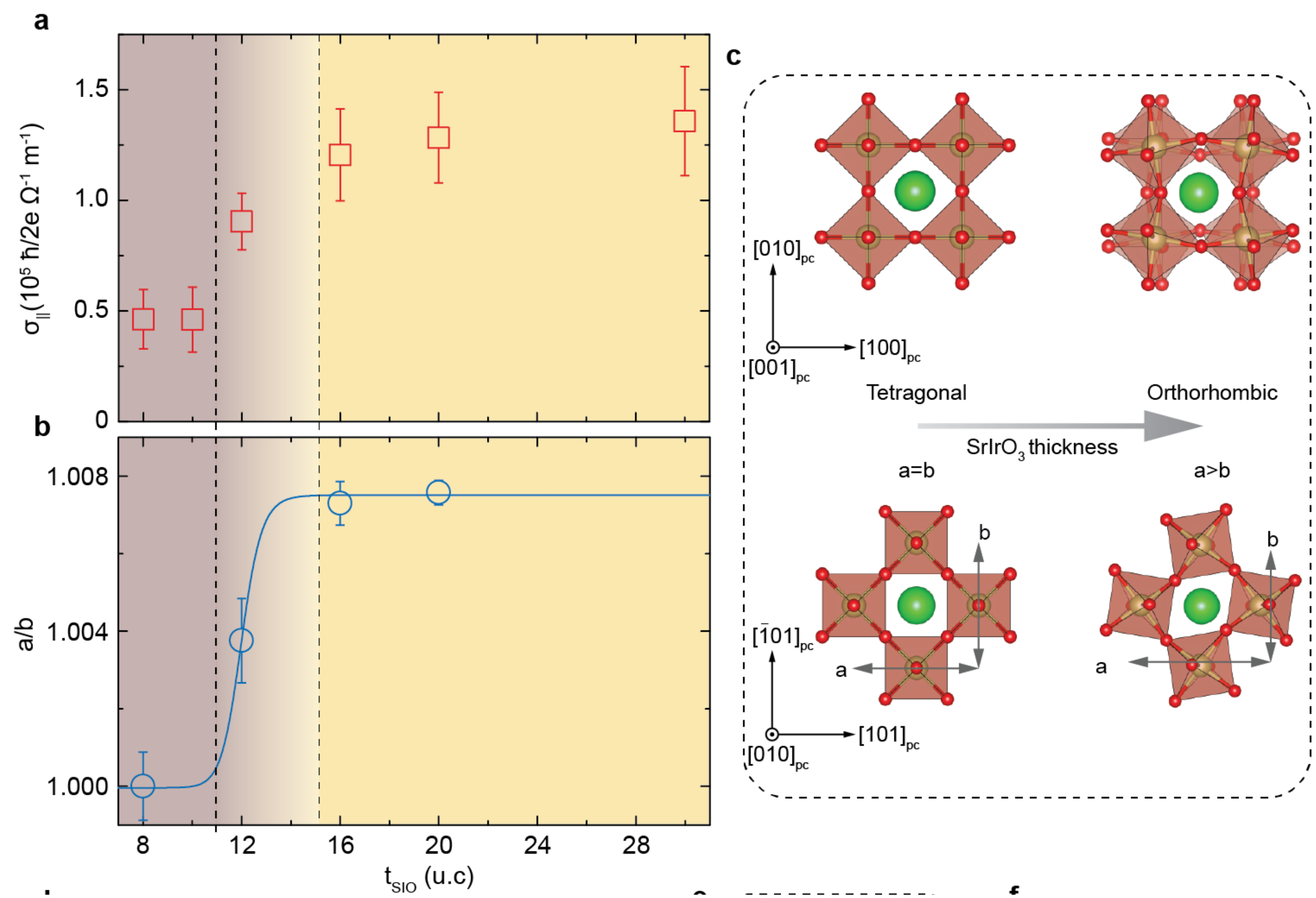
location of surface states

Won't be too sensitive to the interface (with FM)



1nm Al_2O_3
3.5nm Py
8nm (20 uc) $SrIrO_3$

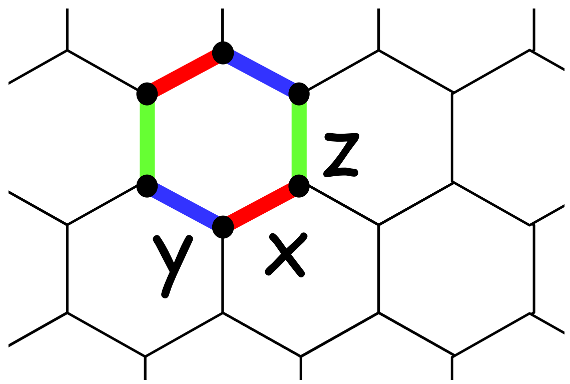
Chang-Bom Eom,
Dan Ralph et al.
(unpublished)



ST-FMR
measurement

Observation of
Large Spin-Hall
Conductivity !

Kitaev Model: Exact Solution



$$\mathcal{H}_{\rm K} = -\sum_{\alpha-links} S_i^\alpha S_j^\alpha$$

$$S_i^\alpha = \frac{1}{2} i b_i^\alpha c_i \qquad \{b_i^x, b_i^y, b_i^z, c\}$$

Four Majorana Fermions

$$\mathcal{H}_K = -\frac{i}{4} \sum_{\alpha-links} u_{ij}^\alpha c_i c_j \qquad u_{ij}^\alpha = i b_i^\alpha b_j^\alpha$$

