Introduction to Heisenberg-Kitaev physics in magnetic fields

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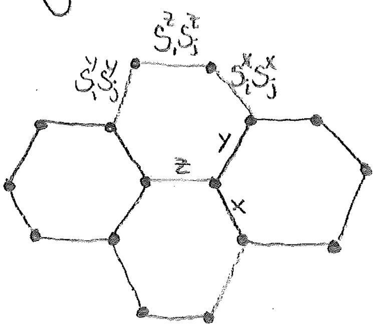
[Janssen et al., PRL 117, 277202 (2016)]

1. Heisenberg-Kitaev model

Hamiltonian:

$$\mathcal{H}_0 = J \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j + 2K \sum_{\gamma = x,y,z} \sum_{\langle ij \rangle_\gamma} S_i^\gamma S_j^\gamma ,$$

defined on honeycomb lattice [large!].

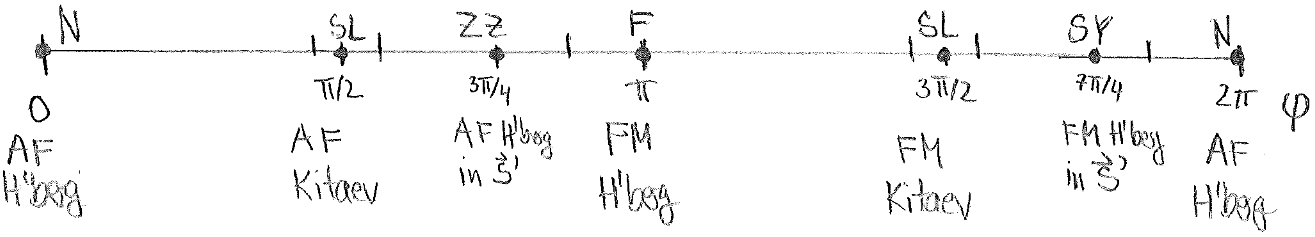


Parametrization:

$$J = \overset{\swarrow \text{ overall energy scale}}{A} \cos\varphi$$

$$K = A \sin\varphi$$

Phase diagram [allow space!]:

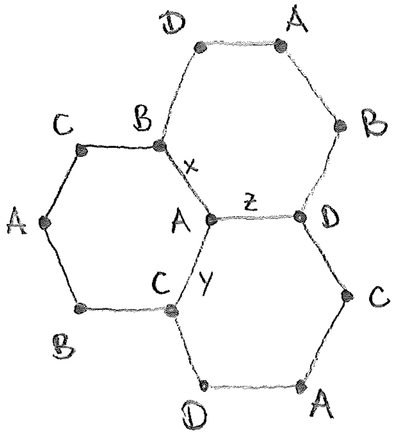


Dual spins:

$$\vec{S}_i' = \begin{cases} \vec{S}_i & \text{, for } i \in A \\ \mathrm{diag}(1,-1,-1)\,\vec{S}_i & \text{, for } i \in B \\ \mathrm{diag}(-1,1,-1)\,\vec{S}_i & \text{, for } i \in C \\ \mathrm{diag}(-1,-1,1)\,\vec{S}_i & \text{, for } i \in D \end{cases}$$

four-sublattice transformation

on



with algebra

$$[S^{x'}, S^{y'}] = i\, S^{z'} \quad \text{etc.}$$

Kitaev term (z-bond):

$$S_i^z S_j^z = S_i^{z'} S_j^{z'} \quad \text{invariant}$$

Heisenberg term (z-bond):

$$\vec{S}_i \cdot \vec{S}_j = S_i^x S_j^x + S_i^y S_j^y + S_i^z S_j^z$$

$$= -S_i^{x'} S_j^{x'} - S_i^{y'} S_j^{y'} - S_i^{z'} S_j^{z'} + S_i^{z'} S_j^{z'} + S_i^{z'} S_j^{z'}$$

$$= -\vec{S}_i' \cdot \vec{S}_j' + 2\, S_i^{z'} S_j^{z'}$$

Klein duality:

$$\mathcal{H}_0 = -J \sum_{\langle ij\rangle} \vec{S}_i' \cdot \vec{S}_j' + 2(K+J) \sum_{\gamma} \sum_{\langle ij\rangle_\gamma} S_i^{\gamma\,\prime} S_j^{\gamma\,\prime}$$

