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Tuesday, November 18, 2014

Density-Matrix Renormalization Group Study of Extended Kitaev-Heisenberg Model

参考：Kazuya Shinjo, *et. al*., ArXiv e-prints (2014), arXiv:1410.4790 [cond-mat.str-el]

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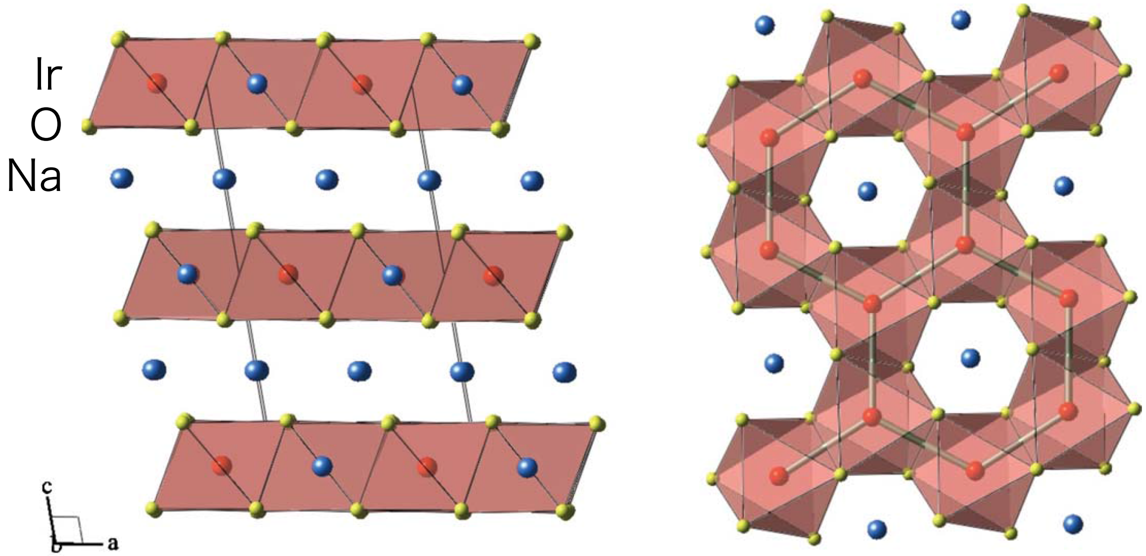
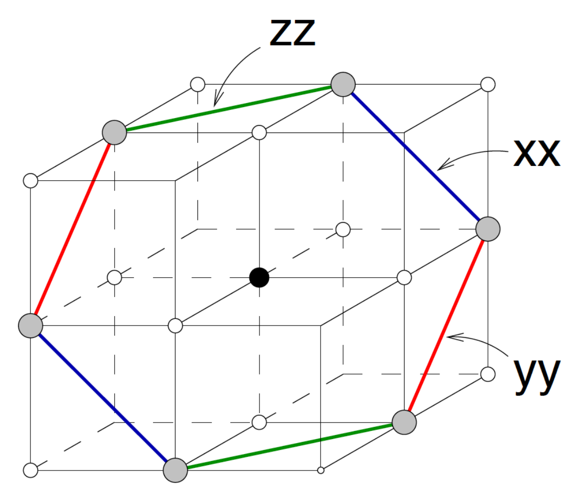
Kitaev-Heisenberg model and Na_2IrO_3



[Y. Singh and P. Gegenwart, Phys. Rev. B **82**, 064412 (2010)]



[G. Jackeli and G. Khaliullin, Phys. Rev. Lett. **102**, 017205 (2009)]

Kitaev-Heisenberg model

$$\mathcal{H}_{ij}^{(\gamma)} = \underbrace{2KS_i^\gamma S_j^\gamma}_{\text{Kitaev term}} + \underbrace{J\boldsymbol{S}_i \cdot \boldsymbol{S}_j}_{\text{Heisenberg term}}.$$