$\mathcal{W}_P = \prod_{\text{loop}} u_{ij}^\alpha$ commute with the Hamiltonian $\Longrightarrow \mathcal{W}_P = \pm 1$

$$W_p = 2^6 S_1^x S_2^y S_3^z S_4^x S_5^y S_6^z$$

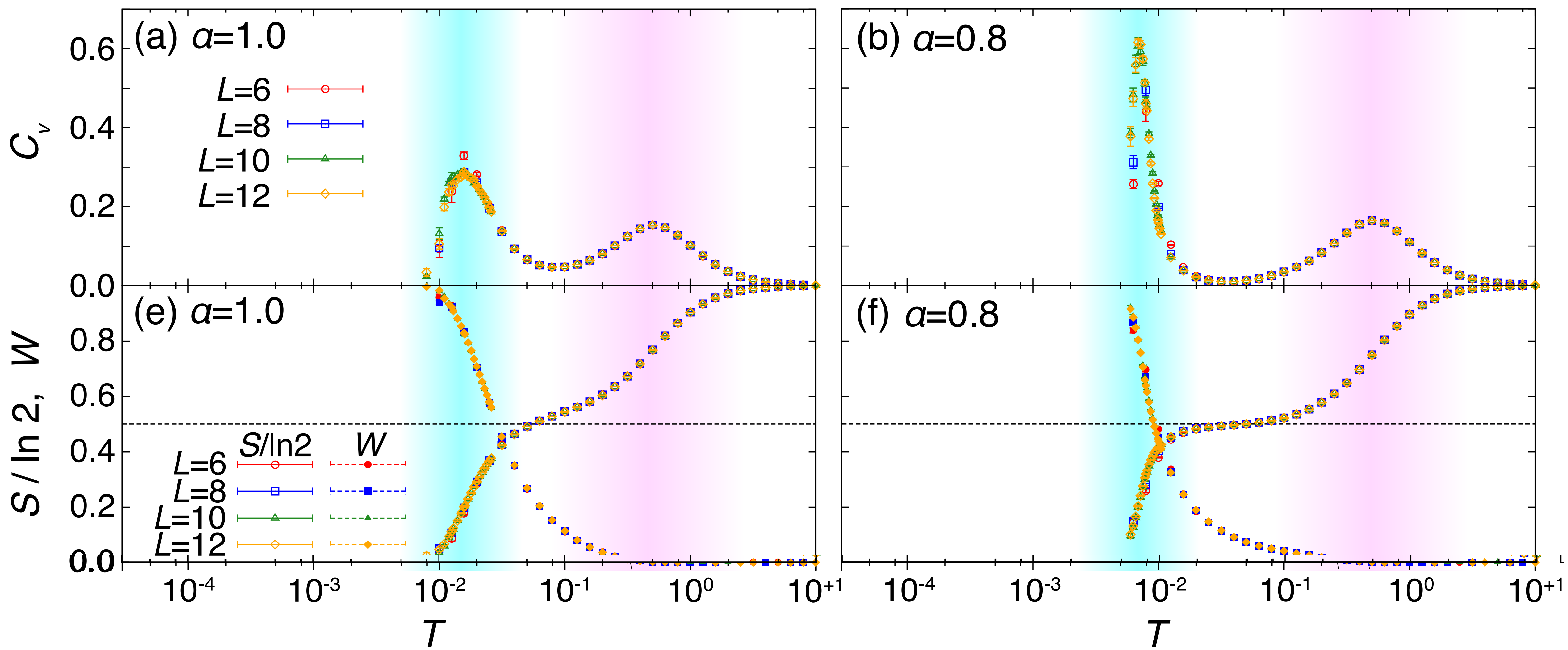
Ground state is in the zero-flux sector $u_{ij}^\alpha = +1 \, (\forall \langle ij \rangle)$

