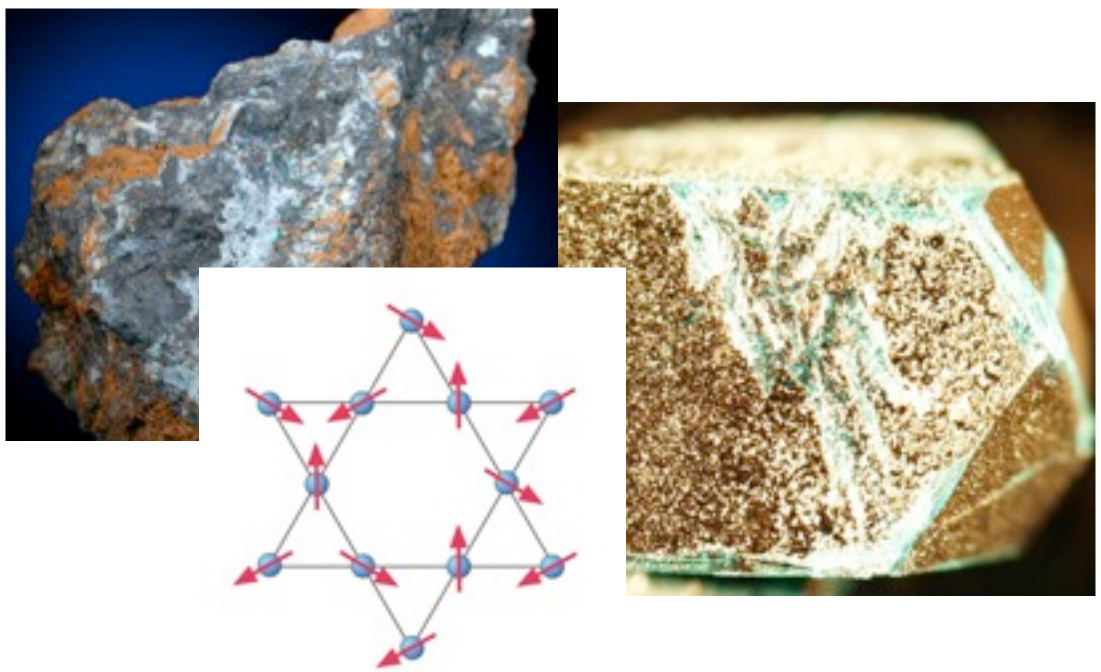
Frustrated magnetism and topology in spin-orbit Mott insulators

Ronny Thomale

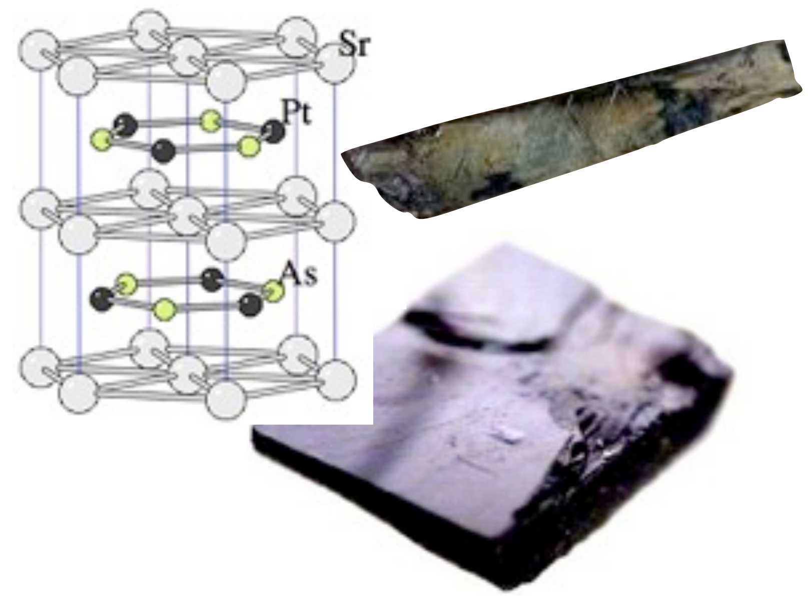
KITP, UC Santa Barbara, LSMATTER, 24th of September 2015

Correlated electron systems

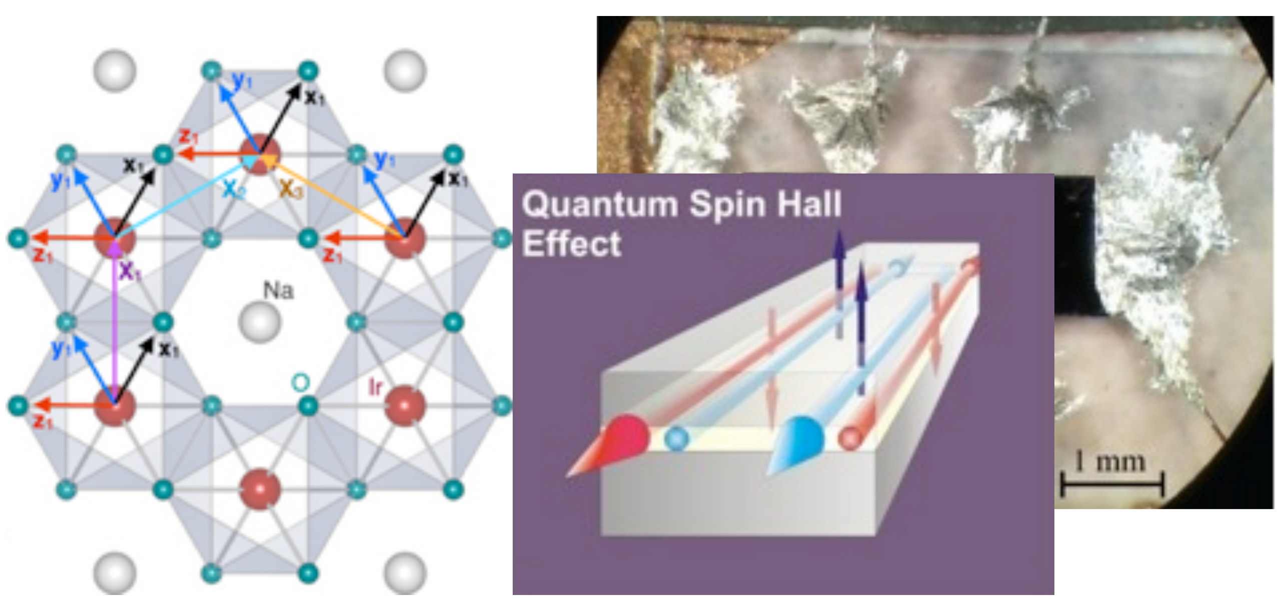
Frustrated Magnetism



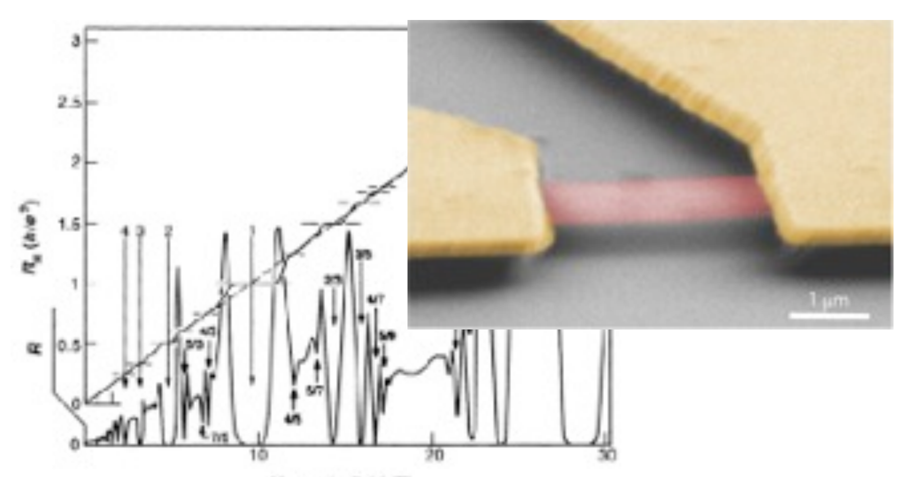
Superconductivity



Spin-orbit Phenomena



Quantum Hall Effect



Correlated electron systems

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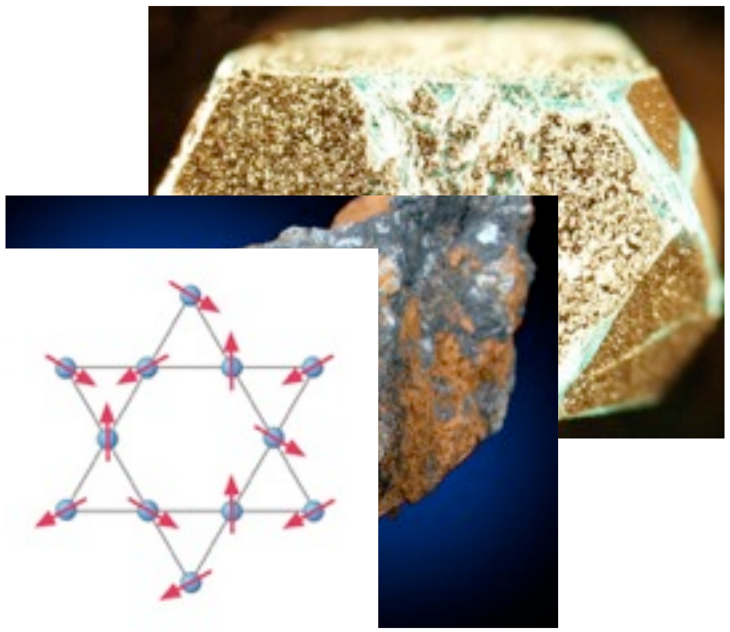

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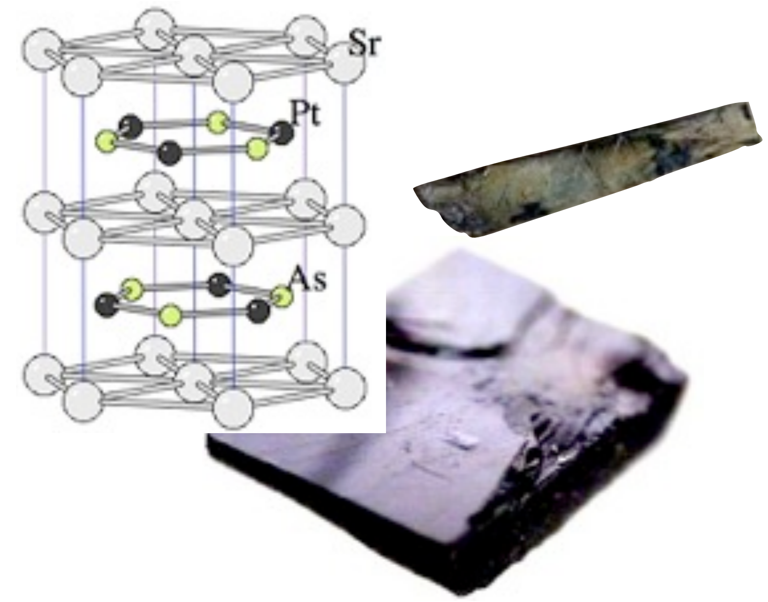

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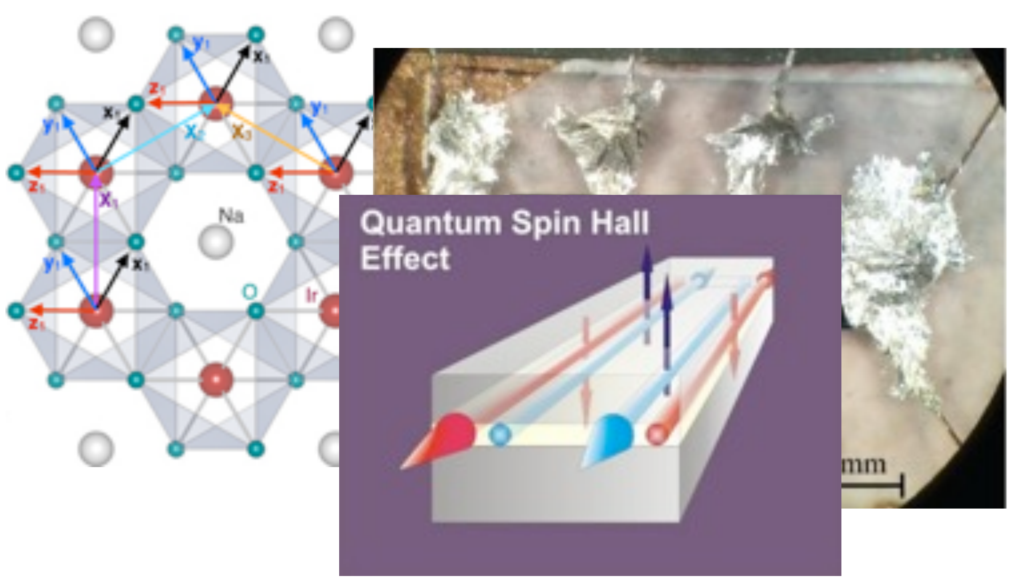

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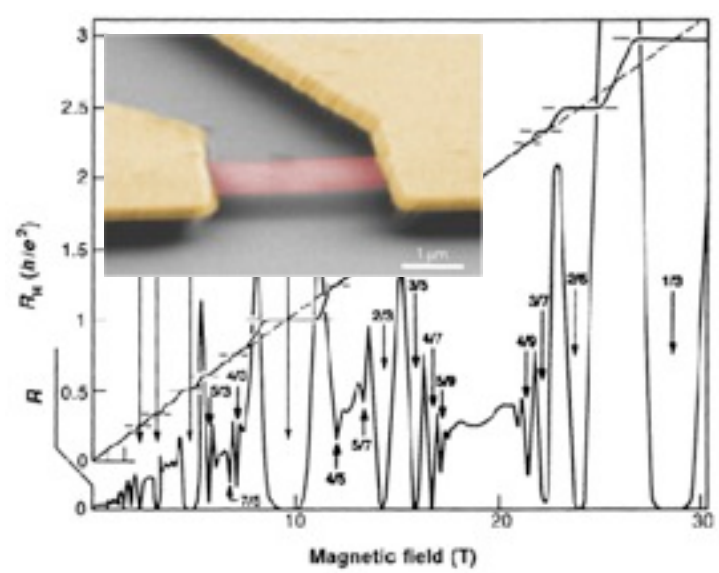

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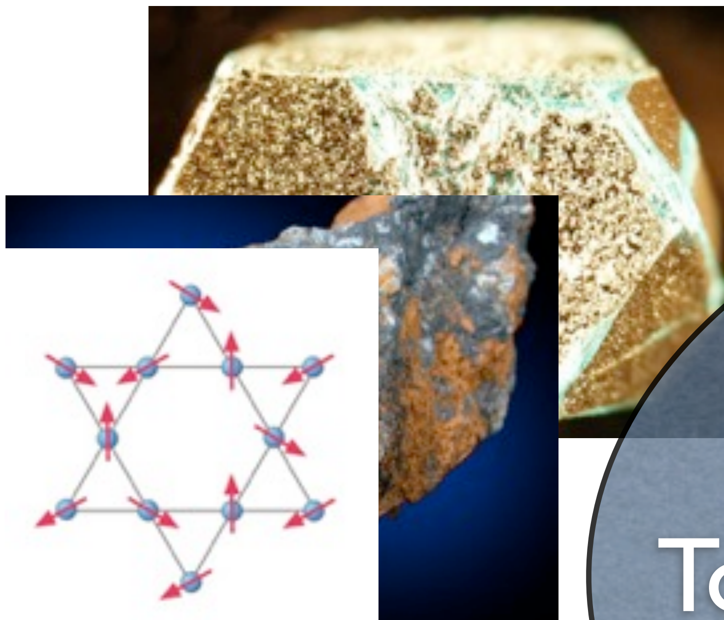

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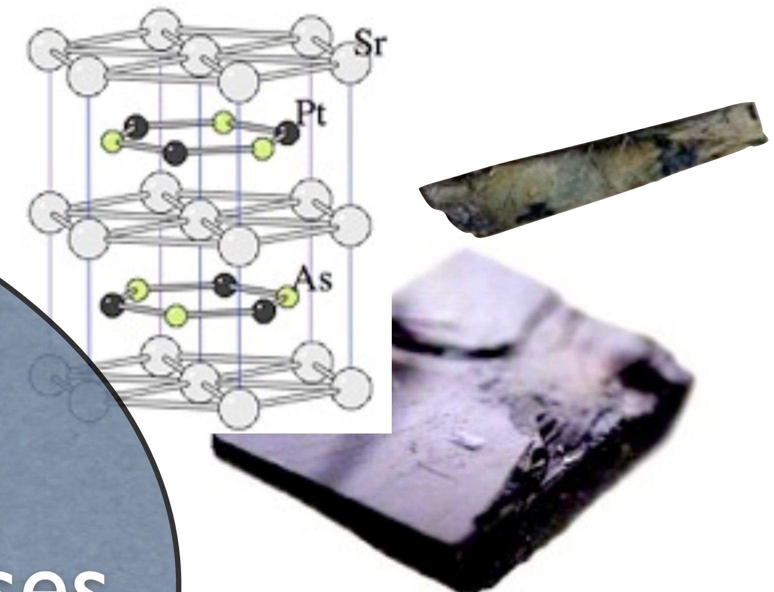
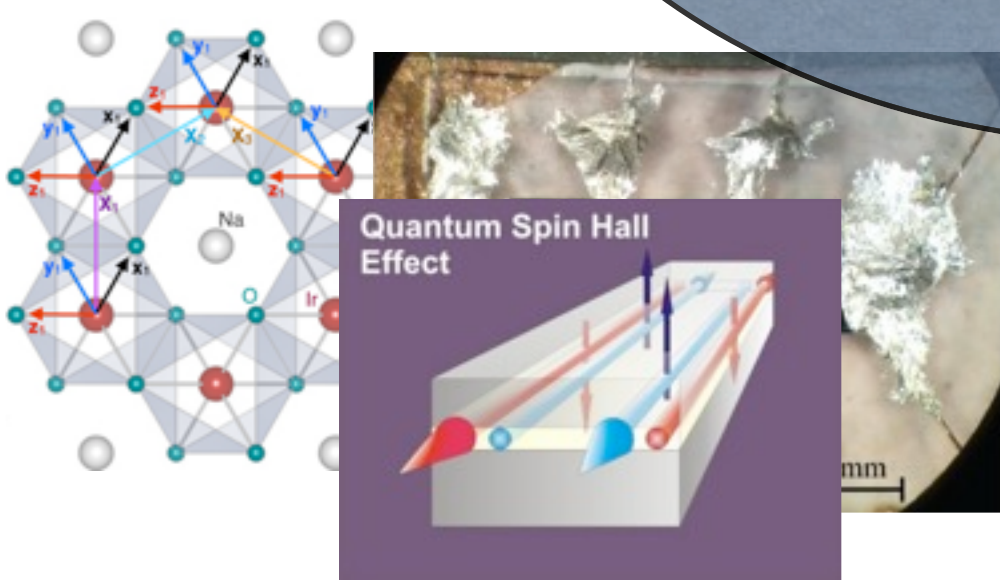
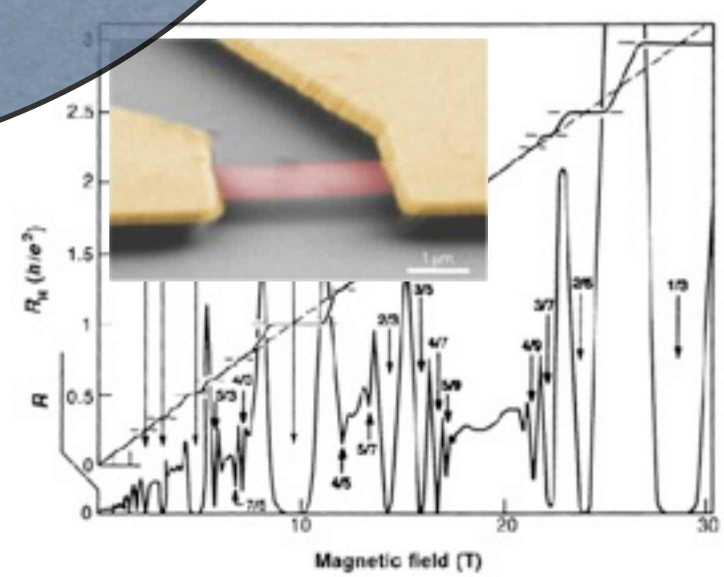