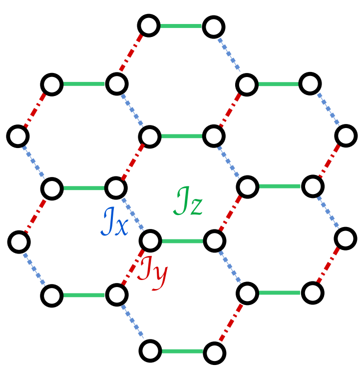
Kitaev term Heisenberg term

Extended Kitaev-Heisenberg model and its phase diagram

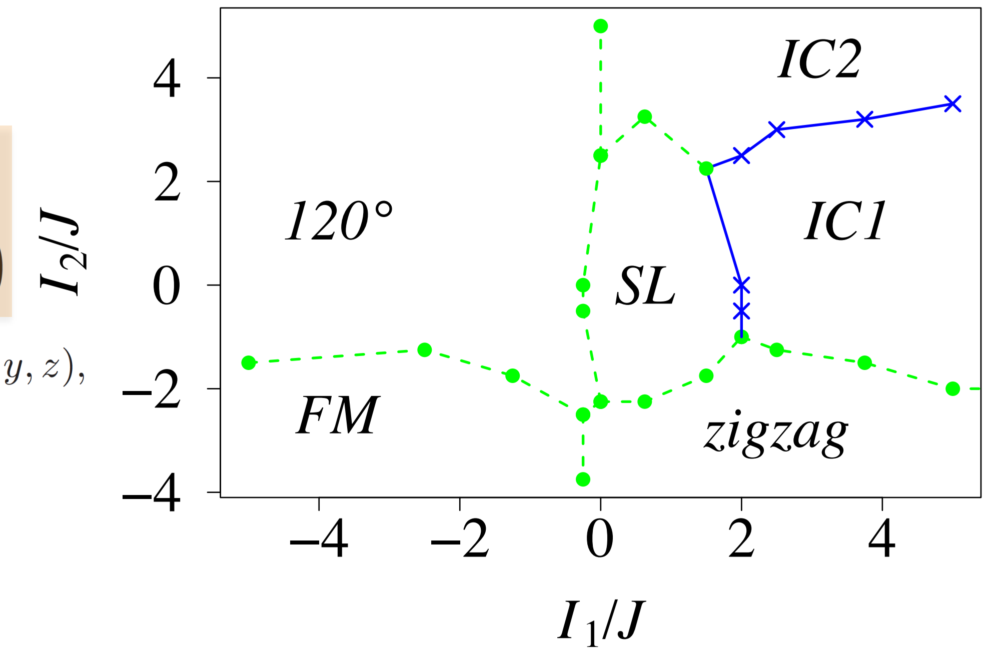
$$\hat{\mathcal{H}} = \sum_{\Gamma} \sum_{\langle lm \rangle \in \Gamma} \hat{\mathcal{H}}_{lm}$$

$$\begin{aligned}\hat{\mathcal{H}}_{lm} &= K S_l^\gamma S_m^\gamma + J\left(S_l^\alpha S_m^\alpha + S_l^\beta S_m^\beta\right) \\ &+ I_1\left(S_l^\alpha S_m^\beta + S_l^\beta S_m^\alpha\right) \\ &+ I_2\left(S_l^\alpha S_m^\gamma + S_l^\gamma S_m^\alpha + S_l^\beta S_m^\gamma + S_l^\gamma S_m^\beta\right)\end{aligned}$$

where Γ represents a combination of $(\alpha, \beta, \gamma) = (x, y, z)$, (z, x, y), and (y, z, x) on the $\mathcal{J}_z$, $\mathcal{J}_y$ and $\mathcal{J}_x$ bond



