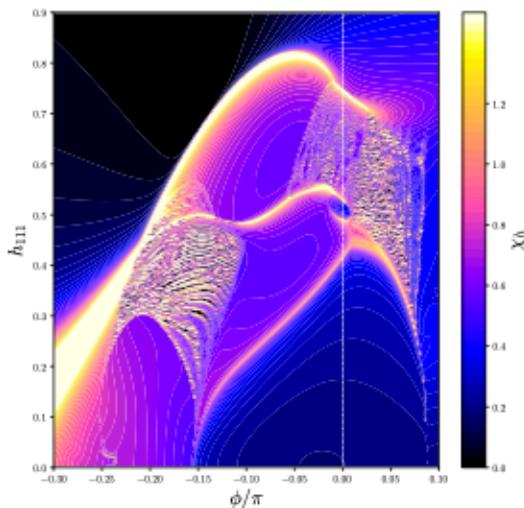


Novel Phases of Kitaev (Chains and) Multileg Ladders



Erik S. Sørensen, McMaster
Hamilton, Canada

- JS Gordon, A Catuneanu, ESS, HY Kee Nature communications 10 (1), 1-8 (2019)
- A Catuneanu, ESS, HY Kee Physical Review B 99 (19), 195112 (2019)
- J Lambert, ESS Physical Review B 102 (22), 224401 (2020)
- ESS, A Catuneanu, JS Gordon, HY Kee Physical Review X 11 (1), 011013 (2021)
- Wang Yang, Alberto Nocera, ESS, Hae-Young Kee, and Ian Affleck Phys. Rev. B **103**, 054437 (2021)
- ESS, JS Gordon, J Riddell, HY Kee, arXiv:2209.06221

RPMBT, Chapel Hill, September 15, 2022

University of Toronto



Hae-Young Kee

Andrei Catuneanu
Jacob S Gordon

UBC



Ian Affleck

Yang Wang
Alberto Nocera

McMaster



Erik Sørensen

Yannick Castonguay-Page
James Lambert
Jonathon Riddell
Addison Richards
Sebastien Avakian

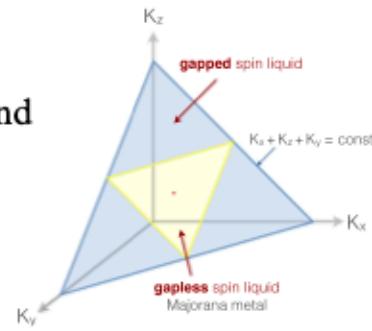
Kitaev Honeycomb Model

Anyons in an exactly solved model and beyond

Alexei Kitaev *

California Institute of Technology, Pasadena, CA 91125, USA

Received 21 October 2005; accepted 25 October 2005



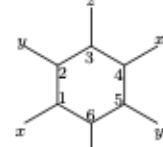
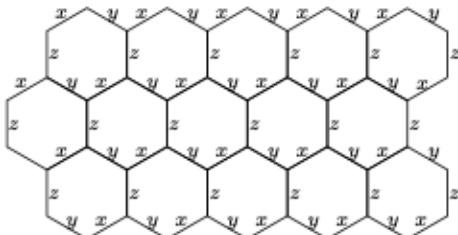
Abstract

A spin-1/2 system on a honeycomb lattice is studied. The interactions between nearest neighbors are of XX, YY or ZZ type, depending on the direction of the link; different types of interactions may differ in strength. The model is solved exactly by a reduction to free fermions in a static \mathbb{Z}_2 gauge

Annals of Physics 321 (2006) 2–111

Toric Code: Annals of Physics 303 (2003) 2–30

$$H = K_x \sum_{x \text{ links}} S_j^x S_k^x + K_y \sum_{y \text{ links}} S_j^y S_k^y + K_z \sum_{z \text{ links}} S_j^z S_k^z$$



$$W_p = \sigma_1^x \sigma_2^y \sigma_3^z \sigma_4^x \sigma_5^y \sigma_6^z$$

$$[H, W_p] = 0$$

Quantum Compass Models (sq lattice) Dorier, Becca, Mila PRB 72, 024448 (2005). Doucot et al PRB (2005)

PRL 102, 017205 (2009)

PHYSICAL REVIEW LETTERS

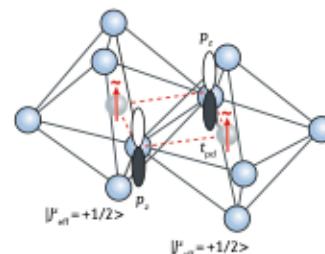
week ending
9 JANUARY 2009

Mott Insulators in the Strong Spin-Orbit Coupling Limit: From Heisenberg to a Quantum Compass and Kitaev Models

G. Jackeli^{1,*} and G. Khaliullin¹

¹Max-Planck-Institut für Festkörperforschung, Heisenbergstrasse 1, D-70569 Stuttgart, Germany
(Received 21 August 2008; published 6 January 2009)

Chaloupka, Jackeli, Khaliullin, PRL 105, 0227204 (2010)
Chaloupka, Jackeli, Khaliullin, PRL 110, 097204 (2013)

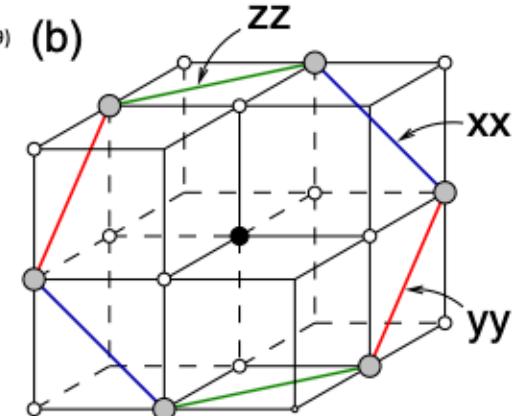


H. Takagi et al
Nature Reviews Physics
volume 1, pages 264–280 (2019)

Edge Sharing Tetrahedra

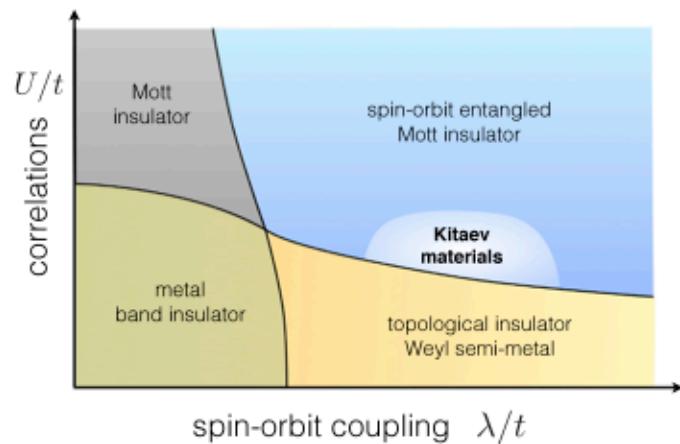
$$H = \sum_{\langle ij \rangle_\gamma} K_\gamma S_i^\gamma S_j^\gamma$$

NN Heisenberg cancels !



[111] is perpendicular

Kitaev Materials



Trebst, Hickey Physics Reports 950, 1 (2022)

Witczak-Krempa, Kim, Chen, Balents Ann Rev Cond Mat 5:57 (2014)

SOC + Strong Correlations

Table 1 | Representative Kitaev candidate materials and a summary of their physical properties

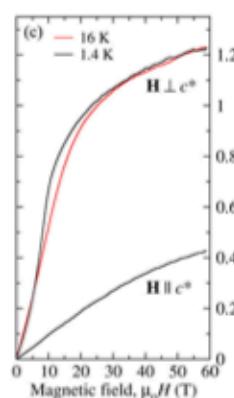
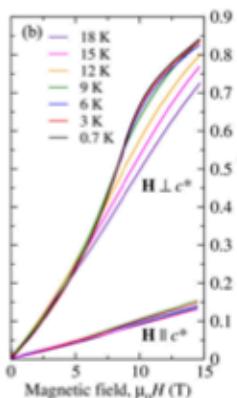
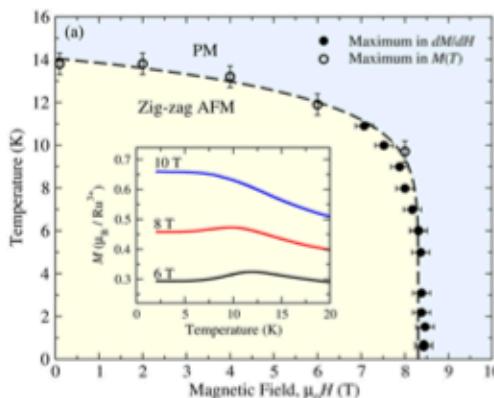
Materials	Crystal structure (space group)	T_{mag}	Anisotropy	$p_{\text{eff}} (\mu_0)$	$\theta_{\text{CW}} (\text{K})$	Magnetic ground state	Refs
Na_xIrO_3	2D ($C2/m$)	15 K	$\chi_z > \chi_{ab}$	1.81 (ab) 1.94 (c)	-176 (θ_{ab}) -40 (θ_z)	Zigzag	41,50,58,89
$\alpha\text{-Li}_x\text{IrO}_3$	2D ($C2/m$)	15 K	$\chi_{ab} > \chi_z$	1.50 (ab) 1.58 (c)	+5 (θ_{ab}) -250 (θ_z)	Spiral	44,56,71
$\text{H}_x\text{LiIr}_2\text{O}_6$	2D ($C2/m$)	-	$\chi_{ab} > \chi_z$	1.60	-105	Spin-liquid	49
Cu_xIrO_3	2D ($C2/c$)	2.7 K	Not known	1.93 (1)	-110	Antiferromagnetic order or spin-glass	42
$\text{Cu}_x\text{LiIr}_2\text{O}_6$	2D ($C2/c$)	15 K	Not known	2.1 (1)	-145	Antiferromagnetic order	49
$\text{Ag}_x\text{LiIr}_2\text{O}_6$	2D ($R-3m^*$)	-12 K	Not known	1.77		Antiferromagnetic order	48
$\alpha\text{-RuCl}_3$	2D ($C2/m$ or $P3_112$, or $R-3$); T and sample dependent	7 K and/or 14 K (see text)	$\chi_{ab} > \chi_z$	2.33 (ab), 2.71 (c)	+39.6 (θ_{ab}), -216.4 (θ_z)	Zigzag	51,28,87, 70,130
$\beta\text{-Li}_x\text{IrO}_3$	3D ($Fddd$)	38 K	$\chi_b > \chi_c > \chi_a$	1.87 (a) 1.80 (b) 1.97 (c)	-90.2 (θ_{ab}) +12.9 (θ_z) +21.6 (θ_c)	Spiral	52,72,83
$\gamma\text{-Li}_x\text{IrO}_3$	3D ($Cccm$)	39.5 K	$\chi_b > \chi_c > \chi_a$	-1.6	+40	Spiral	53,73

