Unconventional pairing and electronic dimerization instabilities in the doped Kitaev-Heisenberg model

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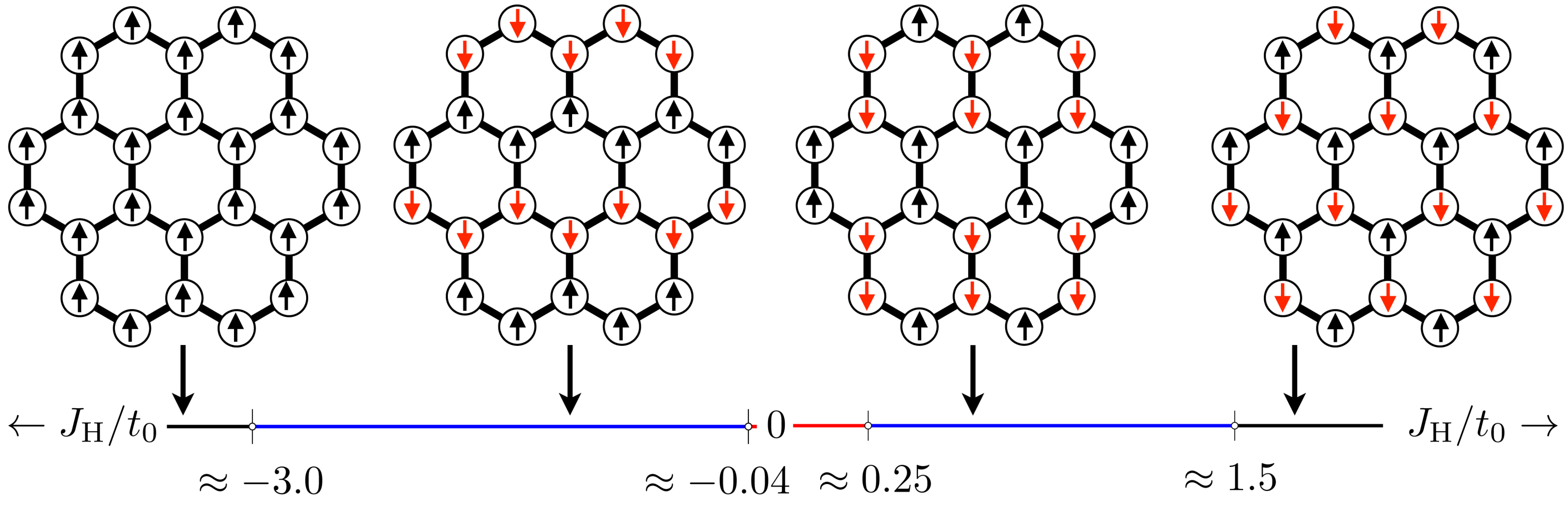
Kitaev-Heisenberg model on the honeycomb

$$H = J_{\mathrm{K}} \sum_{\langle i,j \rangle} S_i^{\gamma(ij)} S_j^{\gamma(ij)} + J_{\mathrm{H}} \sum_{\langle i,j \rangle} \vec{S}_i \cdot \vec{S}_j$$

$J_{\mathrm{K}} > 0, J_{\mathrm{H}} < 0$ $J_{\mathrm{K}}/t_0 = 1$ $J_{\mathrm{K}} < 0, J_{\mathrm{H}} > 0$ $J_{\mathrm{K}}/t_0 = -1$



$J_{\mathrm{K}}/t_0 = 1$ $J_{\mathrm{K}}/t_0 = -1$

FM zigzag $\mathbb{Z}_2$ QSL stripy Néel AF

ground-state manifold as obtained in [Chaloupka et al. (2013)] Phys. Rev. Lett. 110, 097204 (2013) by exact diagonalization, also partly discussed by spin-fRG in [Reuther et al. (2011)] Phys. Rev. B 84, 100406(R) (2011)

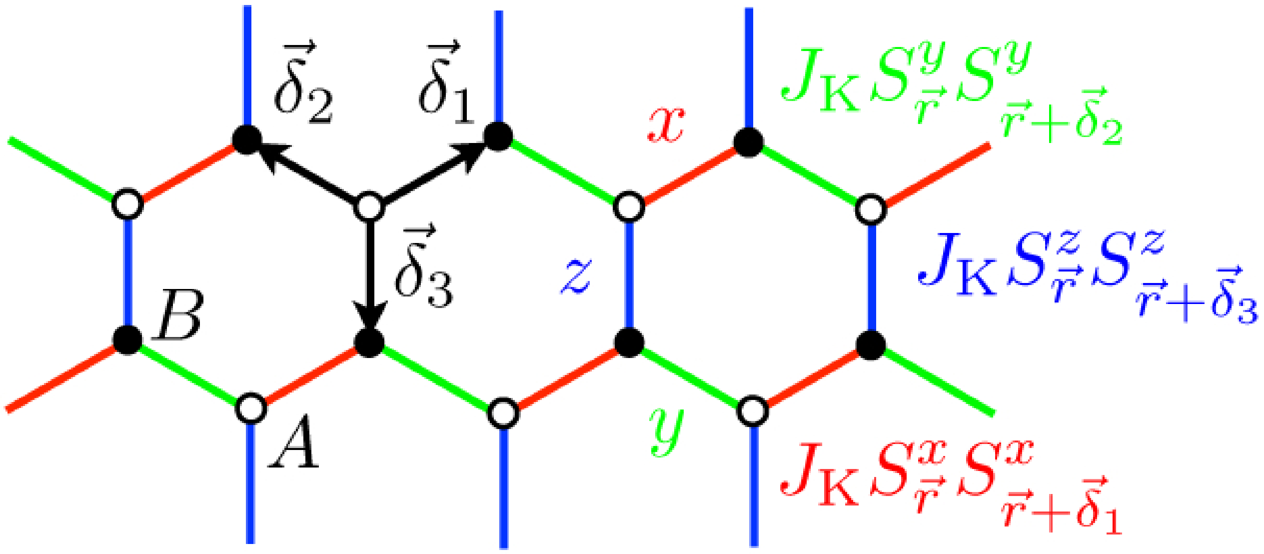
Kitaev limit: Z₂ quantum spin liquid

- quantum spin-1/2 model on honeycomb, strongly frustrated bond-specific Ising-type exchange

