Deconfinement in Heisenberg-perturbed Kitaev models

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References:

1) A. Kumar and V. Tripathi, Kitaev quasiparticles in a proximate spin liquid: A many-body localization perspective, arXiv:1910.00030.

2) S. D. Das et al., Magnetic anisotropy of the alkali iridate Na_2IrO_3 at high magnetic fields: evidence for strong ferromagnetic Kitaev correlations, Phys. Rev. B **99**, 081101(R) (2019).

3) S. D. Das, Kusum Dhochak and V. Tripathi, Kondo route to spin inhomogeneities in the honeycomb Kitaev model, Phys. Rev. B **94**, 024411 (2016).

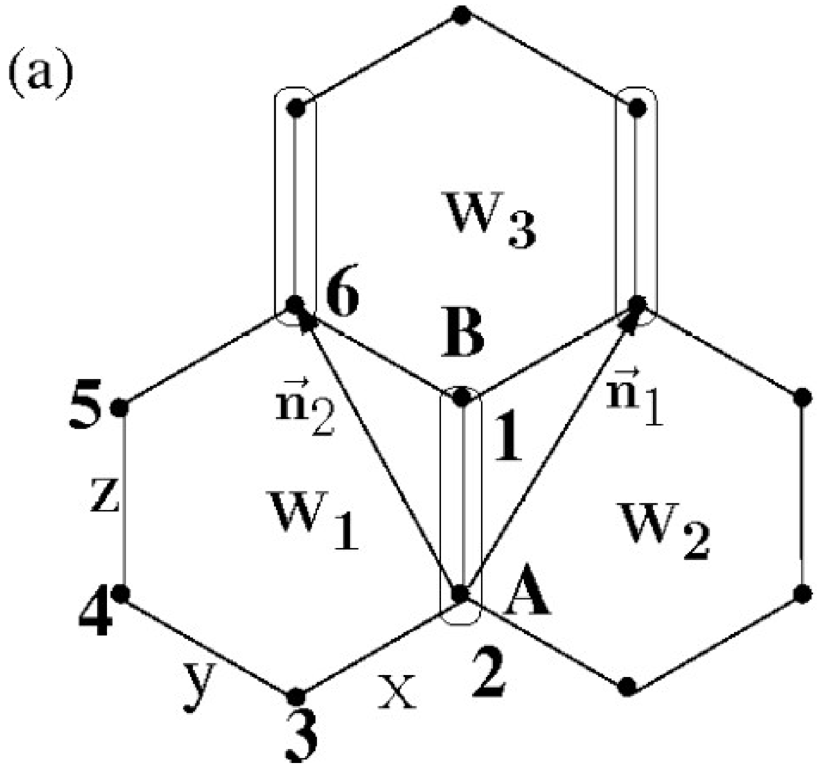
4) Kusum Dhochak, R. Shankar and V. Tripathi, Magnetic impurities in the honeycomb Kitaev model, Phys. Rev. Lett. **105**, 117201 (2010).

Kitaev model in a nutshell

[Kitaev, Ann. Phys. (2006)]

$$H = J_x \sum_{\langle ij \rangle,\, x-bonds} \sigma_i^x \sigma_j^x + J_y \sum_{\langle ij \rangle,\, y-bonds} \sigma_i^y \sigma_j^y + J_z \sum_{\langle ij \rangle,\, z-bonds} \sigma_i^z \sigma_j^z$$

Ising-like model on honeycomb lattice with peculiar Kugel-Khomskii like direction-dependent interactions. Integrable!



Quasiparticles: Not spin-1 magnons but gapped, localized Z_2 vortices (π-fluxes) and deconfined Majorana fermions.

$$W_1 = \sigma_{1x} \sigma_{2y} \sigma_{3z} \sigma_{4x} \sigma_{5y} \sigma_{6z}$$

The vortices are known to be non-Abelian anyons – interesting from the point of view of topological quantum computing.

Excitations in the deconfined phase

Express each spin-1/2 particle on the honeycomb lattice as a bilinear of Majorana fermions:

$$\sigma_x = i b_x c\,,\quad \sigma_y = i b_y c\,,\quad \sigma_z = i b_z c$$

A gauge constraint also needs to be imposed at every site: $D = b_x b_y b_z c \equiv 1$

$$H = \frac{i}{4} \sum_{\langle ij \rangle} \hat{A}_{ij} c_i c_j$$

$$\hat{A}_{ij} = 2 J_{\alpha_{ij}} \hat{u}_{ij}\,,\quad \hat{u}_{ij} = i b^i_{\alpha_{ij}} b^j_{\alpha_{ij}}$$

$$[H, \hat{u}_{ij}] = 0\,,\quad [\hat{u}_{ij}, \hat{u}_{kl}] = 0\,,\quad \hat{u}_{ij}^2 = 1$$

Hilbert space divided into sectors labelled by the eigenvalues of $\hat{u}_{ij}$ – restricting to any such sector gives model of **free** Majorana fermions.

$2^{3N/2}$ possible combinations for the gauge fields, but they do not all correspond to distinct physical states. Physical objects are the (gauge invariant) fluxes.

... Excitations in the deconfined phase

Z_2 fluxes in terms of gauge fields (plaquette Wilson loops):

$$W_p = \prod_{\langle ij \rangle,\ i \in A,\ j \in B} u_{ij} \,,$$

Gauge transformations leave fluxes unchanged:

$$[D_i, W_p] = 0$$

Hamiltonian non-interacting in each flux sector. *N* Majorana fermions ⇒ $2^{N/2}$ degrees of freedom in each sector.