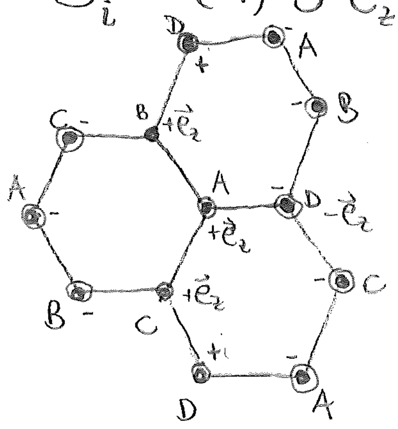
Points with hidden SU(2) symmetry:

$$K = -J \gtrless 0 \quad \Leftrightarrow \quad \varphi = \frac{3\pi}{4} \text{ or } \frac{7\pi}{4}$$

[add to diagram]

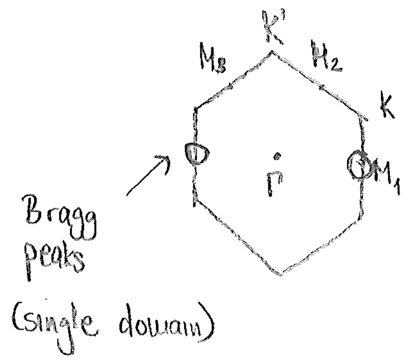
Ground states at $\varphi = \frac{3\pi}{4}$:

- E.g.: $\vec{S}_i' = (-1)^i S \, \vec{e}_z \parallel [001] \Rightarrow \vec{S}_i = \begin{cases} \vec{S}_i' & i \in A \\ -\vec{S}_i' & i \in B \\ -\vec{S}_i' & i \in C \\ \vec{S}_i' & i \in D \end{cases}$



"z-zigzag antiferromagnet" [α-$RuCl_3$, Na_2IrO_3, ...]

Ordering wavevector: $\vec{Q} = \vec{M}_1$



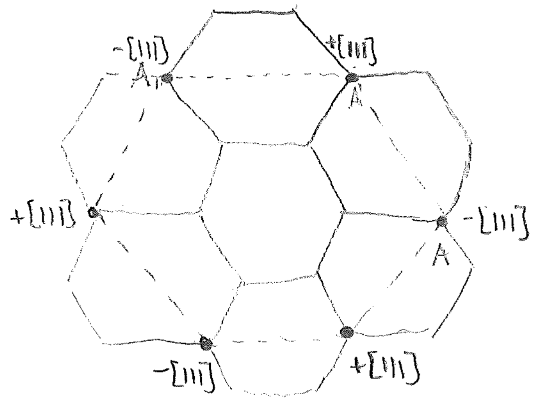
single-Q

- E.g.: $\vec{S}_i' = (-1)^i S \frac{1}{\sqrt{3}}(\vec{e}_x + \vec{e}_y + \vec{e}_z) \parallel [111]$

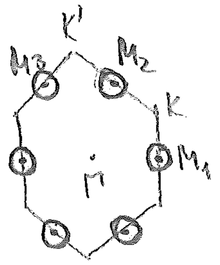
$$\Rightarrow \vec{S}_i \propto \begin{cases} \pm[111] & i \in A \\ \pm[1\bar{1}\bar{1}] & i \in B \\ \pm[\bar{1}1\bar{1}] & i \in C \\ \pm[\bar{1}\bar{1}1] & i \in D \end{cases}$$

non-coplanar w/ 8-site unit cell

"AF star"