[Kitaev (2006)] Annals of Physics 321 (2006) 2-111

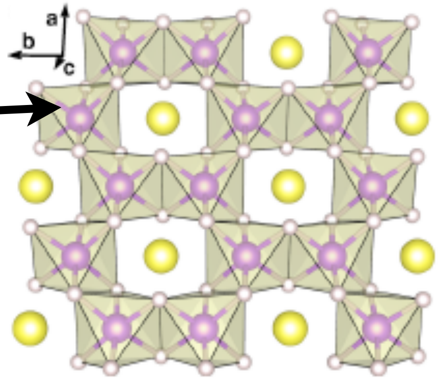
$$\begin{aligned} H &= J_{\mathrm{K}} \sum_{\langle i,j \rangle} S_i^{\gamma(ij)} S_j^{\gamma(ij)} \\ &= J_{\mathrm{K}} \sum_{\langle i,j \rangle : x-\mathrm{bond}} S_i^x S_j^x + J_{\mathrm{K}} \sum_{\langle i,j \rangle : y-\mathrm{bond}} S_i^y S_j^y + J_{\mathrm{K}} \sum_{\langle i,j \rangle : z-\mathrm{bond}} S_i^z S_j^z \end{aligned}$$

- realizes Z₂ quantum spin liquid (QSL)
- Exact solution in terms of Majorana fermions coupled to static Z₂ gauge field
- fermionic excitations above ground state

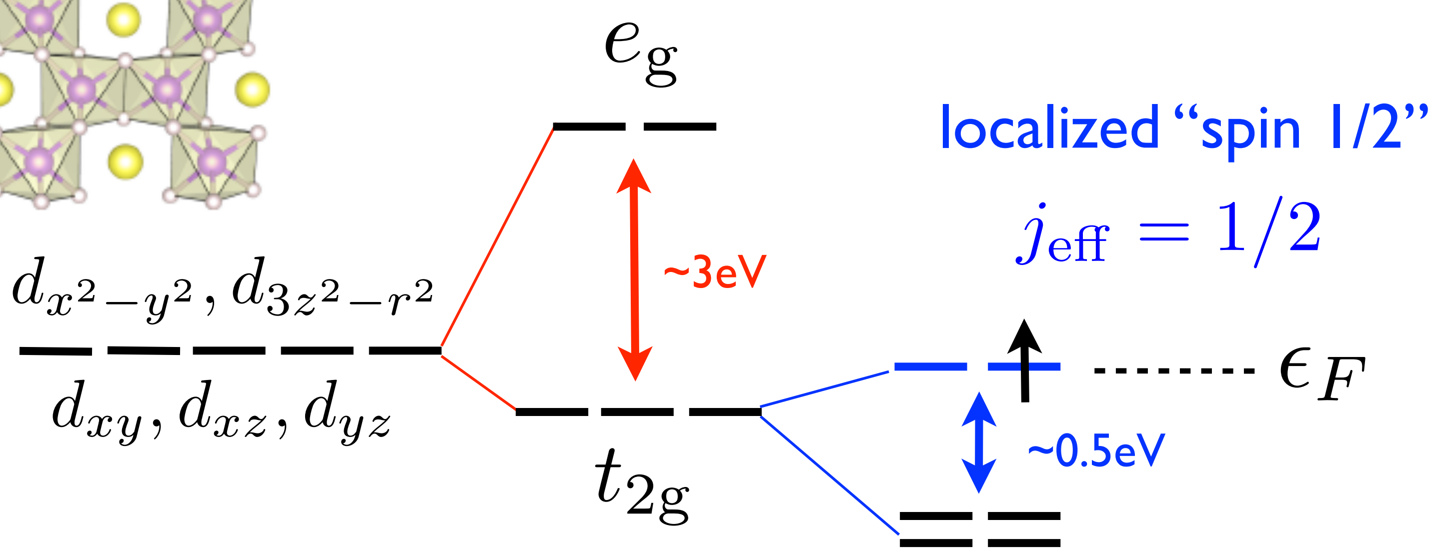


Honeycomb iridate Na_2IrO_3

- layered transition-metal oxide
- Ir^{4+} ions form honeycomb lattice
- electronic structure of d-orbitals:



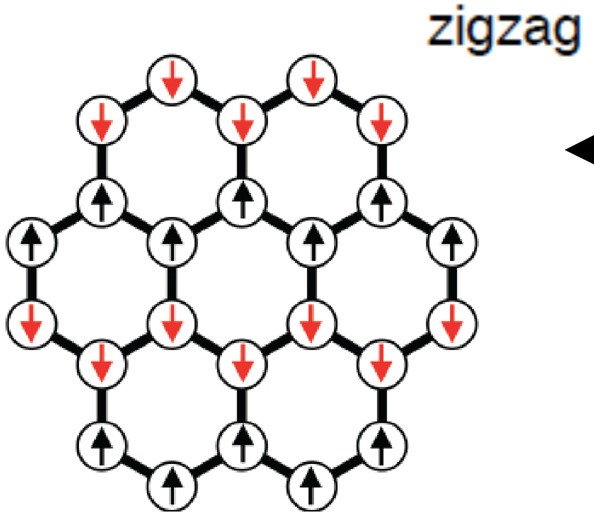
crystal field splitting
spin-orbit coupling



- effective low-energy $j_{\text{eff}} = 1/2$ doublet
- U ~1eV: spin-orbit Mott insulator →

strong coupling expansion:

nearest-neighbor Kitaev-Heisenberg!



theory: [Chaloupka et al. (2013)] Phys. Rev. Lett. 110, 097204 (2013)

AF Kitaev exchange to stabilize zigzag

neutron & X-ray diffraction: [Ye et al. (2012)] Phys. Rev. B 85, 180403(R) (2012), *RIXS*: [Gretarsson et al. (2013)] Phys. Rev. Lett. 110, 076402 (2013), *magnetic depletion*: [Andrade & Vojta] arXiv:1309.2951 & [Manni et al. (2014)] Phys. Rev. B 89, 241102(R), ...

alternative descriptions: *quasimolecular orbitals* [Foyevtsova et al. 2013] Phys. Rev. B 88, 035107 (2013), *quasimolecular crystal* [Mazin et al. (2012)] Phys. Rev. Lett. 109, 197201, *longer-ranged exchange (deduced from spin-wave spectra)* [Choi et al. (2012)] Phys. Rev. Lett. 108, 127204 (2012), *longer-ranged exchange (deduced from susceptibilites & heat capacitites)* [Singh et al. (2012)] Phys. Rev. Lett. 108, 127203 (2012), *superexchange theory* [Sizyuk et al. (2014)] arXiv:1408.3647, ...