Flux excitations can be created at finite temperatures

$W_p = -1$ for some loops

Specific Heat and Thermal Entropy

Kitaev model at finite temperature

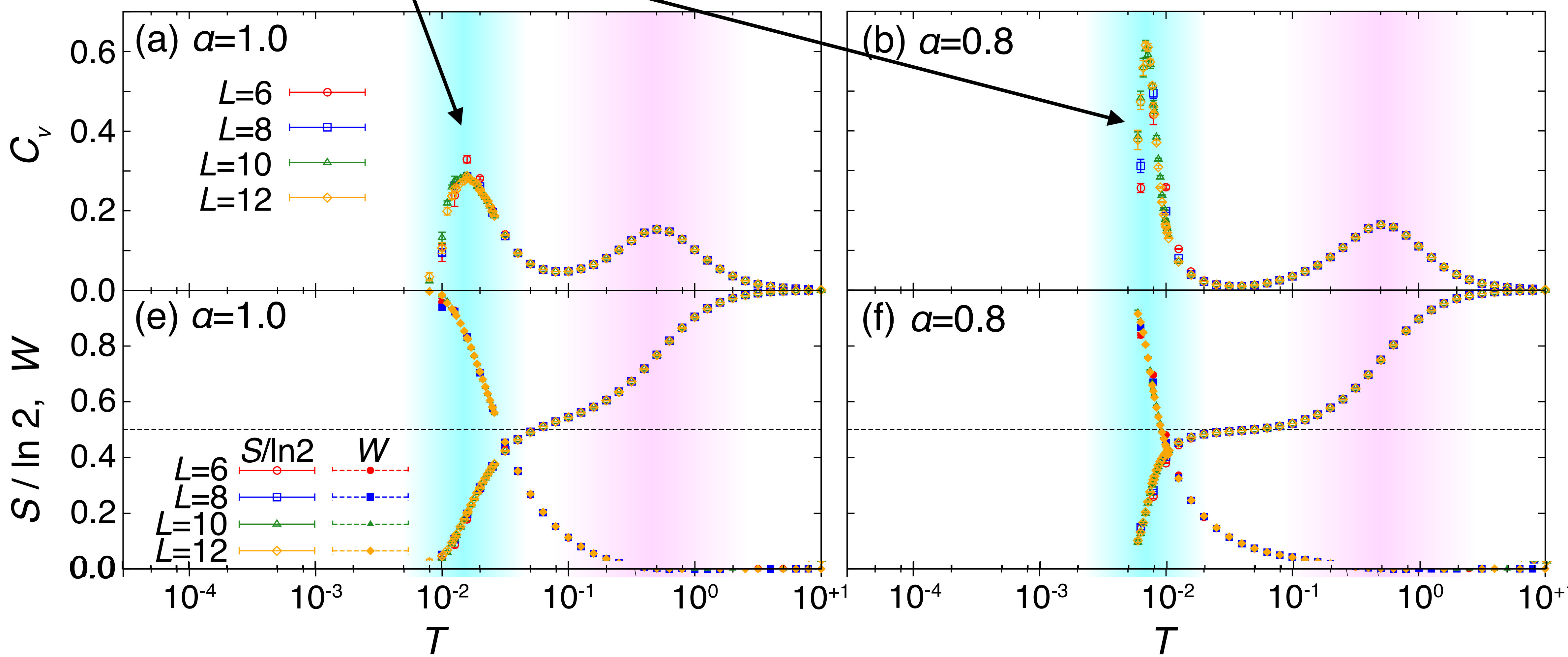


J. Nasu, M. Udagawa, Y. Motome (2015)

Specific Heat and Thermal Entropy

exciting flux
degree of freedom

$$\mathcal{W}_P = \prod_{\text{loop}} u_{ij}^{\alpha} = -1$$



Specific Heat and Thermal Entropy

exciting flux degree of freedom

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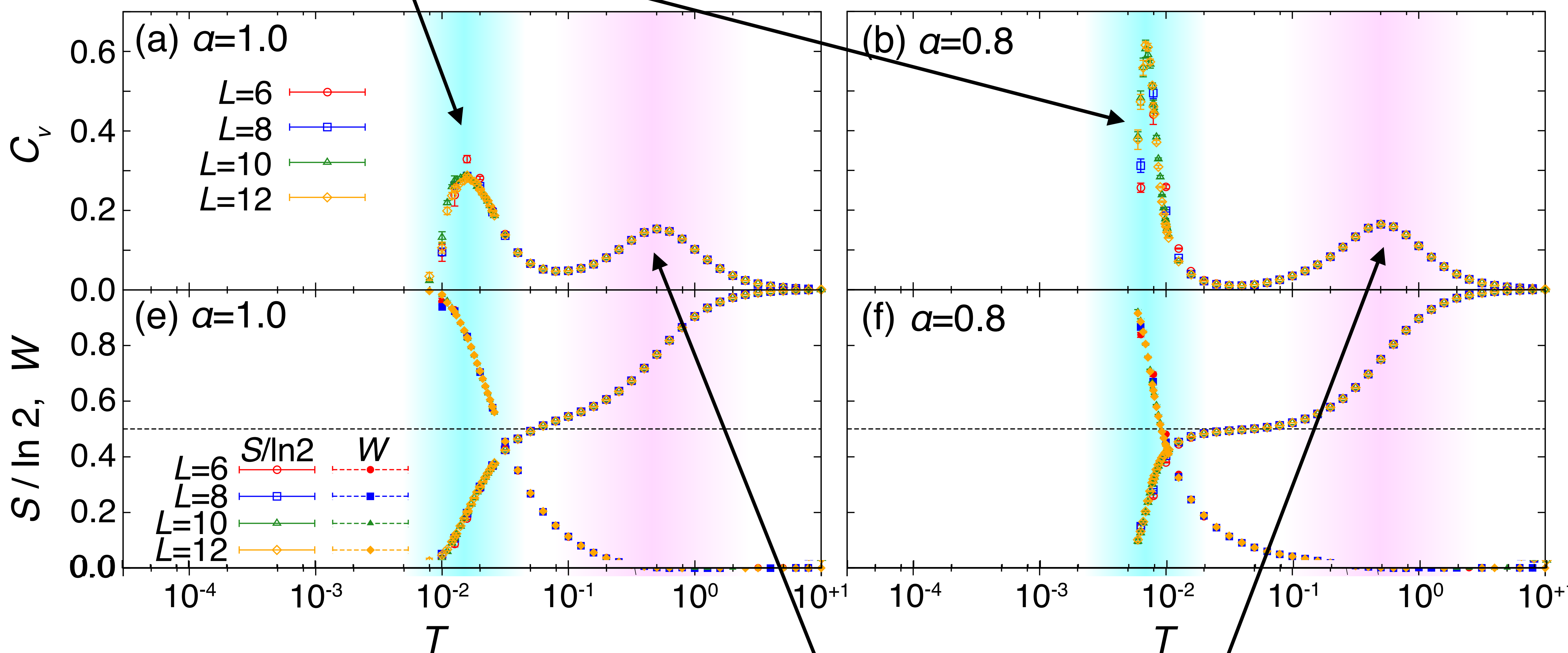
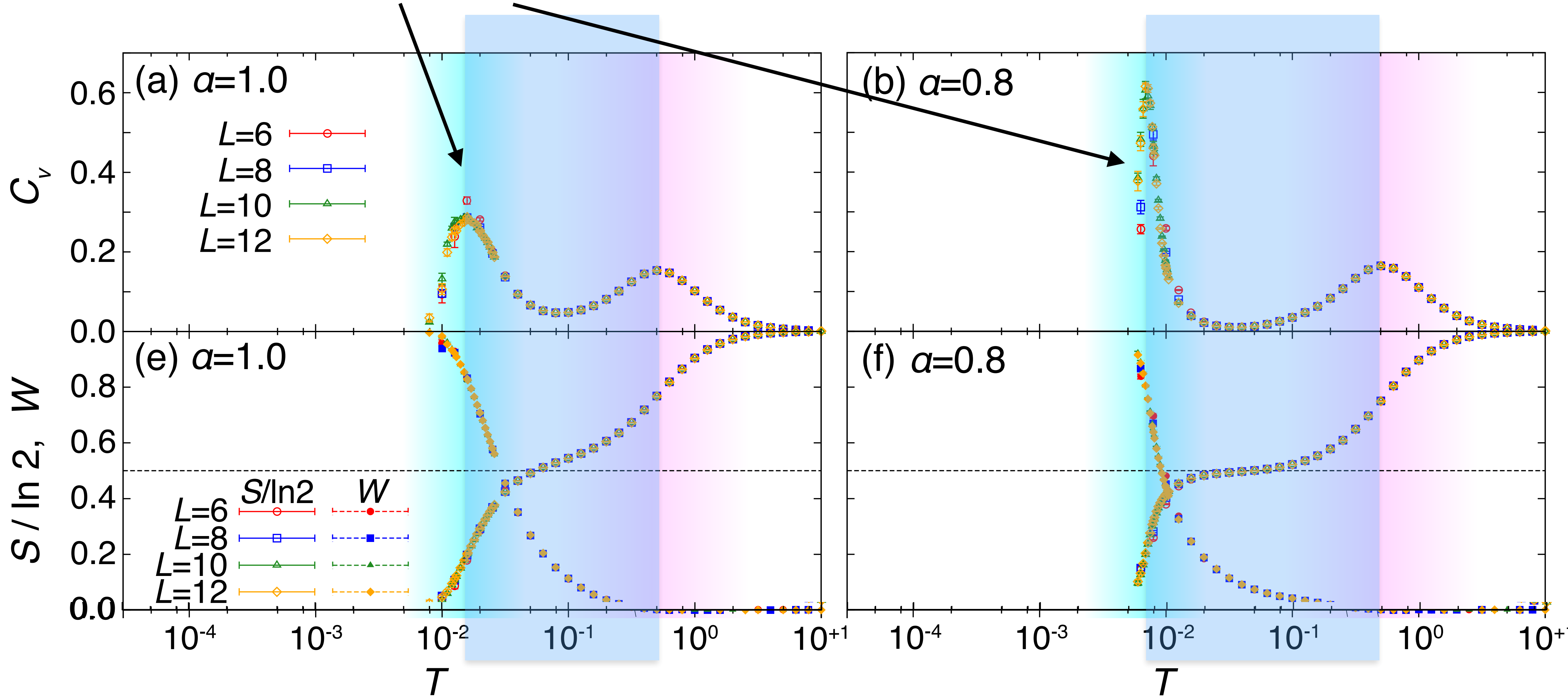


