Extended Quantum Spin Liquid with Spinon-like Excitations in an Anisotropic Kitaev-Gamma Model

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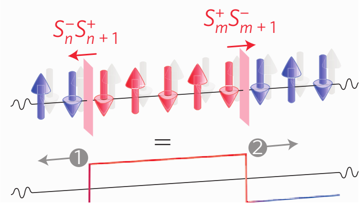
NQS 2022, YITP Kyoto
November 30, 2022

Spinon-like excitations in an anisotropic Kitaev-Gamma model

e.g. AF Heisenberg chain



e.g. Mourigal et al., Nature 9, 435 (2013)

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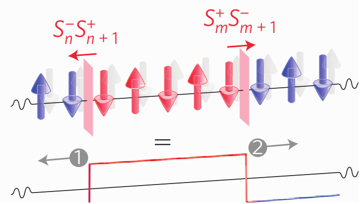

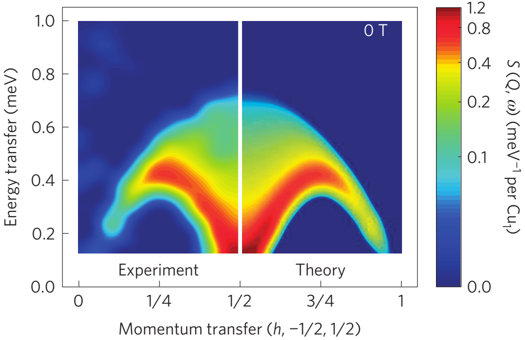

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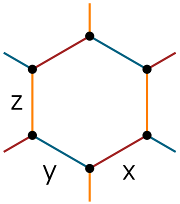
Kitaev model:

- Exactly solvable 2D spin model with bond-dependent $S_i^x S_j^x$, $S_i^y S_j^y$ and $S_i^z S_j^z$
- Quantum spin liquid: itinerant Majorana in a static Z_2-gauge field



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

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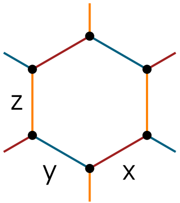
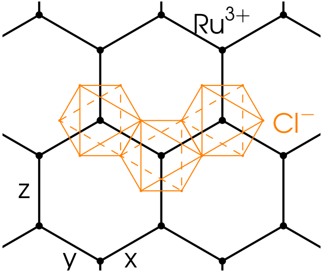
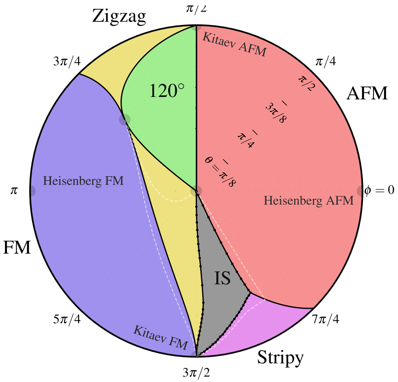




Experiments:

- Potential realization in materials via strong spin-orbit coupling

G. Jackeli, G. Khaliullin, PRL 102, 017205 (2010)



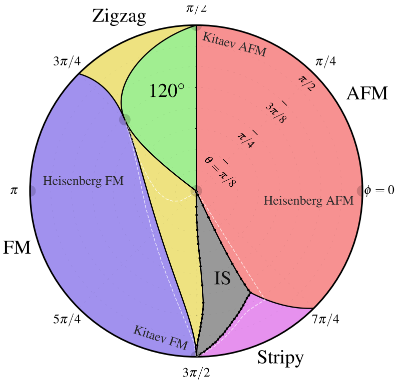
spin-exchange, e.g. on z-bond:

$$\mathcal{H}_{\langle i,j\rangle_z} = \boldsymbol{S}_i J_{ij}^z \boldsymbol{S}_j$$

with

$$J_{ij}^z = \begin{pmatrix} J & \Gamma & \Gamma' \\ \Gamma & J & \Gamma' \\ \Gamma' & \Gamma' & J+K \end{pmatrix}$$

J. Rau, E. K.-H. Lee, H.-Y. Kee, PRL 112, 077204 (2014)
J. Rau, H.-Y. Kee, arXiv:1408.4811



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- α-$RuCl_3$ is zigzag ordered

→ two minimal models:

- Kitaev-Heisenberg
  with $K > 0$, and $J < 0$
- Kitaev-Γ(-Γ′)
  with $K < 0$, $\Gamma > 0$

J. Rau, E. K.-H. Lee, H.-Y. Kee, PRL 112, 077204 (2014)
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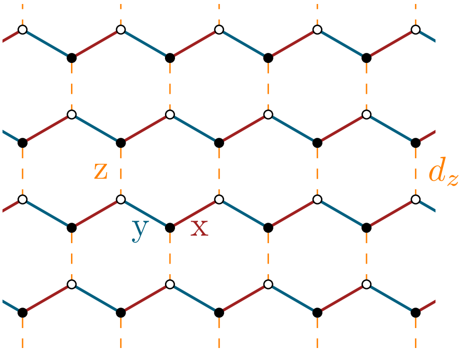
Spinon-like excitations in an anisotropic Kitaev-Gamma model

$$\mathcal{H} = K \sum_{\langle i,j \rangle_\gamma} d_\gamma S_i^\gamma S_j^\gamma + \Gamma \sum_{\langle i,j \rangle_\gamma, \alpha, \beta \neq \gamma} d_\gamma \left(S_i^\alpha S_j^\beta + S_i^\beta S_j^\alpha \right), \quad \text{where} \quad 0 \leq d_z \lesssim 1,\ d_{x,y} = 1$$



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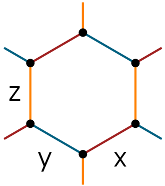
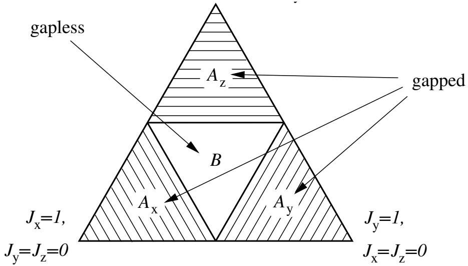


- Here: **gapless** Majorana fermions in a static Z_2 gauge field



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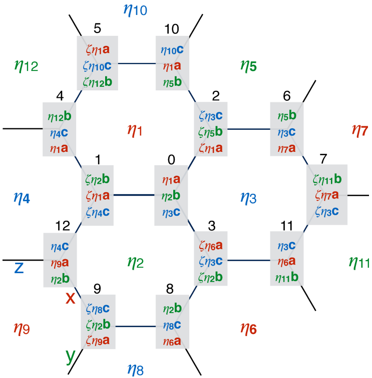

Γ limit

- classical: spin liquid with extensive degeneracy
- quantum: zigzag order? QSL?

I. Rousochatzakis, N. Perkins, PRL 118, 147204 (2017)

Kitaev-Gamma model, isotropic limit $d_z = 1$, numerous results ...