Doping a frustrated spin-orbit Mott insulator

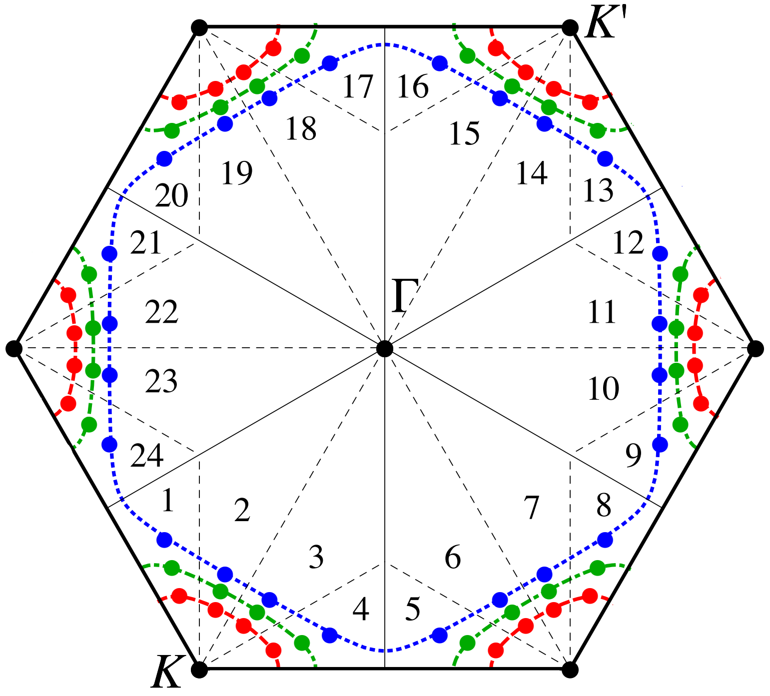
- Kitaev-Heisenberg $t - J_{\mathrm{K}} - J_{\mathrm{H}}$ model to describe doped Mott insulator
- slave-boson theory:

$$c_i \rightarrow b_i^\dagger \, f_{i,\sigma}, \qquad c_i^\dagger \rightarrow f_{i,\sigma}^\dagger b_i$$

$$\vec{S}_i = f_{i,\sigma}^\dagger \vec{\sigma}_{\sigma\sigma'} f_{i,\sigma'}$$

- condensing holons: 'metal of fermionic spinons' with reduced band-width $\sim \delta\, t_0$

$$H_{\mathrm{slave}} = -\delta t_0 \sum_{\langle i,j\rangle} f_{i,\sigma}^\dagger f_{j,\sigma} + \mathrm{h.c.} + J_{\mathrm{K}} \sum_{\langle i,j\rangle} S_i^{\gamma(ij)} S_j^{\gamma(ij)} + J_{\mathrm{H}} \sum_{\langle i,j\rangle} \left(\vec{S}_i \cdot \vec{S}_j - \frac{n_i n_j}{4} \right)$$



- Q: what kind of Fermi surface instabilities will occur for this 'auxiliary metal'?
- A (mean-field): unconventional pairing, topological pairing, ...

[Hyart et al. (2012)] Phys. Rev. B 85, 140510(R) (2012)
[You et al. (2012)], Phys. Rev. B 86, 085145 (2012)
[Okamoto (2013)] Phys. Rev. B 87, 064508 (2013)

A Theorem: topological odd-parity pairing

according to Altland-Zirnbauer, SC states in 2D can be classified according to

- Z_2 invariants (class DIII)
- Z invariants (class D, CI)

[Altland, Zirnbauer (1997)] Phys. Rev. B 55, 1142 (1997)
[Shinsei Ryu et al. (2010)] New J. Phys. 12 065010 (2010)

assumptions:

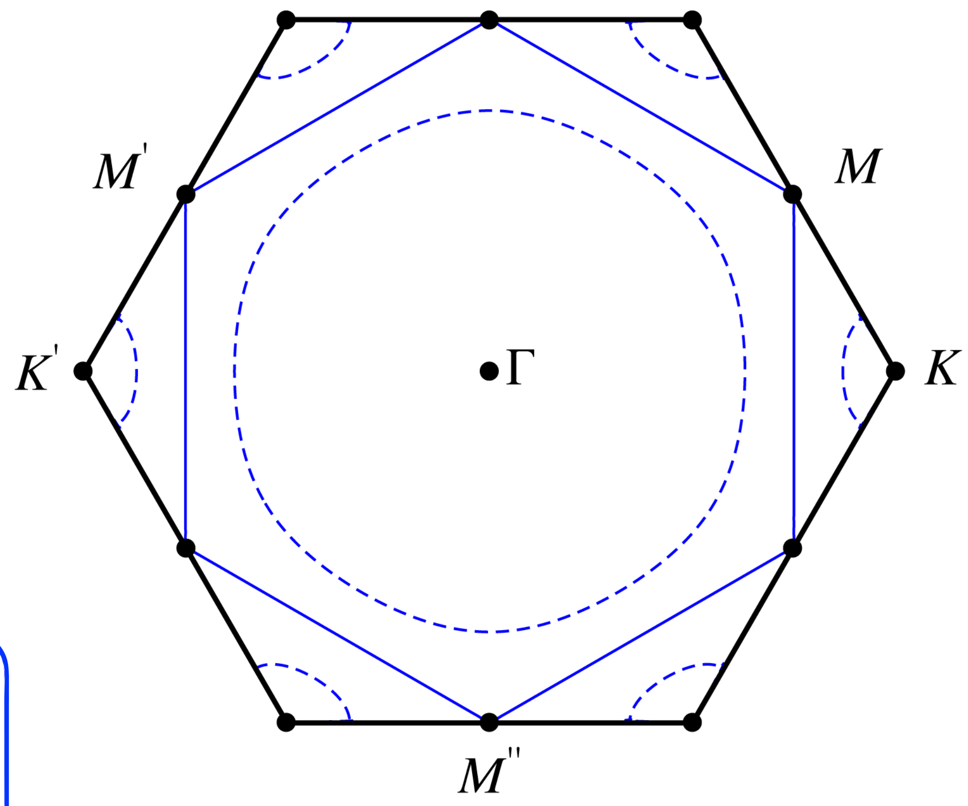
- fully gapped SC state
- odd-parity pairing
- weak-pairing limit

then:

topological non-triviality is determined by number-parity of time-reversal invariant points below Fermi level in the normal state.