emergence of short-range spin correlations

Specific Heat and Thermal Entropy

exciting flux
degree of freedom

$$\mathcal{W}_P = \prod_{\text{loop}} u_{ij}^{\alpha} = -1$$

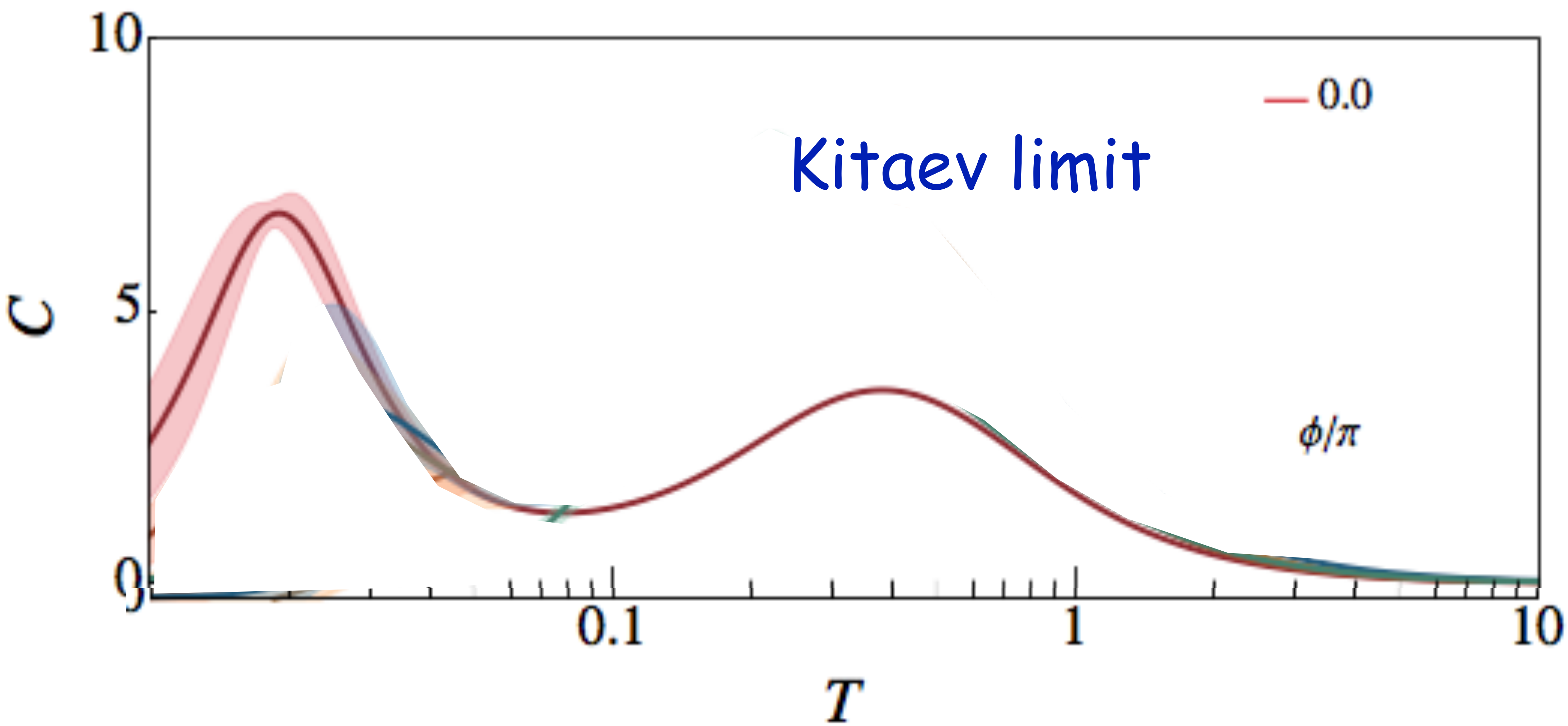


Majorana fermions in the background of thermally excited fluxes

Specific Heat (Yamaji, thermal pure quantum state)