Ground state manifold corresponds to zero flux in all plaquettes (Lieb, 1994):

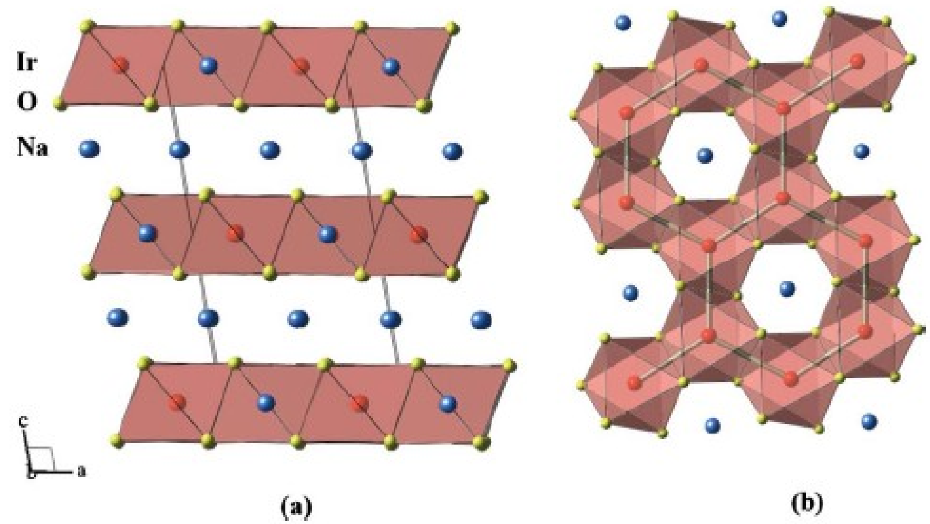
$$W_i = +1$$

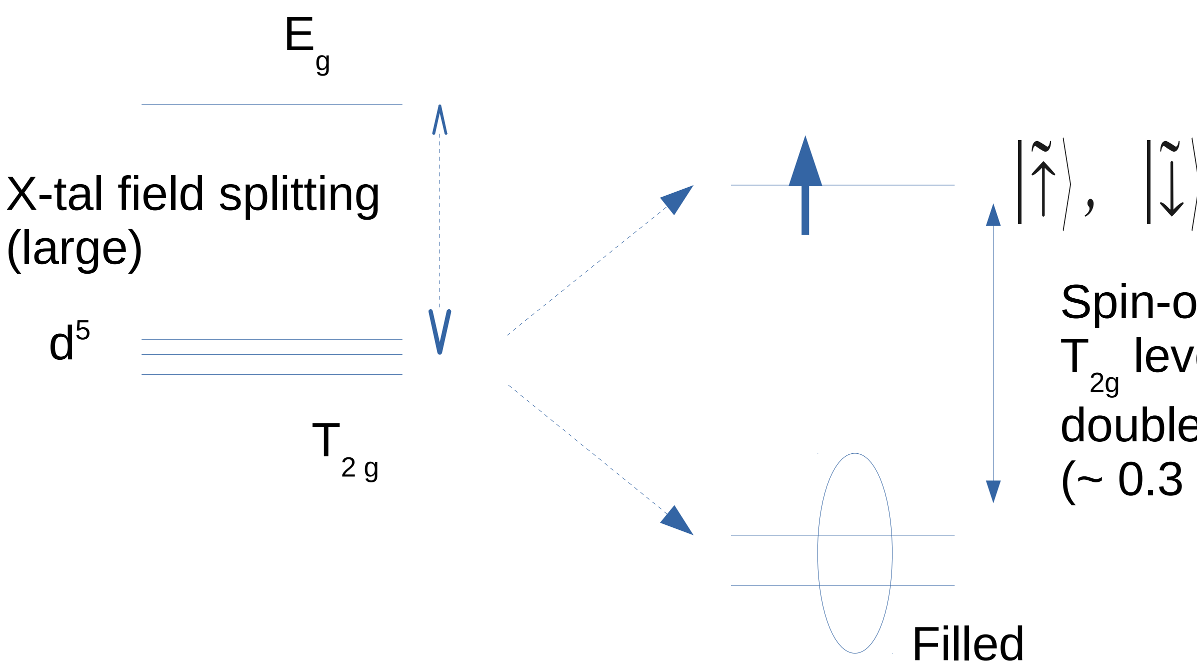
The nonzero expectation value of plaquette Wilson loops and their finite excitation energy are smoking gun signatures of deconfinement.

Real Kitaev materials

The alkali iridate Na_2IrO_3 and α-$RuCl_3$ are the two most studied Kitaev material candidates.

First theoretical proposal:
G. Jackeli & G. Khaliullin, PRL (2009).
Quantum analogue of Kugel-Khomskii classical compass models.





Spin-orbit coupling (~ 0.5 eV) splits T_{2g} levels to give a half-filled Kramers doublet. Local Coulomb correlations (~ 0.3 eV) are smaller.

Real Kitaev materials, competing interactions

Presence of competing spin-spin interactions (which are small) nevertheless drives both the materials to long range magnetic order (zigzag AFM).