odd: non-trivial, even: trivial

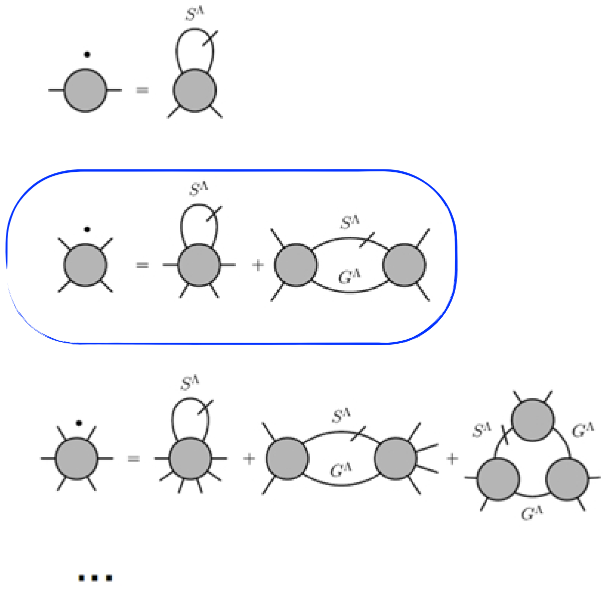
→ Majorana states (at edges or vortex cores)

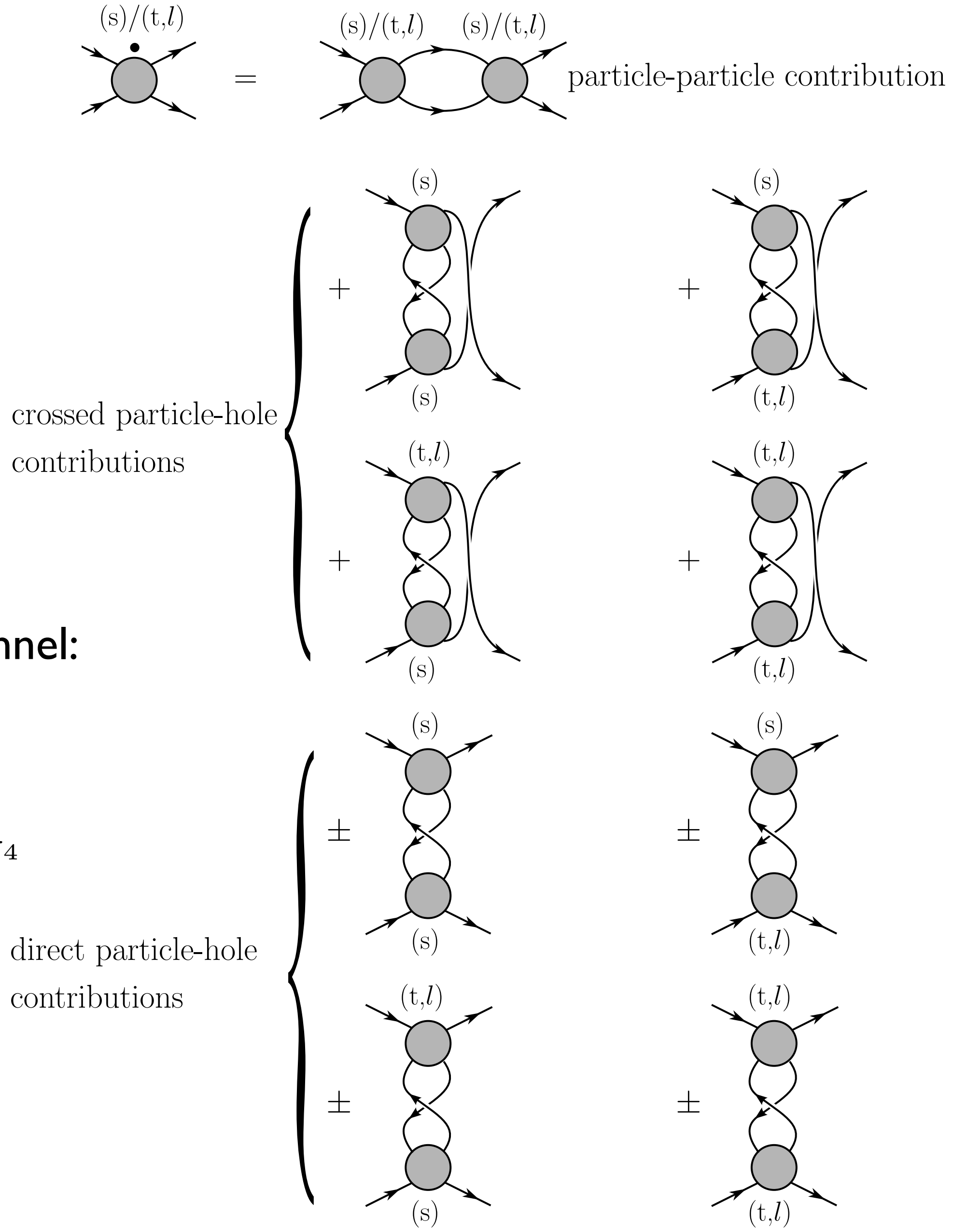


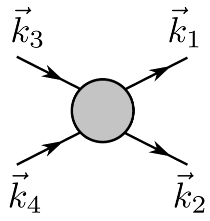
[Sato (2009)] Phys. Rev. B 79, 214526 (2009)
[Sato (2010)] Phys. Rev. B 81, 220504(R) (2010)
[Qi et al. (2010)] Phys. Rev. B 81, 134508 (2010)

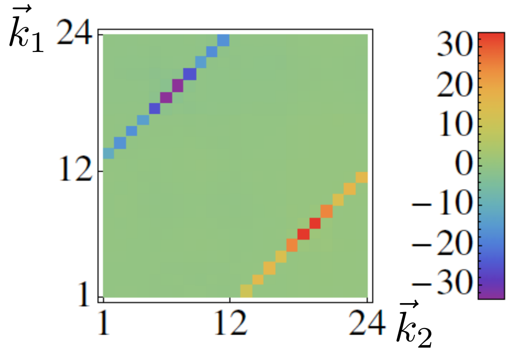
Method: functional Renormalization Group (fRG)