Topological Quantum Phases

Spin-orbit Phenomena

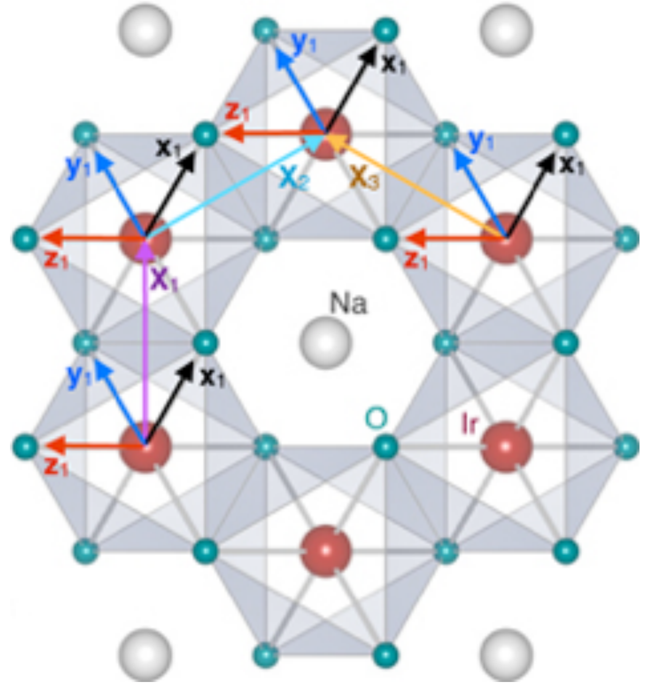


Quantum Hall Effect

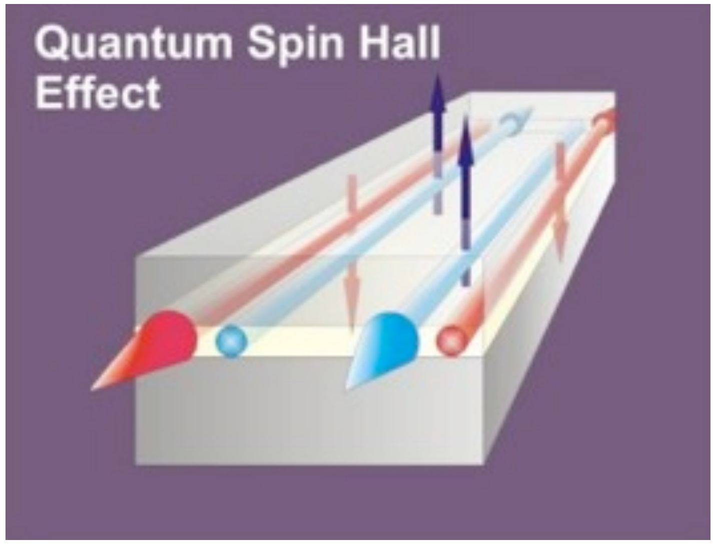


Spin-orbit coupling, correlations, and topology

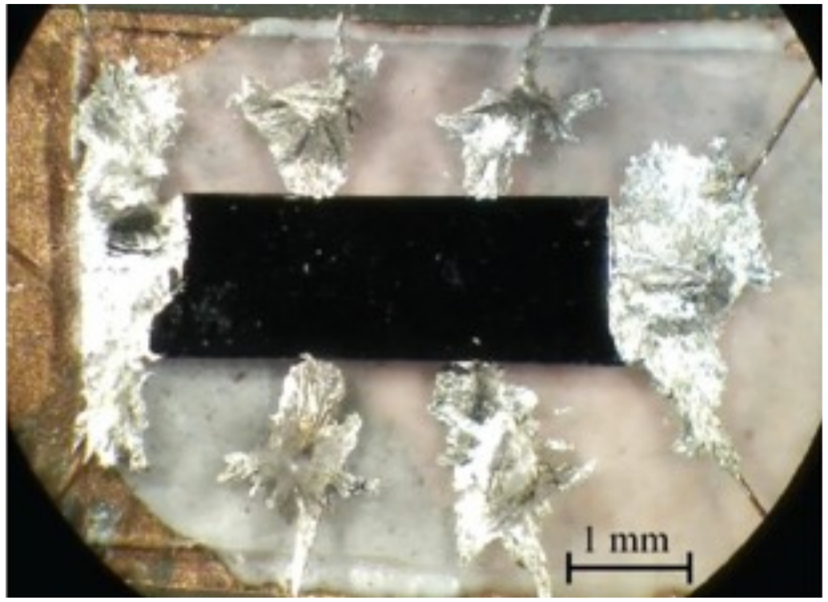
Frustrated anisotropic magnetism



Interacting topological insulators

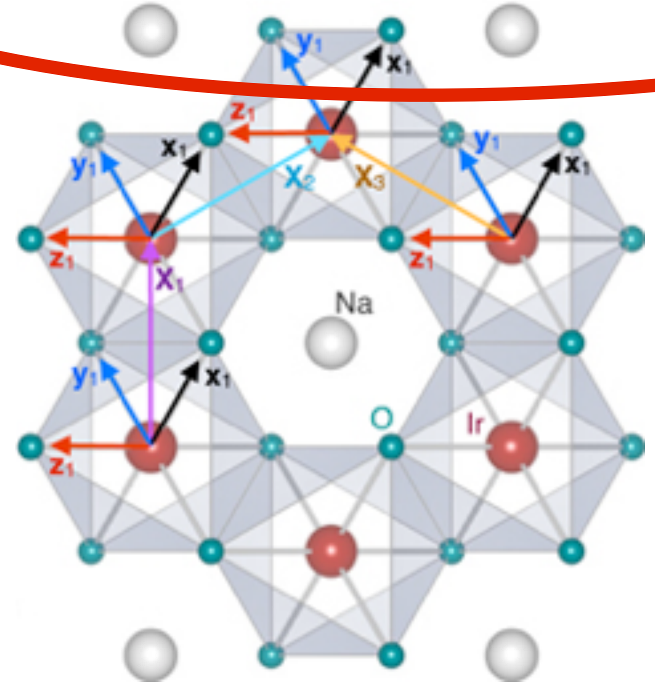


Localized/itinerant topological insulators

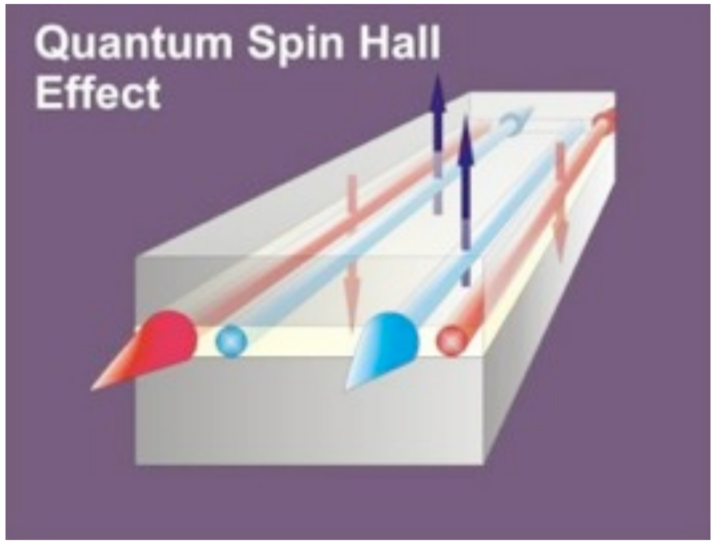


Spin-orbit coupling, correlations, and topology

Frustrated anisotropic magnetism



Interacting topological insulators



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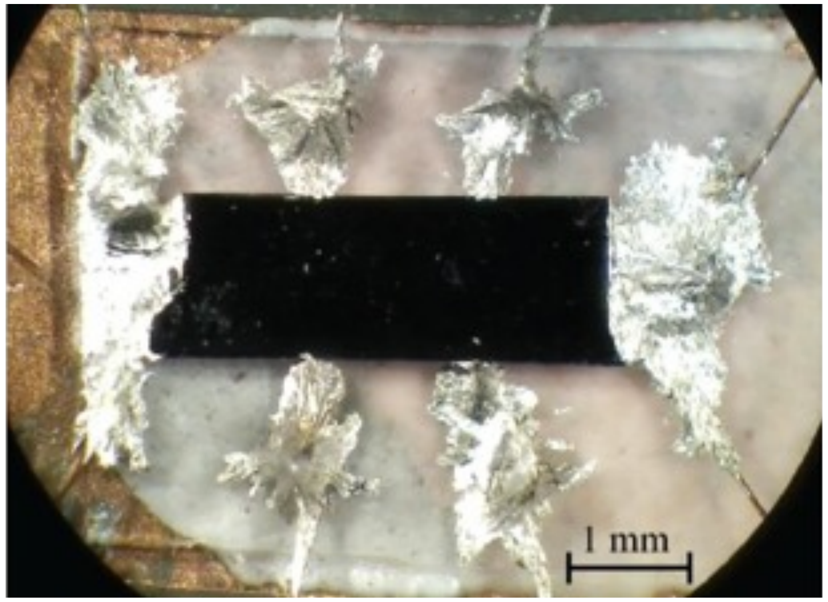

Recent collaborators

Schnells

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DRESDEN

Universität
Augsburg
University

Gegenwart

Outline

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Heisenberg-Kitaev model

- Relevant parameter regime for honeycomb Iridates
- Zig-zag magnetic order revisited

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Strong coupling limit of topological insulators

- XY-AFM in the Kane-Mele model
- Spiral transition and QSH* phase in the Shitade model

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- XY-AFM in the Kane-Mele model
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Chiral spin liquids

- Parent Hamiltonians for the Kalmeyer-Laughlin state
- (Parafermionic) CSLs from anisotropic spin-spin interactions

Pseudofermion functional renormalization group

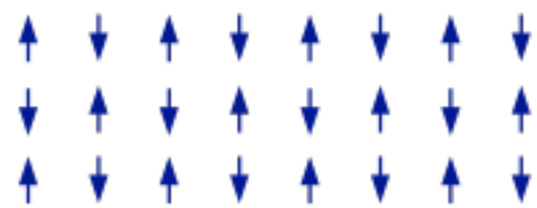
Reuther and Thomale, review in preparation

The scaling problem

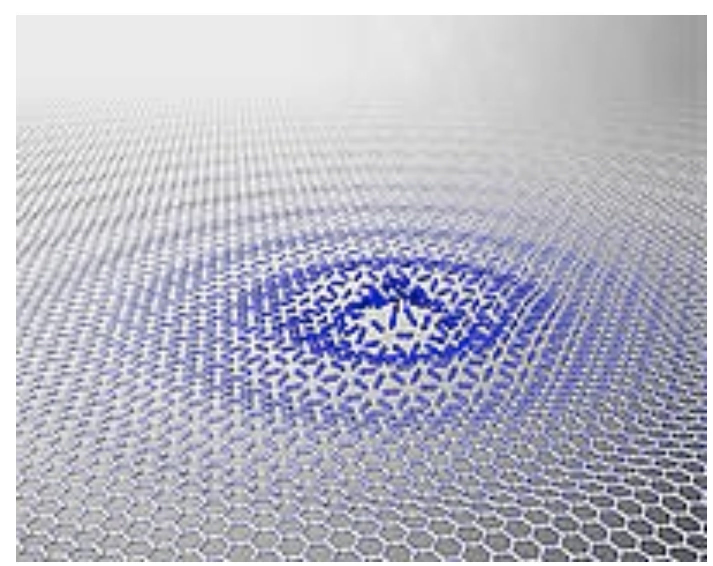
10^5 T[mK]

$$H = J \sum_{\langle i,j \rangle} \vec{S}_i \vec{S}_j$$

10^3 Magnetism

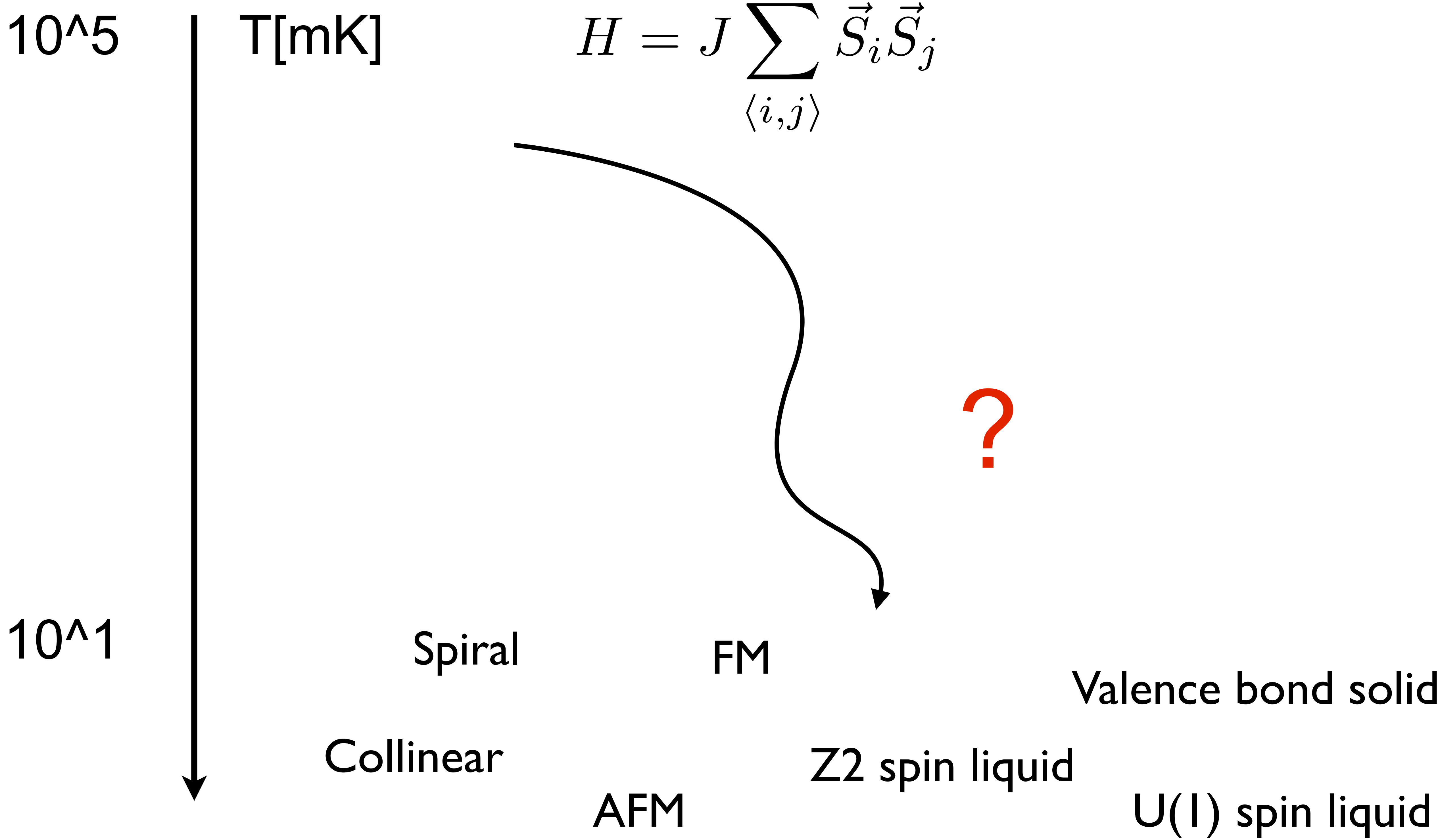


10^1 Frustrated Magnetism



Renormalization group for frustrated magnets

$$H = J \sum_{\langle i,j \rangle} \vec{S}_i \vec{S}_j$$



Short recap on Abrikosov fermions

Spin operator representation by auxiliary fermions:

$$\mathbf{S}_i = \frac{1}{2} \sum_{\alpha,\beta} f_{i\alpha}^{\dagger} \sigma^{\alpha\beta} f_{i\beta}$$

Mean field treatment of single occupancy constraint:

$$Q_i = \sum_{\alpha} f_{i\alpha}^{\dagger} f_{i\alpha} = 1 \qquad \langle Q_i \rangle = \langle Q \rangle = 1$$

Heisenberg model at half filling:

$$H = \sum_{i,j} \mathbf{S}_i \mathbf{S}_i \to \sum_{i,j,\alpha,\beta,\gamma,\delta} V(i,j,\alpha,\beta,\gamma,\delta) f_{i\alpha}^{\dagger} f_{j\beta}^{\dagger} f_{j\gamma} f_{i\delta}$$

Pseudofermion FRG: Cutoff Flow

Λ

$$G_\Lambda(\omega) = \frac{\Theta(|\omega| - \Lambda)}{i\omega + \mu}$$

$\mu = 0 :$ mean single occupancy

$$\Gamma(1', 2'; 1, 2) \sim J_{i_1, i_2} \sigma_{\alpha_{1'}, \alpha_1} \sigma_{\alpha_{2'}, \alpha_2} \delta_{i_{1'}, i_1} \delta_{i_{2'}, i_2}$$

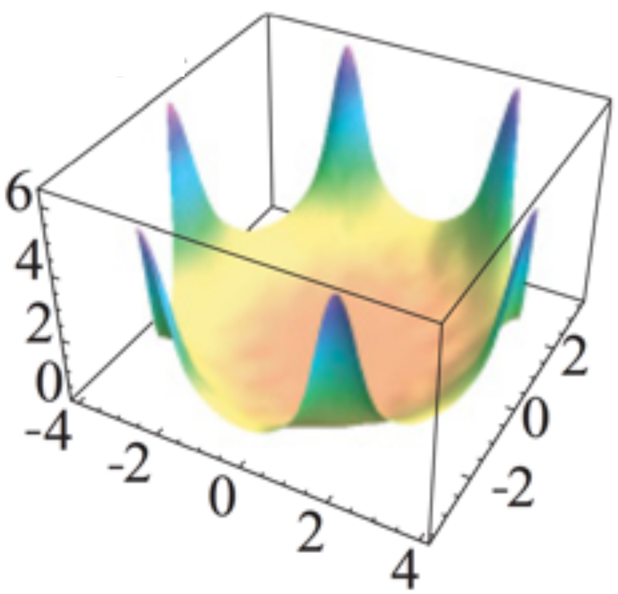
$$G_\Lambda(\omega) = \frac{\Theta(|\omega| - \Lambda)}{i\omega - \Sigma^\Lambda(\omega)}$$

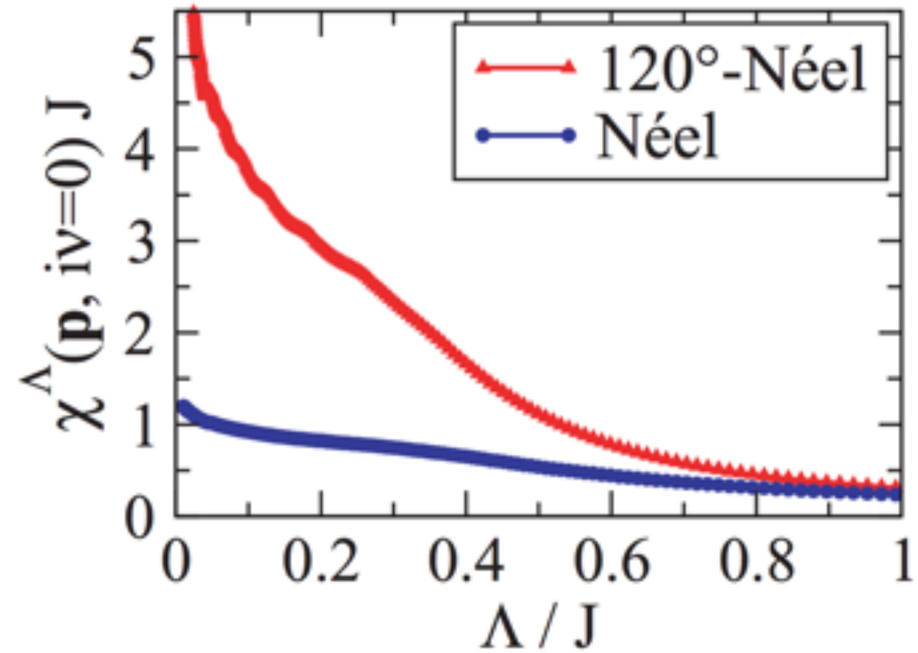
low-energy theory

$$\Gamma_{\mathrm{eff},\Lambda}(1', 2'; 1, 2)$$

Pseudofermion RG

• Flow-driven channels of V(w1, w2, w3, i, j) and a breakdown of the continuous flow specify the type of magnetic order





• Ordering instabilities emerge from the direct particle-hole channel (1/S expansion)

• Paramagnetic phases emerge from the crossed particle-hole channel (1/N expansion)

→ Rather unbiased description of the competition between magnetic order and disorder

Systems studied by PFFRG

J1-J2 model on the square lattice	Reuther and Wölfle Phys. Rev. B 81, 144410 (2010).
J1 model on the anisotropic triangular lattice	Reuther and Thomale Phys. Rev. B 83, 024402 (2011).
J1-J2-J3 model on the square lattice	Reuther, Wölfle, Darradi, Brenig, Arlego, and Richter Phys. Rev. B 83, 064416 (2011).
J1-J2-J3 model on the honeycomb lattice	Reuther, Abanin and Thomale Phys. Rev. B 84, 014417 (2011).
Heisenberg-Kitaev model for Iridates	Reuther, Thomale, and Trebst Phys. Rev. B 84, 100406(R) (2011).
	Singh et al. Phys. Rev. Lett. 108, 127203 (2012).
	Reuther, Thomale, and Rachel Phys. Rev. B 90, 100405(R) (2014).
Interacting Quantum Spin Hall models	Reuther, Thomale, and Rachel Phys. Rev. B 86, 155127 (2012).
Bilayer antiferromagnet	Reuther and Thomale Phys. Rev. B 89, 024412 (2014).
J1-J2-Jd model on the kagome lattice	Suttner, Platt, Reuther, and Thomale Phys. Rev. B 89, 020408(R) (2014).
	Iqbal, Jeschke, Greiter, Reuther, Valenti, Mazin, and Thomale arXiv:1506.03436

Heisenberg-Kitaev model

Reuther, Thomale, and Trebst, Phys. Rev. B 84, 100406(R) (2011).