^aR-3m assumed in REF.⁴⁸ because of strong stacking disorder.

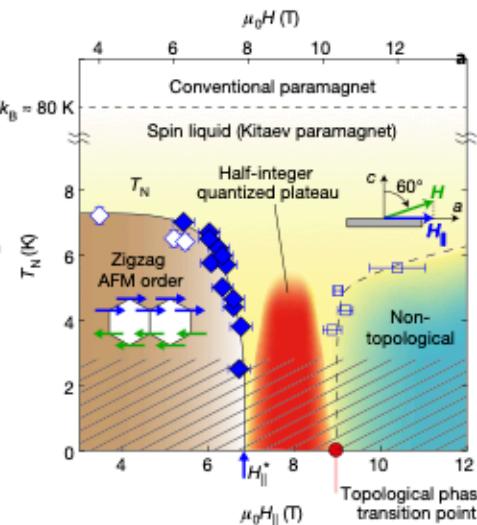
Takagi et al., *Nature Reviews Physics* volume 1, pages 264–280 (2019)

Ordering

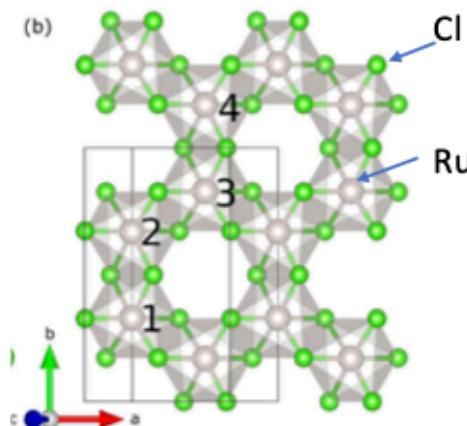
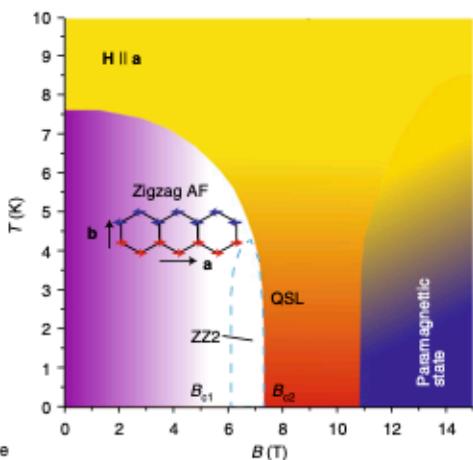
α -RuCl₃



Kasahara, et al, Matsuda, Nature 559, 227 (2018)



Czajka et al, Ong Nature Physics, 17, 915 (2021)



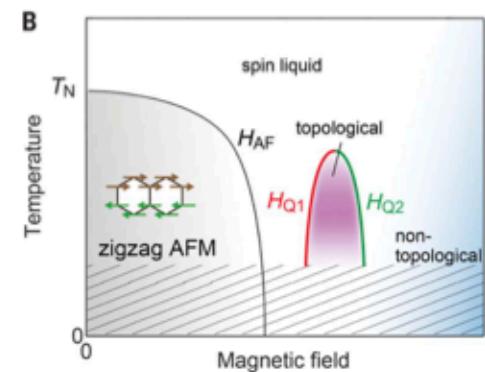
Quantized (or not quantized) thermal hall effect..

PA Lee

www.condmatjclub.org

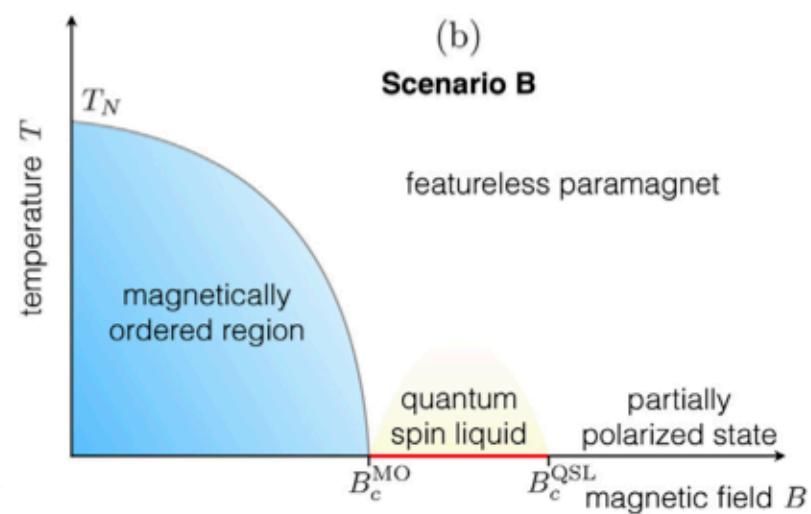
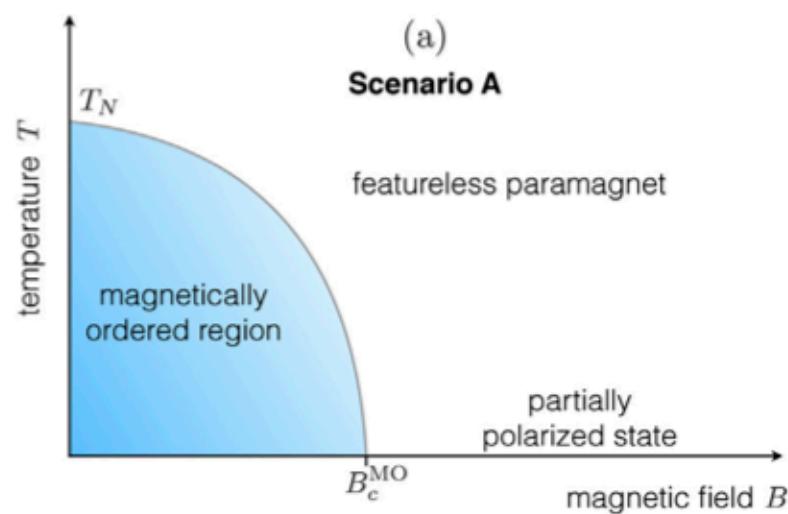
Nov 2021

$\frac{1}{2}$ a fermion
= Majorana edge mode



Yokoi et al, Matsuda Science 373, 568 (2021)

Phase at Intermediate Fields ??



Trebst, Hickey Physics Reports 950, 1 (2022)

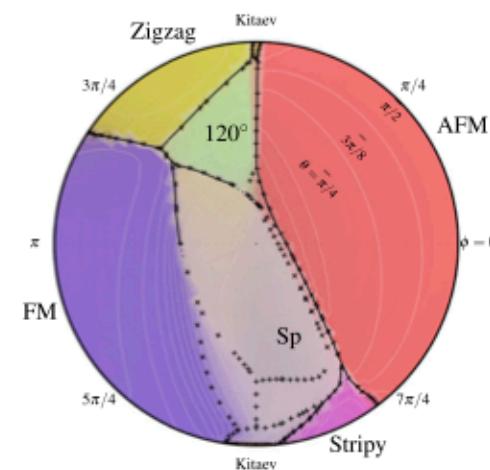
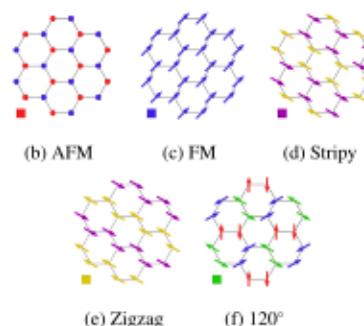
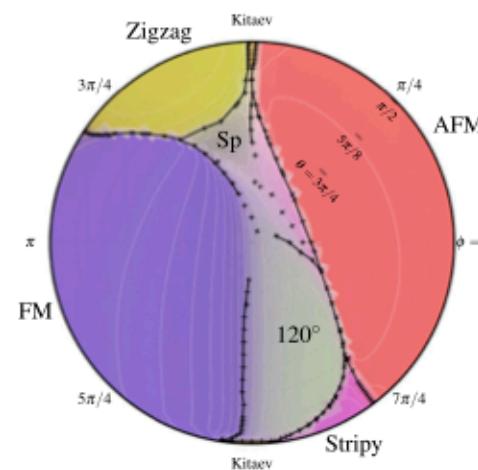
How can a magnetic field increase the entanglement shouldn't it disentangle ?