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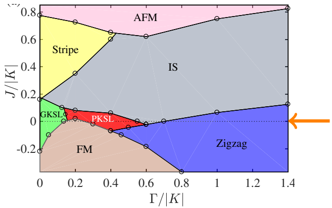
VMC



Wang, Normand, Liu, PRL 123 197201 (2019)

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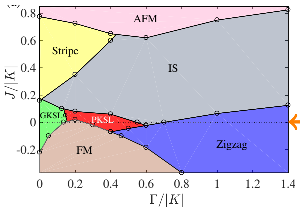
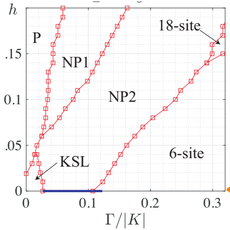
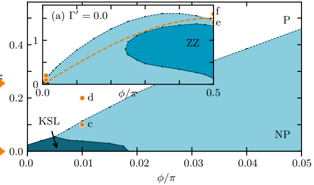


2D Tensor Networks



iDMRG



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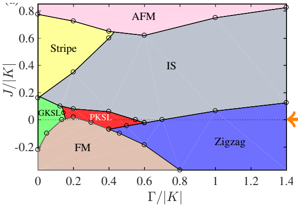

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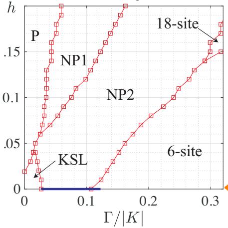

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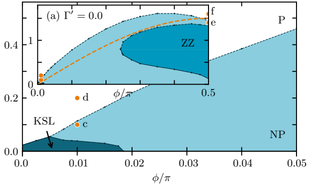
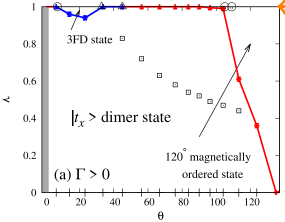


Dimer Series Expansion & ED



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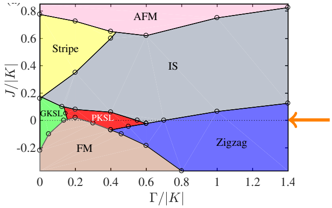

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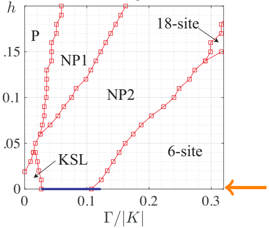

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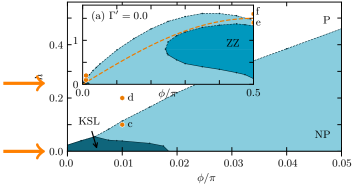

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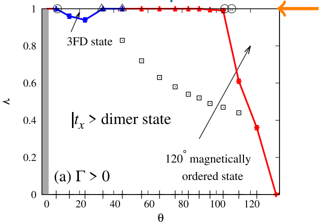
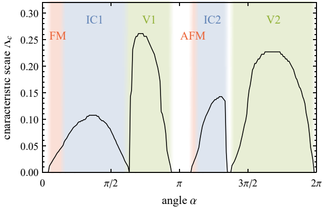


Functional RG (finite-T)



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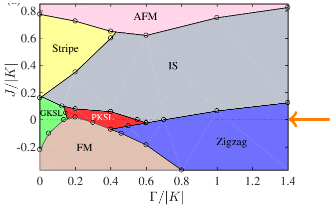

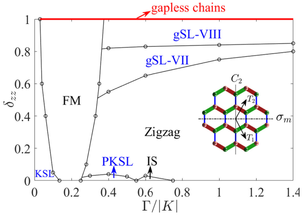

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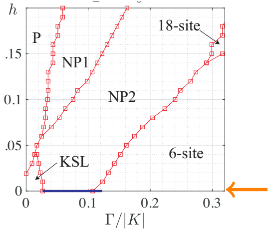

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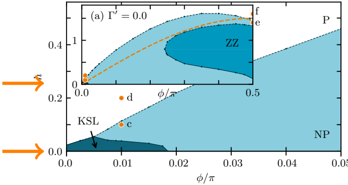

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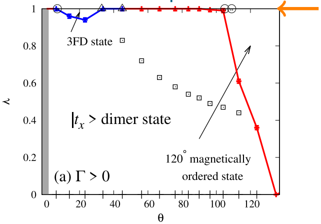

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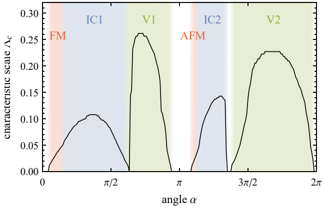

Wang, Normand, Liu, PRL 123 197201 (2019)
Wang, Liu, PRB 102 094416 (2020)

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MG, Chern, Kee, Kim, PRR 2 043023 (2021)
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Anisotropic Kitaev-Gamma model, chain limit $d_z = 0$

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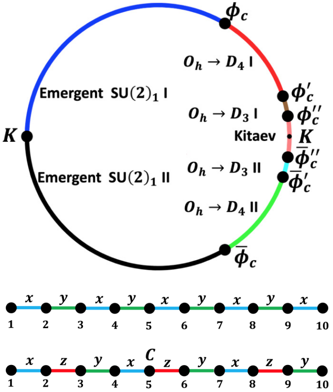

- Sublattice transformation:
  xy-$K\Gamma$ chain $\mapsto$ alternating XXZ-chain

$$\mathcal{H}' = -K \sum_{\langle i,j \rangle_\gamma} S_i^\gamma S_j^\gamma - \Gamma \sum_{\langle i,j \rangle_\gamma, \alpha, \beta \neq \gamma} \left(S_i^\alpha S_j^\alpha + S_i^\beta S_j^\beta \right)$$

Yang, Nocera, Tummuru, Kee, Affleck, PRL 124 147205 (2020)
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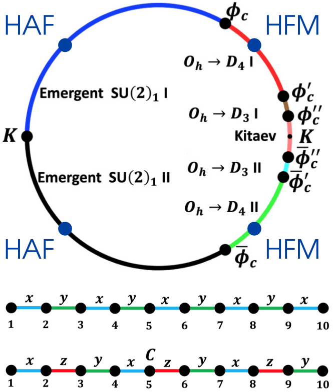

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  $K/|\Gamma| = 1$ is dual to HAF-chain
  $K/|\Gamma| = -1$ is dual to HFM-chain

Yang, Nocera, Tummuru, Kee, Affleck, PRL 124 147205 (2020)
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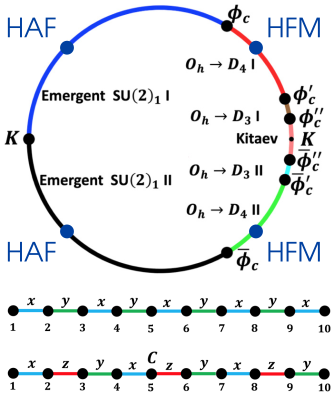

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- Dual points:
  $K/|\Gamma| = 1$ is dual to HAF-chain
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- Tomonaga-Luttinger liquid
  with emergent $SU(2)$ symmetry

Yang, Nocera, Tummuru, Kee, Affleck, PRL 124 147205 (2020)
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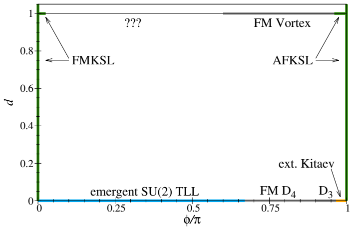
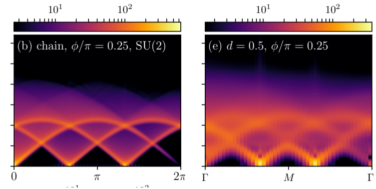
Outline