Singh, Manni, Reuther, Berlijn, Thomale, Ku, Trebst, Gegenwart, Phys. Rev. Lett. 108, 127203 (2012).

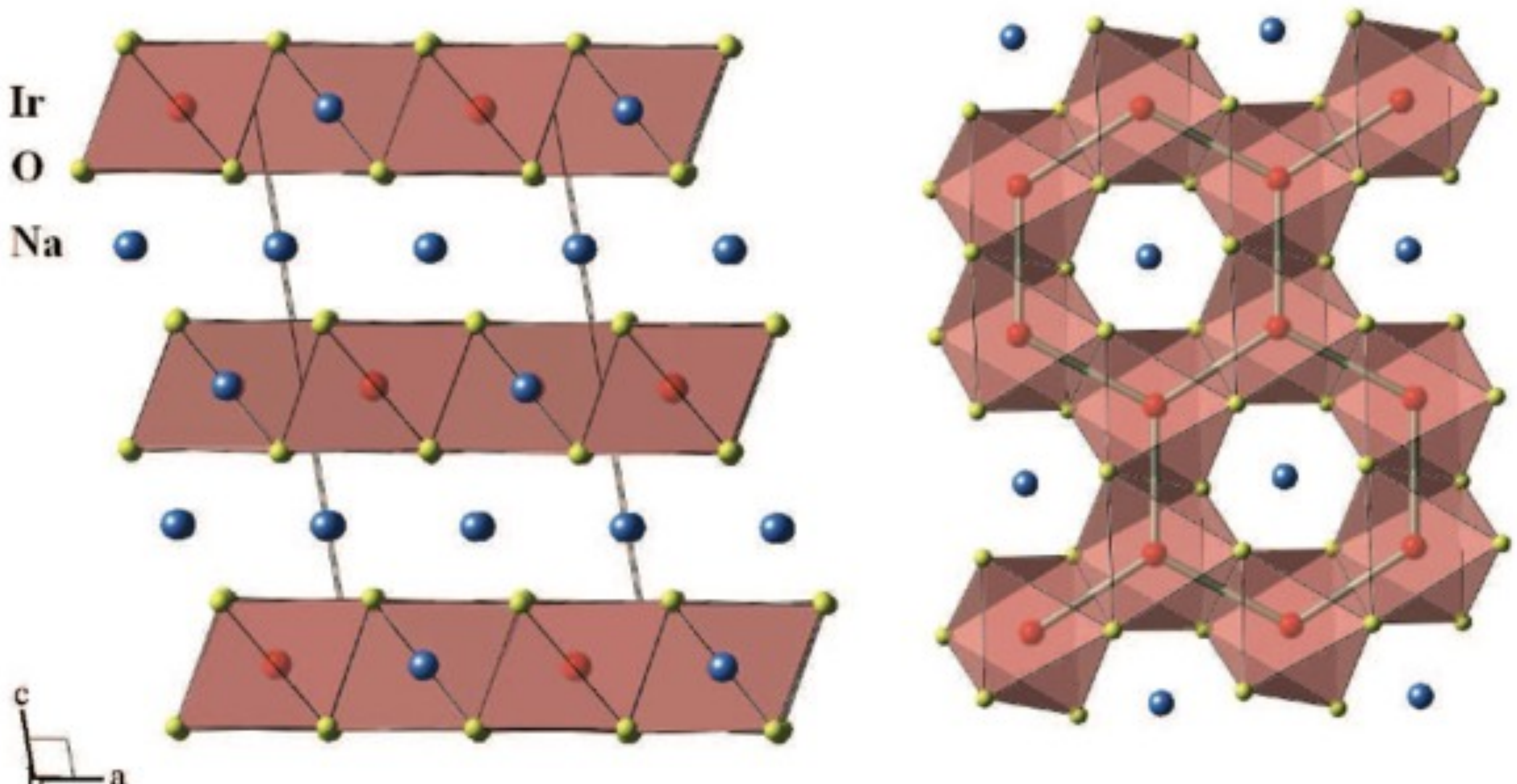
Reuther, Thomale, and Rachel Phys. Rev. B 90, 100405(R) (2014).

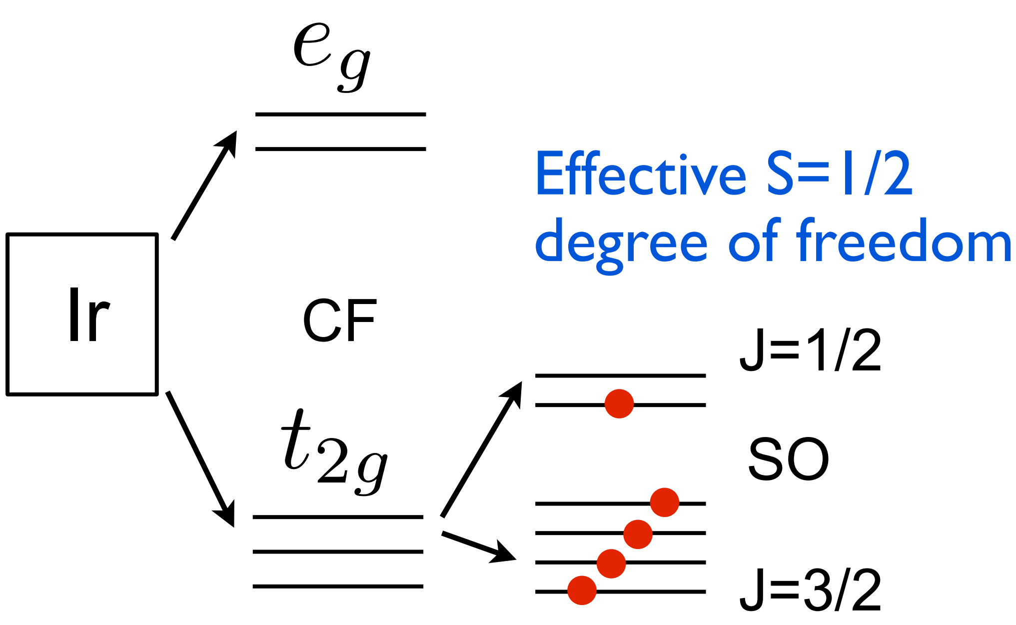
Heisenberg-Kitaev model

Heisenberg, 1928; Kitaev, 2006

Jackeli, Khaliullin et al., 2009/2010

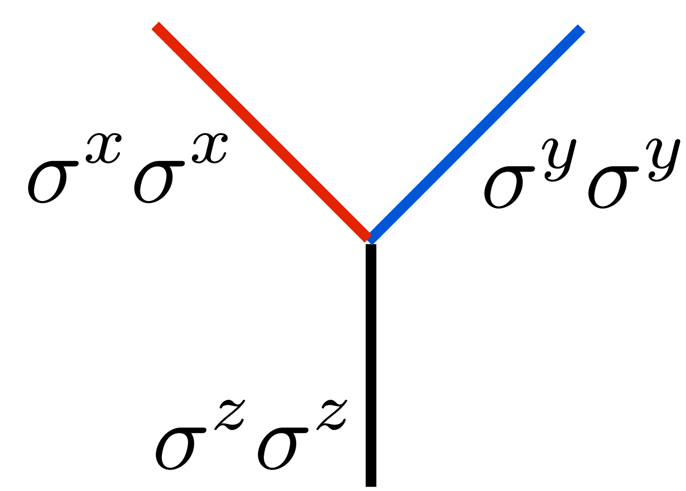
Anisotropic pseudospin models from a Mott spin orbit picture



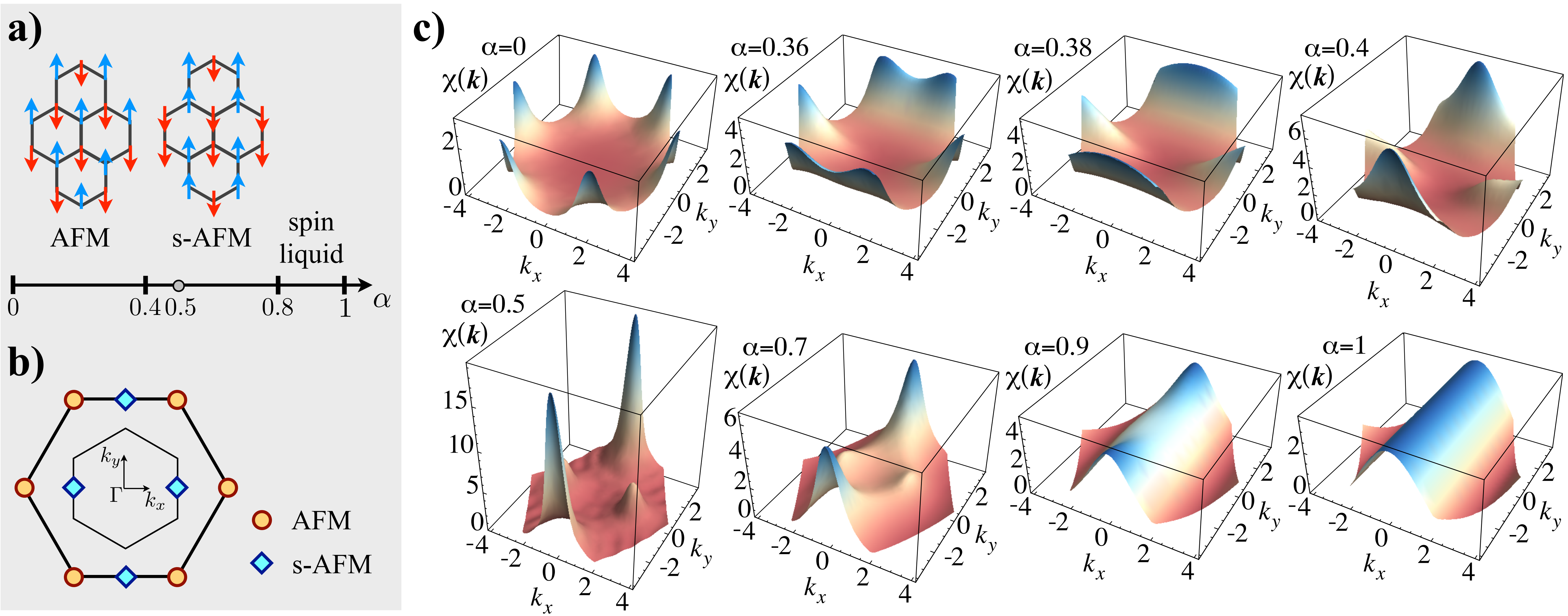


Singh, Gegenwart et al., 2010

$$H_{\mathrm{HK}}[\alpha] = (1-\alpha)\sum_{\langle i,j \rangle} \vec{\sigma}_i \cdot \vec{\sigma}_j - 2\alpha \sum_{\gamma-\mathrm{links}} \sigma_i^\gamma \sigma_j^\gamma$$



Magnetic susceptibilities for the HKM from Spin-FRG



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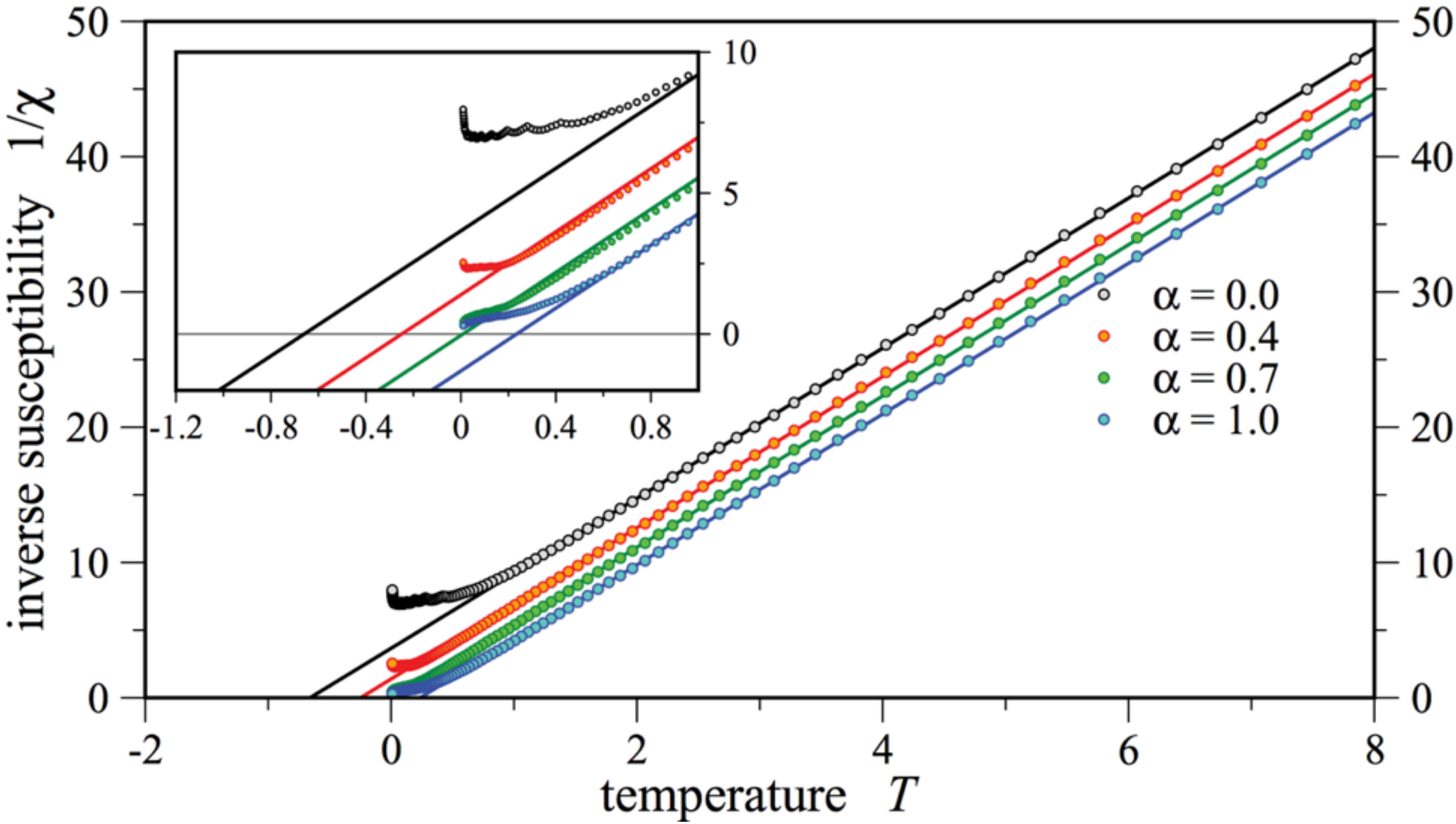
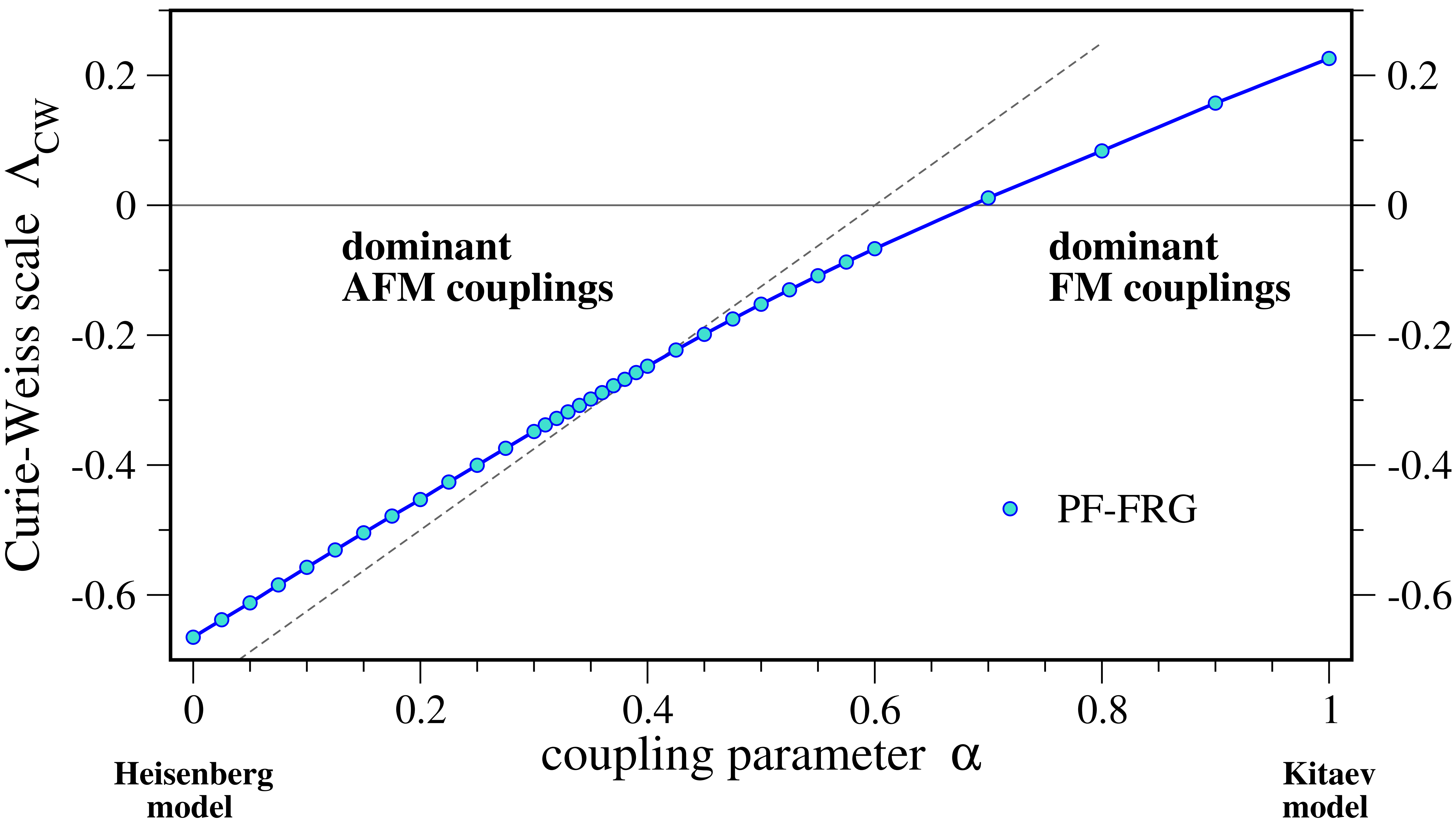
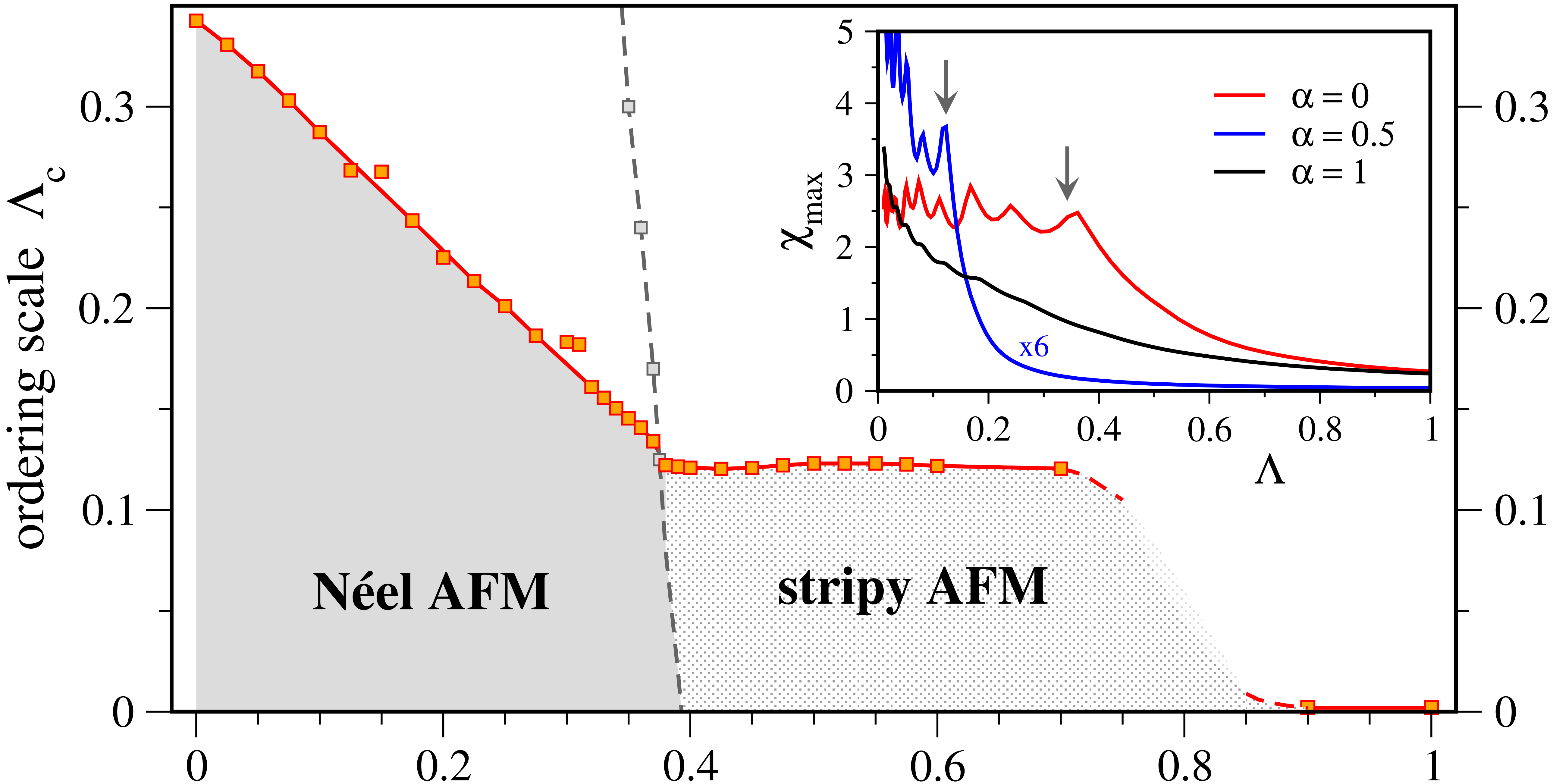
Cutoff flow ~ Temperature flow