[See eg. Y. Singh et al., PRL (2012) F. Ye et al., PRB (2012);
S. Choi et al., PRL (2012); X. Liu et al., PRB (2011)
for the iridate and A. Banerjee et al., Nat. Mater. (2016) for α-$RuCl_3$]

Wide separation of zigzag ordering scale (~ 10K) and Curie termperature (~ -100K) is due to strong frustrating effect of dominant Kitaev interaction.

Ground state not Kitaev QSL but magnetically long-range ordered. However the materials are quite close in parameter space to the QSL state (so-called proximate spin liquid).

Possible to realize Kitaev physics in these materials?
Suppress magnetic order or look at excited states?

Kitaev physics in real Kitaev materials

Both views are not without merit.

- Excited states? Two scenarios.

Dominant interaction in the model is Kitaev. Once zigzag order is destroyed by, say, raising the temperature, shouldn’t the high energy excitations involved be better described as Kitaev quasiparticles? Should look for deconfinement in excited states.

Counter view: Low-energy excitations of a 3D magnet are spin-1 bosons (magnons) and not Majorana fermions. For higher energies, magnon-magnon scattering becomes important leading to their decay. Residual Kitaev interactions in the magnetically ordered state may further enhance magnon scattering, but all within the ambit of interacting spin waves.
No deconfinement here.

- Magnetic field tuning

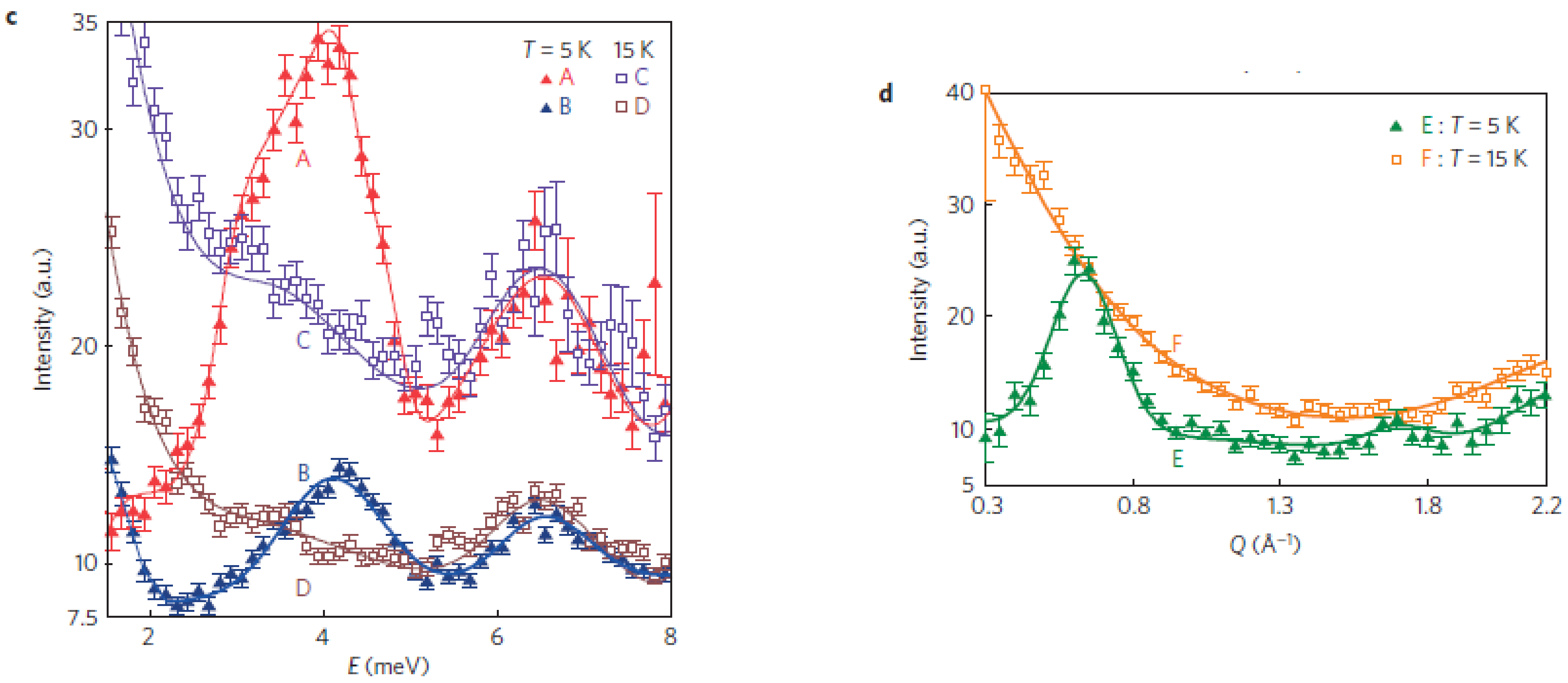
Suppress SDW using magnetic field, possibly reinstating the deconfined phase. A field tuned Kitaev QSL?

Spin-waves: temperature dependence

Proximate Kitaev quantum spin liquid behaviour in a honeycomb magnet

A. Banerjee[1*], C. A. Bridges[2], J.-Q. Yan[3,4], A. A. Aczel[1], L. Li[5], M. B. Stone[1], G. E. Granroth[1,6], M. D. Lumsden[1], Y. Yiu[5], J. Knolle[7], S. Bhattacharjee[8,9], D. L. Kovrizhin[7], R. Moessner[8], D. A. Tennant[10], D. G. Mandrus[3,4] and S. E. Nagler[1,11*]

Nat. Mater. **15**, (2016)



Spin-waves incoherent above zigzag AFM ordering temperature.