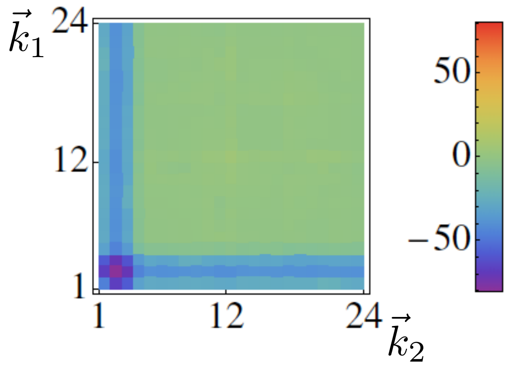
1-PI functional: $\Gamma^{\Lambda}[\psi,\bar{\psi}] = (\bar{\eta}^{\Lambda},\psi) + (\bar{\psi},\eta^{\Lambda}) + \mathcal{G}^{\Lambda}[\eta^{\Lambda},\bar{\eta}^{\Lambda}]$











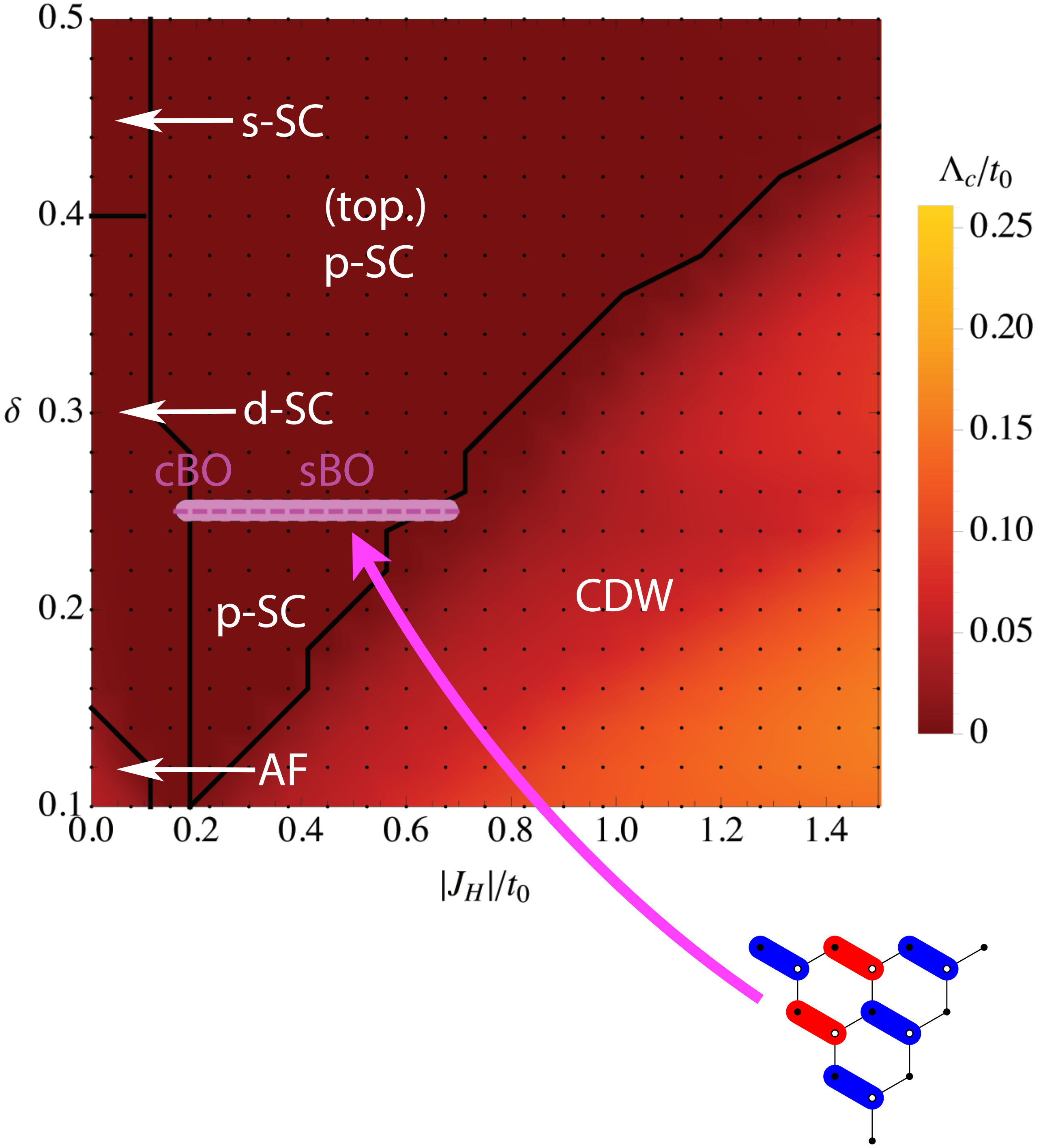
truncate hierarchy, parametrize 4-point vertex function in singlet and triplet channel:

$$V^{\Lambda} = -V^{(\mathrm{s})}[\Gamma_0^{\dagger}]_{\sigma_1\sigma_2}[\Gamma_0]_{\sigma_3\sigma_4} + \sum_{l\in\{x,y,z\}} V_l^{(\mathrm{t})}[\Gamma_l^{\dagger}]_{\sigma_1\sigma_2}[\Gamma_l]_{\sigma_3\sigma_4}$$