Curie Weiss temperature



Neel temperature

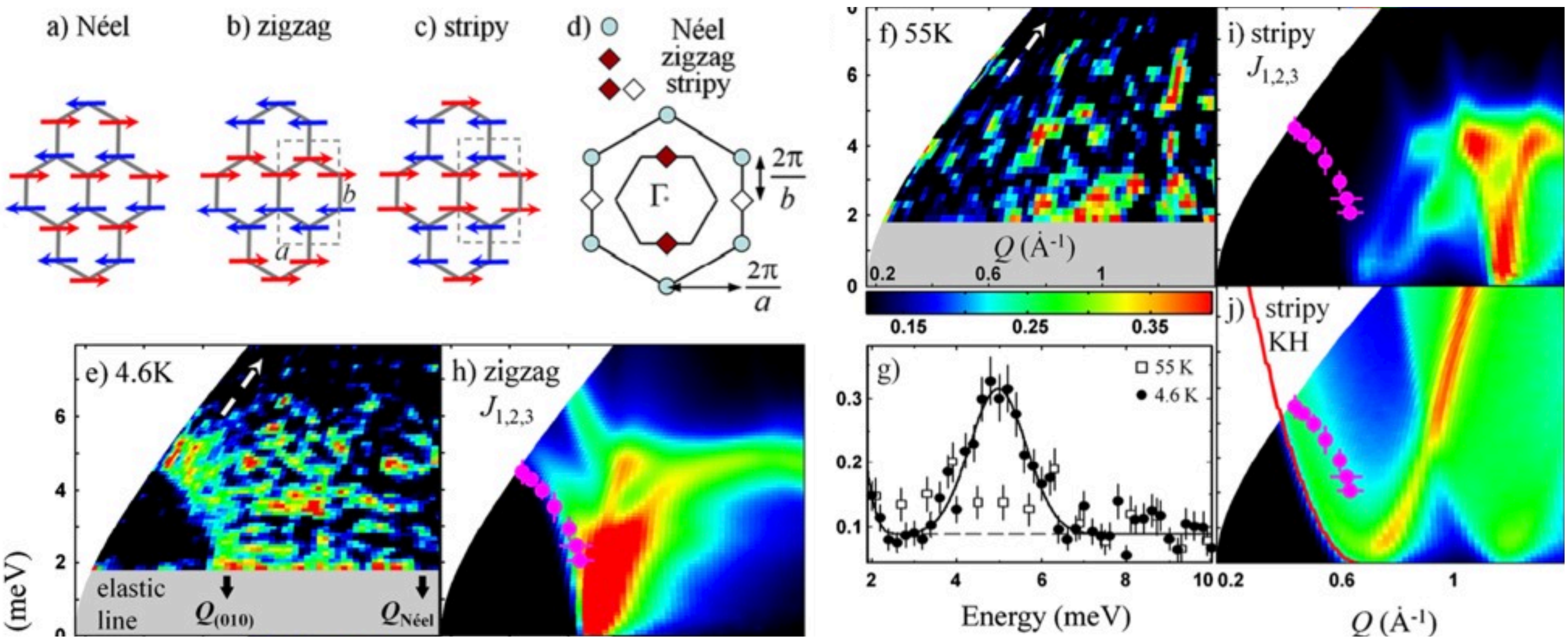


Heisenberg model

Kitaev model

Finding from experiment: nature of magnetism in Na-Iridate

Choi, Taylor et al., 2012, Ye, Cao et al., 2012



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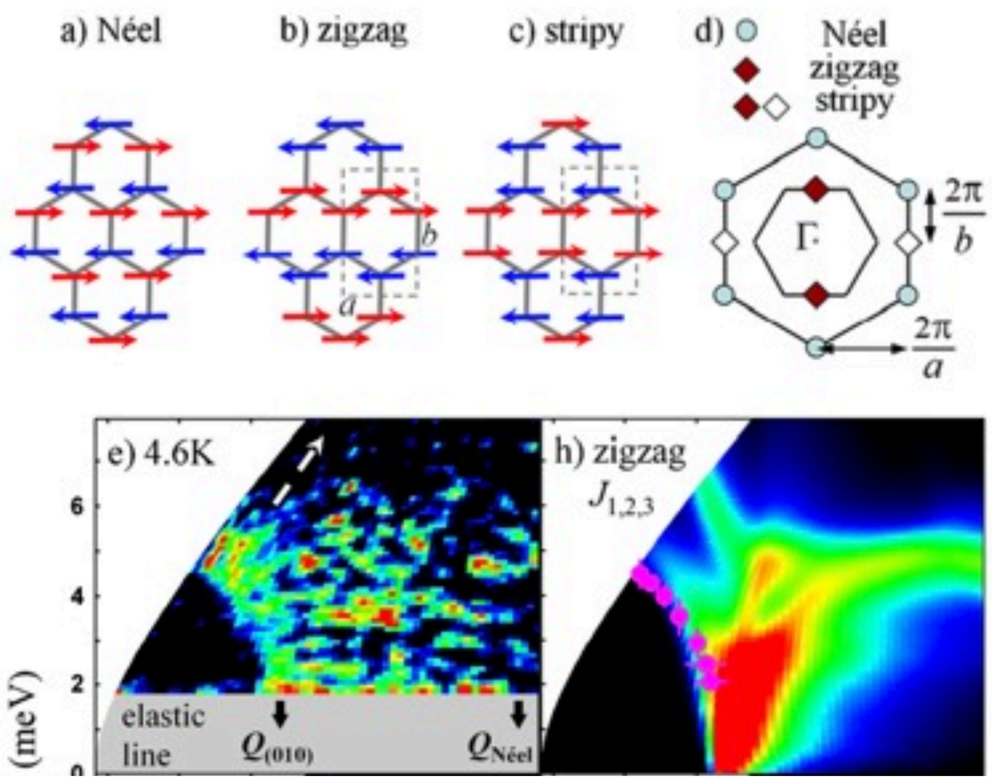

Magnetic order: indication to be of zig-zag type

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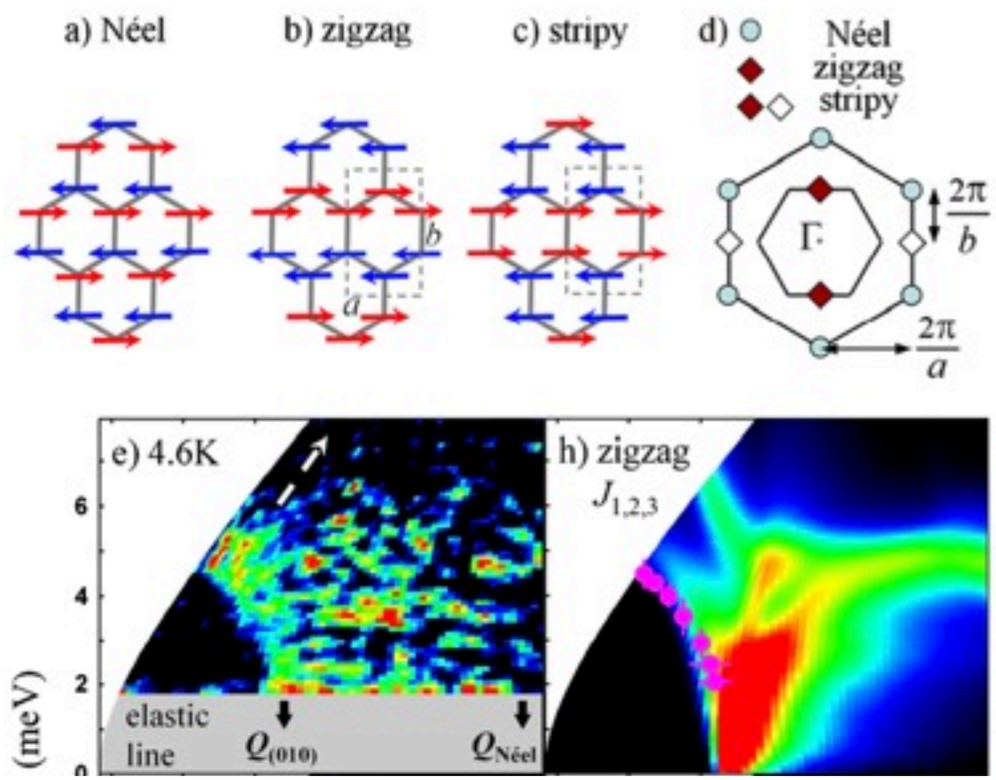

Magnetic order: indication to be of zig-zag type

How can we reconcile this from theory?

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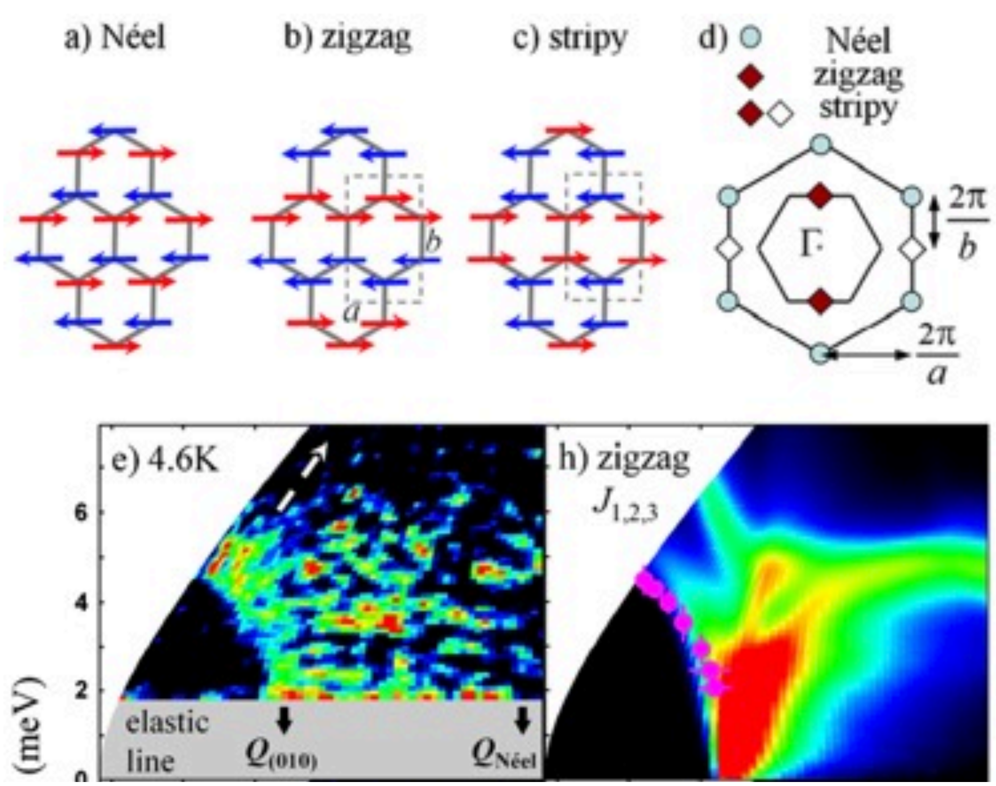

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Option 1: Reverse sign of nearest neighbor Heisenberg-Kitaev couplings

Chaloupka, Jackeli, Khaliullin, PRL 2013

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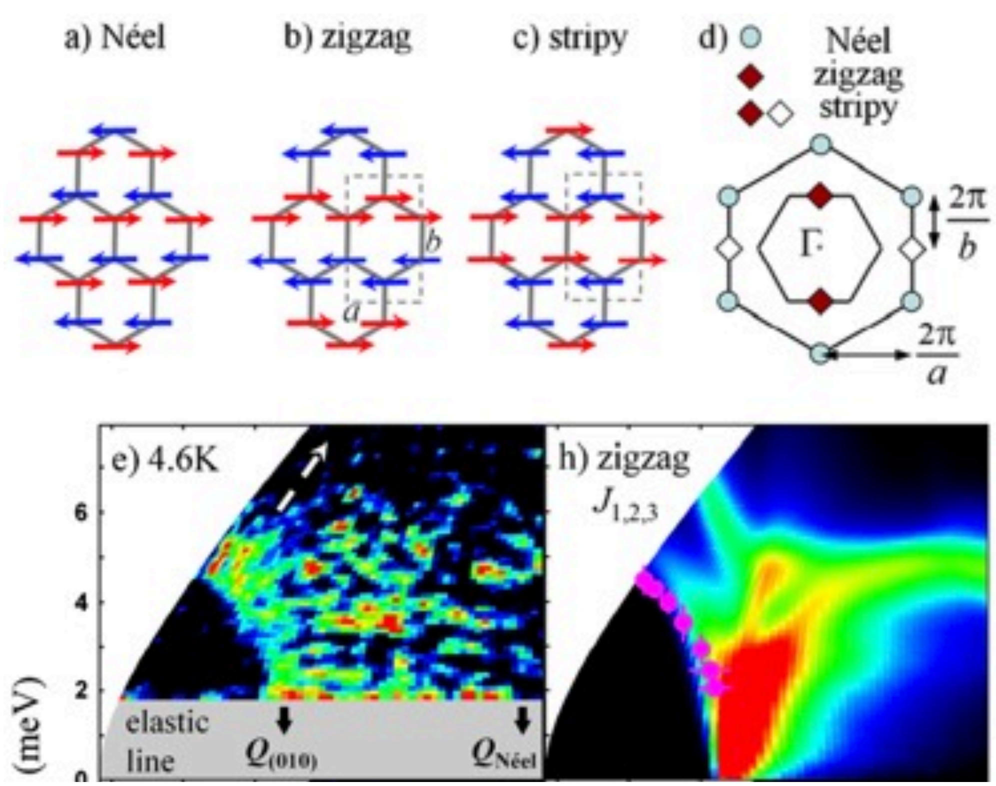

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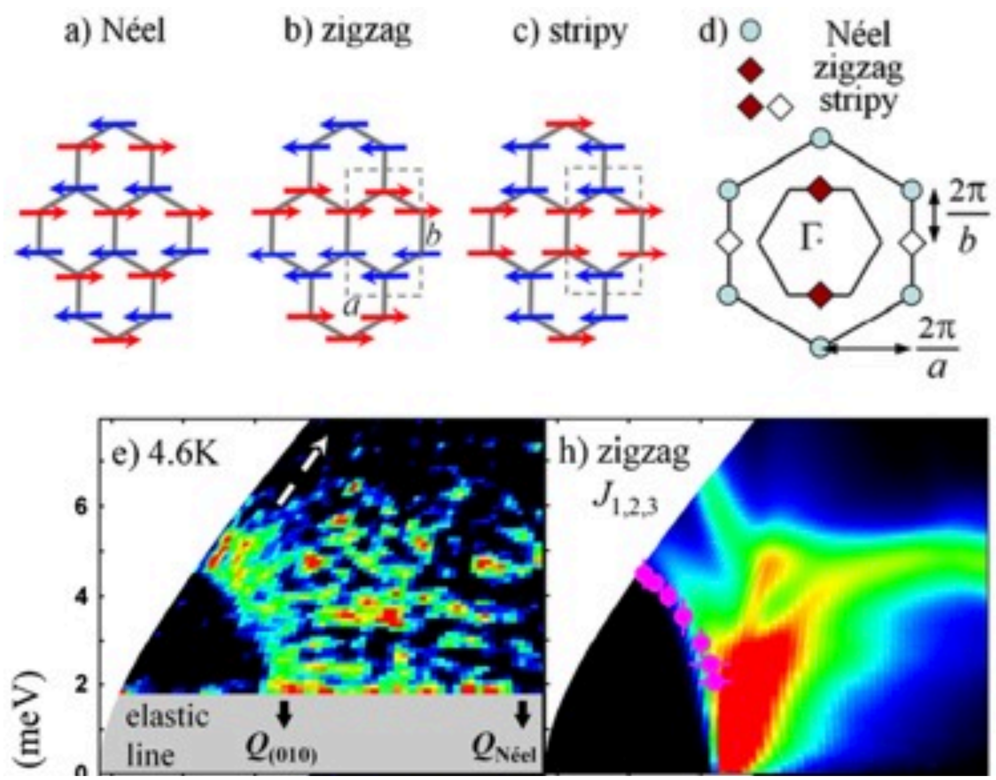

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Reuther, Thomale, and Rachel
Phys. Rev. B 90, 100405(R) (2014).