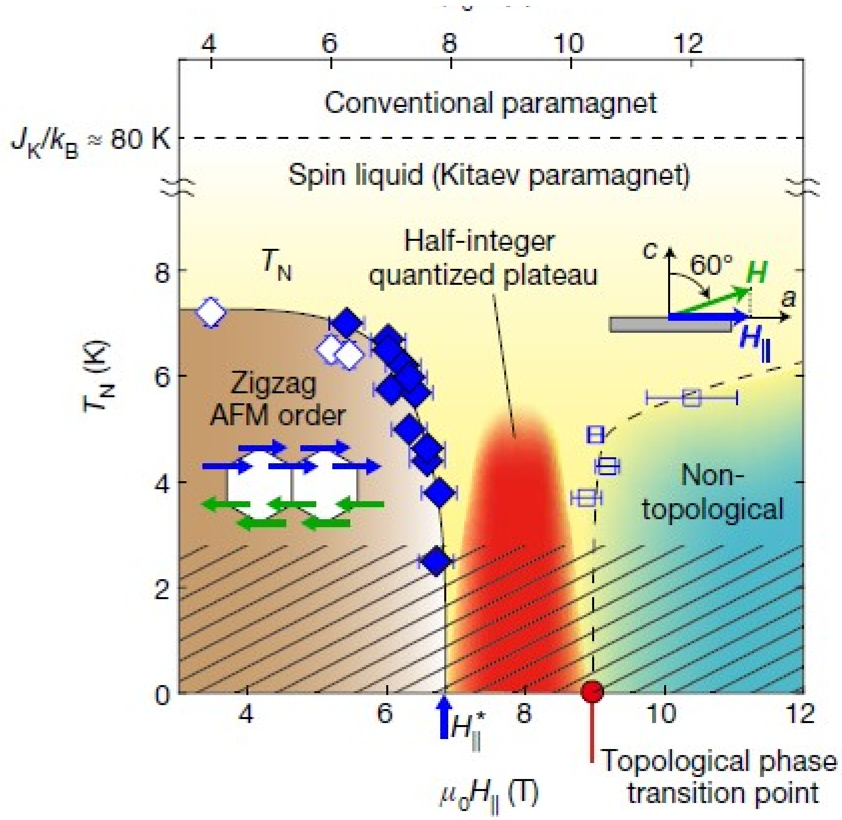
Field induced Kitaev spin liquid?

Majorana quantization and half-integer thermal quantum Hall effect in a Kitaev spin liquid

Y. Kasahara[1], T. Ohnishi[1], Y. Mizukami[2], O. Tanaka[2], Sixiao Ma[1], K. Sugii[3], N. Kurita[4], H. Tanaka[4], J. Nasu[4], Y. Motome[5], T. Shibauchi[2] & Y. Matsuda[1]*

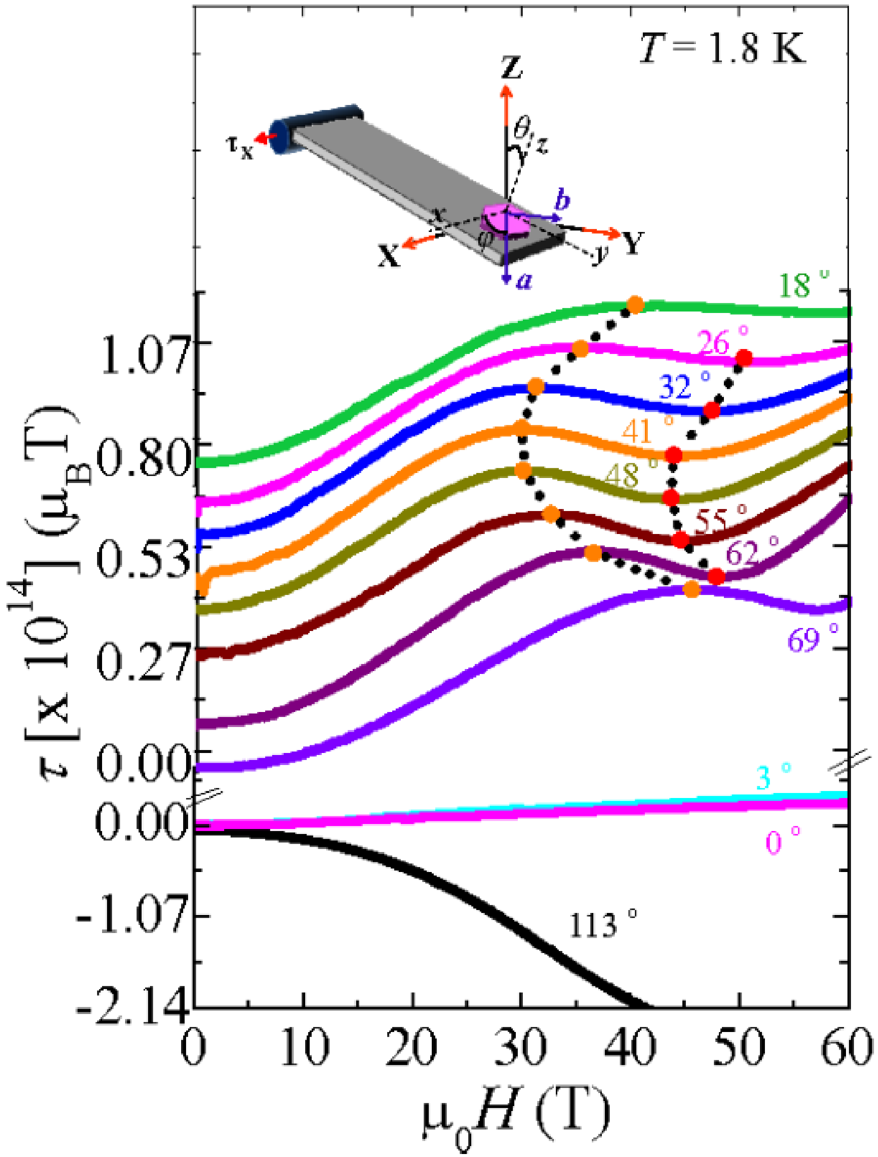
Nature **559** (2018)