$$K^z = -(1+2a)\cos\phi$$
$$K^x = K^y = -(1-a)\cos\phi$$
$$\Gamma = \sin\phi$$

a = 0.1



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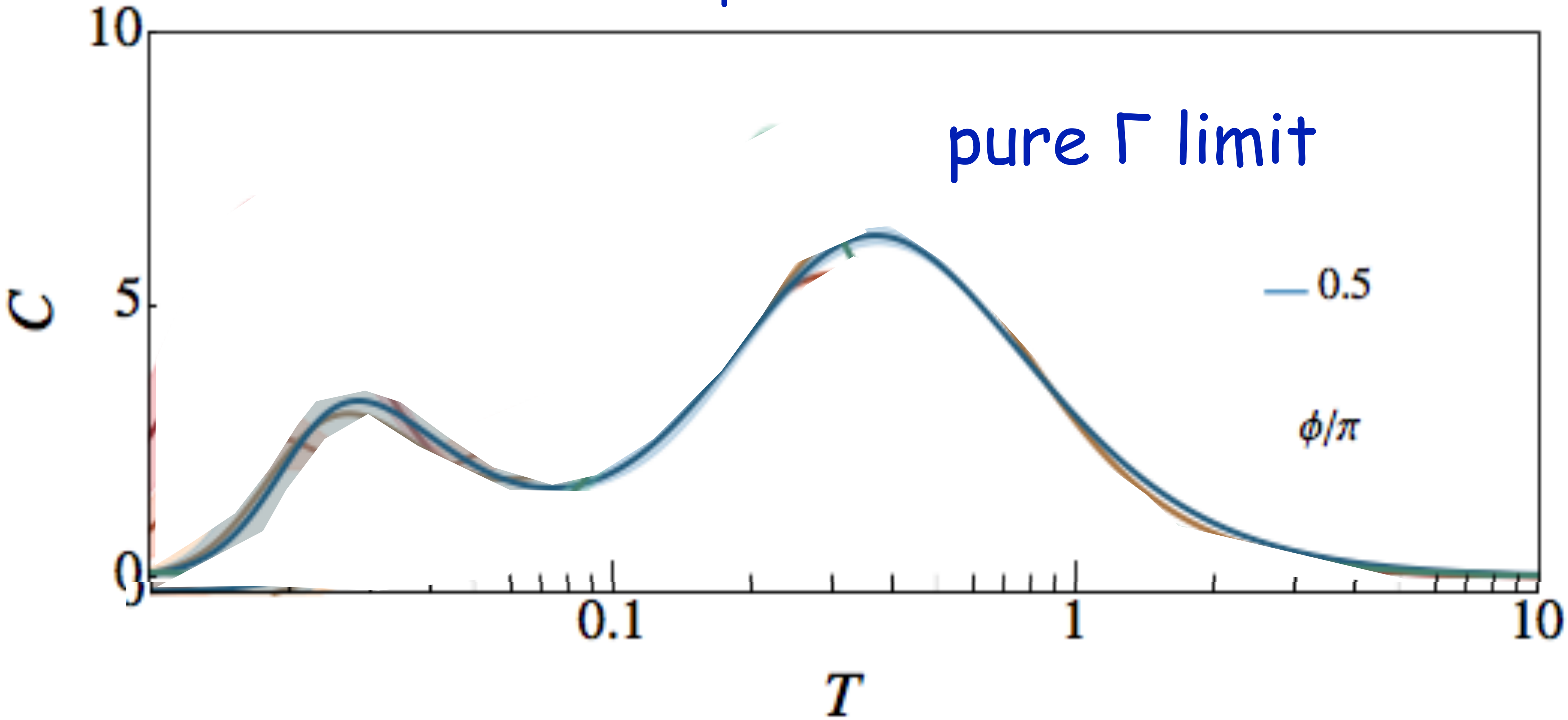
two-peak structure survives !



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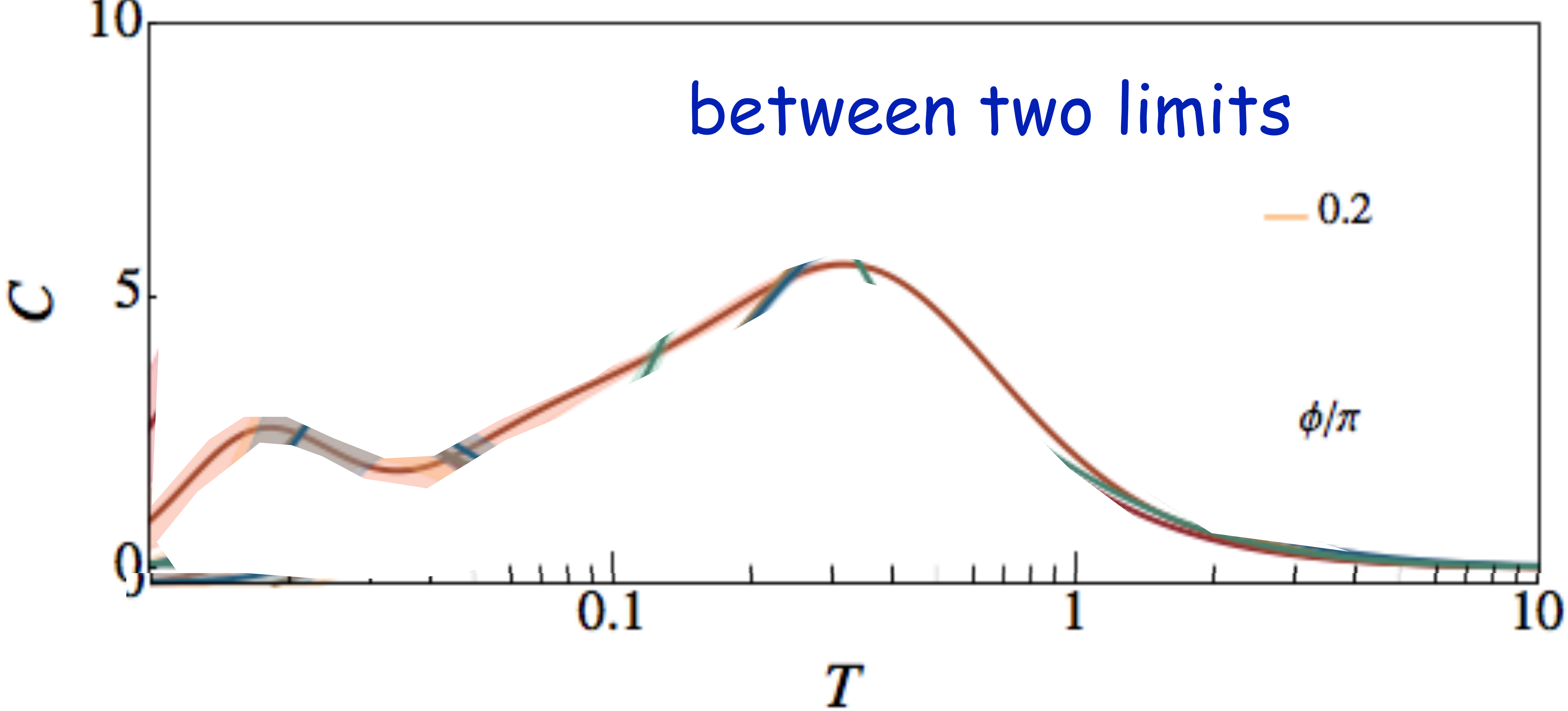