Why should there be an intermediate phase ?

Kitaev-Heisenberg-Gamma Model

Rau, Lee, Kee PRL 112, 077204 (2014)

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



$$-\hbar |\sum_j \hat{h} \cdot \vec{S}_j|$$

Hickey, Trebst
Nat. Comm. 10, 530 (2019)

24 site Exact
Diagonalization

TABLE I. The representative sets of parameters of the generalized KH model (1) for α -RuCl₃ (in meV). The values that come close to the ranges proposed in this work are highlighted in bold. The common acronyms include linear spin-wave theory (LSWT), density-functional theory (DFT), spin-orbit coupling (SOC), inelastic neutron scattering (INS), exact diagonalization (ED), and terahertz spectroscopy (THz); structures of P3 and C2 symmetry are referred to as “P3” and “C2” for brevity.

Reference	Method	K	Γ	Γ'	J	J_3	$\Gamma+2\Gamma'$	$J+3J_3$
Banerjee <i>et al.</i> [22]	LSWT, INS fit	+7.0			-4.6		-4.6	
Kim <i>et al.</i> [29]	DFT+ t/U , P3	-6.55	5.25	-0.95	-1.53		3.35	-1.53
	DFT+SOC+ t/U	-8.21	4.16	-0.93	-0.97		2.3	-0.97
	Same+fixed lattice	-3.55	7.08	-0.54	-2.76		6.01	-2.76
	Same+ U + zigzag	+4.6	6.42	-0.04	-3.5		6.34	-3.5
Winter <i>et al.</i> [30]	DFT+ED, C2	-6.67	6.6	-0.87	-1.67	2.8	4.87	6.73
	Same, P3	+7.6	8.4	+0.2	-5.5	2.3	8.8	+1.4
Yadav <i>et al.</i> [24]	Quantum chemistry	-5.6	-0.87		+1.2		-0.87	+1.2
Ran <i>et al.</i> [34]	LSWT, INS fit	-6.8	9.5				9.5	
Hou <i>et al.</i> [31]	DFT+ t/U , $U=2.5$ eV	-14.43	6.43		-2.23	2.07	6.43	+3.97
	Same, $U=3.0$ eV	-12.23	4.83		-1.93	1.6	4.83	+2.87
	Same, $U=3.5$ eV	-10.67	3.8		-1.73	1.27	3.8	+2.07
Wang <i>et al.</i> [32]	DFT+ t/U , P3	-10.9	6.1		-0.3	0.03	6.1	-0.21
	Same, C2	-5.5	7.6		+0.1	0.1	7.6	+0.4
Winter <i>et al.</i> [35]	<i>Ab initio</i> + INS fit	-5.0	2.5		-0.5	0.5	2.5	+1.0
Suzuki <i>et al.</i> [36]	ED, C_p fit	-24.41	5.25	-0.95	-1.53		3.35	-1.53
Cookmeyer <i>et al.</i> [37]	Thermal Hall fit	-5.0	2.5		-0.5	0.11	2.5	-0.16
Wu <i>et al.</i> [38]	LSWT, THz fit	-2.8	2.4		-0.35	0.34	2.4	+0.67
Ozel <i>et al.</i> [39]	Same, $K > 0$	+1.15	2.92	+1.27	-0.95		5.45	-0.95
	Same, $K < 0$	-3.5	2.35		+0.46		2.35	+0.46
Eichstaedt <i>et al.</i> [33]	DFT+Wannier+ t/U	-14.3	9.8	-2.23	-1.4	0.97	5.33	+1.5
Sahasrabudhe <i>et al.</i> [42]	ED, Raman fit	-10.0	3.75		-0.75	0.75	3.75	1.5
Sears <i>et al.</i> [40]	Magnetization fit	-10.0	10.6	-0.9	-2.7		8.8	-2.7
Laurell <i>et al.</i> [41]	ED, C_p fit	-15.1	10.1	-0.12	-1.3	0.9	9.86	+1.4
	“Realistic” range	[-11 , -3.8]	[3.9, 5.0]	[2.2, 3.1]	[-4.1 , -2.1]	[2.3, 3.1]	[9.0, 11.4]	[4.4, 5.7]
This work	Point 1	-4.8	4.08	2.5	-2.56	2.42	9.08	4.7
	Point 2	-10.8	5.2	2.9	-4.0	3.26	11.0	5.78
	Point 3	-14.8	6.12	3.28	-4.48	3.66	12.7	6.5

Third neighbor

$$K < 0, \Gamma > 0, \Gamma' < 0, J < 0$$

$$|\Gamma| > J$$

Matrix Product States (Tensor Networks)

$$|\Psi\rangle = \sum_{j_1, \dots, j_n} c_{j_1, \dots, j_N} |j_1, \dots, j_N\rangle \quad n^N$$

Variational Ansatz

$$|\Psi\rangle = \sum_{j_1, \dots, j_n} A^{[1]j_1} A^{[2]j_2} \dots A^{[N]j_N} |j_1, \dots, j_N\rangle$$

$S = 1/2 : j = \uparrow, \downarrow$

A: D x D Matrix

$N \times n \times D^2$

Eigenvalues of reduced density matrix: $\lambda_1 \geq \lambda_2 \geq \lambda_3 \dots \lambda_D$

Finite DMRG OBC

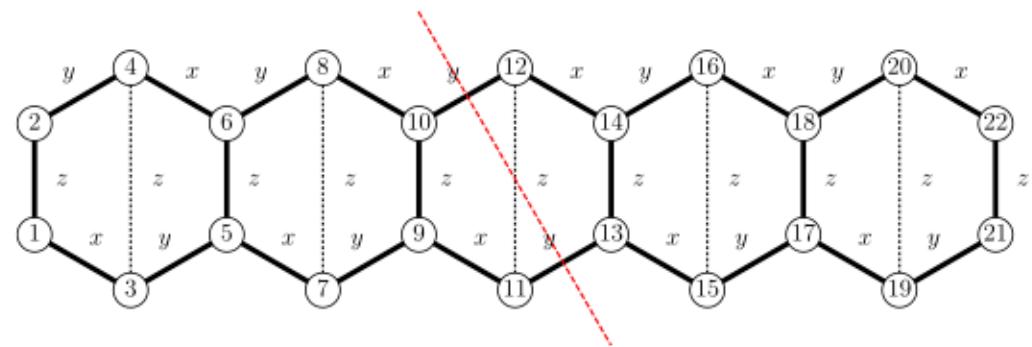
Translationally invariant form, iDMRG, OBC

$$\chi^e \sim L^{2/\nu - (d+z)}$$

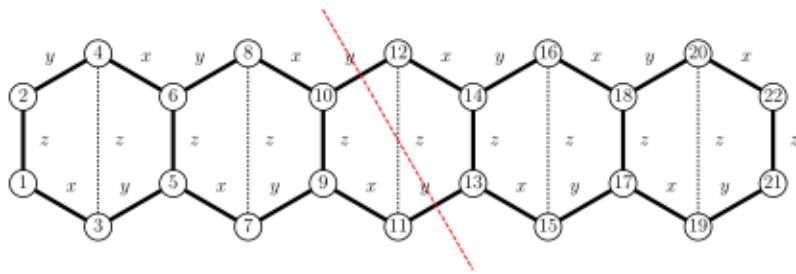
$$\chi_h^e = -\frac{\partial^2 e_0}{\partial h^2}$$

$$\chi_h^{\lambda_1} = -\frac{\partial^2 \lambda_1}{\partial h^2}$$

Two Leg Ladders K-J



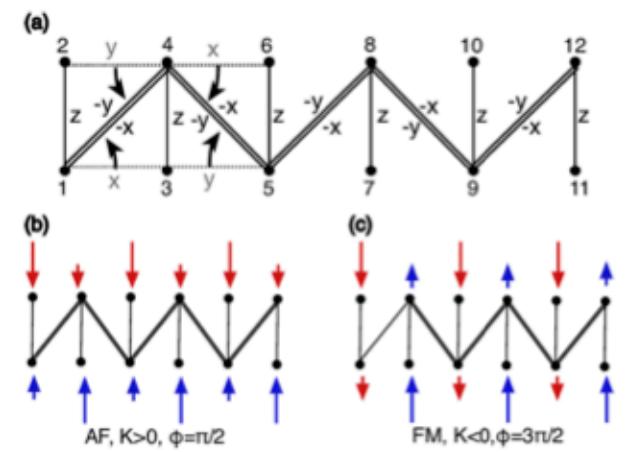
$$J = \cos(\phi)$$
$$K = \sin(\phi)$$


 H

"Hidden" String order

 \xrightarrow{V}
 \tilde{H}

Local Order



Exact for $J=0$ w OBC!