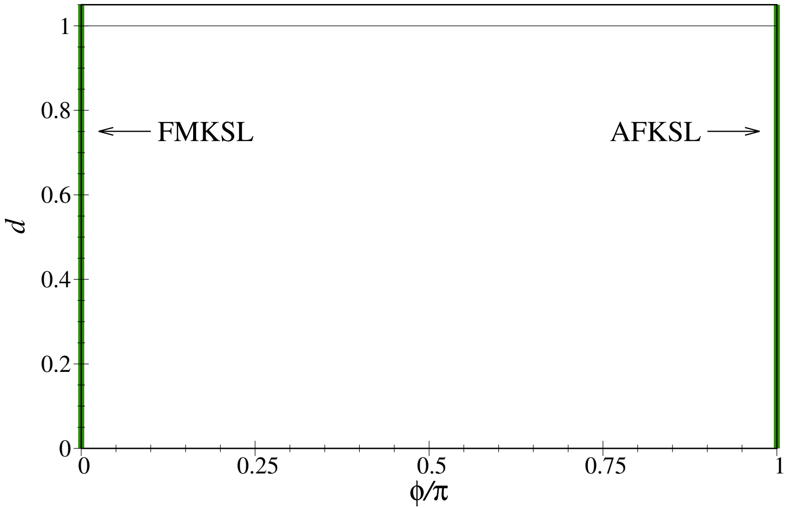
1. Phase diagram as a function of anisotropy and $K/|\Gamma|$



2. Properties of the extended QSL
   - Frustration suppresses effective inter chain coupling
   - Scaling of spectral gap and magnetization
   - Dynamics

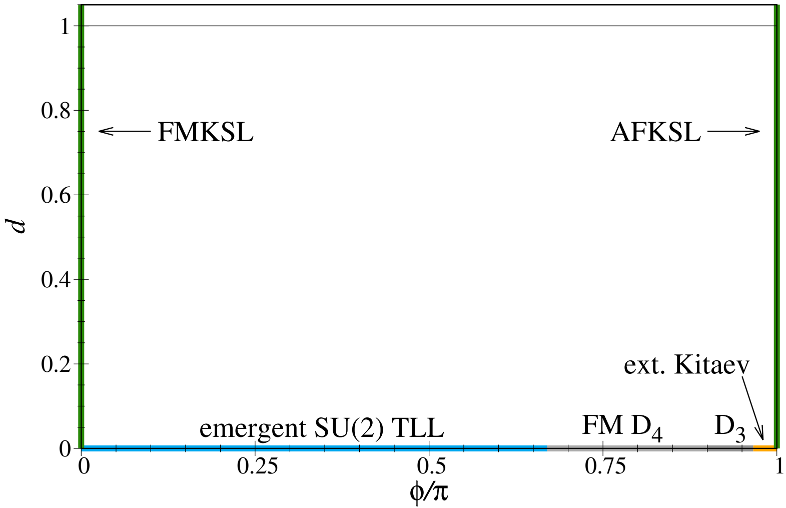


Phase diagram, known limits



$K = -\cos\phi$
$\Gamma = \sin\phi$
$0 \leq \phi \leq \pi$
$0 \leq d \lesssim 1$

Phase diagram, known limits



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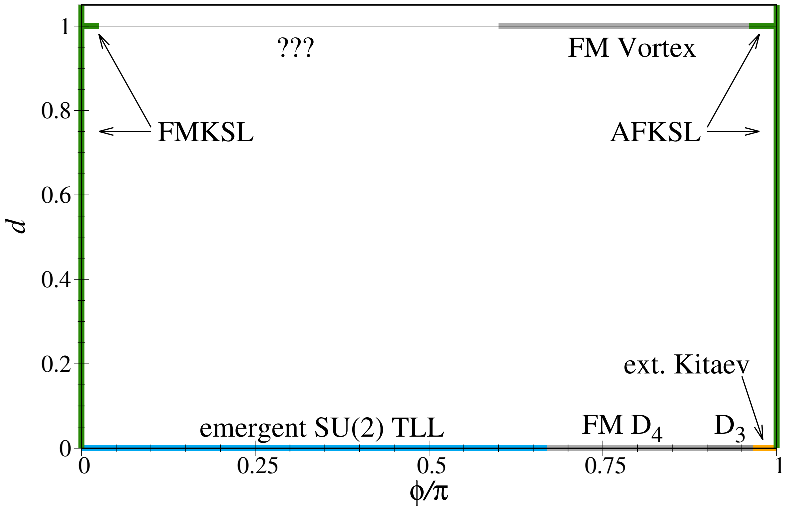

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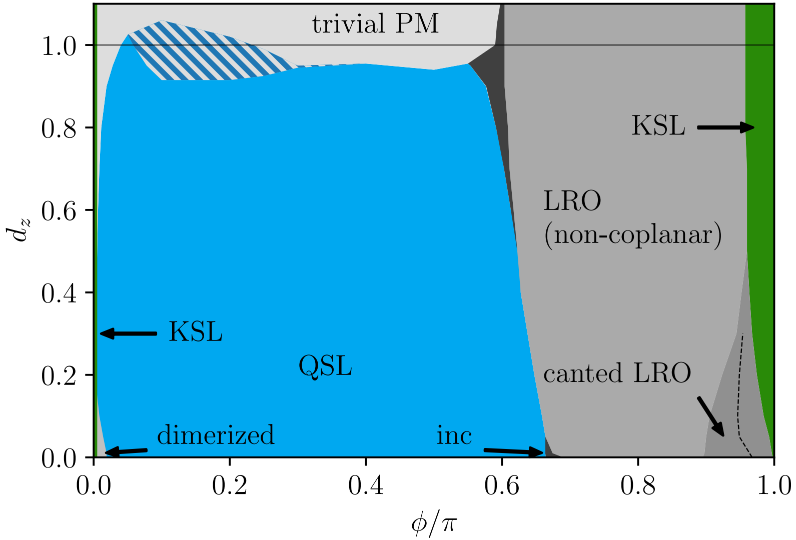

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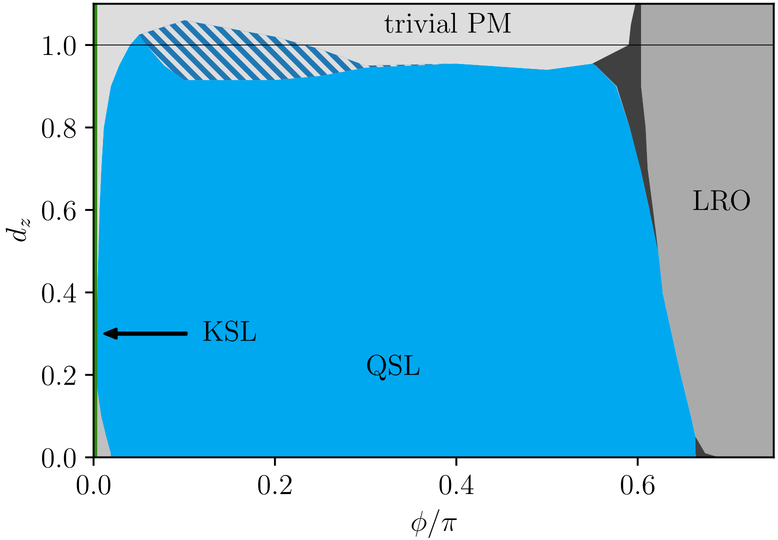