Ordering wavevectors: $Q = \vec{M}_1, \vec{M}_2,$ and $\vec{M}_3$



multi-Q!
(single domain)

Implications for phase diagram:

- At $\varphi = \frac{3\pi}{4}$ ground state has SU(2) degeneracy
- (Only) three are zigzag states, others are generically non coplanar
- In the vicinity of (but not right at!) $\varphi = \frac{3\pi}{4}$, quantum fluctuations favor coplanar zigzag states
- Similar story $\varphi = \frac{7\pi}{4}$: "stripy" antiferromagnet

2. Effects of magnetic field : Heisenberg limit

Zeeman term:

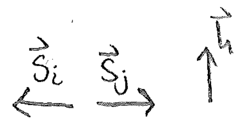
$$\mathcal{H}_h = - \vec{h} \cdot \sum_i \vec{S}_i$$

Energy:

$$\varepsilon(\vec{h}) = \varepsilon(0) - \underbrace{\vec{m}(0) \cdot \vec{h}}_{=0 \ (\text{AFM})} - \frac{1}{2} \chi(0) h^2 + \mathcal{O}(h^3)$$

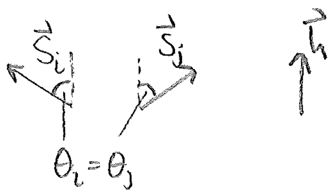
Small h:

Spins will align such that χ is maximized : $\vec{S}_i \perp \vec{h}$



Finite h:

Spins <u>cant</u> towards $\vec{h}$:



3. Effects of magnetic field: Heisenberg-Kitaev model

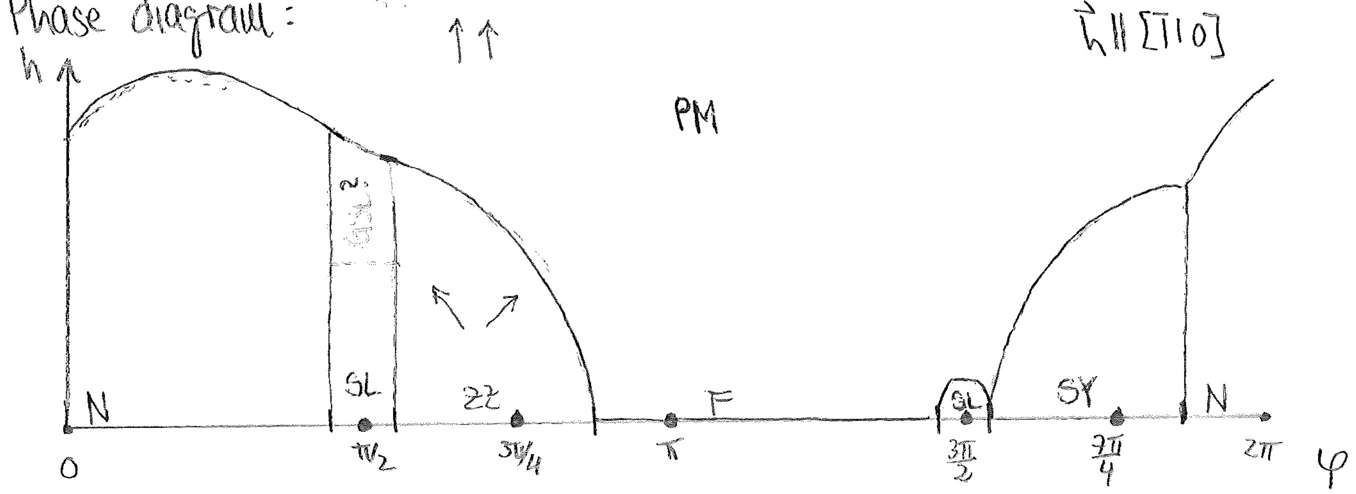
Small h:

Orthogonal alignment only for selected field directions

Example ($\vec{h} \parallel [\bar{1}10] \propto b$):