V is non-local

$$\Gamma = 0$$

The Kitaev-Heisenberg (KJ) Ladder

$$H = \cancel{J} \cos(\phi) \sum_{\langle i,j \rangle} \vec{S}_i \cdot \vec{S}_j + \cancel{K} \sin(\phi) \sum_j (S_{2j-1}^x S_{2j}^x + S_{2j}^z S_{2j+1}^z + S_{2j}^y S_{2j+3}^y)$$

A Catuneanu, ESS, HY Kee Physical Review B 99 (19), 195112 (2019)

Non-local Unitary Operator

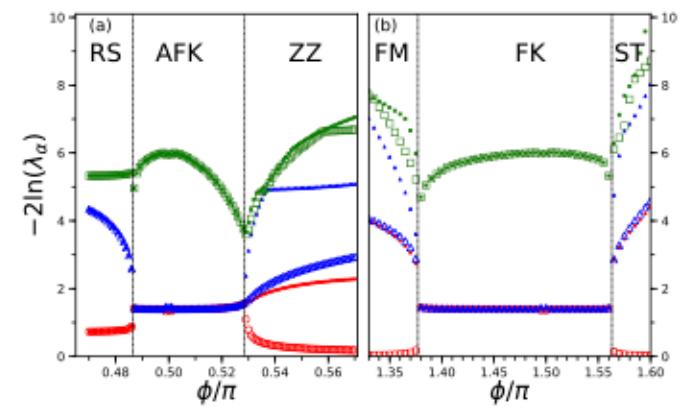
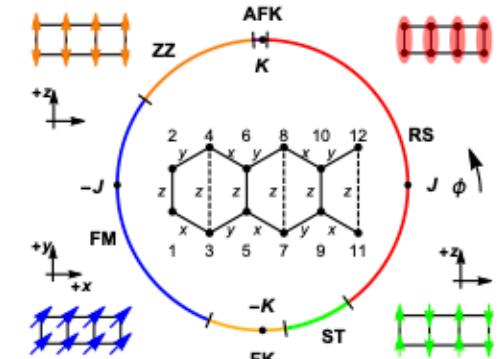
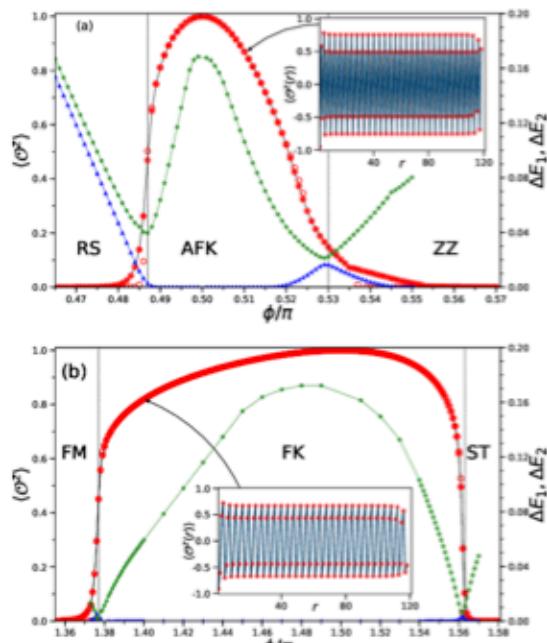
$$V = \prod_{\substack{j+1 < k \\ j \text{ odd, } k \text{ odd} \\ j=1, \dots, N-3 \\ k=3, \dots, N-1}} U(j, k).$$

$$U(j, k) = e^{i\pi(S_j^y + S_{j+1}^y) \cdot (S_k^x + S_{k+1}^x)}$$

String Order !!

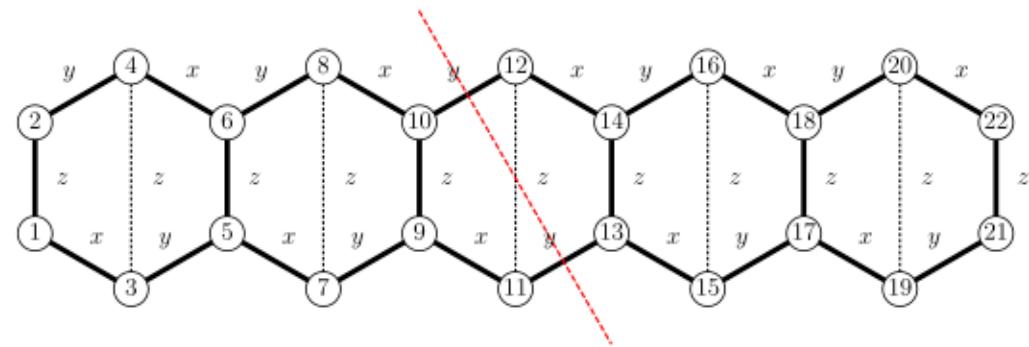
$$\langle \mathcal{O}^z(r) \rangle = 4 \langle \tilde{S}_2^z \tilde{S}_{2+r}^z \rangle = (-1)^{\lfloor (r+1)/2 \rfloor}$$

$$\times \begin{cases} \left\langle \sigma_1^y \sigma_2^x \left(\prod_{k=3}^r \sigma_k^z \right) \sigma_{r+1}^x \sigma_{r+2}^y \right\rangle & r \text{ even} \\ \left\langle \sigma_1^y \sigma_2^x \left(\prod_{k=3}^{r+1} \sigma_k^z \right) \sigma_{r+2}^y \sigma_{r+3}^x \right\rangle & r \text{ odd.} \end{cases}$$



Symmetry Protected
Topological Phase (SPT)

Two Leg Ladders $\kappa\text{-}\Gamma$



$$K = \cos(\phi), \quad \Gamma = \sin(\phi), \quad J = 0$$

Kitaev-Gamma Ladder

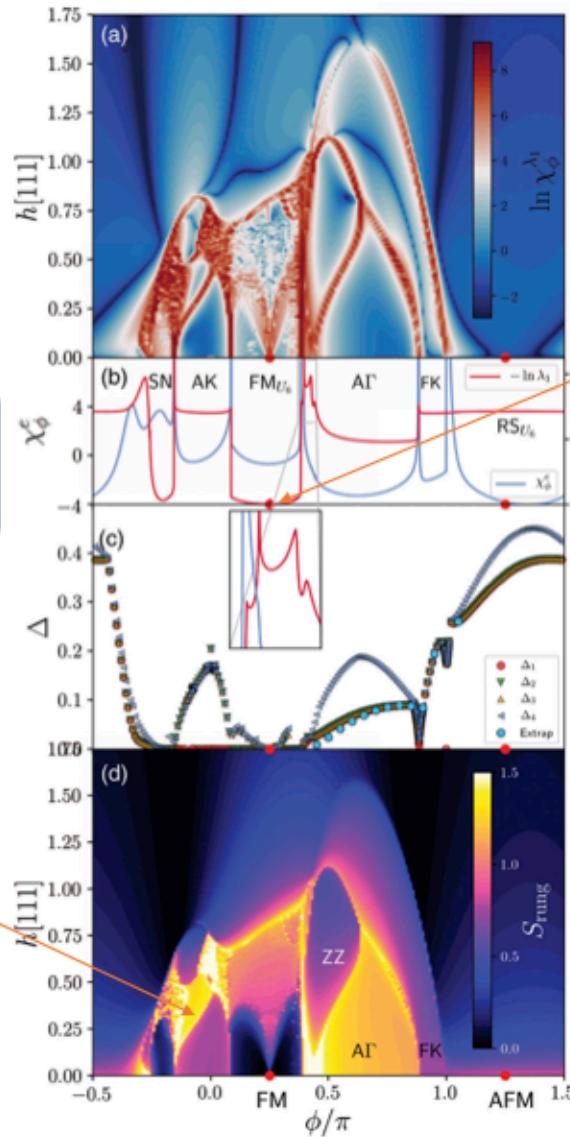
$$H_{KG} = \sum_{\langle ij \rangle, \gamma \in (x,y,z)} K S_i^\gamma S_j^\gamma + \Gamma (S_i^\alpha S_j^\beta + S_i^\beta S_j^\alpha)$$

$$K = \cos(\phi) \quad \Gamma = \sin(\phi)$$

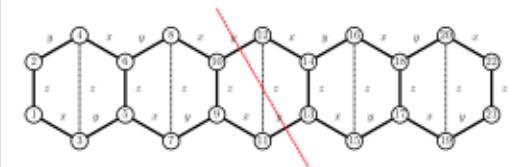
$$-\frac{h[111]}{\sqrt{3}}(S^x + S^y + S^z)$$

Highly Entangled

ESS, A Catuneanu, JS Gordon, HY Kee
Physical Review X 11 (1), 011013 (2021)