SUGGESTION RAPID

Option 3: Longer-range Heisenberg couplings

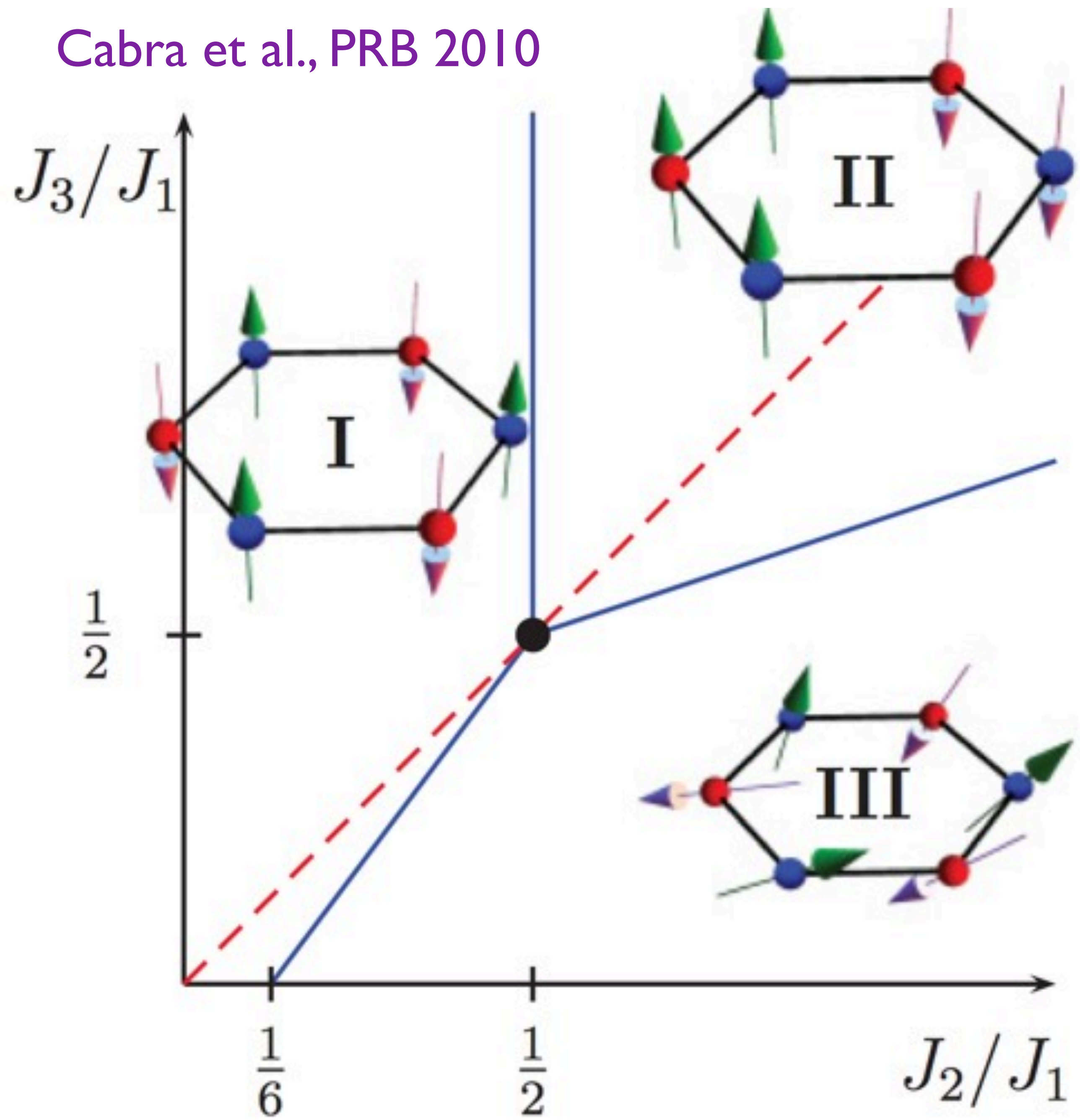
Singh, Gegenwart et al.
Phys. Rev. Lett. 108, 127203 (2012).

Classical phase diagram of the long-range honeycomb antiferromagnet

$$H_{\mathrm{HCM}} = J_1 \sum_{\langle i,j \rangle} \vec{S}_i \vec{S}_j + J_2 \sum_{\langle\langle i,j \rangle\rangle} \vec{S}_i \vec{S}_j + J_3 \sum_{\langle\langle\langle i,j \rangle\rangle\rangle} \vec{S}_i \vec{S}_j$$

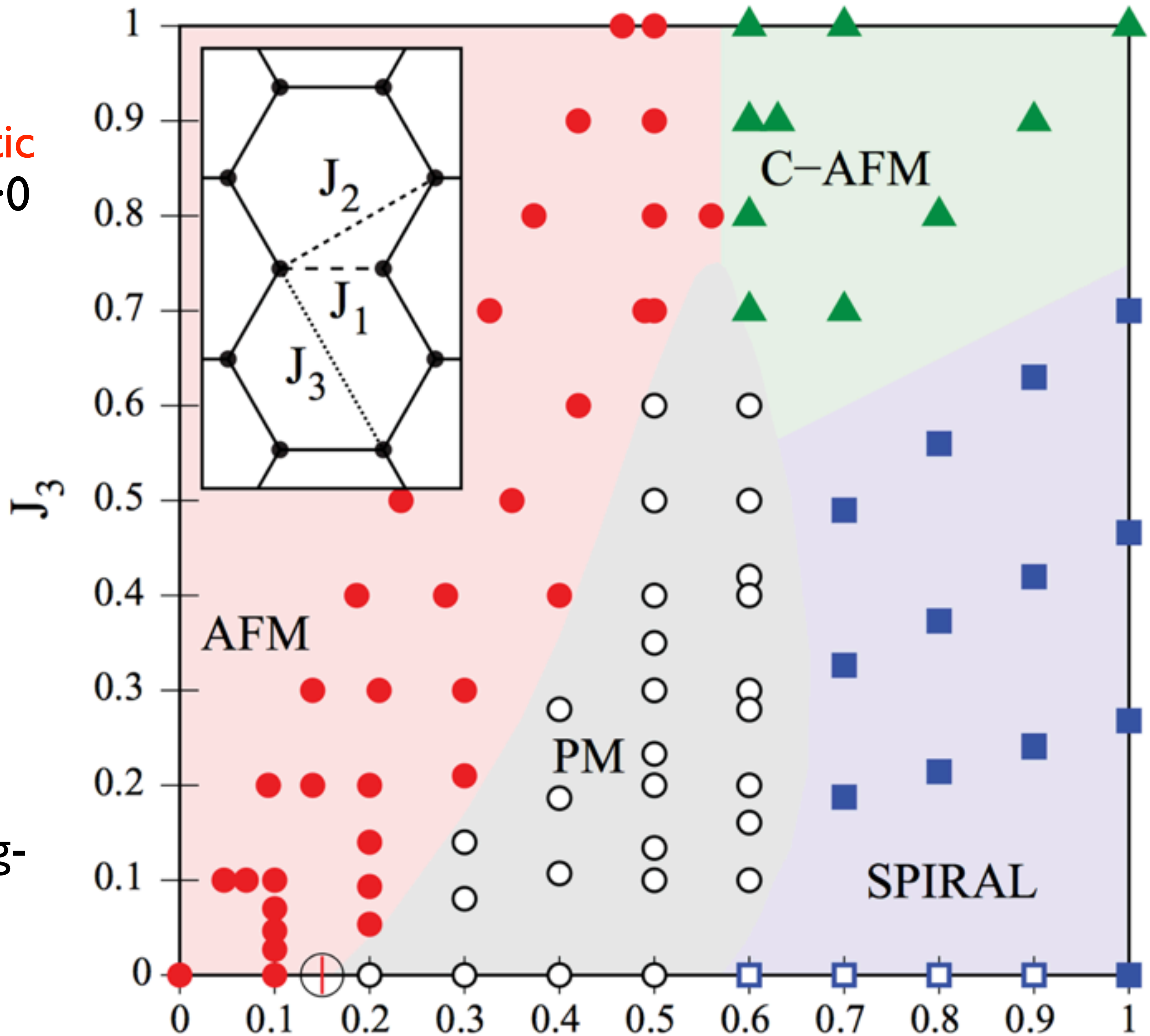
- AFM order (Region I)
- Zig-zag order (Region II)
- Spiral order (Region III)
- Tricritical point at J2=J3=0.5 J1

Cabra et al., PRB 2010

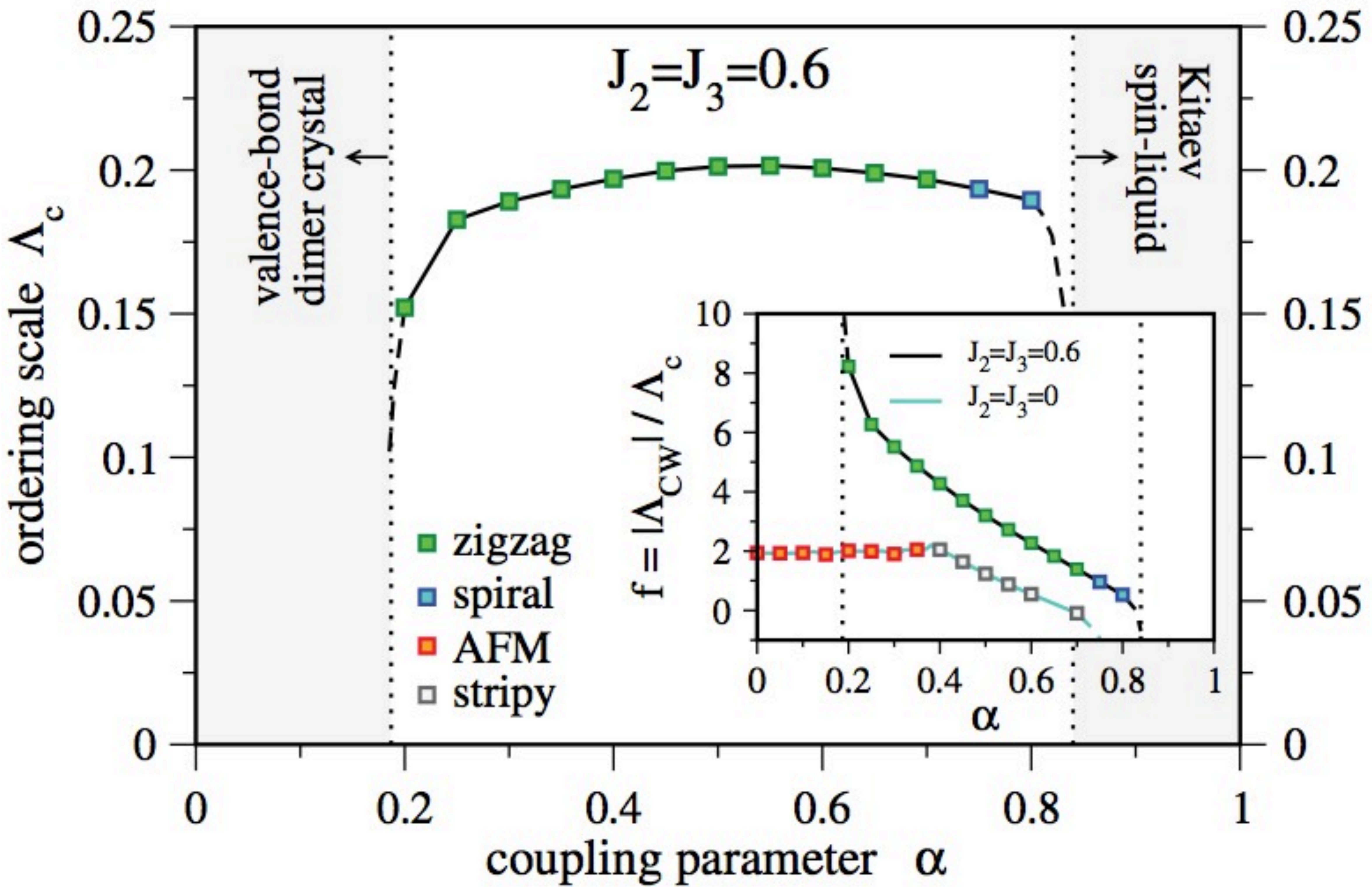


Quantum phase diagram from PFFRG

- Extended para-magnetic phase for J2 ~ 0.5, J3 >0
- J3=0: extended paramagnetic regime for 0.15 < J2 < 0.7
- 1st order transition AFM to zig-zag
- 2nd order transition zig-zag to spiral



Long-range Heisenberg terms in the Iridates?

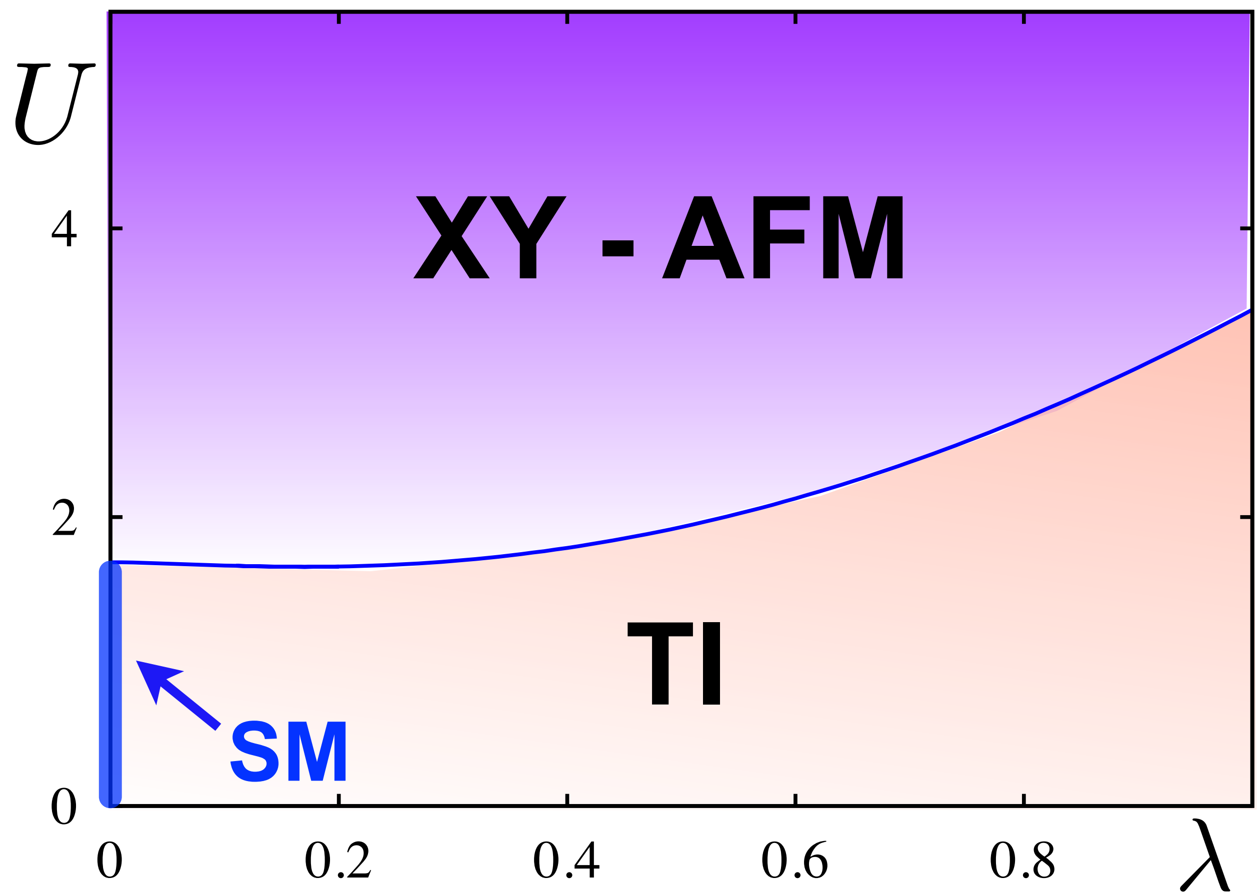


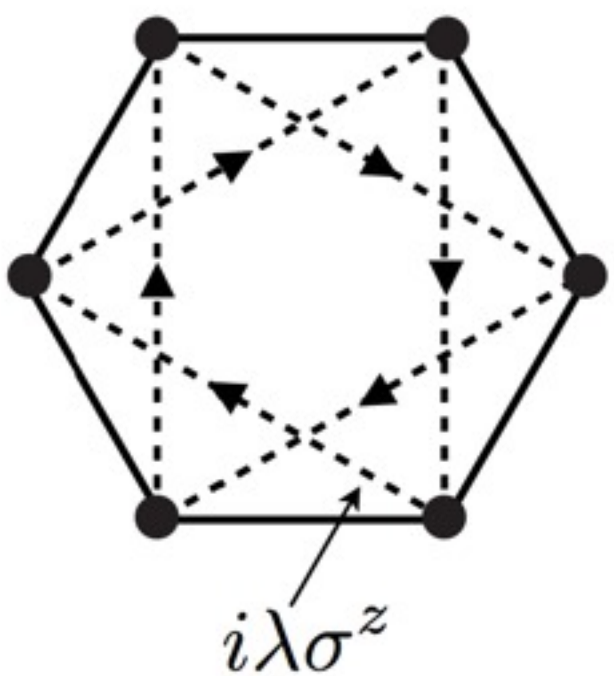
Strong coupling limit of topological insulators

Reuther, Thomale, and Rachel, Phys. Rev. B 86, 155127 (2012).

Minimal Kane Mele Hubbard model

$$H_{\text{KM-U}} = -t \sum_{\langle ij \rangle \sigma} c^\dagger_{i\sigma} c_{j\sigma} + i\lambda \sum_{\langle\langle ij \rangle\rangle} \sum_{\alpha\beta} v_{ij} c^\dagger_{i\alpha} \sigma^z_{\alpha\beta} c_{j\beta} + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

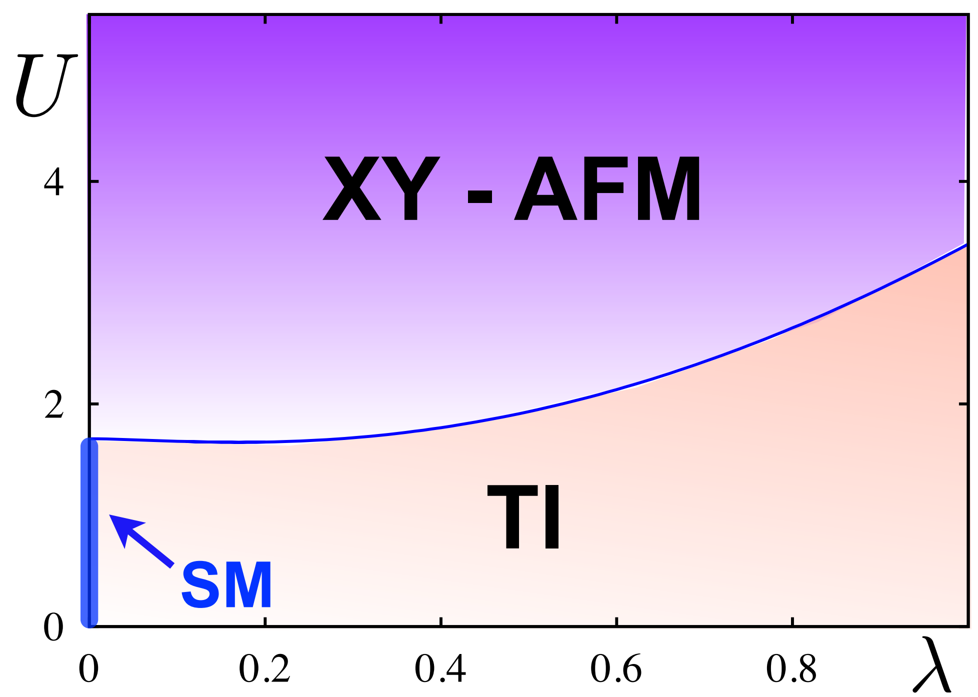


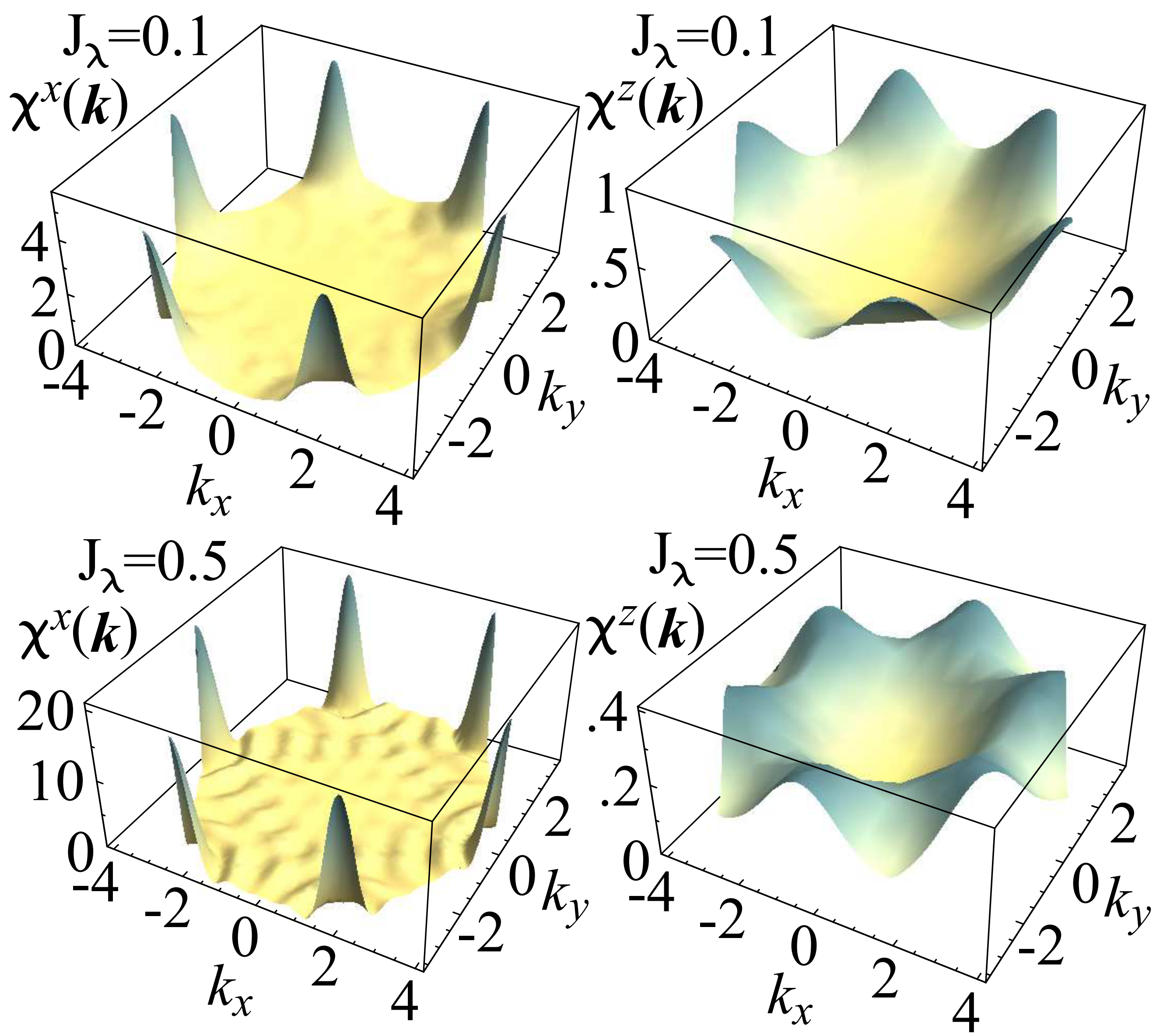


Only U(1) conserving spin-orbit coupling: Hubbard interaction only drives a magnetic phase transition