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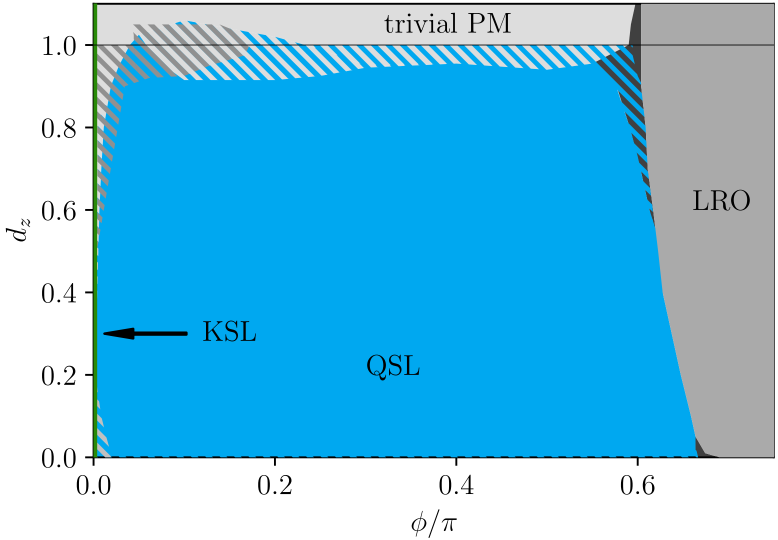

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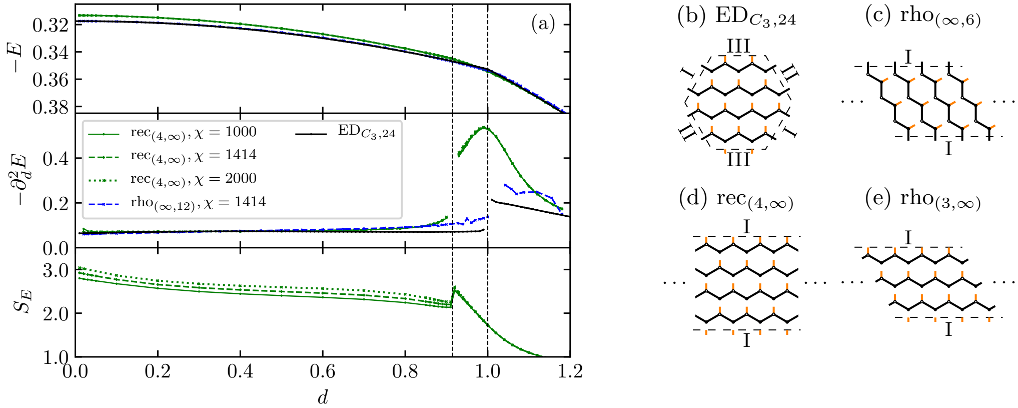
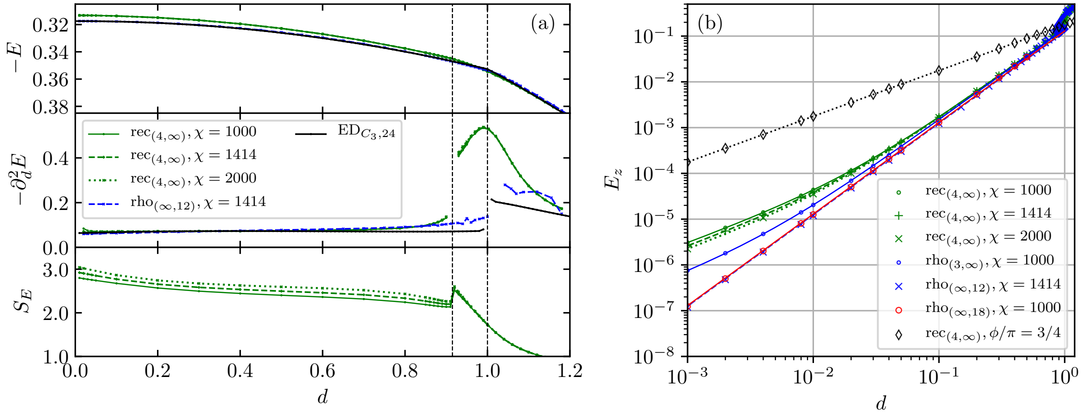
Single cut at $\phi/\pi = 1/4$



Single cut at $\phi/\pi = 1/4$: reduced eff. inter-chain coupling



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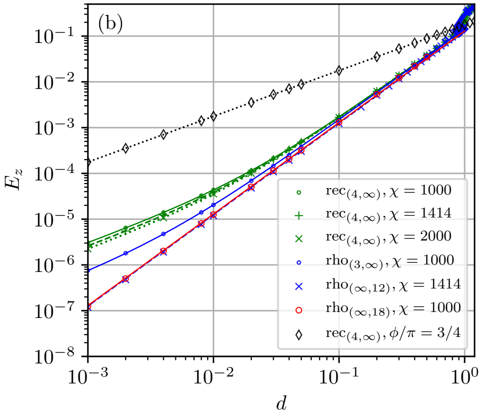
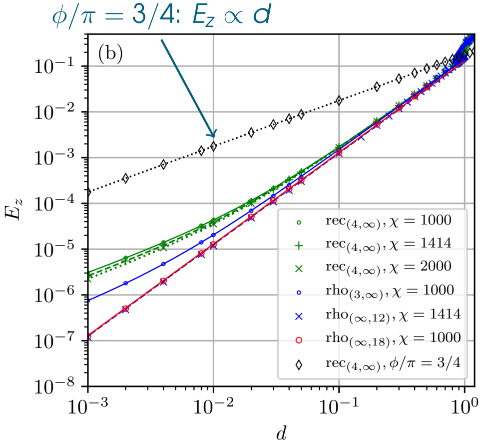


$f_{\mathrm{fit}}(x) = c_1 x^2 + c_2 x$	c_1	c_2
$\mathrm{rec}_{(4,\infty)}, \chi = 1000$	0.1425(4)	0.002928(11)
$\mathrm{rec}_{(4,\infty)}, \chi = 1414$	0.1440(2)	0.002468(5)
$\mathrm{rec}_{(4,\infty)}, \chi = 2000$	0.14521(15)	0.002101(3)
$\mathrm{rho}_{(3,\infty)}, \chi = 1000$	0.1440(17)	0.000607(18)
$\mathrm{rho}_{(\infty,12)}, \chi = 1414$	0.1265(20)	0.00000(8)
$\mathrm{rho}_{(\infty,18)}, \chi = 1000$	0.1293(15)	0.00000(5)
$\mathrm{rec}_{(4,\infty)}, \phi/\pi = 3/4$	0.00000(6)	0.176794(16)

(c) fitting parameter for (b)