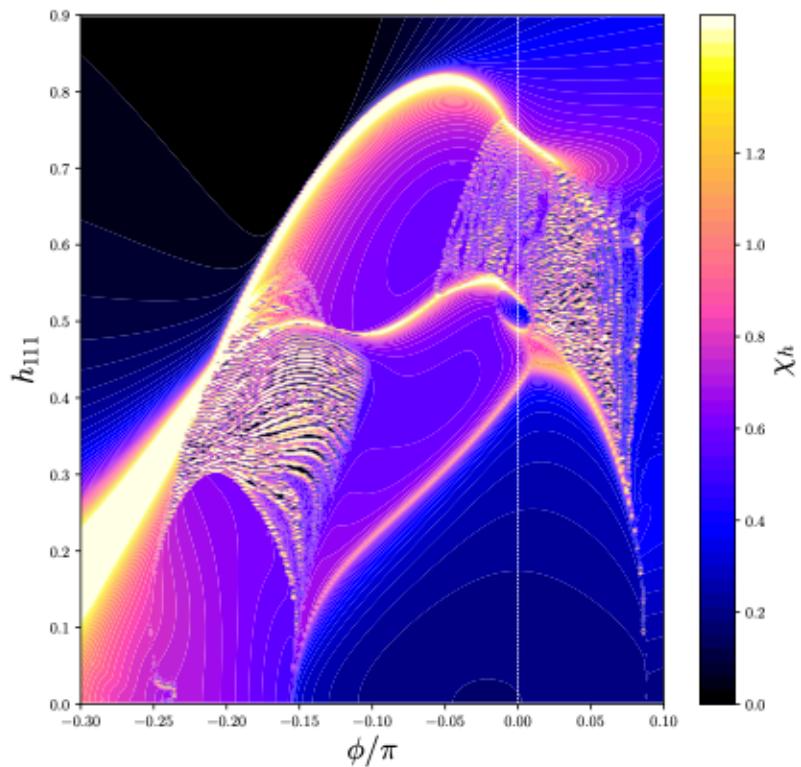
Product State



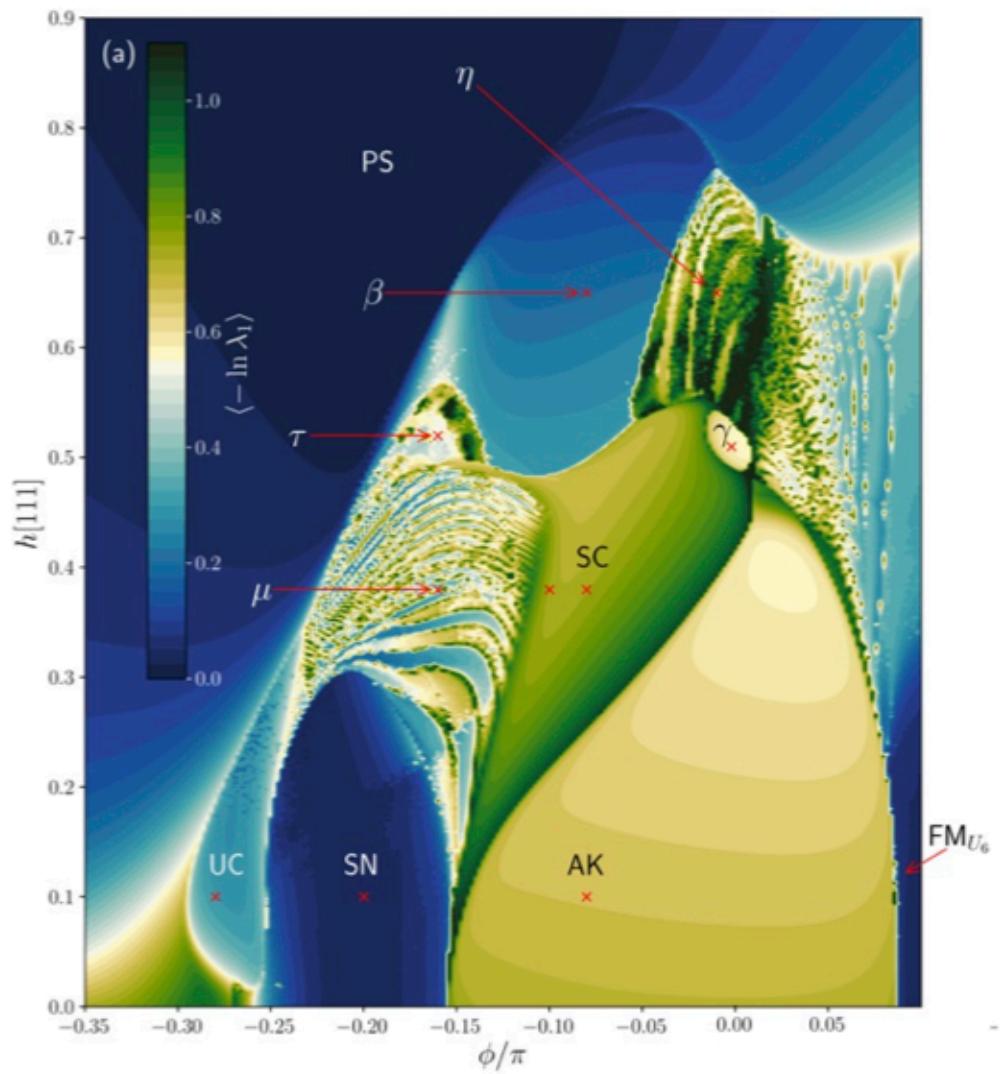
Vicinity of AF Kitaev Point

Vicinity of AFK

ESS, A Catuneanu, JS Gordon, HY Kee
Physical Review X 11 (1), 011013 (2021)

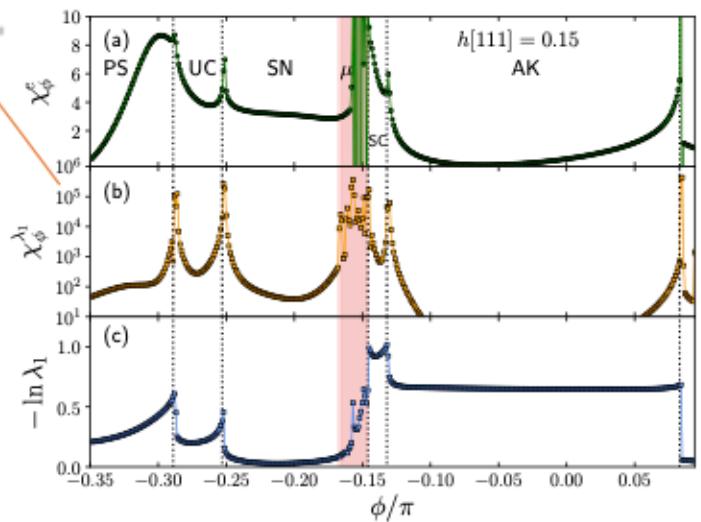
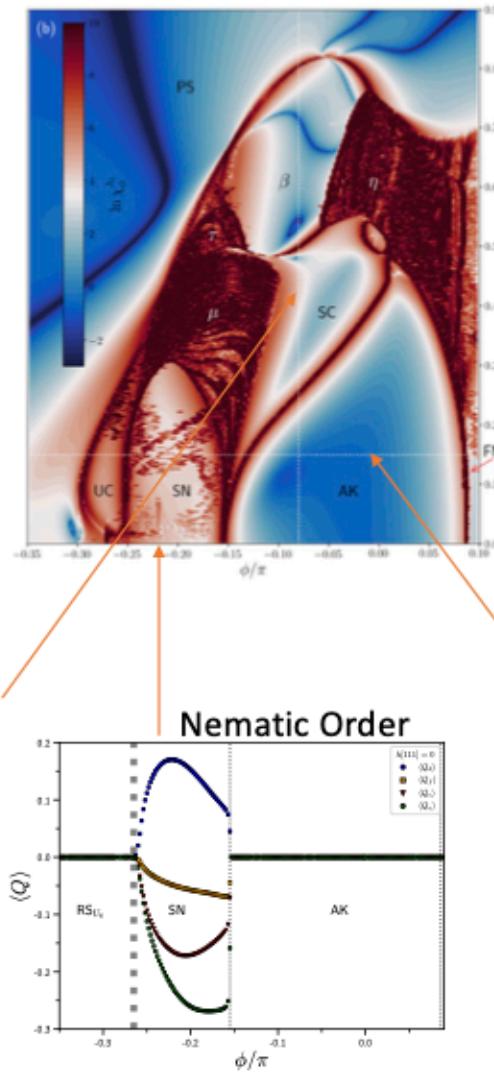
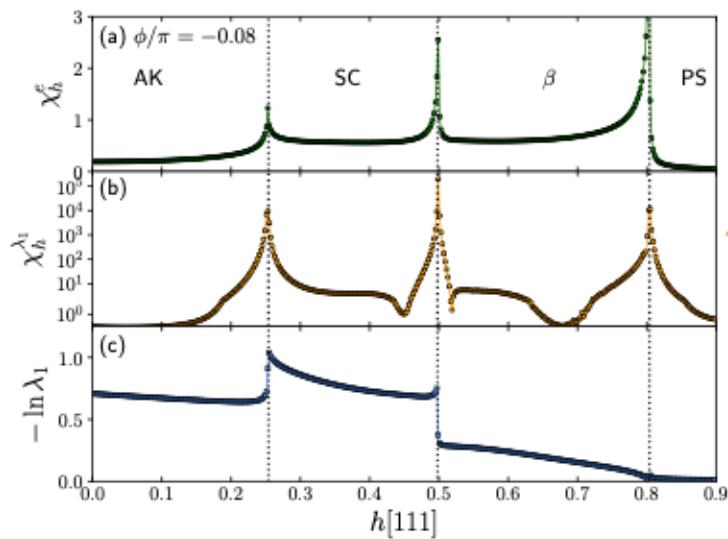


$$\chi_h^e = -\frac{\partial^2 e_0}{\partial h^2}$$
$$\chi_\phi^{\lambda_1} = -\frac{\partial^2 \lambda_1}{\partial \phi^2}$$