Minimal Kane Mele Heisenberg limit

$$\mathcal{H}_{\mathrm{KM}} = J_1 \sum_{\langle ij \rangle} \boldsymbol{S}_i \boldsymbol{S}_j + J_\lambda \sum_{\langle\langle ij \rangle\rangle} [-S_i^x S_j^x - S_i^y S_j^y + S_i^z S_j^z]$$





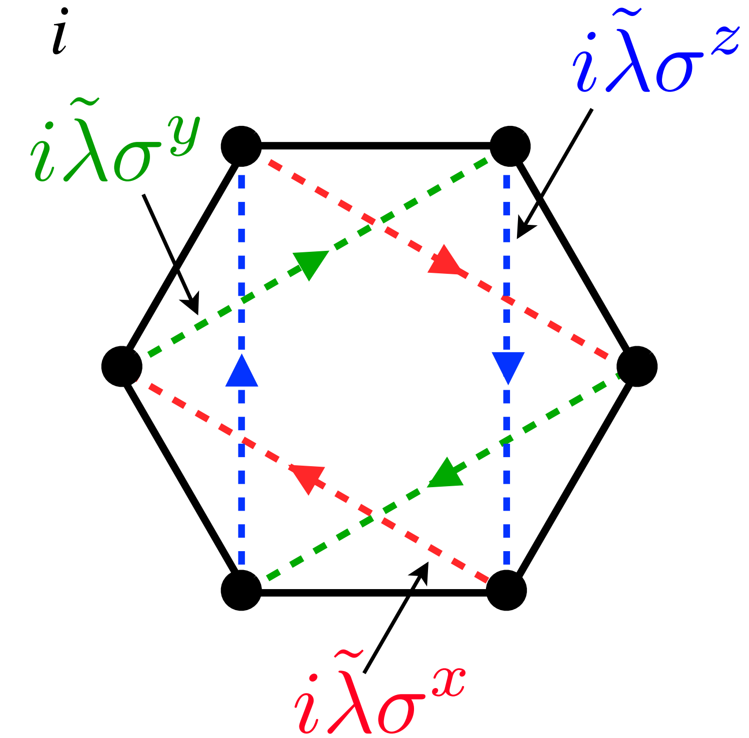
AFM avoids SO frustration by rotating into the XY plane.

Extended spin-orbit honeycomb model

Strong coupling limit of a kinetic model with multiple SO terms...

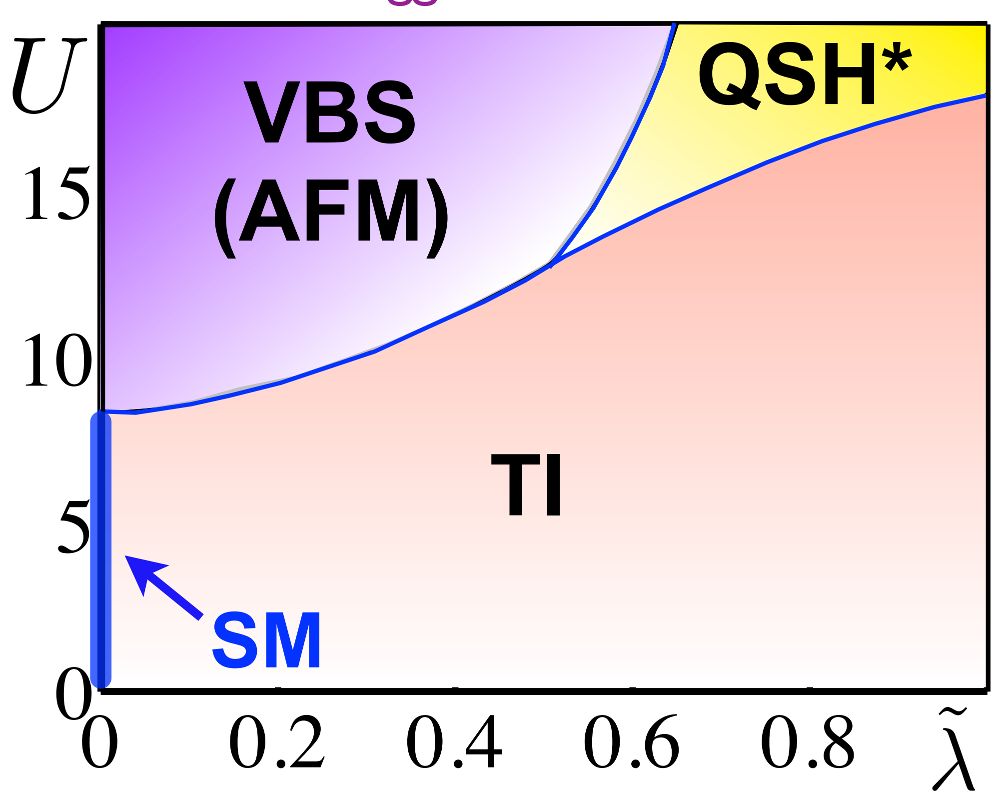
Shitade et al., 2009

$$H_S = -t \sum_{\langle ij \rangle \sigma} c^\dagger_{i\sigma} c_{j\sigma} + i\tilde{\lambda} \sum_{\langle\langle ij \rangle\rangle} \sum_{\alpha\beta} c^\dagger_{i\alpha} \sigma^\gamma_{\alpha\beta} c_{j\beta} + U \sum_i n_{i\uparrow} n_{i\downarrow}$$



...yields a spin model with broken axial U(1) symmetry:

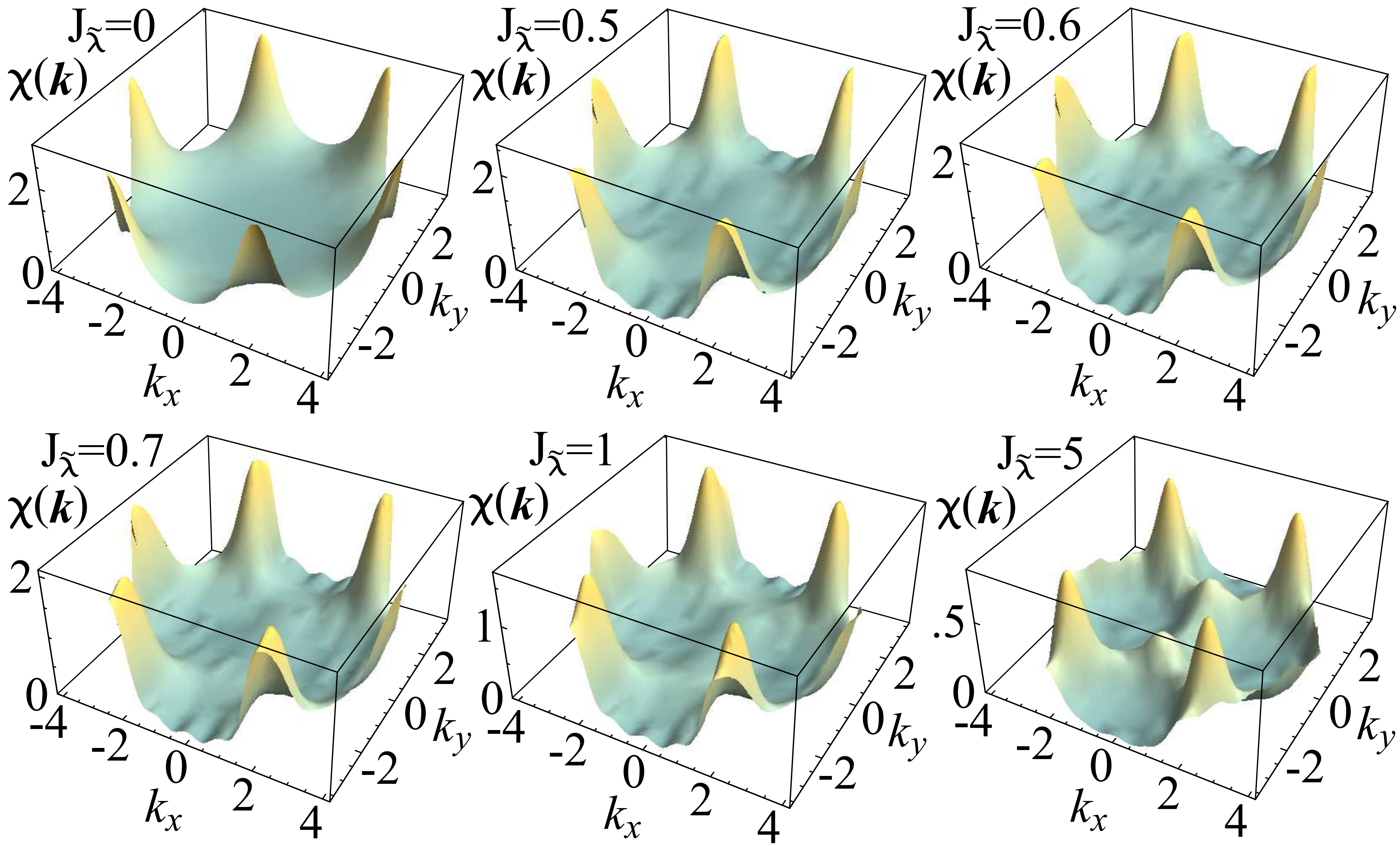
Rüegg, Fiete, 2011



$$\mathcal{H}_{\rm S} = J_1 \sum_{\langle ij \rangle} \boldsymbol{S}_i \boldsymbol{S}_j - J_{\tilde{\lambda}} \sum_{\langle\langle ij \rangle\rangle} \boldsymbol{S}_i \boldsymbol{S}_j + 2J_{\tilde{\lambda}} \sum_\gamma S^\gamma_i S^\gamma_j$$

Magnetic susceptibility of the extended SO spin model

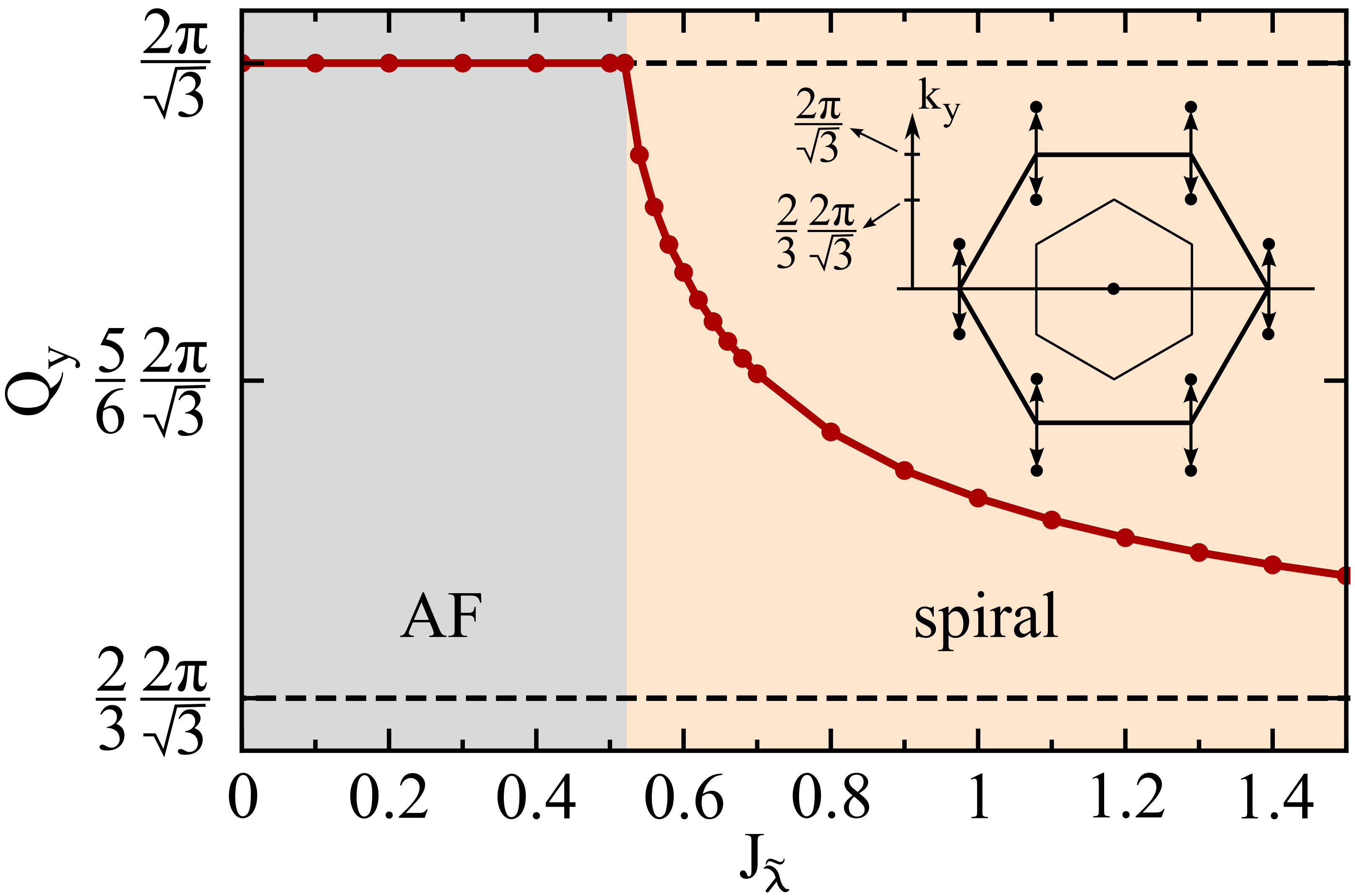
$$\mathcal{H}_{\mathrm{S}} = J_1 \sum_{\langle ij \rangle} \boldsymbol{S}_i \boldsymbol{S}_j - J_{\tilde{\lambda}} \sum_{\langle\langle ij \rangle\rangle} \boldsymbol{S}_i \boldsymbol{S}_j + 2 J_{\tilde{\lambda}} \sum_{\gamma} S_i^{\gamma} S_j^{\gamma}$$



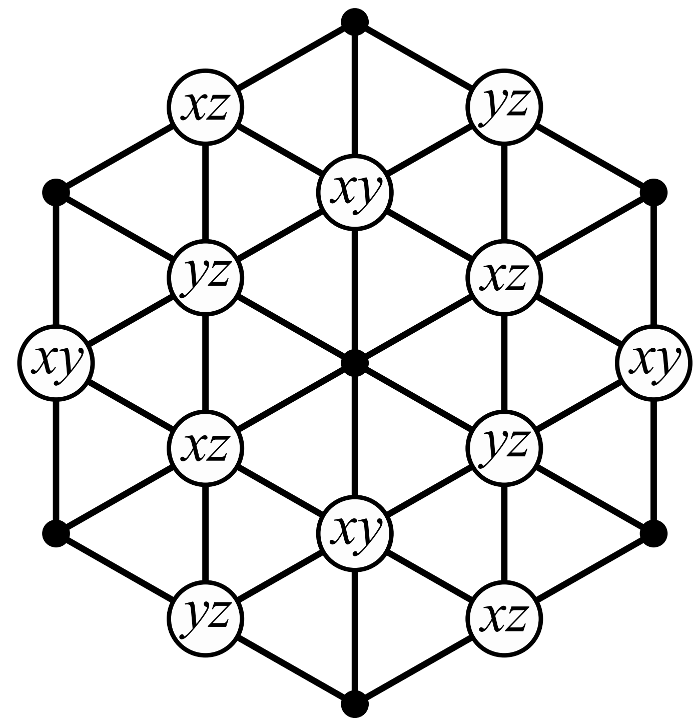
Magnetic phase diagram of the extended SO spin model

$$\mathcal{H}_{\rm S} = J_1 \sum_{\langle ij \rangle} \boldsymbol{S}_i \boldsymbol{S}_j - J_{\tilde{\lambda}} \sum_{\langle\langle ij \rangle\rangle} \boldsymbol{S}_i \boldsymbol{S}_j + 2J_{\tilde{\lambda}} \sum_{\gamma} S_i^{\gamma} S_j^{\gamma}$$

$$J_{\tilde{\lambda}} \to \infty$$



Decoupled triangular sublattices mapping to the Heisenberg model

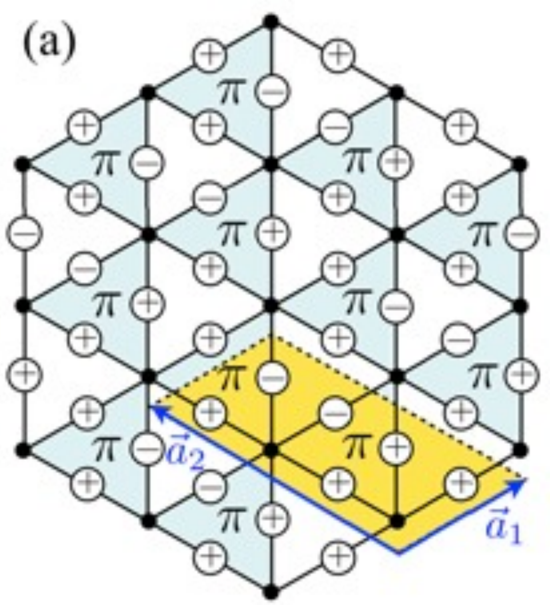


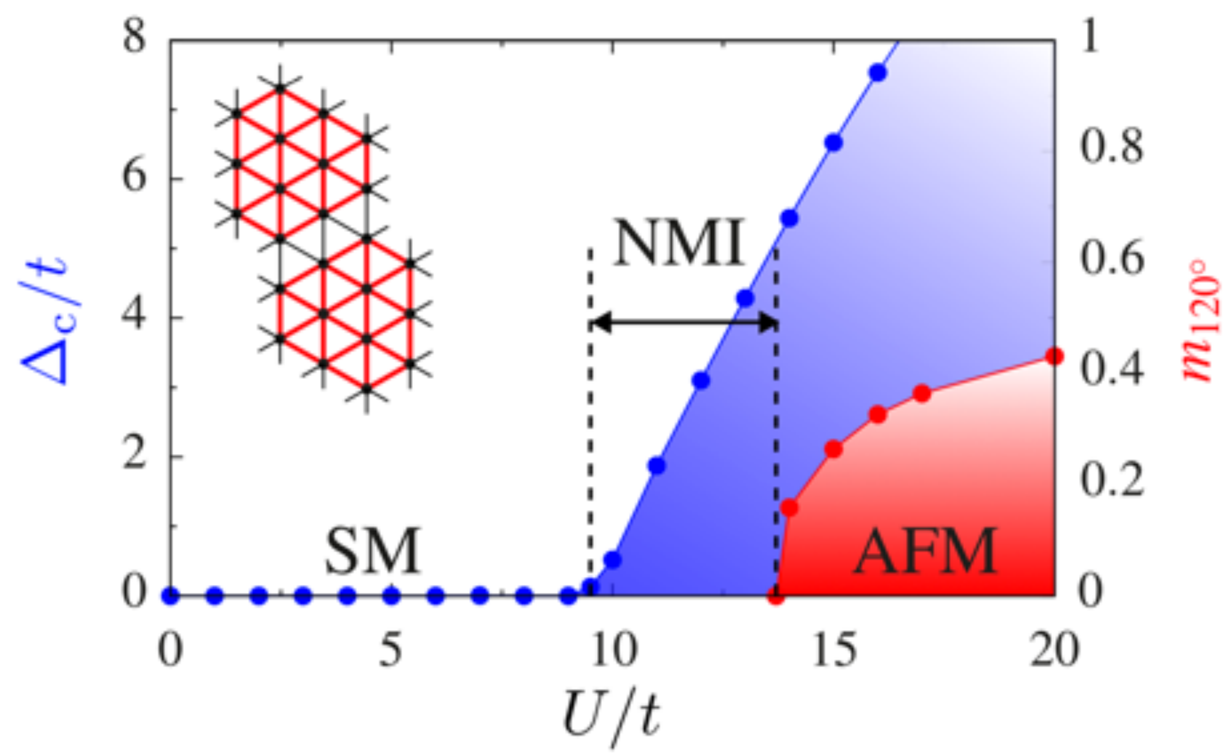
Generalized Klein duality in Hubbard models