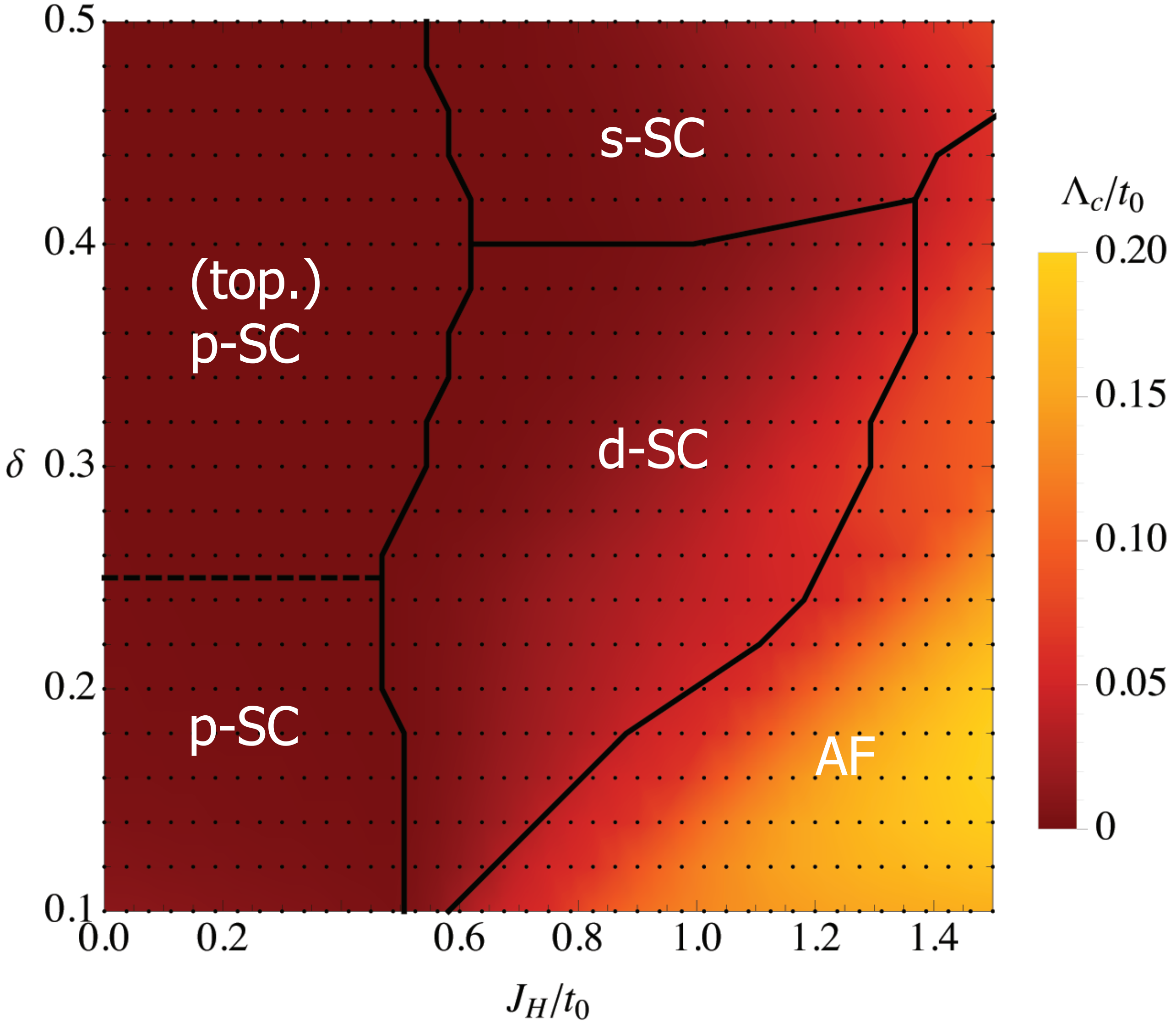
for review: [Metzner et al. (2012)] Rev. Mod. Phys. 84, 299 (2012)

Results: Phase diagram for doped Kitaev-Heisenberg model

$J_{\mathrm{K}} > 0, J_{\mathrm{H}} < 0 \qquad J_{\mathrm{K}}/t_0 = 1$

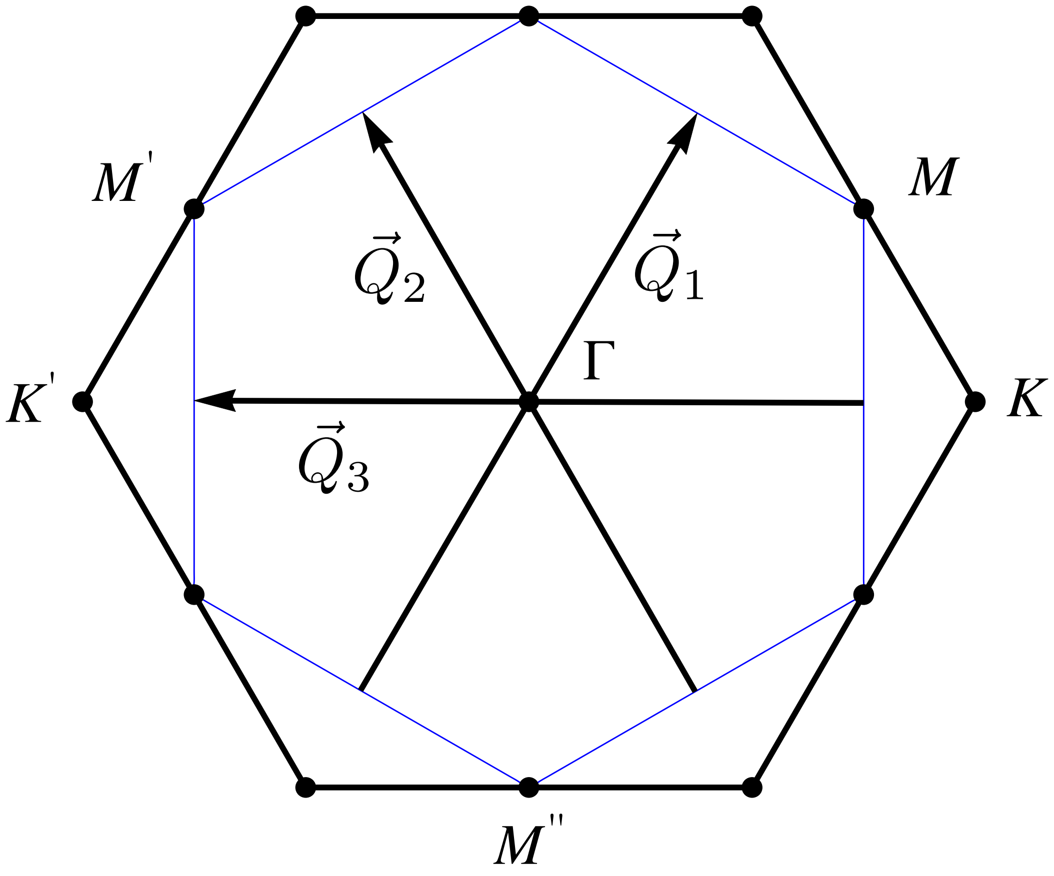


$J_{\mathrm{K}} < 0, J_{\mathrm{H}} > 0 \qquad J_{\mathrm{K}}/t_0 = -1$



Results: bond-order instabilities

$J_{\mathrm{K}} > 0, J_{\mathrm{H}} < 0 \qquad J_{\mathrm{K}}/t_0 = 1$



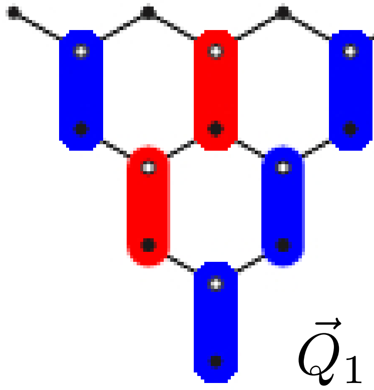
- charge bond-order:

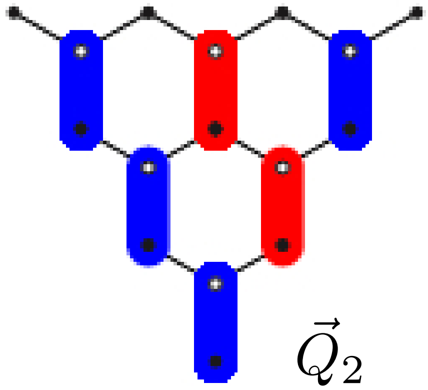
$$\Phi_{\vec{Q}} \propto \sum_{\vec{k},\sigma} \sum_{o,o'} \tilde{\epsilon}_{o,o'} t^{o,o'}_{\vec{k}}(\vec{Q}) f^{\dagger}_{o,\vec{k},\sigma} f_{o',\vec{k}-\vec{Q},\sigma}$$

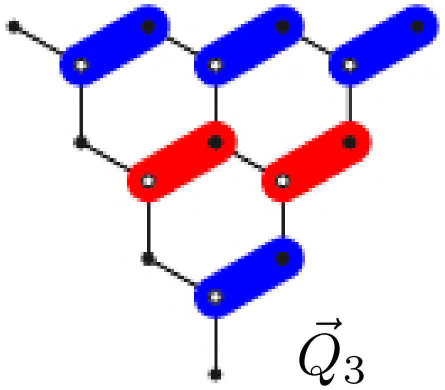
- spin bond-order:

$$\Phi_{l,\vec{Q}} \propto \sum_{\vec{k},\sigma,\sigma'} \sum_{o,o'} \tilde{\epsilon}_{o,o'} t^{o,o'}_{l,\vec{k}}(\vec{Q}) f^{\dagger}_{o,\vec{k},\sigma} [\sigma_l]_{\sigma\sigma'} f_{o',\vec{k}-\vec{Q},\sigma'}$$

wavevector	σ_x	σ_y	σ_z
$\vec{Q}_1$	✓	–	✓
$\vec{Q}_2$	–	✓	✓
$\vec{Q}_3$	✓	✓	–

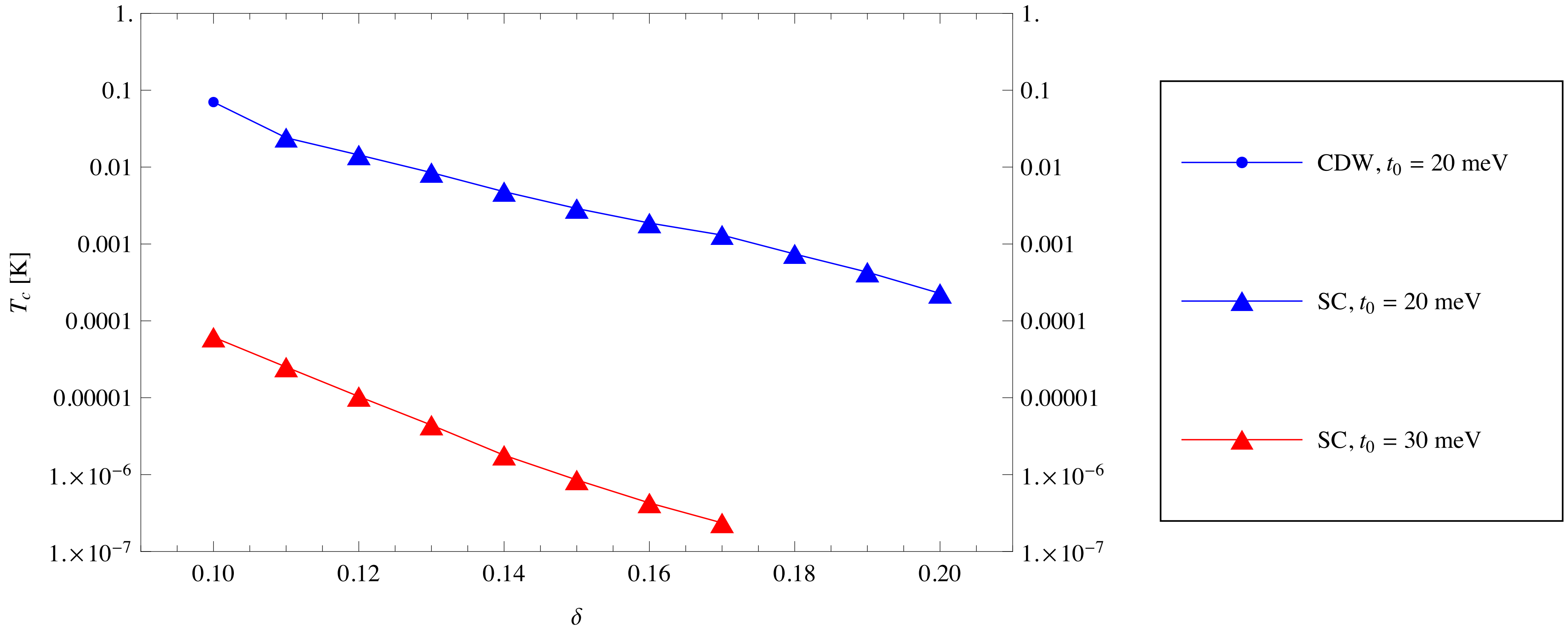






Is a topological p-wave state to be expected?