Quantization of thermal Hall conductance at intermediate fields in α-$RuCl_3$



Field-tuned Kitaev QSL: High field torque magnetometry

[Our work: S. Das et al., PRB(R) (2019)]



Torque measured as a function of field (as high as 60T) as well as orientation.

Distinctive nonmonotonous torque response observed for a wide range of field orientation at intermediate fields (25-45 T).

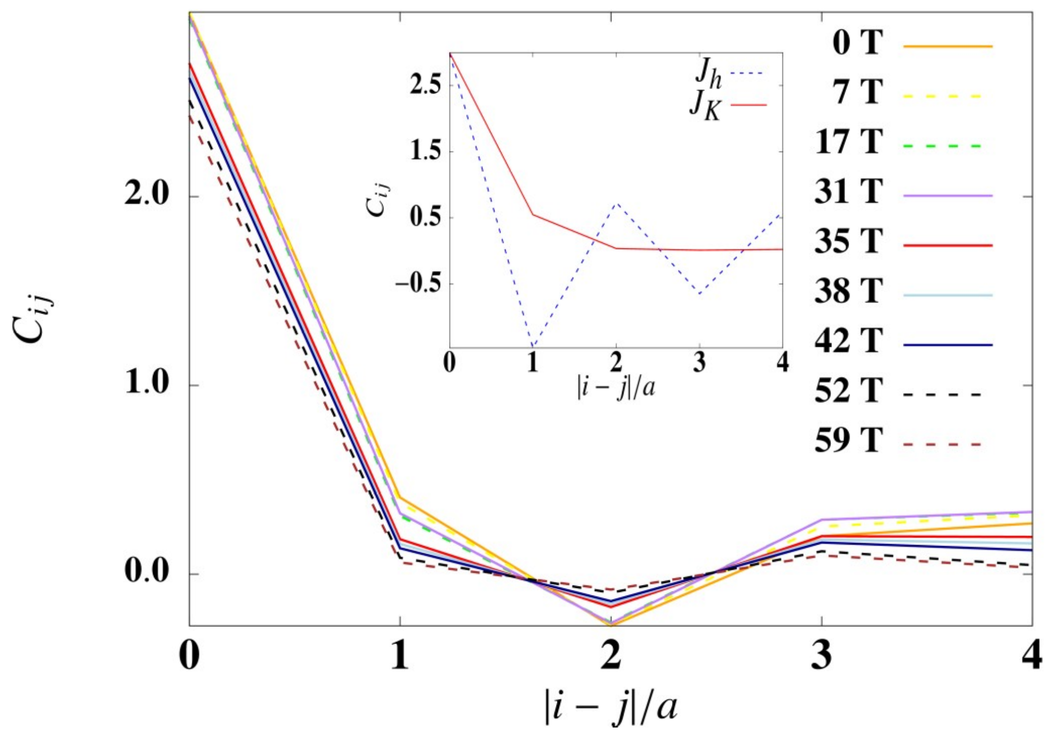
Feature observed only below the zigzag ordering temperature.

Essentially the same feature is also observed (but not explained) in α-$RuCl_3$.
[I. A. Leahy et al., PRL (2017)]

Nonmonotonous field dependence of torque severely constrains parameters in effective Kitaev-Heisenberg models.

Field tuning to Kitaev QSL [S. Das et al., PRB(R) (2019)]

Using the magnetometry constrained models, we computed distance dependence of the spin-correlation function for different field values.



Correlation functions decay much faster as a function of separation at higher values of the applied field, and the amplitude of their oscillation falls off rapidly with increasing fields, in particular above the zigzag ordering scale.

Deconfinement in SDW phase

How good are Kitaev quasiparticles in the presence of perturbations such that the ground state has magnetic SDW order?

Model with FM Kitaev (K>0) and AFM Heisenberg (J>0) interactions:
[J. Chaloupka et al. PRL (2010)]

$$H = -K \sum_{\langle ij \rangle, \gamma-bonds} \sigma_i^\gamma \sigma_j^\gamma + J \sum_{\langle ij \rangle} \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j$$

Phases:
Kitaev QSL (0 < J/K < 0.12); Stripy AFM (0.12 < J/K < 0.75);
Neel AFM (J/K > 0.75).

Stripy AFM order peaks at J/K=1/2, a sublattice transformation maps it to a Heisenberg ferromagnet.

The regime 0.12 < J/K < 0.5 is the so-called proximate spin liquid (**PSL**).