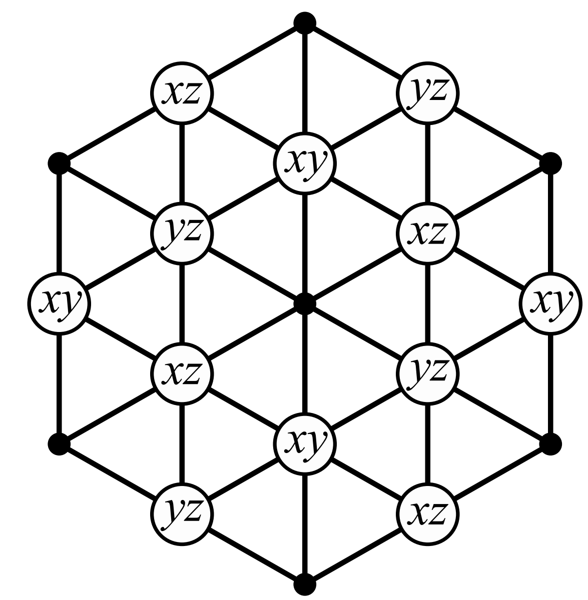
PRL **114**, 167201 (2015) PHYSICAL REVIEW LETTERS week ending 24 APRIL 2015

Quantum Paramagnet in a π Flux Triangular Lattice Hubbard Model

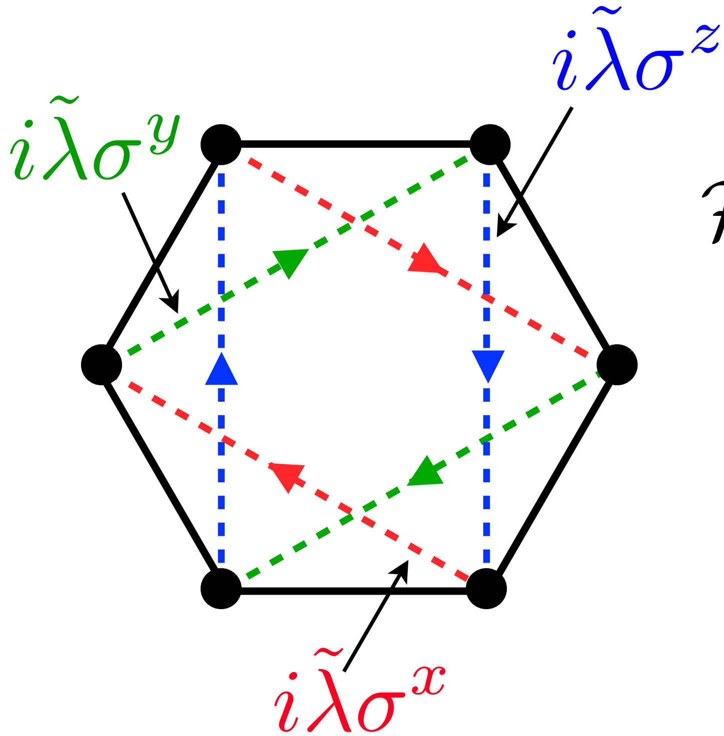
Stephan Rachel,[1] Manuel Laubach,[2] Johannes Reuther,[3,4] and Ronny Thomale[2]
[1]*Institute for Theoretical Physics, Technische Universität Dresden, 01062 Dresden, Germany*
[2]*Institute for Theoretical Physics, University of Würzburg, 97074 Würzburg, Germany*
[3]*Dahlem Center for Complex Quantum Systems and Fachbereich Physik, Freie Universität Berlin, 14195 Berlin, Germany*
[4]*Helmholtz-Zentrum Berlin für Materialien und Energie, 14109 Berlin, Germany*
(Received 4 December 2014; published 23 April 2015)







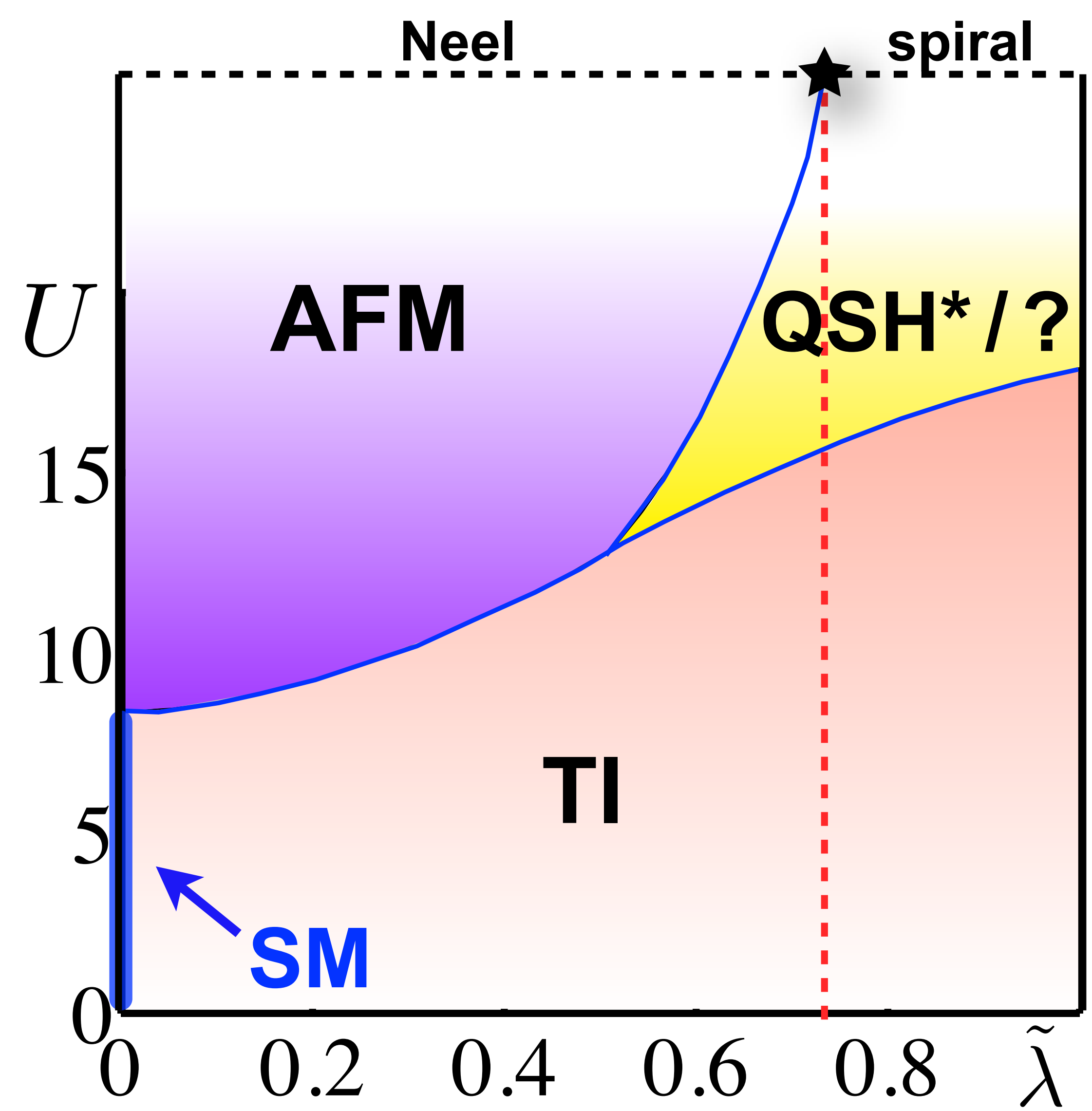
General spin-orbit spin exchange model: Possibility of a fractional (chiral) spin liquid?



$$\mathcal{H}_{\mathrm{S}} = J_1 \sum_{\langle ij \rangle} \boldsymbol{S}_i \boldsymbol{S}_j - J_{\tilde{\lambda}} \sum_{\langle\langle ij \rangle\rangle} \boldsymbol{S}_i \boldsymbol{S}_j + 2J_{\tilde{\lambda}} \sum_{\gamma} S_i^\gamma S_j^\gamma$$

Phase boundary in mean field theory extrapolated to strong coupling matches the magnetic phase transition

The incommensurate fluctuation regime might be particularly susceptible to exotic phases upon charge fluctuations



Chiral spin liquids

Schroeter, Kapit, Thomale, and Greiter, Phys. Rev. Lett. 99, 097202 (2007)

Greiter and Thomale, Phys. Rev. Lett. 102, 207203 (2009)

Greiter, Schroeter, and Thomale, Phys. Rev. B 89, 165125 (2014)

Meng, Neupert, Greiter, and Thomale, Phys. Rev. B 91, 241106 (2015).

Fractionalization of spin

AKLT spin chain: S=1 bulk spin, S=1/2 edge

 $= \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$

 $= |+\rangle\langle\uparrow\uparrow| + |0\rangle\frac{\langle\uparrow\downarrow| + \langle\downarrow\uparrow|}{\sqrt{2}} + |-\rangle\langle\downarrow\downarrow|$

Chiral spin liquid: S=1 spin flip particle constituents, S=1/2 quasiparticles

$$|\Psi\rangle = \sum_{\{z_j\}} \Psi(z_1,\ldots,z_M) S^+_{z_1}\ldots S^+_{z_M}|\downarrow\ldots\downarrow\rangle$$

$$\Psi^0_{\mathrm{CSL}} \sim \prod_{j<k}^{M}(z_j - z_k)^2 \qquad \Psi^\eta_{\mathrm{CSL}} \sim \prod_{j=1}^{M}(\eta - z_j)\prod_{j<k}^{M}(z_j - z_k)^2$$

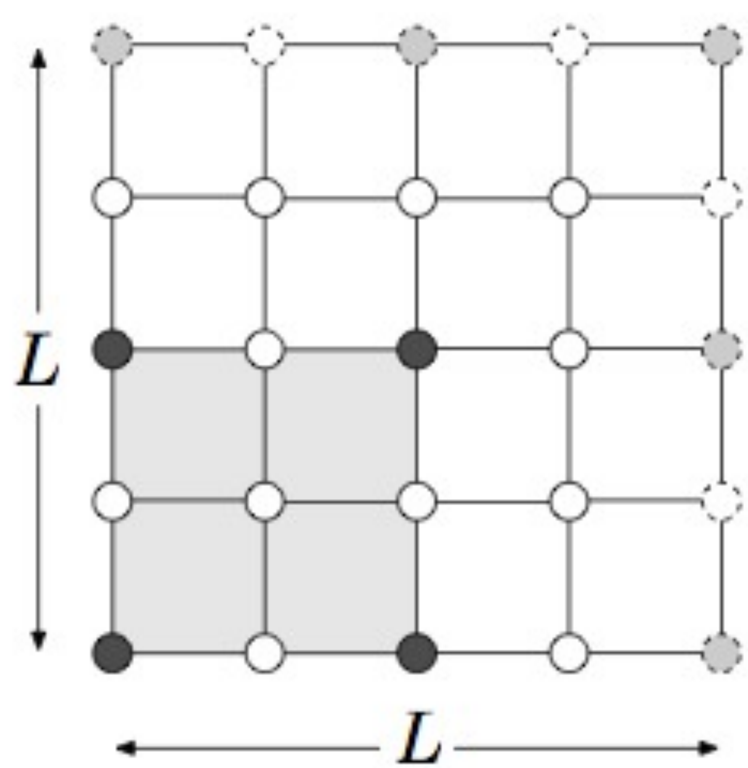
Chiral spin liquid: ν=1/2 bosonic fractional Chern insulator

Kalmeyer, Laughlin 87

$$|\Psi_{\rm CSL}\rangle = \sum_{\{z\}} \Psi_{\rm CSL}(z_1,\ldots,z_M) S^\dagger_{z_1} S^\dagger_{z_2} \ldots S^\dagger_{z_M} |\downarrow\downarrow\ldots\downarrow\rangle$$

$$M = N/2 \to \nu = 1/2$$

$$\Psi_{\rm CSL} = \prod_{j<k}^{M} (z_j - z_k)^2 \prod_{j=1}^{M} G(z_j) \exp^{-\frac{\pi}{2}|z_j|^2}$$



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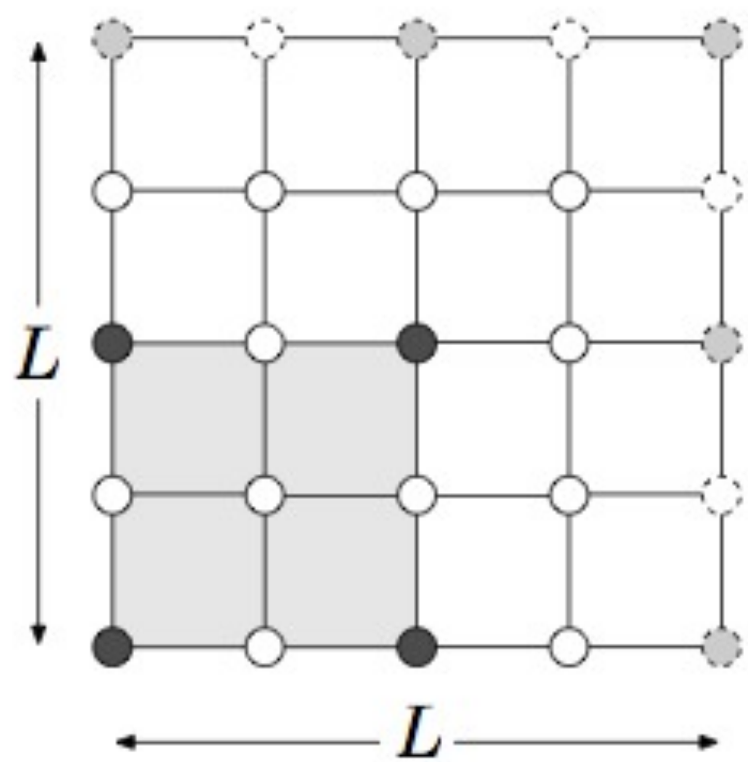

(deconfined) S=1/2 spinon excitations with half-Fermi statistics

Wilczek 82; Kalmeyer, Laughlin 87

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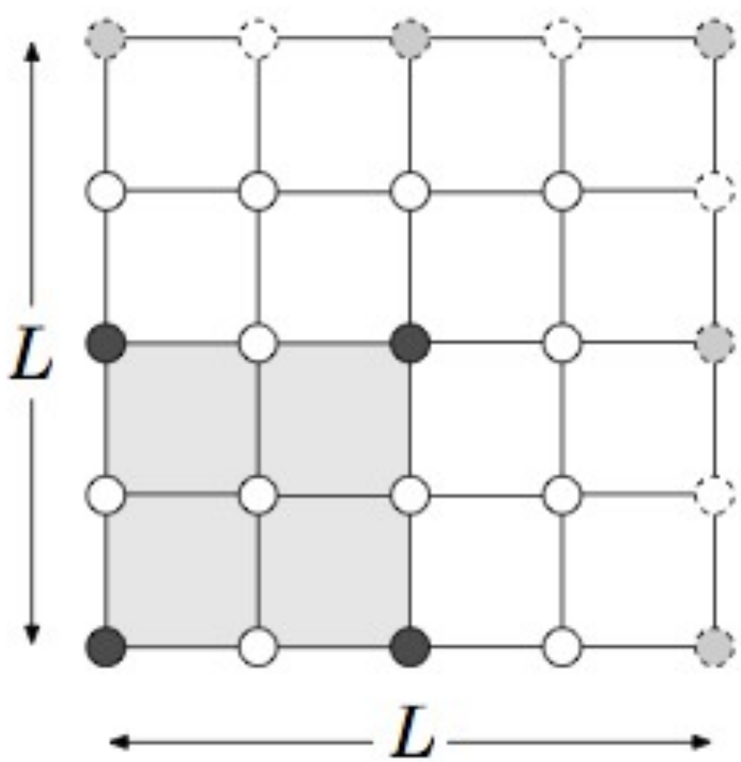

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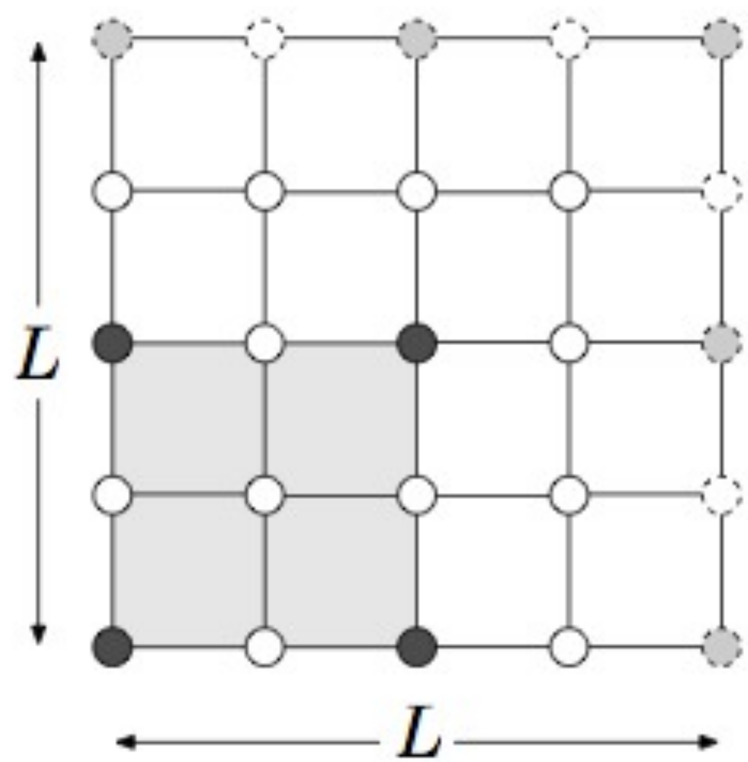

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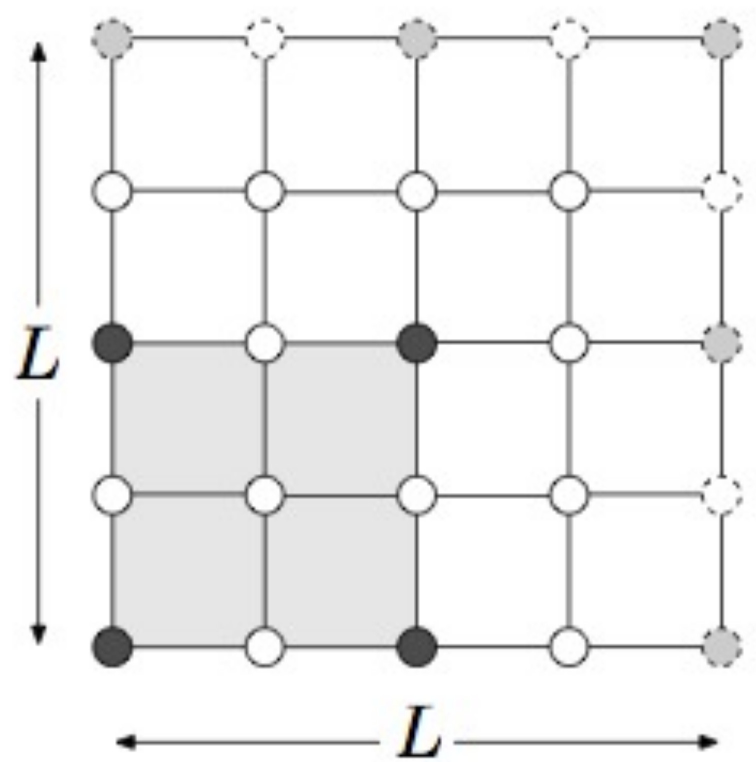

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microscopic model prediction: 6-spin operators