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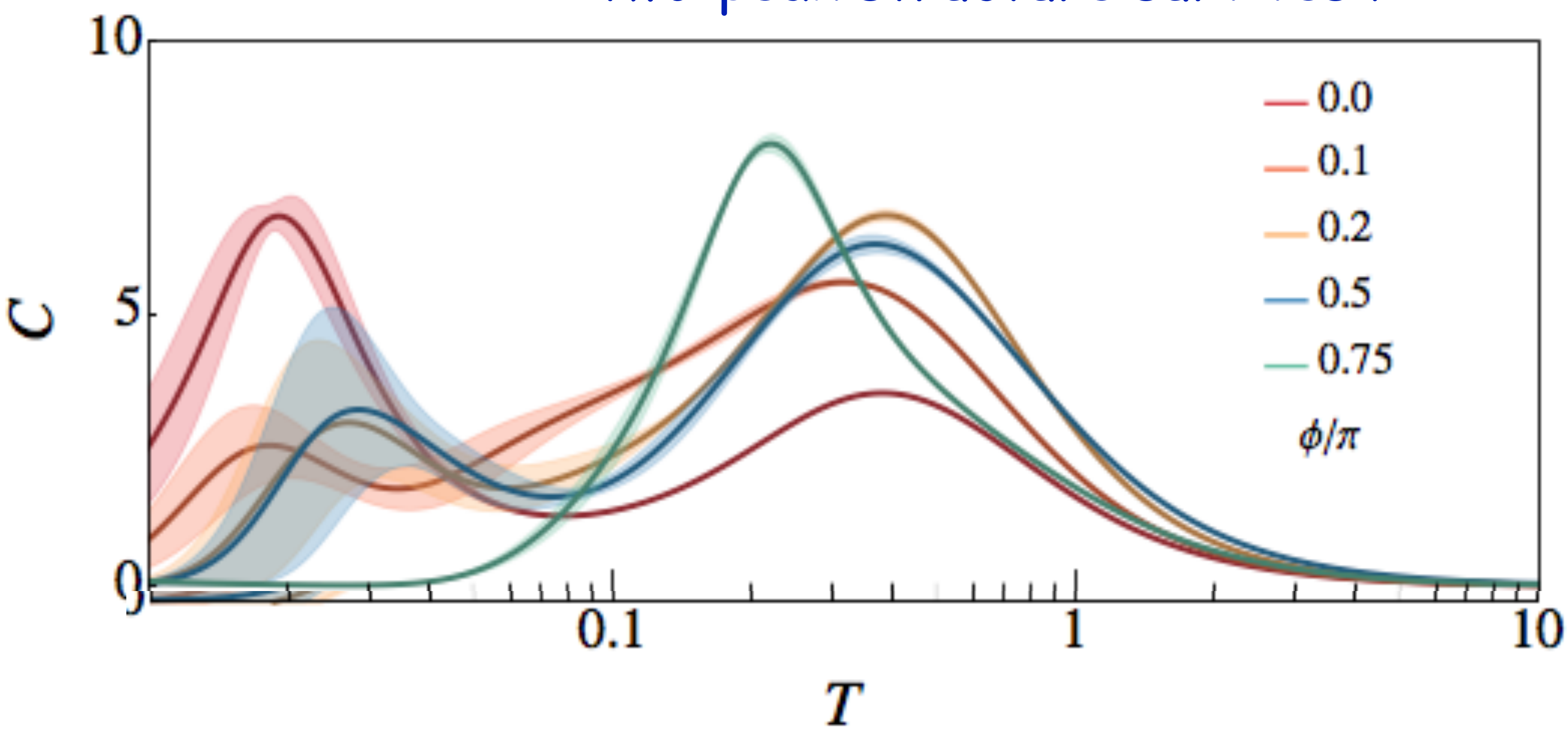