Scaling analysis for quasiparticle stability

[B. Altshuler et al., PRL (1997)]

- Calculate "support size" ξ of Kitaev quasiparticle states in Fock space of the exact states of J-K model. Inverse Participation Ratio (IPR).

- Obtain the scaling of support size with number of spins, N.

  If $\xi \sim 2^N$, the Kitaev state is unstable, i.e., not a "good" approximation to the exact eigenstate. This many-body wavefn is fully delocalized in the Fock space!

  If $\xi \sim 2^{cN}$, $c < 1$, the Kitaev state does not decay even though the wavefn is delocalized in Fock space. [Fractal scaling]

  If ξ scales weaker than exponential, then the Kitaev state is stable. An example of many-body localization.

Exact diagonalization strategy

[A. Kumar, VT, arXiv:1910.00030]

To describe the delocalized states, we essentially need an exponentially large number of exact eigenstates. If all eigenstates are computed, and no symmetries are exploited, then N=16 is about the best we can do with our computing resources.

Lanczos or Davidson algorithms based on shift-inverse strategies do not give more than a few tens of states at a time. Besides, it involves inversion of singular matrices – numerically unstable.

Our method: **FEAST**

- Contour integration based algorithm
- Yields eigenstates in arbitrary, user-specified eigenvalue ranges
- Allows parallelization at multiple levels.

Unlike Lanczos and Davidson, FEAST is able to handle degeneracies.

FEAST eigensolver

[E. Polizzi, Phys. Rev. B (2009)]

Basic idea – a countour integration based projector

$$\frac{1}{2\pi i}\oint_C \frac{dE}{EI - H} = \sum_{n \in C} |n\rangle\langle n|$$

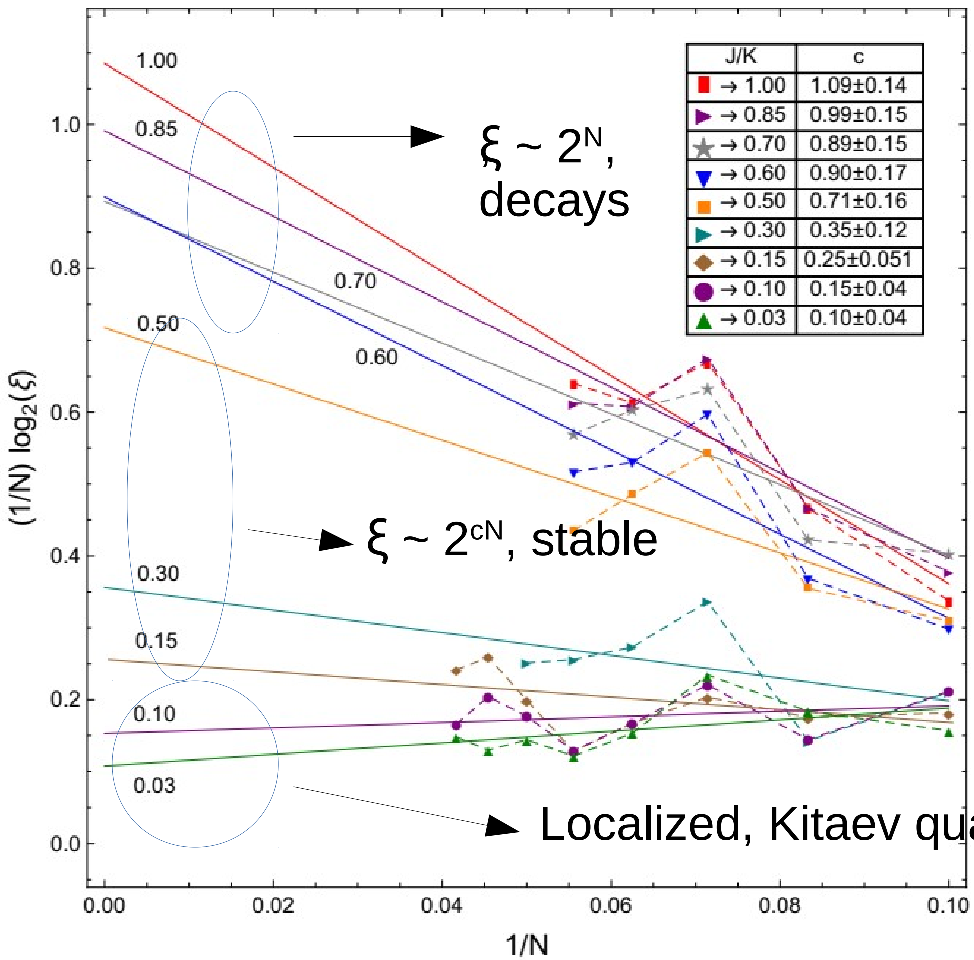
Projects large sparse Hamiltonian to subspace spanned by eigenfunctions whose corresponding eigenvalues are enclosed by C.

Exact diagonalization of the projected lower-dimensional Hamiltonian yields the eigenstates enclosed by C. Contour integration performed approximately by quadratures.

Although FEAST also involves a shift-inverse, the matrix being inverted is not singular over much of C, except for points very close to the real axis.

Decay of a low-lying 2-vortex Kitaev state

Finite size scaling of logarithm of support size vs 1/N.



