UNIVERSITY OF CAMBRIDGE

TCM

CAVENDISH LABORATORY

Dynamic structure factor of a 2D quantum spin liquid

Dima Kovrizhin

TCM, Cavendish Laboratory

Collaboration

Johannes Knolle, Roderich Moessner (MPIPKS)

John Chalker (Oxford University)

Phys. Rev. Lett. 112, 207203

Selected for a Viewpoint in *Physics*

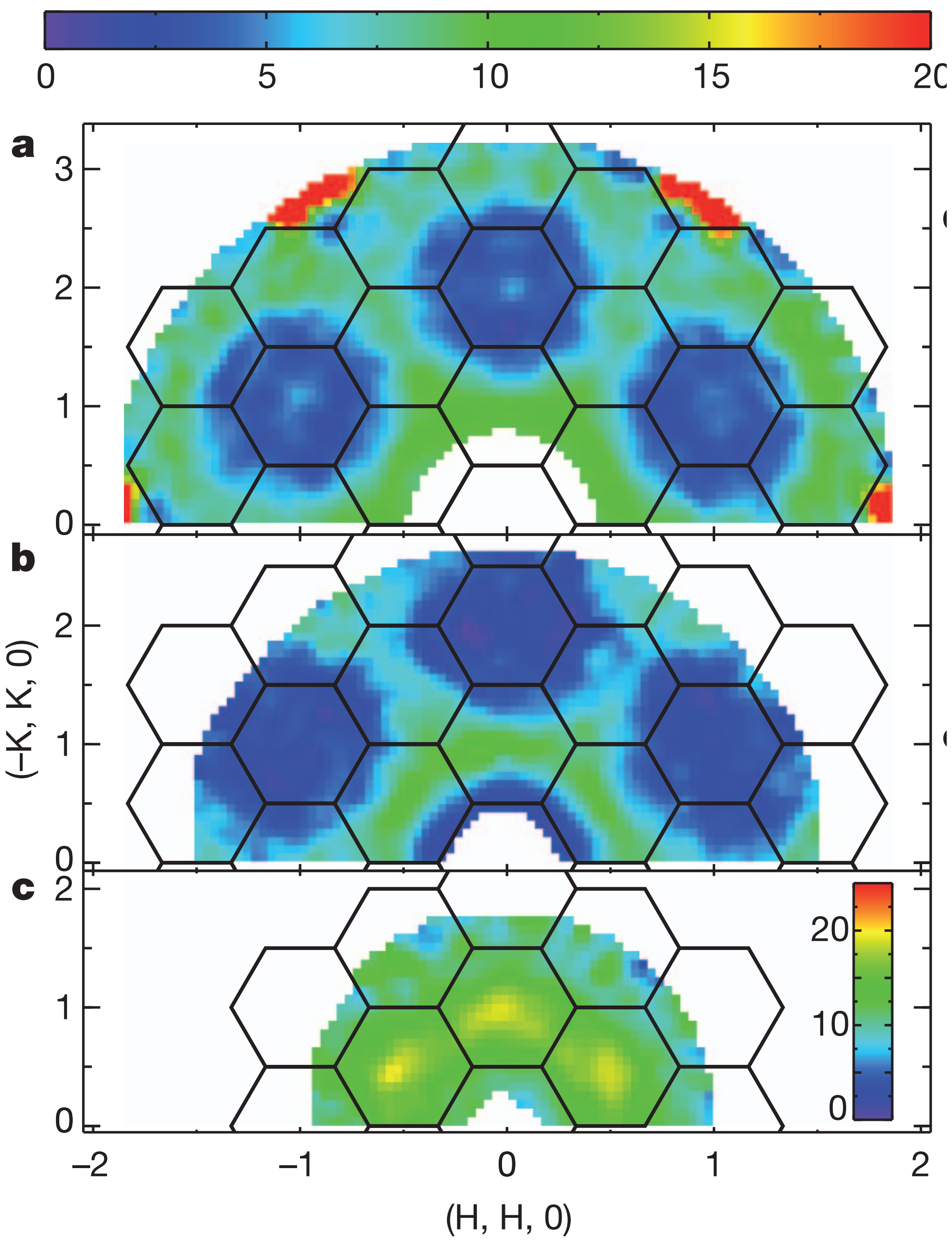
see a viewpoint by Alexei Tsvelik

HFM 2014, July 10, 2014

Dynamic structure factor of a 2D QSL - experiment

Observation of spin-excitation continuum — c.f. with sharp dispersive features for spin-waves