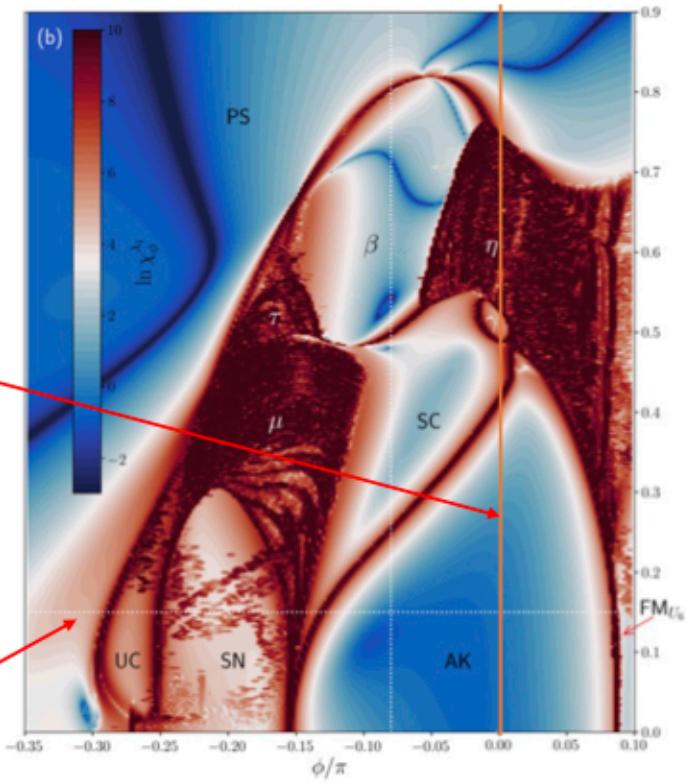
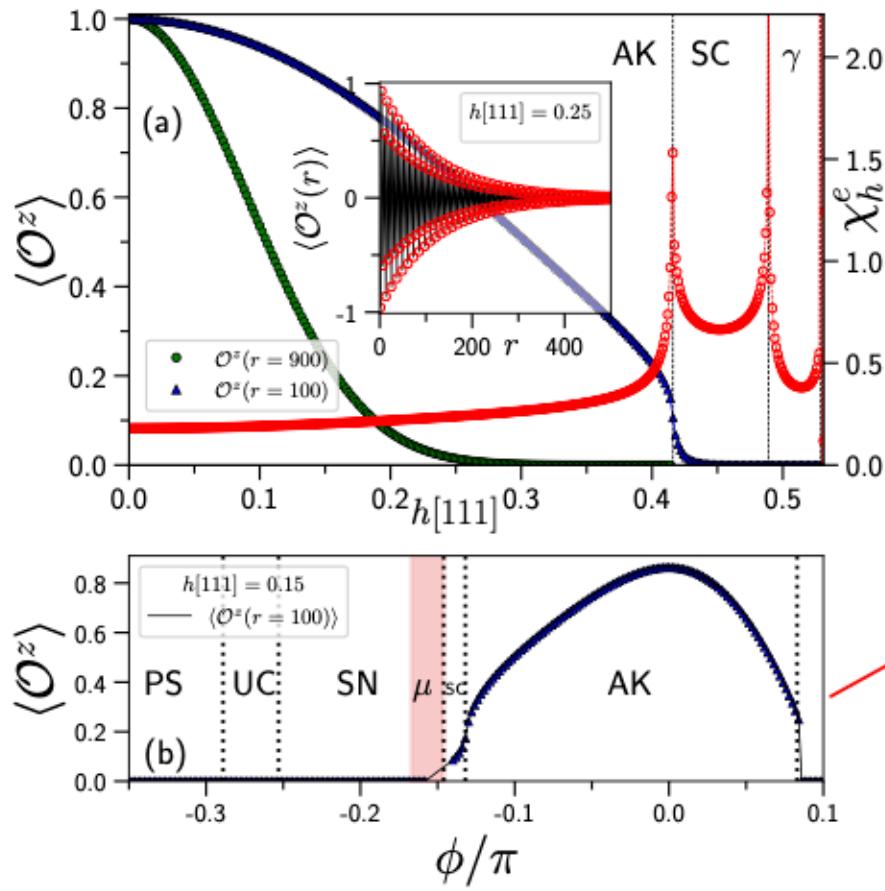


Vicinity of AFK

ESS, A Catuneanu, JS Gordon, HY Kee
 Physical Review X 11 (1), 011013 (2021)

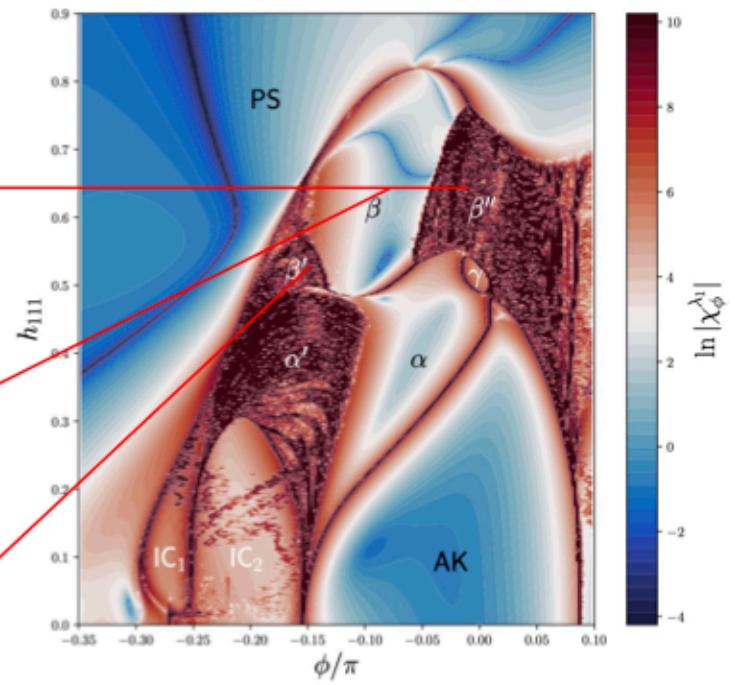
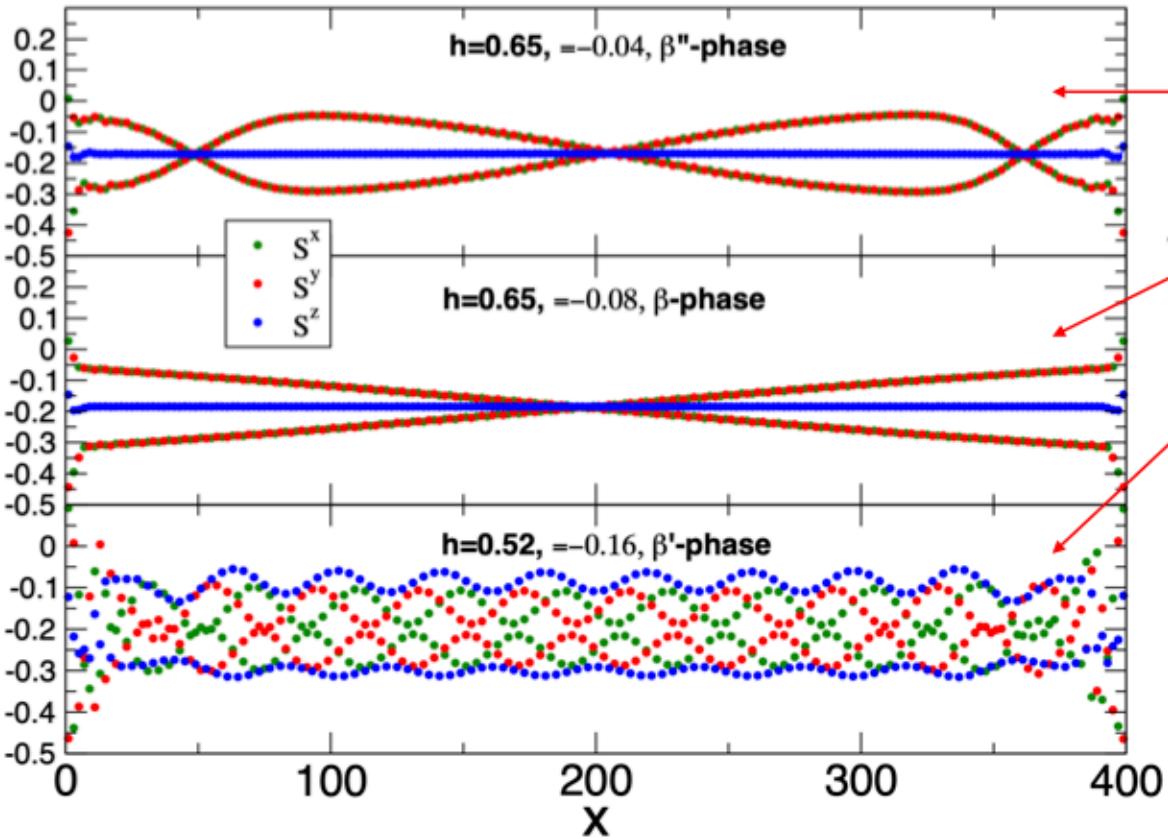