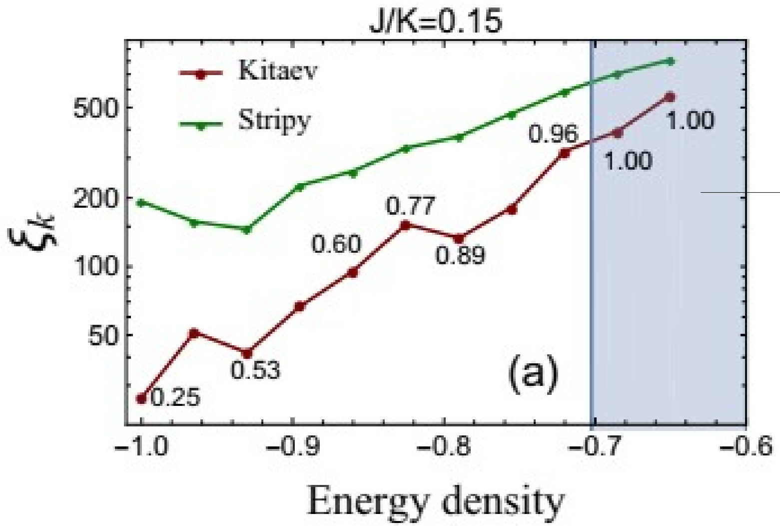
Y-intercept gives exponent for exponentially scaling delocalized states.

Localized to fractal transition at J/K ~ 0.12, the Kitaev-zigzag boundary.

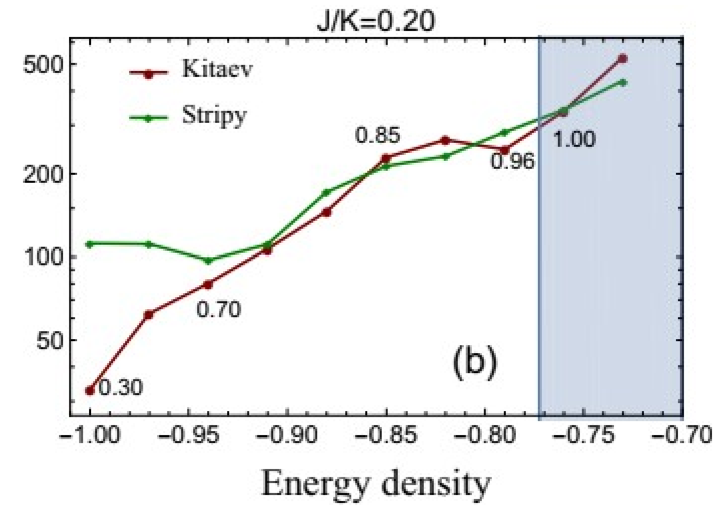
Kitaev quasiparticles unstable only for J/K > 0.5, deep *within* the stripy phase.

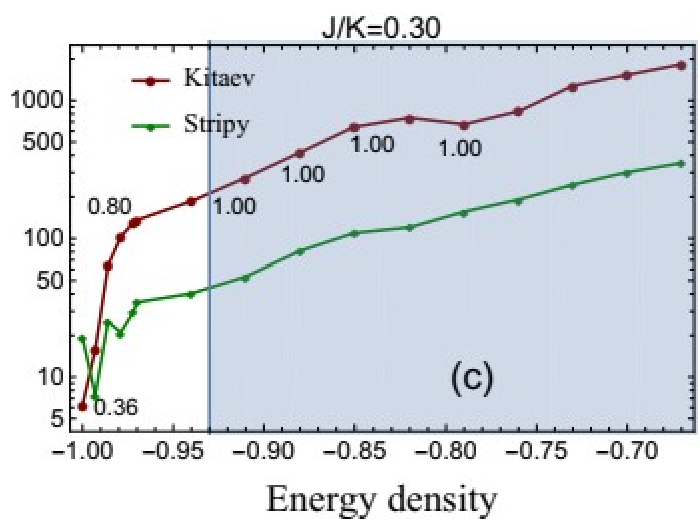
Excited states in PSL: Kitaev or magnons?

What's better: Magnon-like excitations of the stripy phase at J/K=0.5 or Kitaev?