Single cut at $\phi/\pi = 1/4$: reduced eff. inter-chain coupling



$f_{\mathrm{fit}}(x) = c_1 x^2 + c_2 x$	c_1	c_2
$\mathrm{rec}_{(4,\infty)}, \chi = 1000$	0.1425(4)	0.002928(11)
$\mathrm{rec}_{(4,\infty)}, \chi = 1414$	0.1440(2)	0.002468(5)
$\mathrm{rec}_{(4,\infty)}, \chi = 2000$	0.14521(15)	0.002101(3)
$\mathrm{rho}_{(3,\infty)}, \chi = 1000$	0.1440(17)	0.000607(18)
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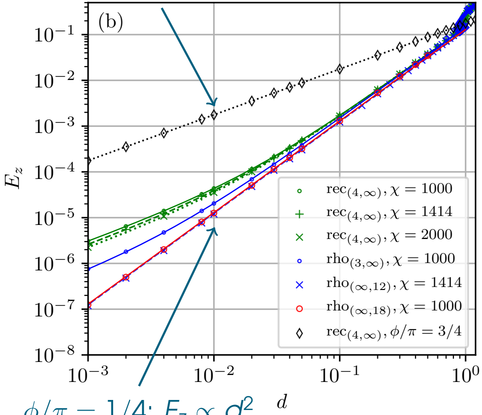
$\mathrm{rec}_{(4,\infty)}, \phi/\pi = 3/4$	0.00000(6)	0.176794(16)

(c) fitting parameter for (b)

Single cut at $\phi/\pi = 1/4$: reduced eff. inter-chain coupling

$\phi/\pi = 3/4$: $E_z \propto d$



$\phi/\pi = 1/4$: $E_z \propto d^2$

$f_{\mathrm{fit}}(x) = c_1 x^2 + c_2 x$	c_1	c_2
$\mathrm{rec}_{(4,\infty)}, \chi = 1000$	0.1425(4)	0.002928(11)
$\mathrm{rec}_{(4,\infty)}, \chi = 1414$	0.1440(2)	0.002468(5)
$\mathrm{rec}_{(4,\infty)}, \chi = 2000$	0.14521(15)	0.002101(3)
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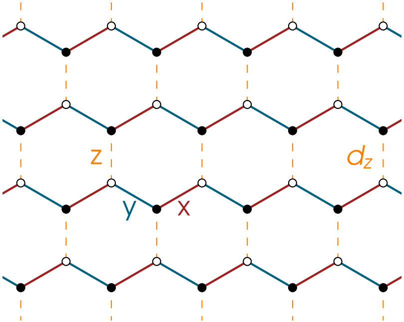
$\mathrm{rec}_{(4,\infty)}, \phi/\pi = 3/4$	0.00000(6)	0.176794(16)

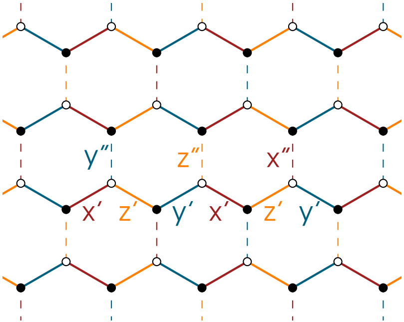
(c) fitting parameter for (b)

Reduced eff. inter-chain coupling due to frustration

Original KΓ model



Dual model with HAF-like chains



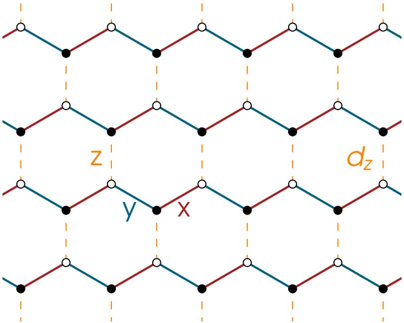
$$\mathcal{H}_{i,j}^{\gamma} = K S_i^{\gamma} S_j^{\gamma} + \Gamma(S_i^{\alpha} S_j^{\beta} + S_i^{\alpha} S_j^{\beta})$$

$$\mathcal{H}_{i,j}^{\gamma'} = -K S_i^{\gamma} S_j^{\gamma} + \Gamma(S_i^{\alpha} S_j^{\alpha} + S_i^{\beta} S_j^{\beta})$$

$$\mathcal{H}_{i,j}^{\gamma''} = -K S_i^{\gamma} S_j^{\gamma} - \Gamma(S_i^{\alpha} S_j^{\alpha} + S_i^{\beta} S_j^{\beta})$$

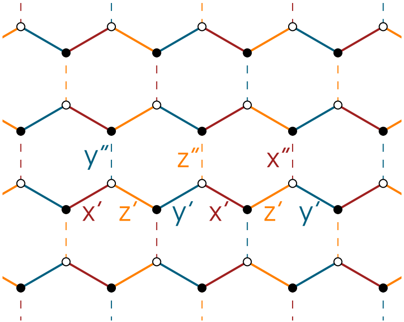
Reduced eff. inter-chain coupling due to frustration

Original KΓ model



$$\mathcal{H}^{\gamma}_{i,j} = K S_i^{\gamma} S_j^{\gamma} + \Gamma(S_i^{\alpha} S_j^{\beta} + S_i^{\alpha} S_j^{\beta})$$

Dual model with HAF-like chains



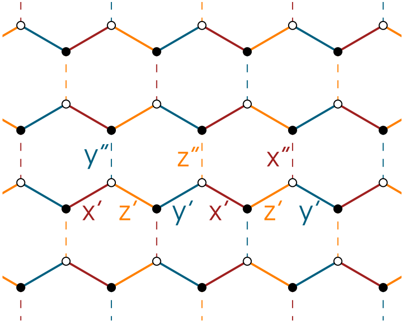
here: $0 < \phi < \pi/2 \rightarrow K < 0 < \Gamma$

$$\mathcal{H}^{\gamma'}_{i,j} = |K| S_i^{\gamma} S_j^{\gamma} + |\Gamma|(S_i^{\alpha} S_j^{\alpha} + S_i^{\beta} S_j^{\beta})$$

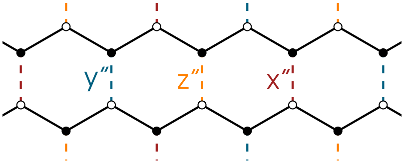
$$\mathcal{H}^{\gamma''}_{i,j} = |K| S_i^{\gamma} S_j^{\gamma} - |\Gamma|(S_i^{\alpha} S_j^{\alpha} + S_i^{\beta} S_j^{\beta})$$

Reduced eff. inter-chain doupling due to frustration

Dual model with HAF-like chains



Suppose $J = |K| = |\Gamma|$ $(\phi/\pi = 1/4)$



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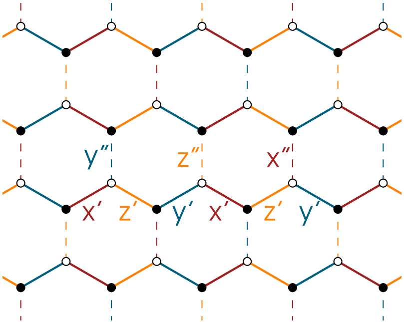
$$\mathcal{H}^{\gamma''}_{i,j} = |K| S_i^{\gamma} S_j^{\gamma} - |\Gamma| (S_i^{\alpha} S_j^{\alpha} + S_i^{\beta} S_j^{\beta})$$

$$\mathcal{H}^{\gamma'}_{i,j} = \mathcal{H}^{\mathrm{HAF}}_{i,j} = J \boldsymbol{S}_i \cdot \boldsymbol{S}_j$$

$$\mathcal{H}^{\gamma''}_{i,j} = J \left[S_i^{\gamma} S_j^{\gamma} - S_i^{\alpha} S_j^{\alpha} - S_i^{\beta} S_j^{\beta} \right]$$