$\vec{h} \perp \vec{e}_z \parallel \vec{S}_i(h=0)$ (z-zigzag)

Phase diagram:

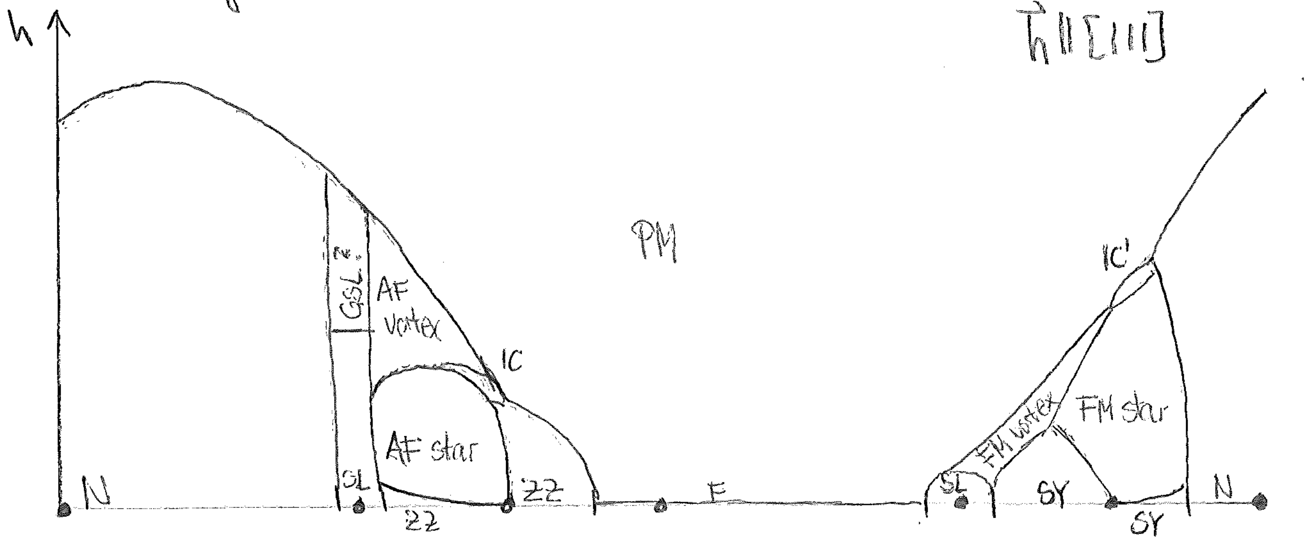


But: Generic field direction $\vec{h} \not\parallel \vec{S}_i$ $\Rightarrow$ no simple canting!

Example ($\vec{h} \parallel [111] \propto c^*$):

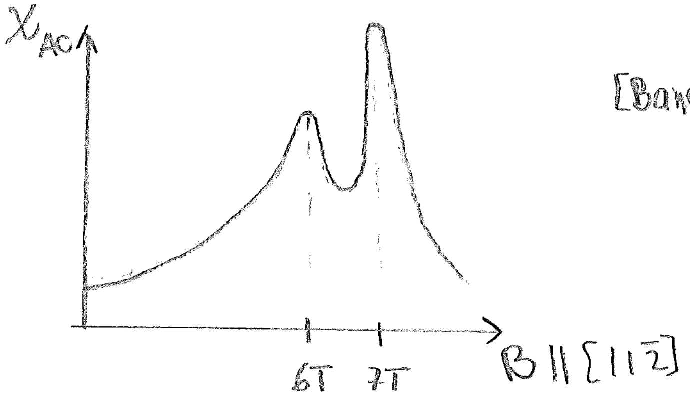
For $\varphi \lesssim \frac{3\pi}{4}$: small h favors "star" over "zigzag"

Phase diagram:



Conclusions:

- Broken SU(2): complex magnetization process
- Strong frustration: field-induced intermediate phases
- α-$RuCl_3$?



[Banerjee et al., npj QM (2018)]