$J_{\mathrm{K}} > 0, J_{\mathrm{H}} < 0$ $|J_{\mathrm{K}}/J_{\mathrm{H}}| \simeq 5$ [Chaloupka et al. (2013)] Phys. Rev. Lett. 110, 097204 (2013)



- critical temperatures: mK regime and below
- realistic hopping possibly (much) greater than 30 meV, topological p-wave seems out of reach in Na_2IrO_3*

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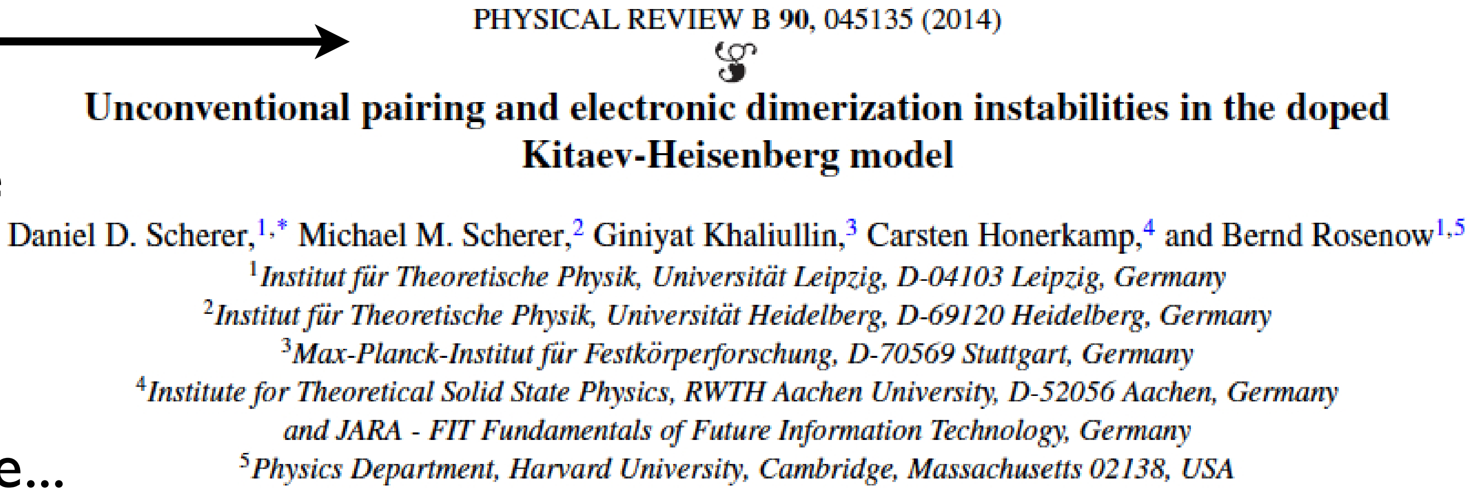
* if Na_2IrO_3 can be described by AF-Kitaev and FM-Heisenberg nearest-neighbor exchange

Conclusions & Outlook

- for fRG details and more results →



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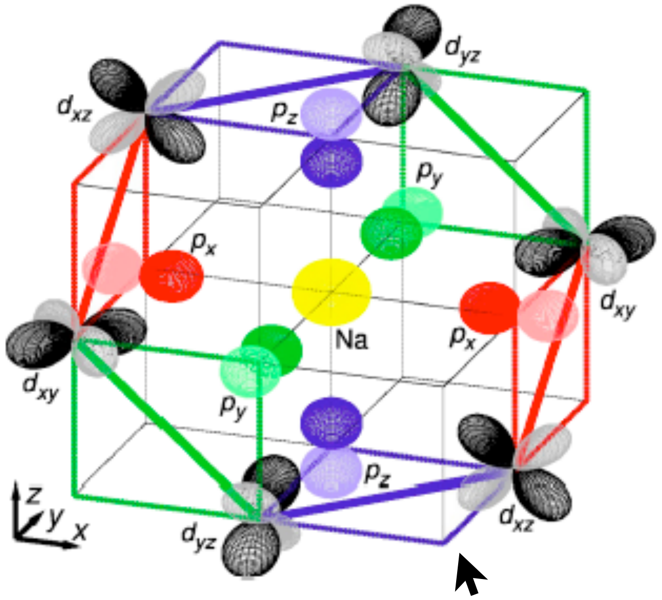
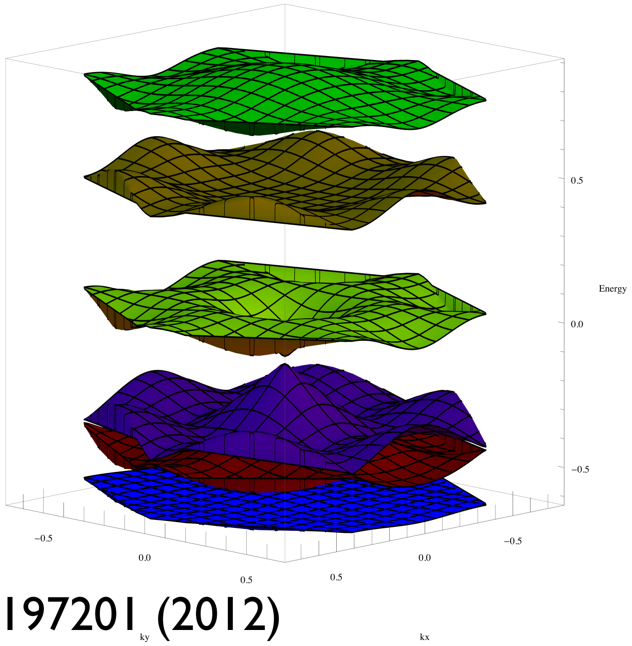
- fRG valuable tool to uncover rich phase diagram for doped Kitaev-Heisenberg model

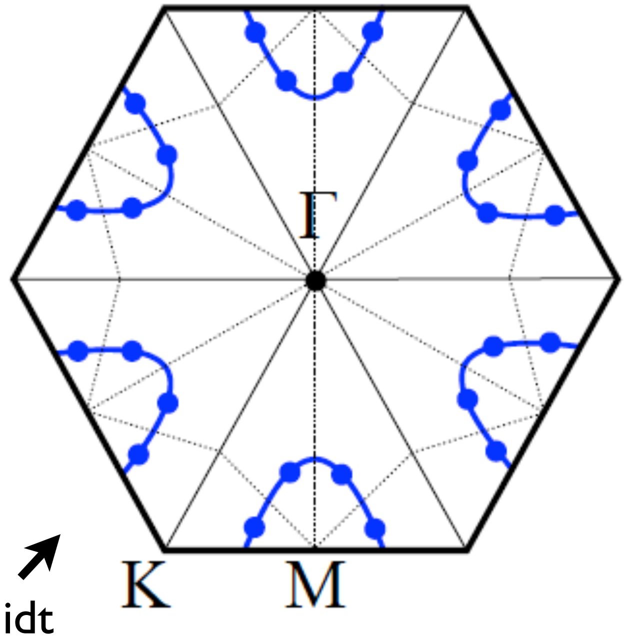
- yet, applicability to Na_2IrO_3 questionable...

Thank you for your attention!

- ... therefore, study interplay of realistic DFT-derived tight-binding band structure with Kitaev-Heisenberg exchange:







from [Mazin et al. (2012)] Phys. Rev. Lett. 109, 197201 (2012)

J. Schmidt