Reduced eff. inter-chain doupling due to frustration

Dual model with HAF-like chains



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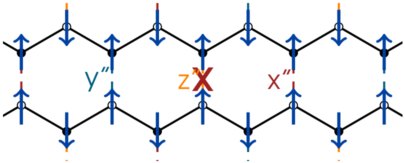


$$\mathcal{H}_{i,j}^{\gamma'} = |K| S_i^{\gamma} S_j^{\gamma} + |\Gamma| (S_i^{\alpha} S_j^{\alpha} + S_i^{\beta} S_j^{\beta})$$

$$\mathcal{H}_{i,j}^{\gamma''} = |K| S_i^{\gamma} S_j^{\gamma} - |\Gamma| (S_i^{\alpha} S_j^{\alpha} + S_i^{\beta} S_j^{\beta})$$

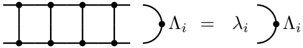
$$\mathcal{H}_{i,j}^{\gamma'} = \mathcal{H}_{i,j}^{\mathrm{HAF}} = J \boldsymbol{S}_i \cdot \boldsymbol{S}_j$$

$$\mathcal{H}_{i,j}^{\gamma''} = J \left[S_i^{\gamma} S_j^{\gamma} - S_i^{\alpha} S_j^{\alpha} - S_i^{\beta} S_j^{\beta} \right]$$

iDMRG: scaling with bond dimension χ, transfer matrix and spectral gap

Consider transfer matrix of iMPS:

$\mathcal{T}$:



- $\lambda_0 = 1, \quad \forall i > 0 : \lambda_i < 1$
- quasi-energies:
  $\epsilon_i = -\ln \lambda_i$

Zauner, Draxler, Vanderstraeten, et al., New J. Phys. 17 053002 (2015)

MG, Wachtel, Yamaji, et al., PRB 97 075126 (2018)

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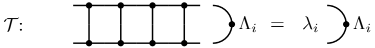

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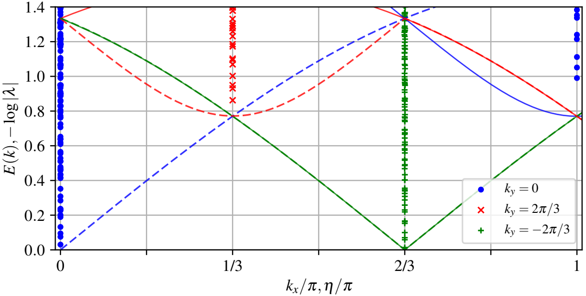
Example: TM spectrum of Kitaev model

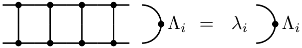


Zauner, Draxler, Vanderstraeten, et al., New J. Phys. 17 053002 (2015)

MG, Wachtel, Yamaji, et al., PRB 97 075126 (2018)

Consider transfer matrix of iMPS:

$\mathcal{T}$:



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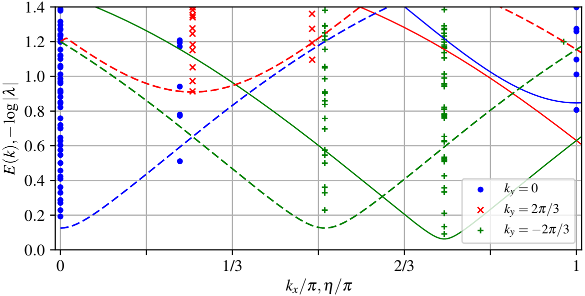

Zauner, Draxler, Vanderstraeten, et al., New J. Phys. 17 053002 (2015)

MG, Wachtel, Yamaji, et al., PRB 97 075126 (2018)

iDMRG: scaling with bond dimension χ, transfer matrix and spectral gap

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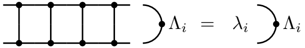

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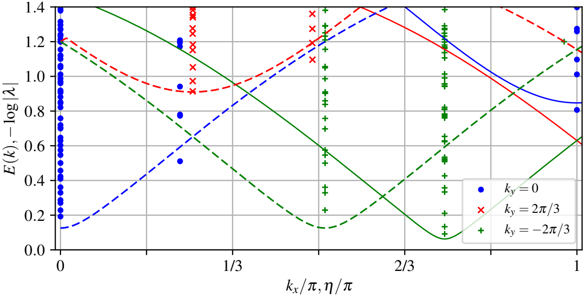
  $\epsilon_i = -\ln \lambda_i$
- $\delta = \sum_i c_i \epsilon_i$
  with choice c_i such that
  $\sum c_i = 0$
- plot $\epsilon_1(\chi) \propto \Delta(\chi)$ vs. $\delta(\chi)$

Example: TM spectrum of Kitaev model

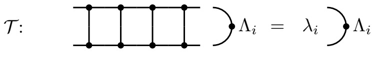


Zauner, Draxler, Vanderstraeten, et al., New J. Phys. 17 053002 (2015)
Rams, Czarnik, Cincio, PRX 8, 041033 (2018)
Vanhecke, Haegeman, Van Acoleyen, Vanderstraeten, Verstraete, PRL 123 250604 (2019)

MG, Wachtel, Yamaji, et al., PRB 97 075126 (2018)

iDMRG: scaling with bond dimension χ, chain

Consider transfer matrix of iMPS:



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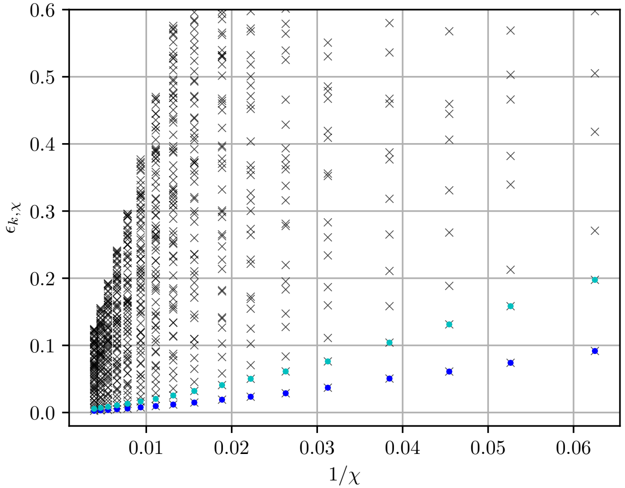

Rams, Czarnik, Cincio, PRX 8, 041033 (2018)
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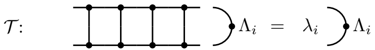

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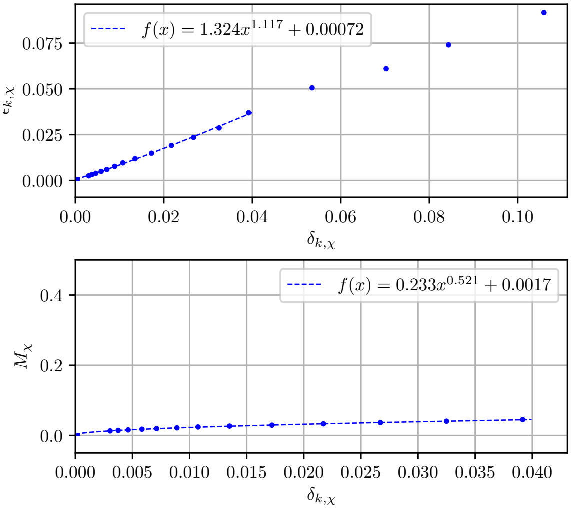
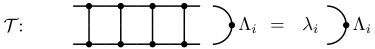