String Order



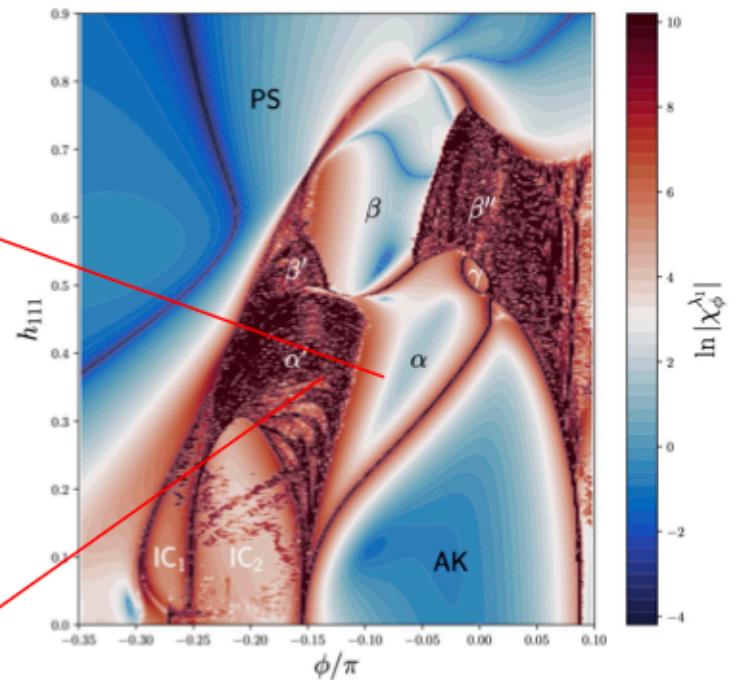
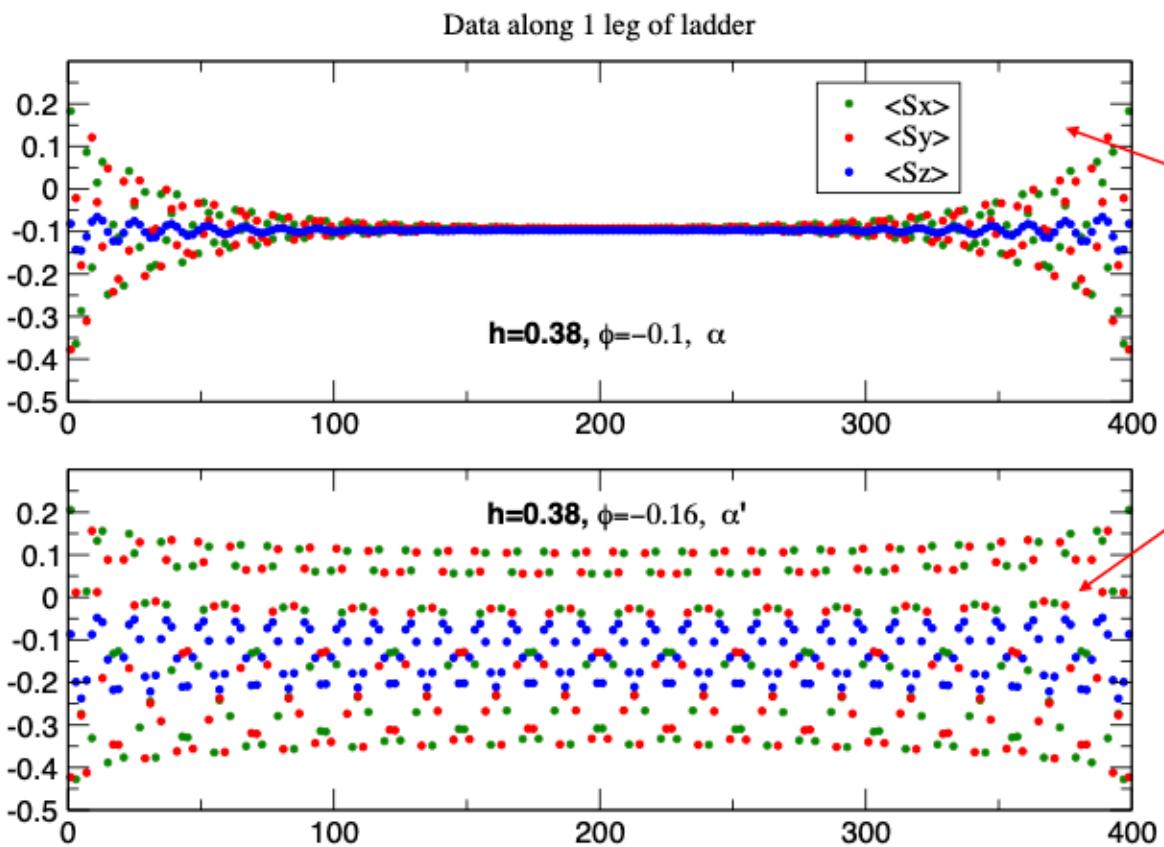
SOP is Fragile !!

Magnetic Order



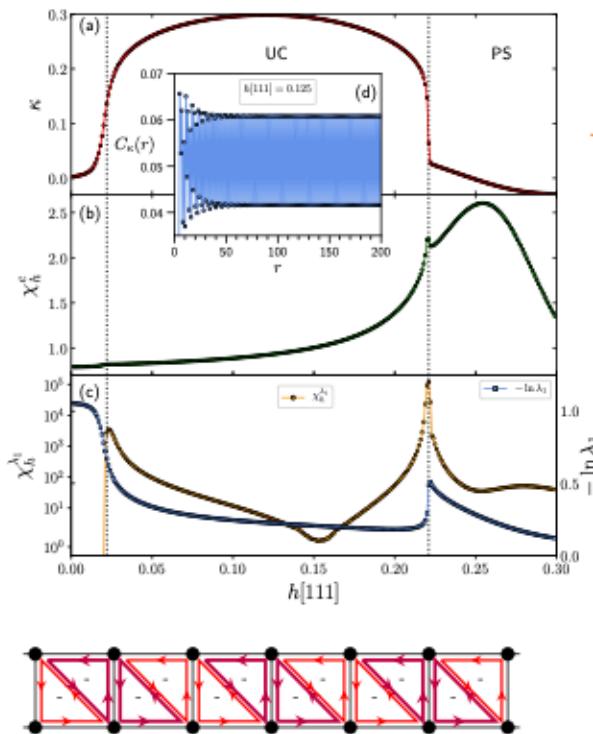
Expectation values along
1 Leg of the ladder

Magnetic Order



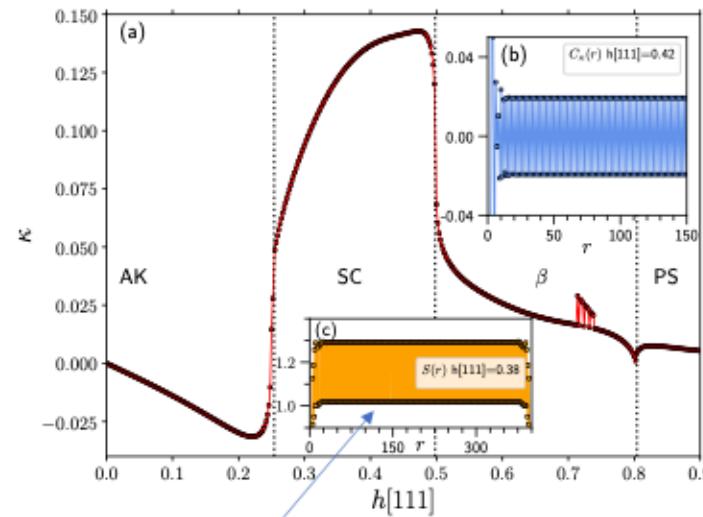
Scalar Chirality

ESS, A Catuneanu, JS Gordon, HY Kee
 Physical Review X 11 (1), 011013 (2021)

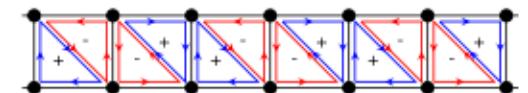
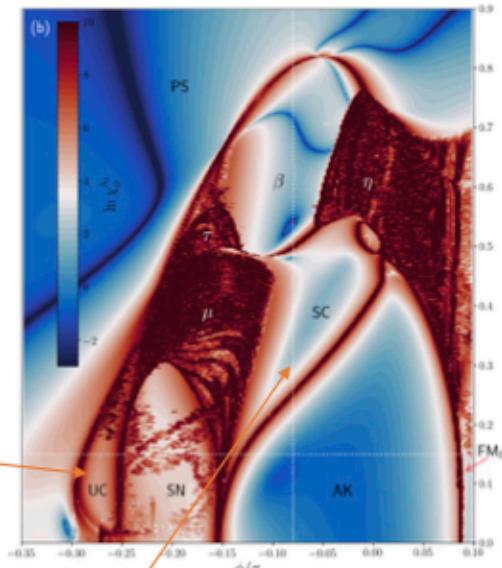


$$\kappa = \langle \sigma_{i,1} \cdot (\sigma_{i,2} \times \sigma_{i+1,1}) \rangle$$

Clock-wise around a triangle



Bipartite Entanglement \rightarrow Gap



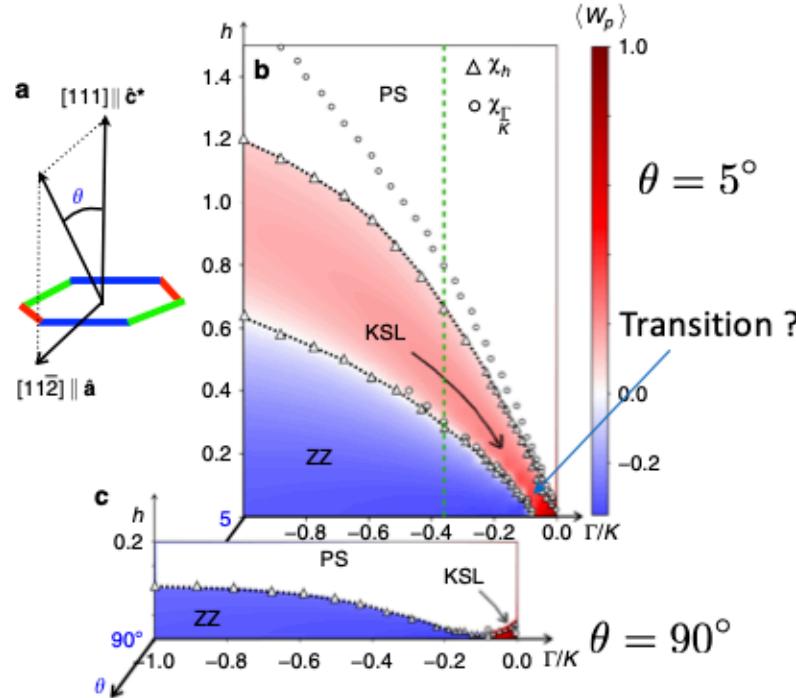


Intermediate Phase ?