Exact Diagonalization

24-site cluster

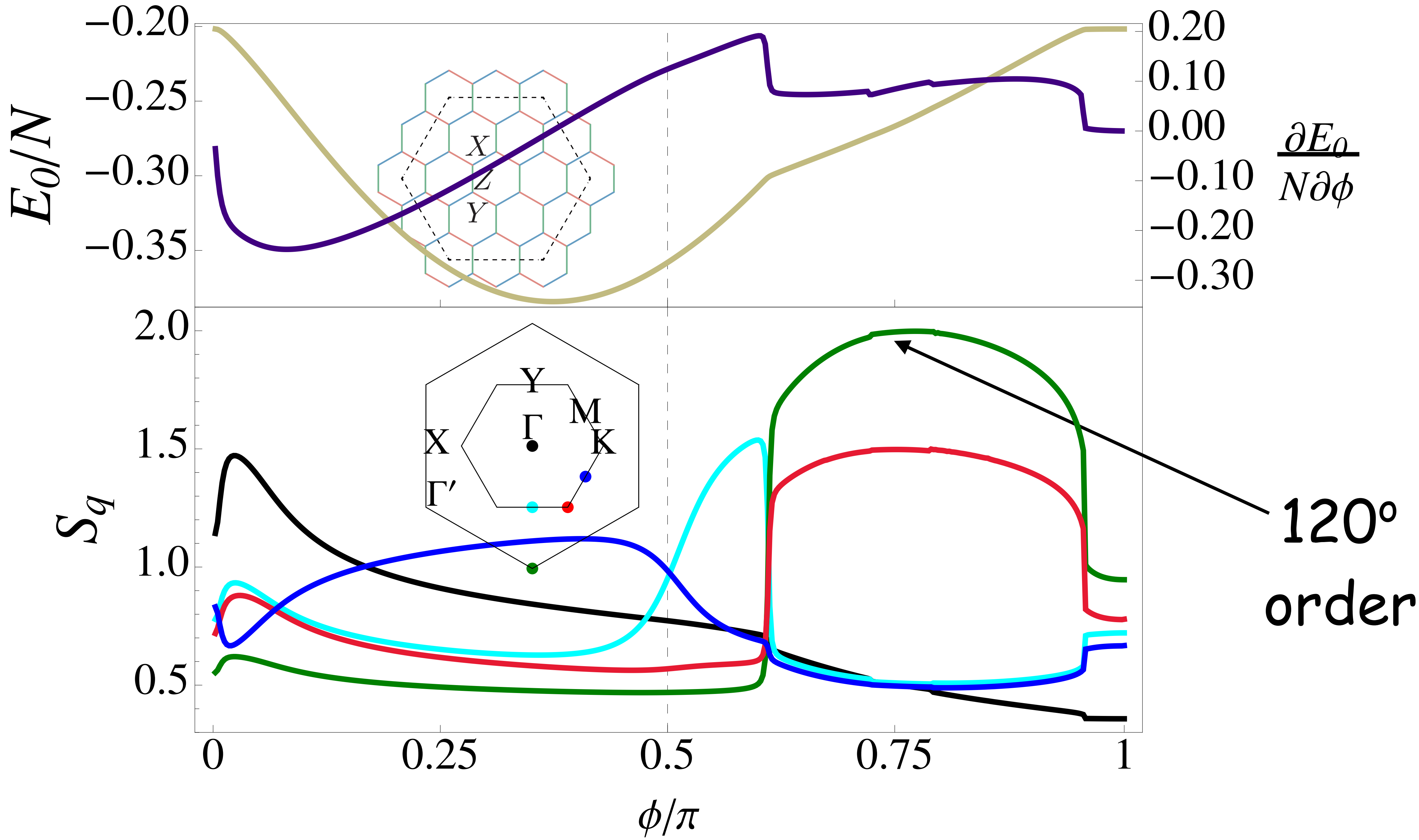
(Catuneanu, Yamaji)

a = 0.1

$$K^z = -(1+2a)\cos\phi$$

$$K^x = K^y = -(1-a)\cos\phi$$

$$\Gamma = \sin\phi$$



Exact Diagonalization

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(Catuneanu, Yamaji)