Rams, Czarnik, Cincio, PRX 8, 041033 (2018)
Vanhecke, Haegeman, Van Acoleyen, Vanderstraeten, Verstraete, PRL 123 250604 (2019)

iDMRG: scaling with bond dimension χ, 4-coupled chains, $d = 0.5$

Consider transfer matrix of iMPS:



- $\lambda_0 = 1, \quad \forall i > 0 : \lambda_i < 1$
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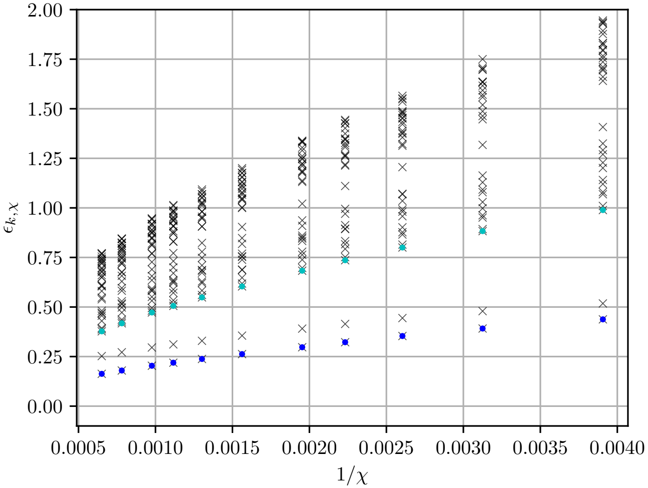

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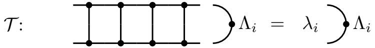
Consider transfer matrix of iMPS:



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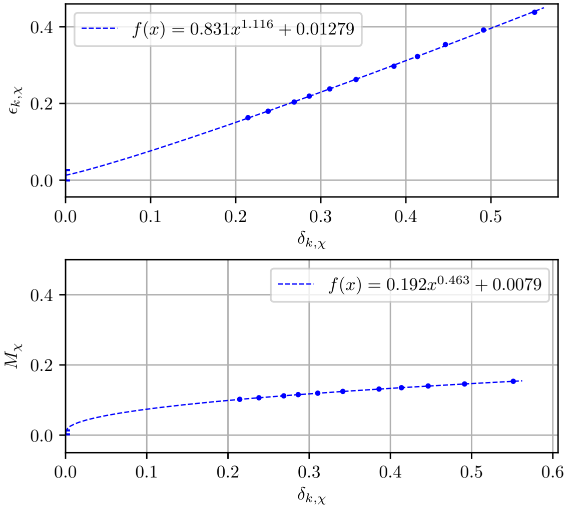
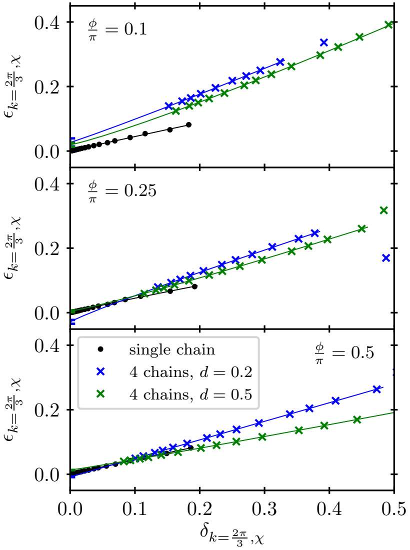
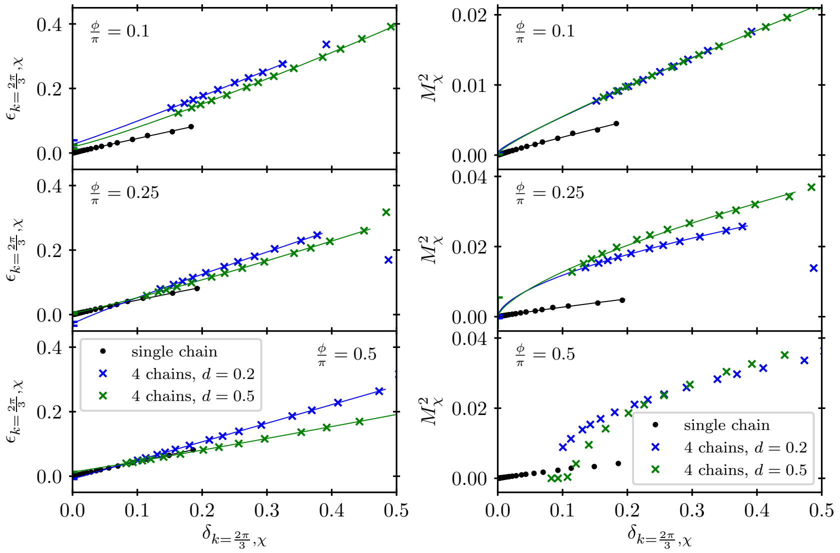


Rams, Czarnik, Cincio, PRX 8, 041033 (2018)
Vanhecke, Haegeman, Van Acoleyen, Vanderstraeten, Verstraete, PRL 123 250604 (2019)

iDMRG: scaling with bond dimension χ, 4-coupled chains, at various K/Γ and d



iDMRG: scaling with bond dimension χ, 4-coupled chains, at various K/Γ and d



Dynamics: $\mathcal{S}(\mathbf{q},\omega)$ in chain limit, $d=0$, TLL phase

→ Spatio-temporal Fourier transform of spin-spin correlations:

$$\mathcal{S}^{\gamma\gamma}(\boldsymbol{k},\omega) = \frac{1}{2\pi}\sum_{\mathbf{r}}\int_{-\infty}^{\infty} e^{i(\omega t - \mathbf{k}\cdot\mathbf{r})} C^{\gamma\gamma}(\mathbf{r},t)\,\mathrm{d}t,$$

where $C^{\gamma\gamma}_{i,j}(\mathbf{r},t) = \langle\psi_0|S^{\gamma}_j U(t) S^{\gamma}_i|\psi_0\rangle$ computed using tMPO

Zaletel et al. PRB 91, 165112 (2015)

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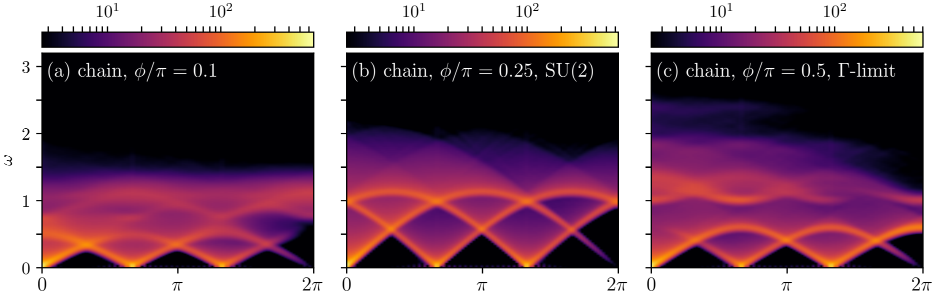