Phase diagram when $K/J = -25$



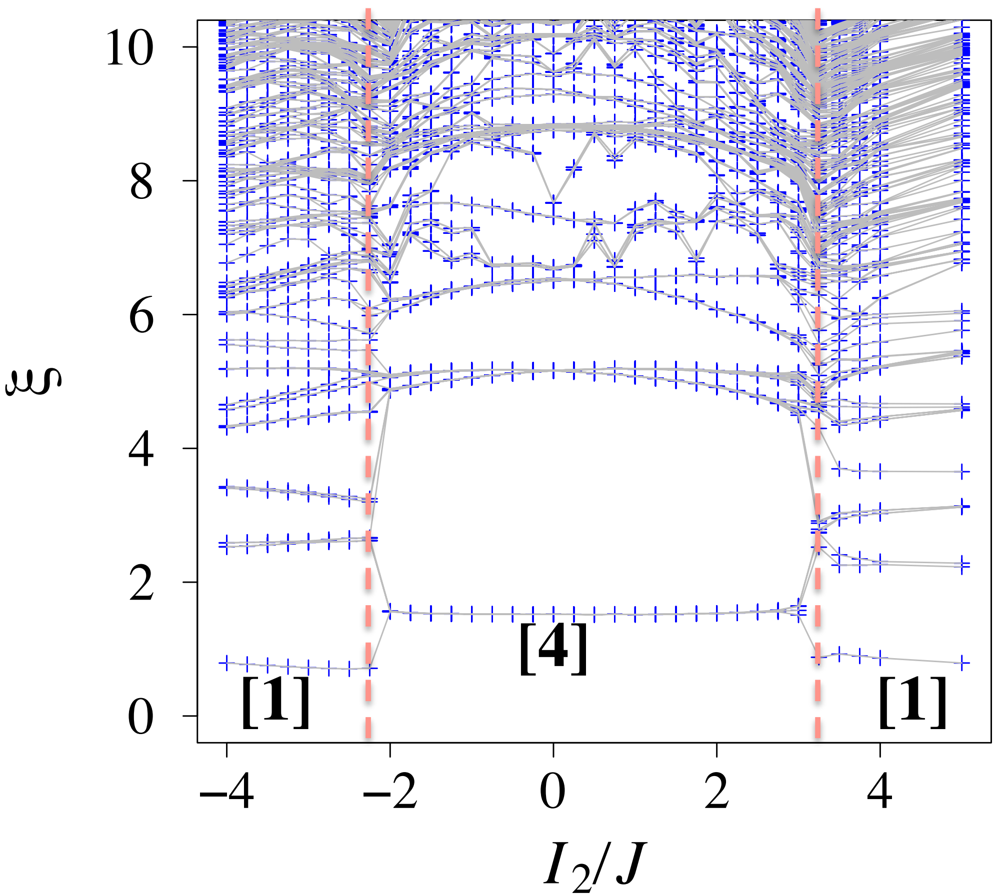
Blue : 1st order
Green : 2nd order

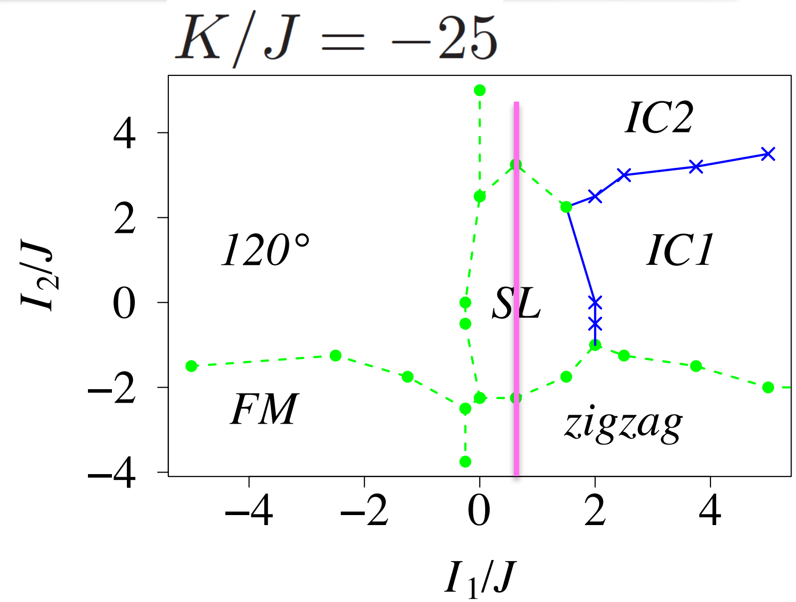
I_1 : coming from crystal structure of Na_2IrO_3

I_2 : coming from trigonal distorion

Entanglement spectrum (E. S.)