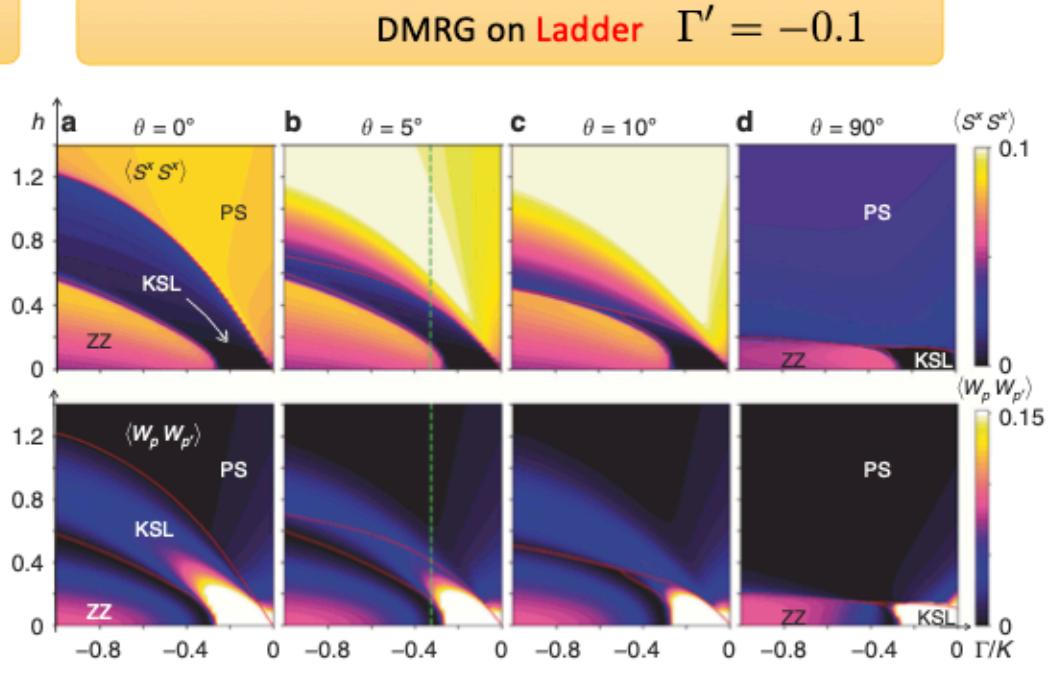
Vicinity of FK point $K<0 \Gamma>0$

JS Gordon, A Catuneanu, ESS, HY Kee Nature communications 10 (1), 1-8 (2019)

24 site ED on Two-dimensional cluster $\Gamma' = -0.03$



DMRG on Ladder $\Gamma' = -0.1$



The spin-spin correlator $\langle S_j^x S_k^x \rangle$ at $k-j=50$
plaquette-plaquette correlator $\langle W_p W_{p'} \rangle$ at $p'-p=30$

$K - J - \Gamma - \Gamma'$ Model: Li et al, Nat Comm 12:4007 (2021)

See also H.-Y. Lee Nat Comm, 11, 1639 (2020)

Zhou et al, Tanaka ArXiv:2201.04597

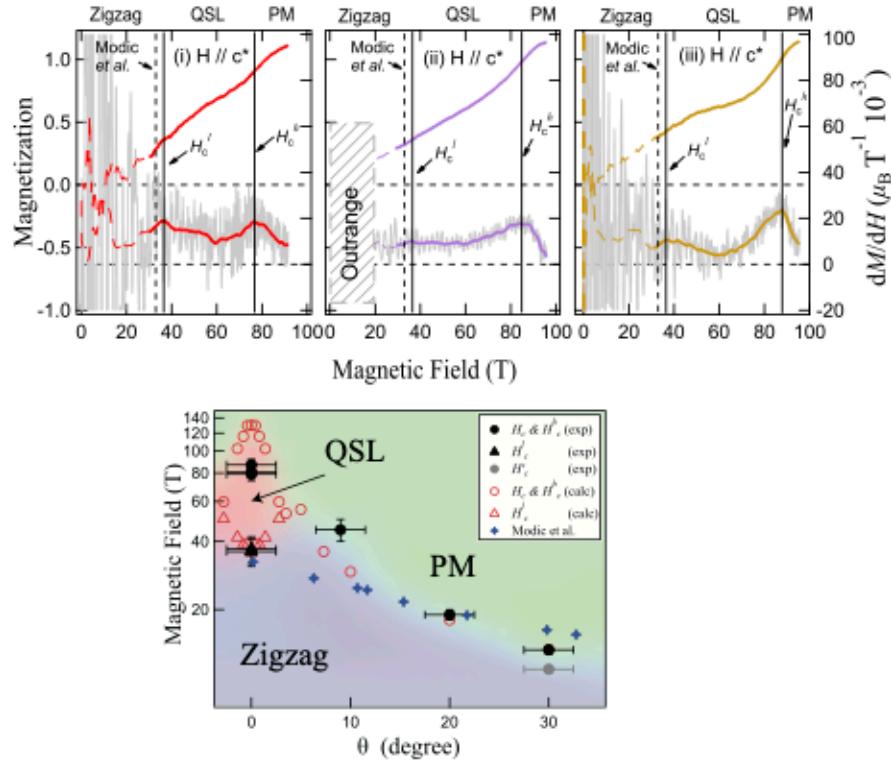
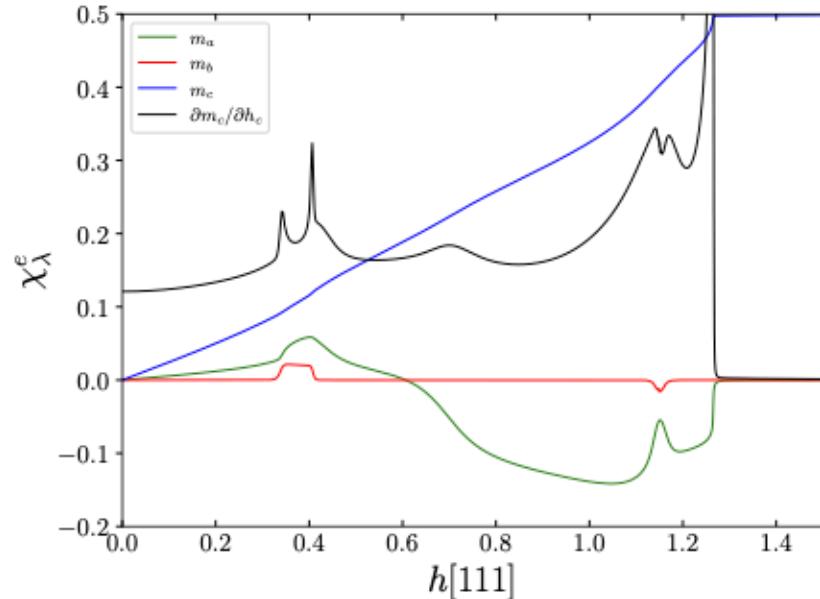


FIG. 4. The field-angle phase diagram that summarizes the values of transition fields determined from both the experimental (black and grey solid markers) and the calculated data (red open ones). We also plot the low-field results (blue stars) taken from Ref. [43] as a supplement. The zigzag antiferromagnetic, paramagnetic (PM), and the quantum spin liquid (QSL) phases are indicated.



- 4 Leg K- Γ Ladder
- $K/\Gamma = -0.73$
- $\Gamma' = 0.0$

Parameters from H. Li et al, Nat. Comm. 12, 407 (2021)

Thanks !

- Phase Diagram sensitive to small changes in parameters
- Several different SPT (QSL) phases at finite field
- Fragile String Order

- JS Gordon, A Catuneanu, ESS, HY Kee Nature communications 10 (1), 1-8 (2019)
- A Catuneanu, ESS, HY Kee Physical Review B 99 (19), 195112 (2019)
- J Lambert, ESS Physical Review B 102 (22), 224401 (2020)
- ESS, A Catuneanu, JS Gordon, HY Kee Physical Review X 11 (1), 011013 (2021)
- Wang Yang, Alberto Nocera, ESS, Hae-Young Kee, and Ian Affleck Phys. Rev. B **103**, 054437 (2021)
- ESS, JS Gordon, J Riddell, HY Kee, arXiv:2209.06221