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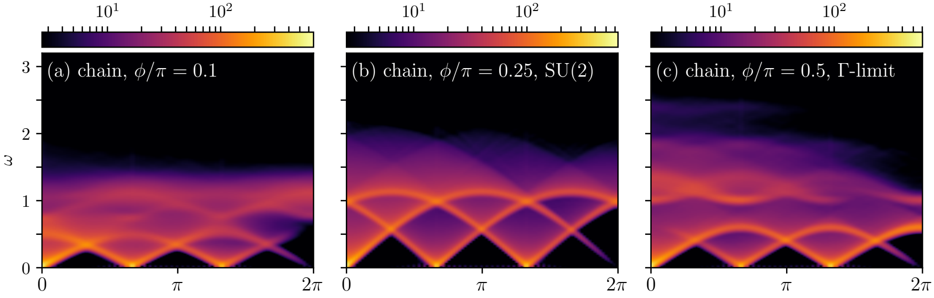
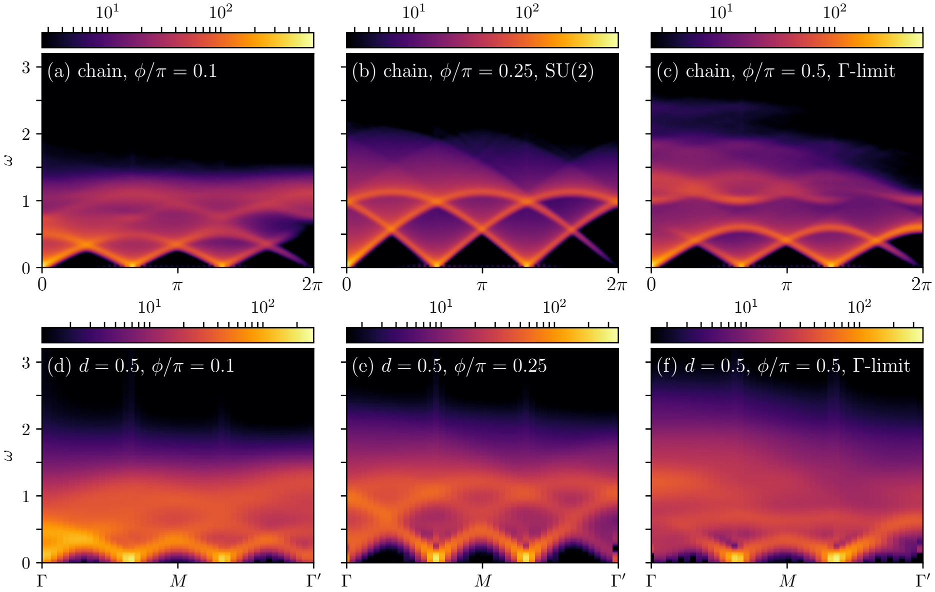


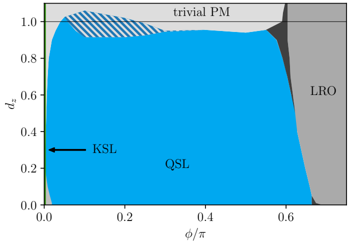
→ three copies of HAF-chain spinon continuum.

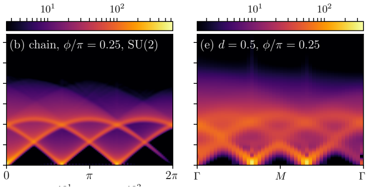
Dynamics: $\mathcal{S}(\mathbf{q},\omega)$ for 3-coupled chains, $d = 0.5$, pTLL phase



Summary

1. Extended QSL phase next to TLL:
   - gapless
   - 'survives' up to isotropic limit due to frustration suppressing eff. inter-chain coupling
   - Spinons of HAF-chain survive significant inter-chain coupling





Coupled wire approach ... recent arXiv 2207.02188

Counter-rotating spiral, zigzag, and 120° orders from coupled-chain analysis of Kitaev-Gamma-Heisenberg model, and relations to honeycomb iridates

Wang Yang,[1] Alberto Nocera,[1] Chao Xu,[2] Hae-Young Kee,[3,4] and Ian Affleck[1]

[1] *Department of Physics and Astronomy and Stewart Blusson Quantum Matter Institute, University of British Columbia, Vancouver, B.C., Canada, V6T 1Z1*
[2] *Kavli Institute for Theoretical Sciences, University of Chinese Academy of Sciences, Beijing 100190, China*
[3] *Department of Physics, University of Toronto, Toronto, Ontario M5S 1A7, Canada*
[4] *Canadian Institute for Advanced Research, CIFAR Program in Quantum Materials, Toronto, Ontario M5G 1M1, Canada*

On page 18:

On the other hand, as discussed in Ref. [61], the 1D Kitaev-Gamma model has an intricate symmetry group G_0, which is nonsymmorphic and satisfies $G_0/\mathbb{Z} \cong O_h$, where O_h is the full octahedral group, or the largest 3D crystalline point group. Therefore, within a coupled-chain approach, there are many more possibilities of magnetic orders and symmetry breaking patterns in 2D Kitaev-Gamma model because of the much larger symmetry group, which is worth for future studies. Indeed, classical analysis and machine-learning-based method have revealed the great complexity of the phase diagram of the 2D Kitaev-Gamma model [51, 52], where magnetic orders having a unit cell of 18, 24, or even 48 sites are found. In addition, it cannot be ruled out the possibility that the Kitaev-Gamma model hosts some disordered phases such as nematic paramagnets [42, 46, 47, 50, 51].

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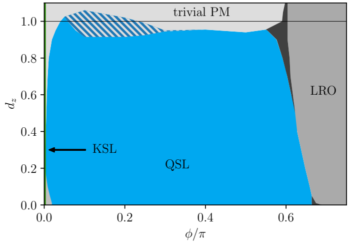
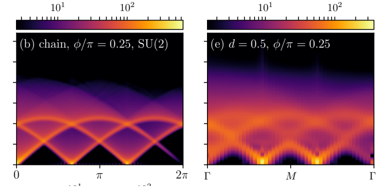
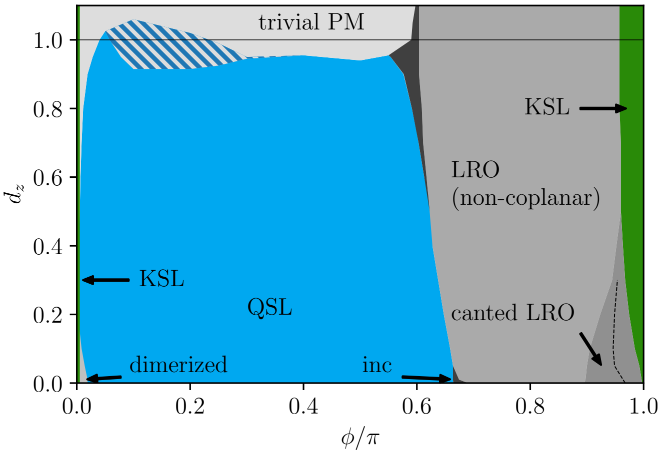


2. Questions/issues:
   - Extended QSL related to Lattice-nematic paramagnetic phase in (111) field?
   - Previous studies: proximity to phase transition reason for (many) different results?



Phase diagram is very rich beyond the QSL phase ...



- $d \to 0$, $\phi/\pi \approx 0.66$: region with strong incommensurate correlations, survives small d
- $d \approx 1$, $\phi/\pi \approx 0.55$: gapless, no dipolar LRO
- $d \approx 0$ to 0.4, $\phi/\pi \approx 0.95$: dipolar LRO: canted Vortex (120°) and doubled unit cell
- $d \approx 0$ to 0.2, $\phi/\pi \to 0$: dimerized phase (also for single chain)