$I_1/J = 0.63$





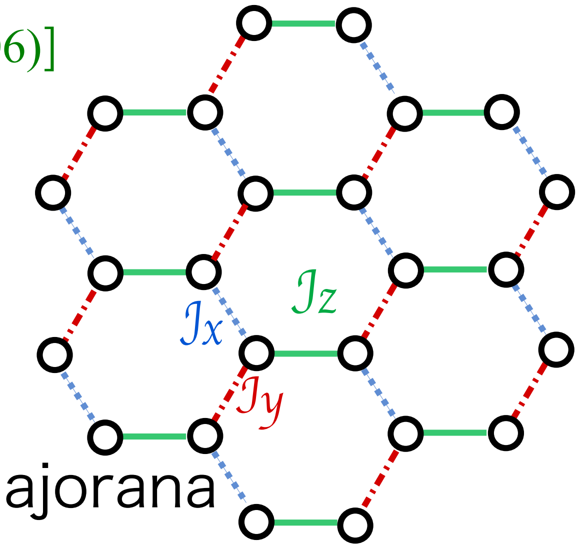
- ✓ Kitaev spin liquid shows degeneracy of E. S.
- ✓ Phase boundaries between the Kitaev spin-liquid and the magnetically ordered phases is determined by examining the Schmidt gap defined as $\Delta\xi = \xi_1 - \xi_2$

Kitaev honeycomb lattice model

[A. Kitaev, Ann. Phys. **321**, 2 (2006)]

$$\hat{\mathcal{H}}_{ij}^{\gamma} = -J_\gamma S_i^\gamma S_j^\gamma$$

$$= \begin{cases} -J_x S_i^x S_j^x & (\text{at } \mathcal{J}_x-\text{bond}) \\ -J_y S_i^y S_j^y & (\text{at } \mathcal{J}_y-\text{bond}) \\ -J_z S_i^z S_j^z & (\text{at } \mathcal{J}_z-\text{bond}) \end{cases}$$



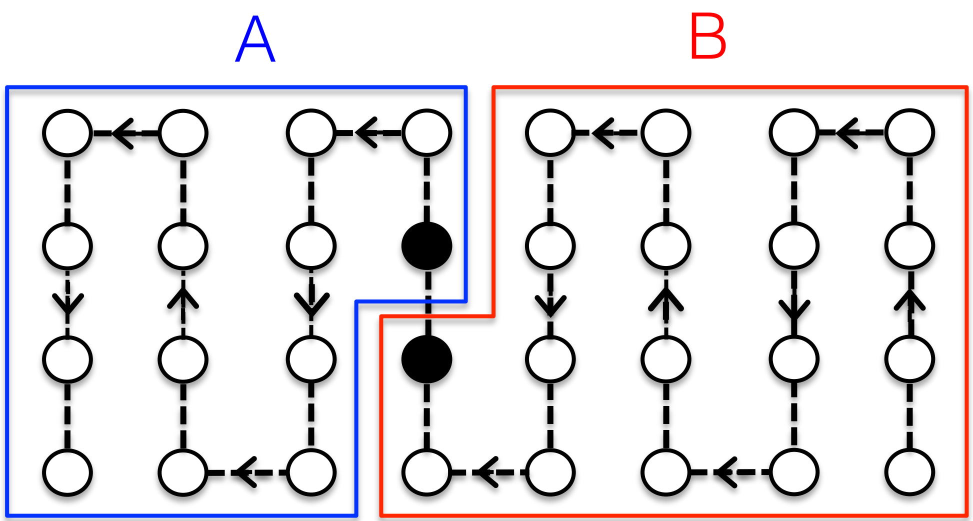
✓ ground state: spin liquid with gapless Majorana excitation

✓ When $|J_z| >> |J_{x,y}|$, the model can be mapped to toric-code model.

✓ If time reversal symmetry is broken, fermions acquires an energy gap and vortices obey non-Abelian anyon

⟶ Topological quantum computation

Density-matrix renormalization group (DMRG)



Schmidt decomposition

$$|\psi\rangle = \sum_{i,j} \psi_{i,j} |i\rangle_A |j\rangle_B$$

$$= \sum_{a=1}^{m} p_a |p_A^a\rangle |p_B^a\rangle$$

打ち切り次数 m が大きいほど、正確になる

Entanglement entropy

$$S_{\mathrm{E}} = -\sum_i p_i \ln p_i = \sum_i \xi_i e^{-\xi_i}$$

Entanglement spectrum

$$\xi_i = -\ln p_i$$

[H. Li and F. D. M. Haldane, Phys. Rev. Lett. **101**, 010504 (2008)]