a = 0.1

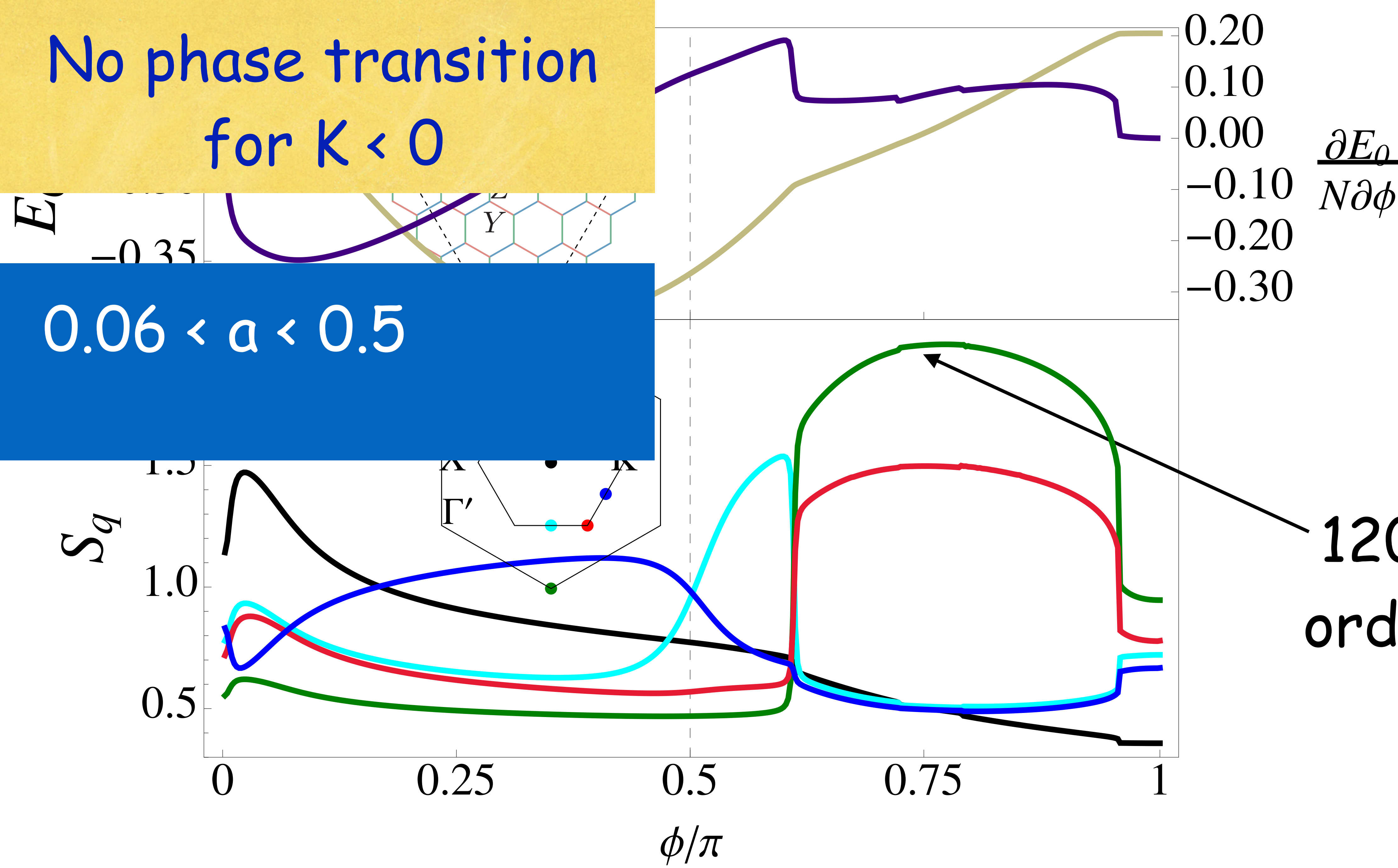
$$K^z = -(1+2a)\cos\phi$$

$$K^x = K^y = -(1-a)\cos\phi$$

$$\Gamma = \sin\phi$$

No phase transition for K < 0

0.06 < a < 0.5



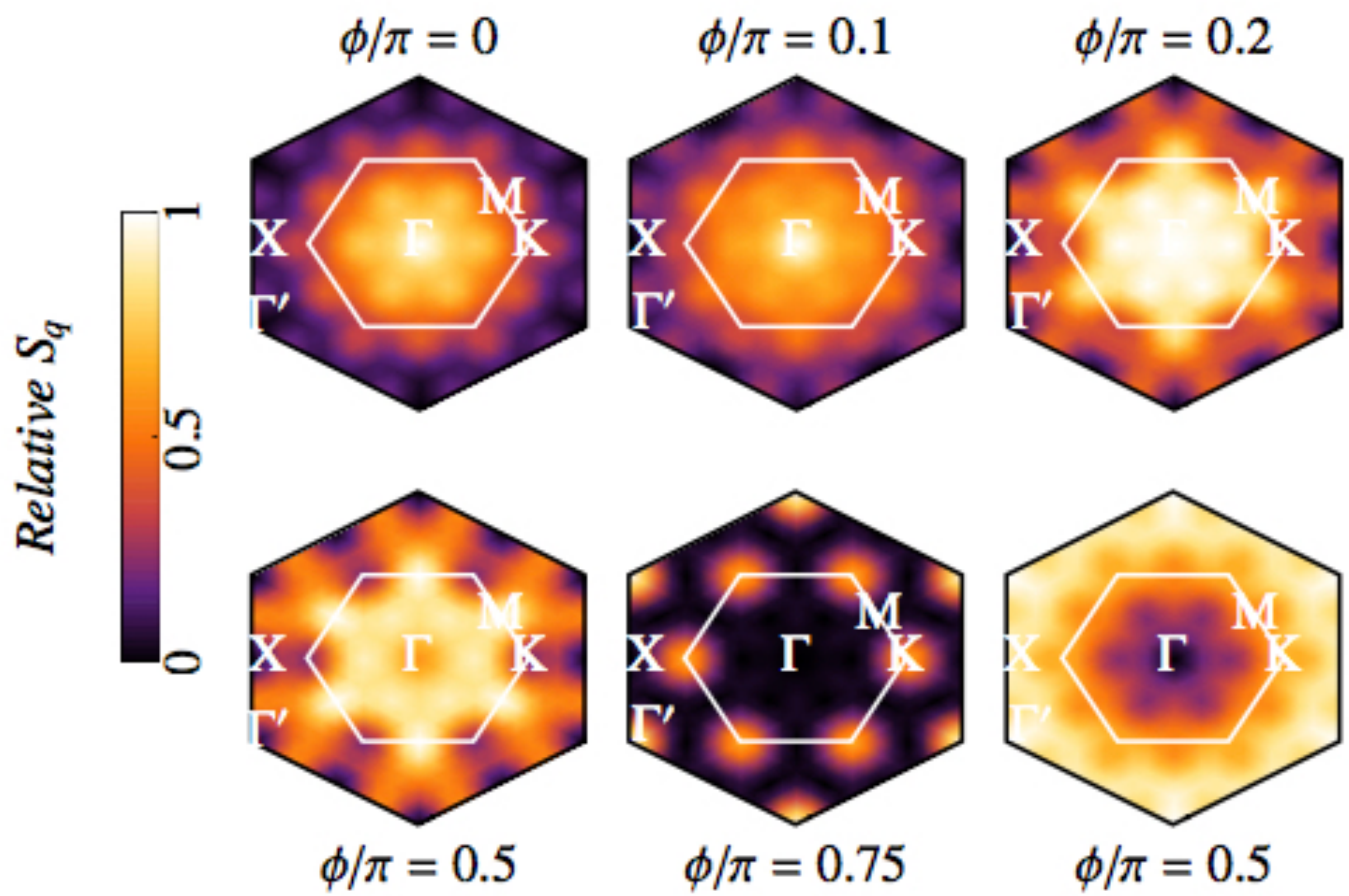
120° order

Static Structure Factor

$$S_{\mathbf{q}} = \frac{1}{N}\sum_{i,j} e^{i(\mathbf{r}_i - \mathbf{r}_j)\cdot\mathbf{q}}\langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle$$

ED 24-site cluster

a = 0.1



Enhanced spin correlation at M point as Γ increases when K is negative (Ferro-like)

$\phi = 0.2\pi$ similar to dynamical structure factor at low energy in experiment