Wen Wilczek Zee 89

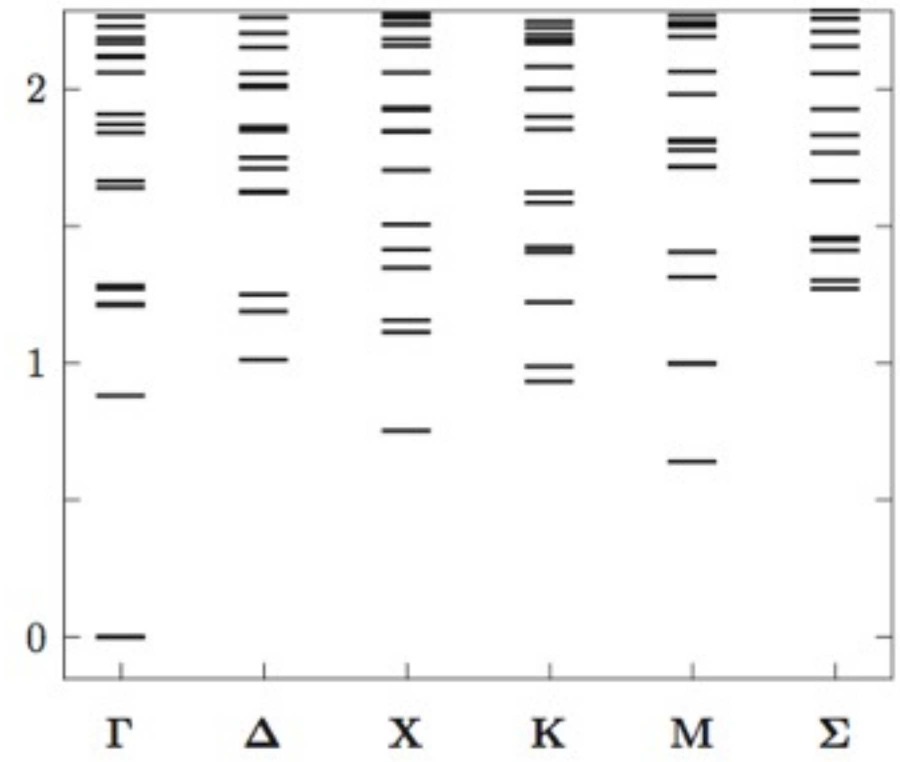
Exact models for the chiral spin liquid

First exact model (2007):

6-spin operators

explicit P,T breaking

SU(2) symmetric



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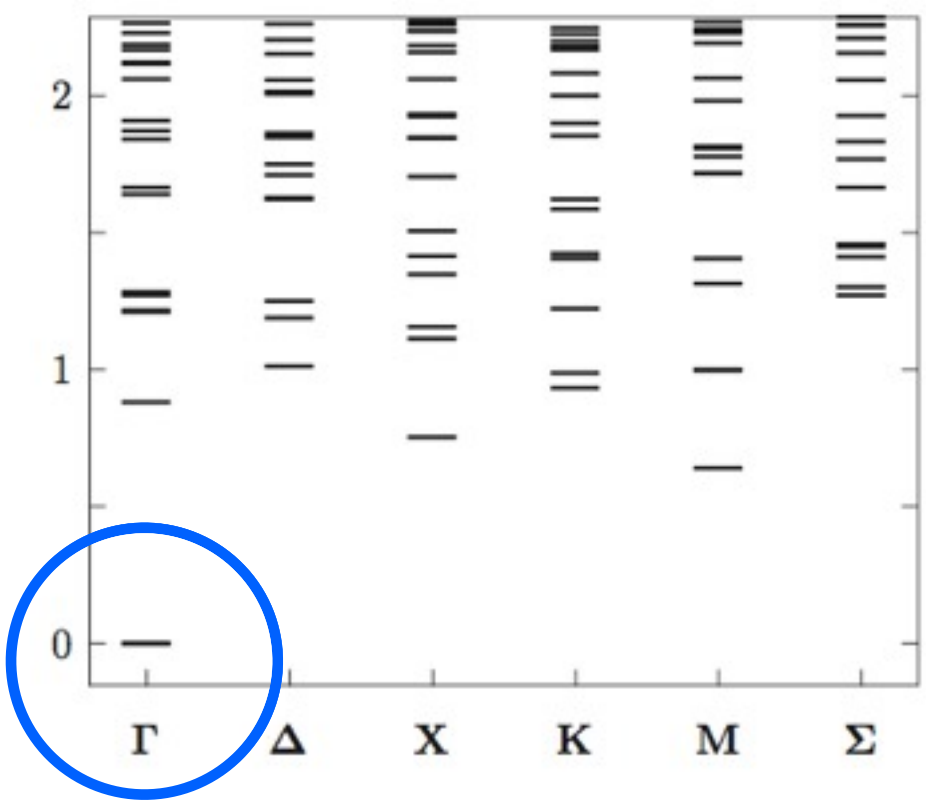

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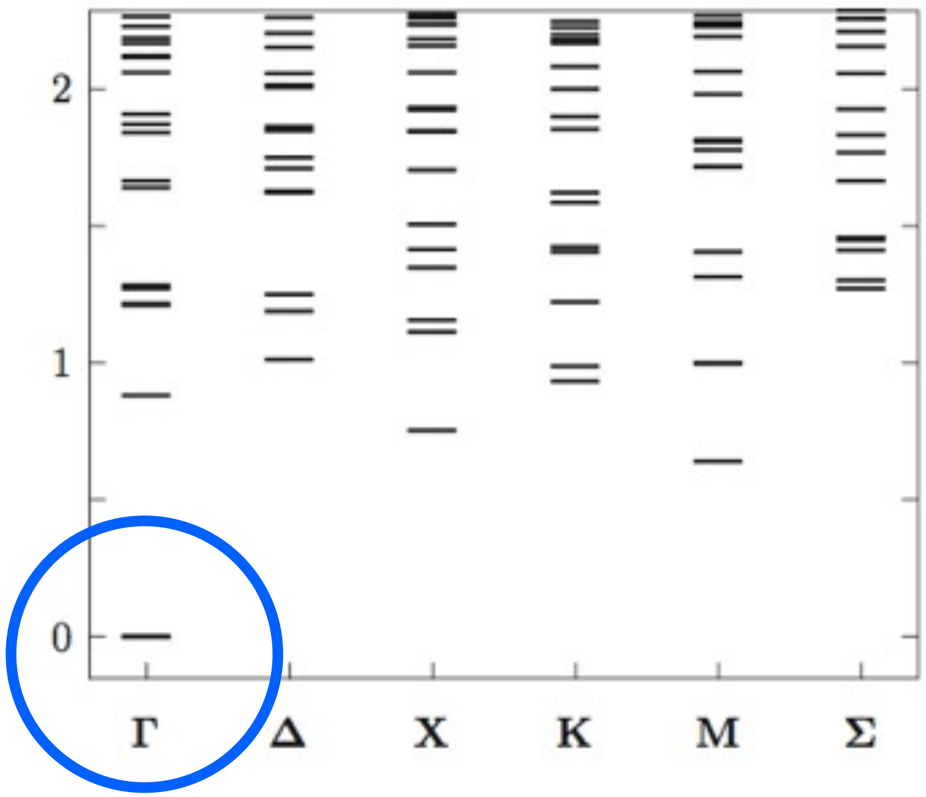

Second exact model (2012):

$$H_{\rm CSL} = \sum_{\alpha\neq\beta} \omega_{\alpha\beta\beta}[S_\alpha S_\beta] + \sum_{\alpha\neq\beta\neq\gamma\neq\alpha} \omega_{\alpha\beta\gamma}[S_\beta S_\gamma - iS_\alpha(S_\beta \times S_\gamma)]$$

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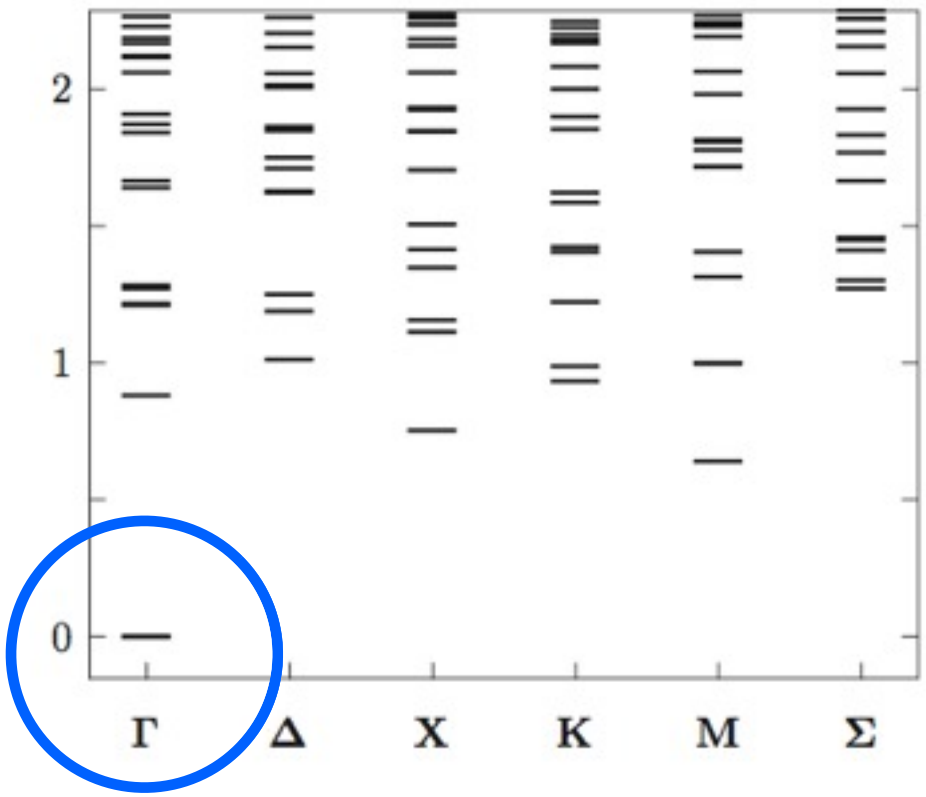

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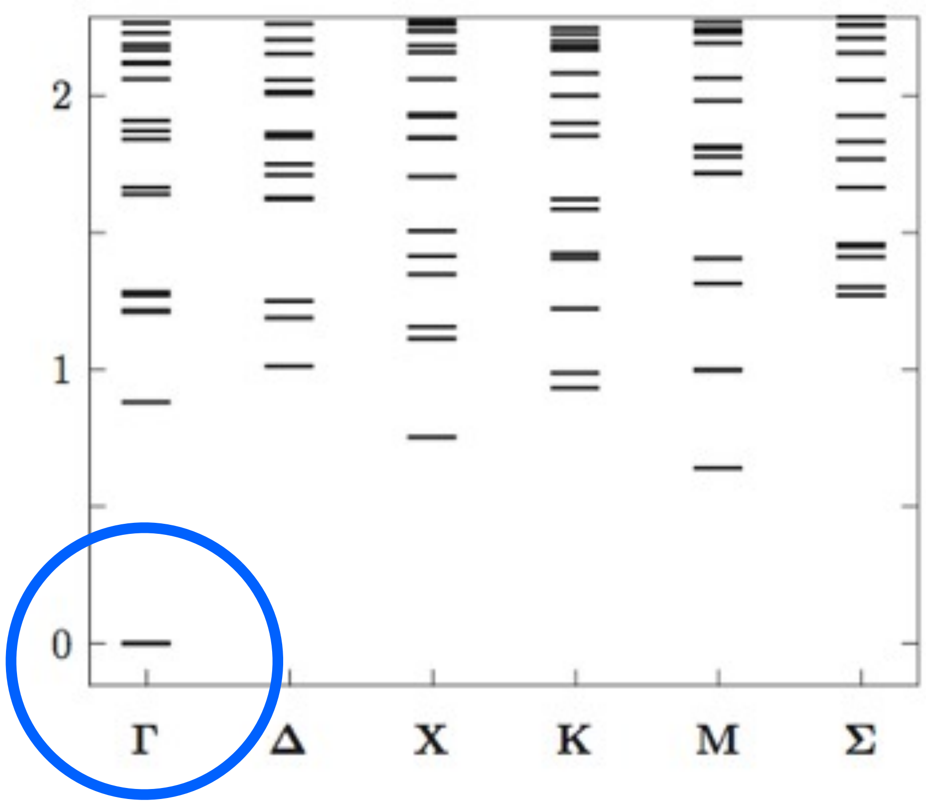

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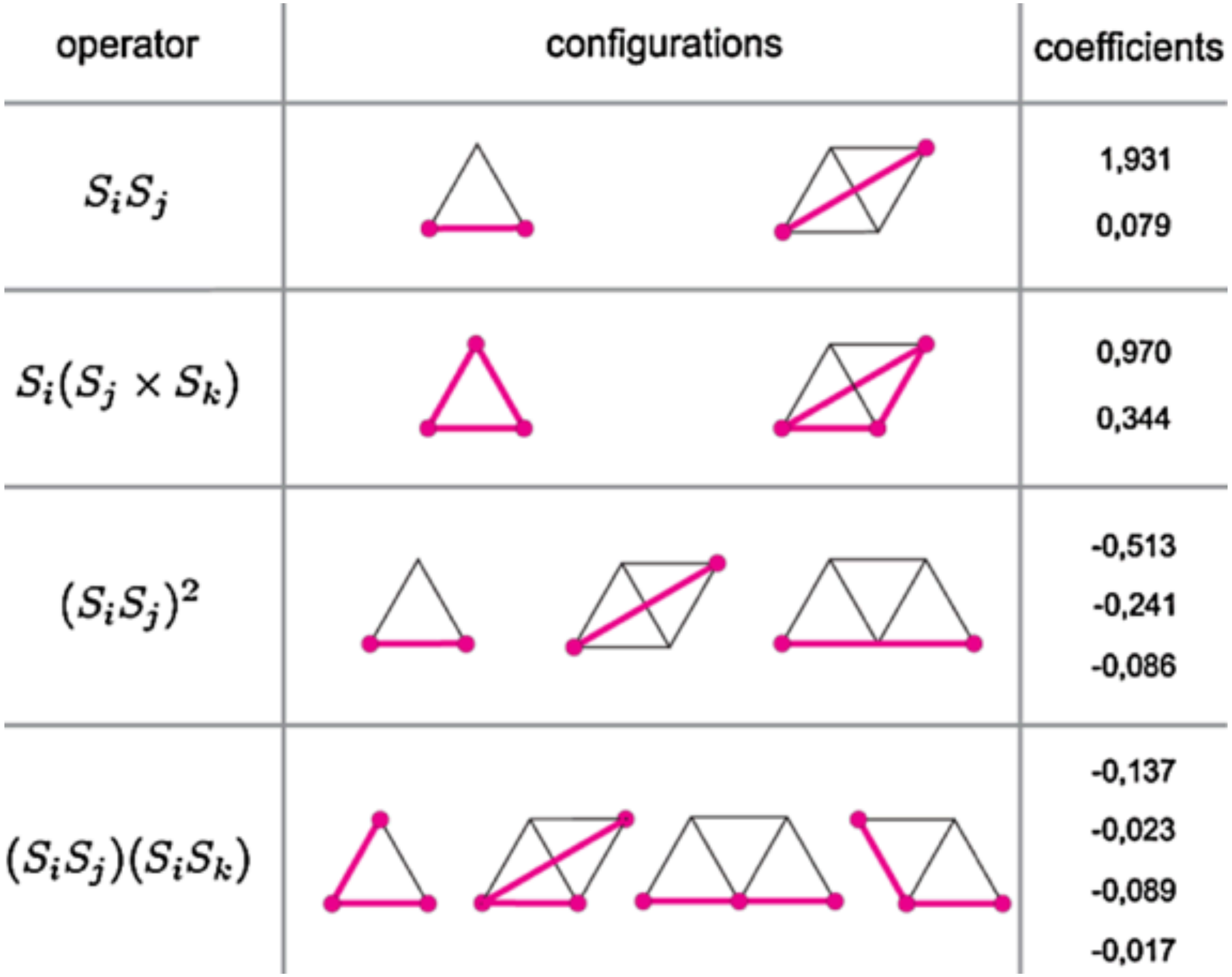
Supported by 2d DMRG calculations on the Kagome lattice

Bauer, Keller, Dolfi, Trebst, Ludwig, Nat. Comm. 2014

Non-Abelian Chiral spin liquid (2009)

$$|\psi_0\rangle = \sum_{z_1,\ldots,z_N} \psi_0(z_1,\ldots,z_N)\tilde{S}^\dagger_{z_1}\ldots\tilde{S}^\dagger_{z_N}\,|-1\rangle_N$$

$$\psi_0 \sim \mathrm{Pf}\left(\frac{1}{z_j - z_k}\right)\prod_{i<j}(z_i - z_j) \qquad \mathrm{Pf}\left(\frac{1}{z_j - z_k}\right) \equiv \mathcal{A}\left[\frac{1}{z_1 - z_2}\ldots\frac{1}{z_{N-1} - z_N}\right]$$



operator	configurations	coefficients
$S_i S_j$		1,931 0,079
$S_i(S_j \times S_k)$		0,970 0,344
$(S_i S_j)^2$		-0,513 -0,241 -0,086
$(S_i S_j)(S_i S_k)$		-0,137 -0,023 -0,089 -0,017

Recent numerical developments

Chiral spin liquids are preferably found for SU(2) breaking spin Hamiltonians:

PRL 112, 137202 (2014) PHYSICAL REVIEW LETTERS week ending 4 APRIL 2014

Chiral Spin Liquid in a Frustrated Anisotropic Kagome Heisenberg Model

Yin-Chen He,[1] D. N. Sheng,[2] and Yan Chen[1,3]

PRL 114, 037201 (2015) PHYSICAL REVIEW LETTERS week ending 23 JANUARY 2015

Distinct Spin Liquids and Their Transitions in Spin-1/2 *XXZ* Kagome Antiferromagnets

Yin-Chen He[1,*] and Yan Chen[1,2]

arXiv:1509.03070

Kagome chiral spin liquid as a gauged $U(1)$ symmetry protected topological phase

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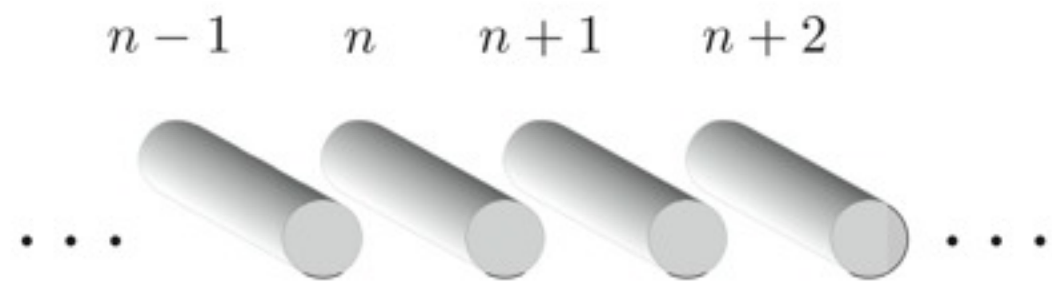
Can SO-induced anisotropic spin interactions help to stabilize a CSL?

Wire construction of the chiral spin liquid

Starting from spinful wires, induce a Mott gap to single out low-energy spin fields.



$$\rho_\sigma(x) = -\frac{1}{\pi}\partial_x \phi_\sigma \qquad \phi_s = \frac{1}{\sqrt{2}}(\phi_\uparrow - \phi_\downarrow) \qquad \theta_s = \frac{1}{\sqrt{2}}(\theta_\uparrow - \theta_\downarrow)$$

Assume S-S coupling between the wires and adjust intrinsic spin-orbit coupling and Zeeman field such that only desired couplings prevail.

$$h_t^i = \frac{J}{(2\pi\alpha)^2}\cos(\sqrt{2}(\phi_s^i - \theta_s^i + \phi_s^{i+1} + \theta_s^{i+1}))$$

$$H_{\mathrm{CSL}} = \sum_i \int dx [h_0^i(x) + h_t^i(x)]$$

Bulk is gapped; edge mode commutator yields $K = \pm 2$

2π kinks in the bulk sine-Gordon term relate to $S^z = \pm 1/2$

Summary

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The specific kind of SO coupling significantly affects the strong coupling limit description of interacting topological insulators. U(1) breaking models are more amenable to exotic phases.

Summary

Pinning down the accurate spin Hamiltonian for Iridate spin-orbit Mott insulators is subtle, and likely involves next nearest neighbor terms.

The specific kind of SO coupling significantly affects the strong coupling limit description of interacting topological insulators. U(1) breaking models are more amenable to exotic phases.

Abelian and non-Abelian parafermionic chiral spin liquids can be constructed from coupled wires through anisotropic spin-spin interactions only. Parafermionic spin liquids exist, and are within numerical reach for higher spin S scenarios.