Kitaev
delocalized



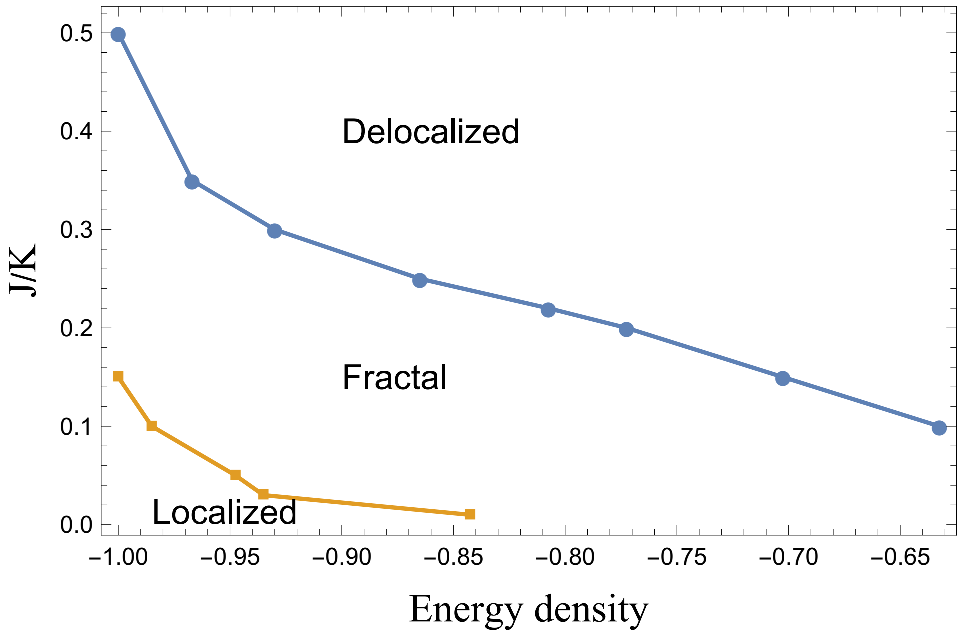


At higher energy densities, both Kitaev
And magnon excitations unstable! So junk
does not imply Kitaev.

At the lowest energy densities, Kitaev is
better than magnon practically everywhere
In PSL even though SDW order is there!

MBL phase diagram for Kitaev states

Result of finite-size scaling analysys in interaction vs energy density plane.



Kitaev quasiparticles stable in localized and fractal scaling Phases.

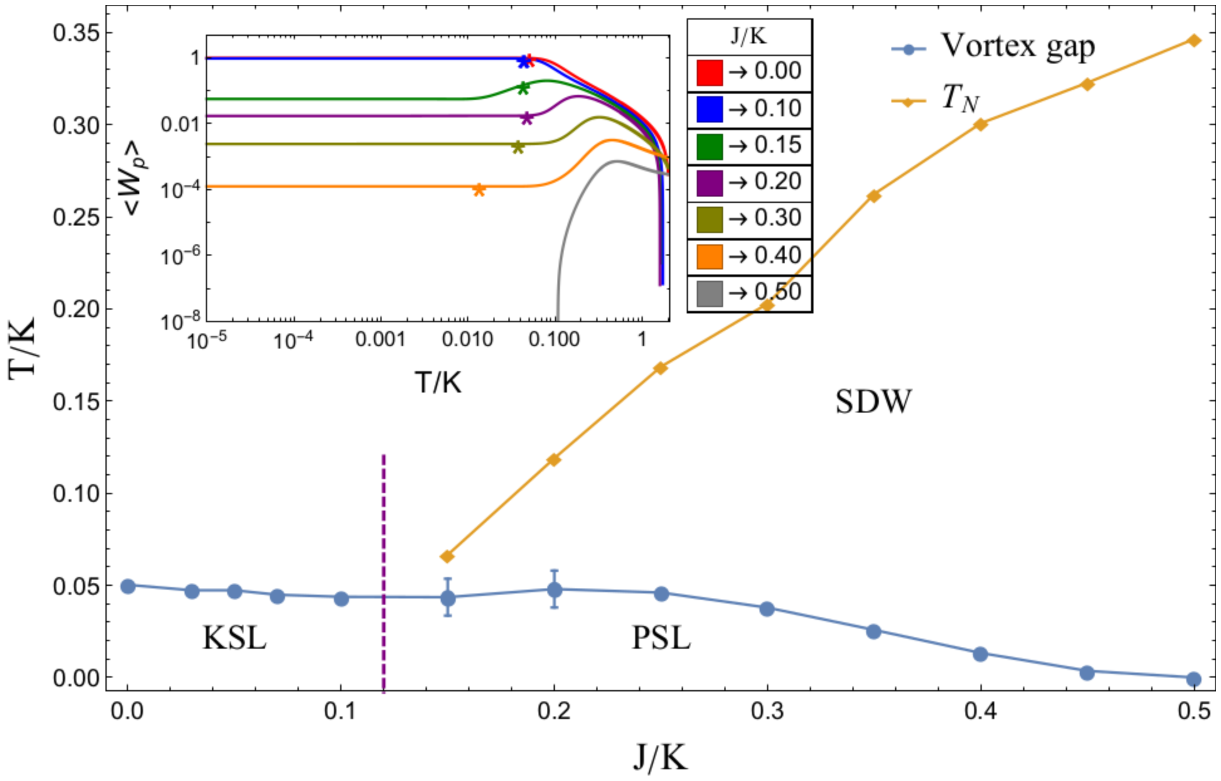
Concomitant SDW order present in the fractal phase.

Low-lying Kitaev states are more robust against Heisenberg perturbation than higher ones.

Looking for Kitaev physics at higher energies not recommended.

Finite temperature phase diagram

Broadly agrees with energy density vs interaction phase diagram from MBL analysis.



Nonzero expectation of plaquette Wilson loop (Kitaev fluxes) and finite vortex gap suggests deconfinement in PSL phase at low temperatures. Higher temperatures – more like SDW. Above T_N – no magnetic order.

Conclusions

We studied the stability of Kitaev quasiparticles in the presence of a perturbing Heisenberg interaction as a Fock space localization phenomenon.

We identified parameter regimes where Kitaev states are localized, fractal or delocalized in the Fock space of exact eigenstates. Delocalization implies quasiparticle instability.

Our finite temperature calculations show that a vison gap, and a nonzero plaquette Wilson loop at low temperatures, both characteristic of the deconfined Kitaev spin liquid phase, persist far into the neighboring proximate spin liquid phase that has a concomitant stripy spin-density wave order.

Kitaev quasiparticle excitations are stable for low-energy states over a signicant parameter range in the stripy phase.