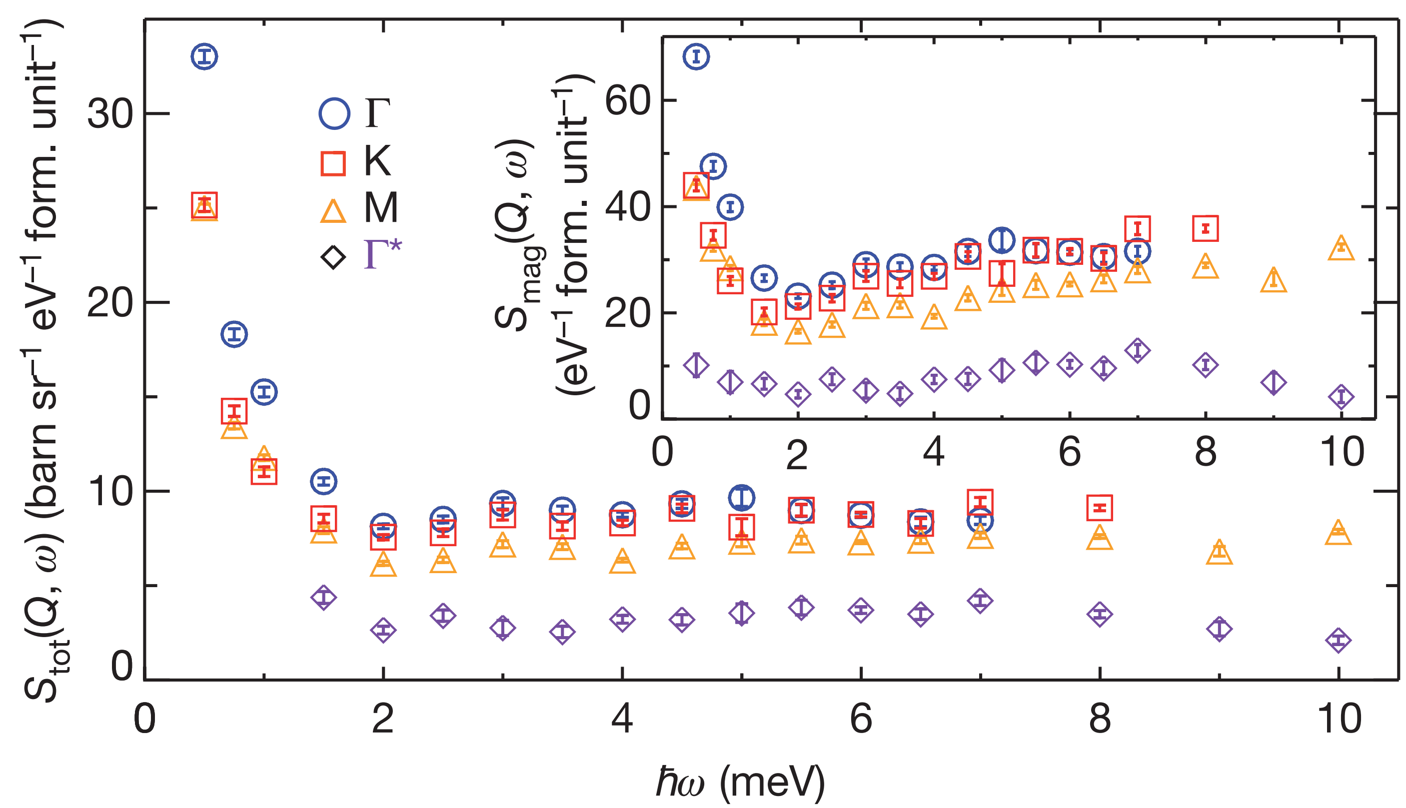
Interpretation in terms of fractionalization of spin degrees of freedom



Dynamic structure factor at fixed energies

ZnCu3(OD)6Cl2

(herbertsmithite)



Integrated dynamic structure factor

T. Han, J. Helton, S. Chu, D. Nocera, J. Rodriguez-Rivera, Collin Broholm & Y. Lee, Nature 492, 406 (2012)

Outline

- How one can test in experiment if one has a quantum spin-liquid ?

  Shortage of experimental signatures due to lack of local order
  Exotic quasiparticles do not couple directly to experimental probes

- What are the signatures of emergent (fractionalised) excitations in e.g. inelastic neutron scattering experiments ?

- Kitaev model as a toy-model of a quantum spin liquid

- Exact dynamic structure factor for an interacting 2D system

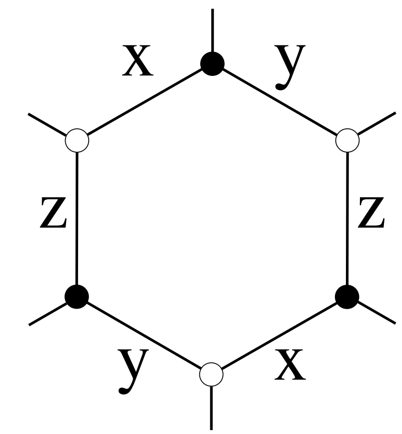
- Interesting connections to quantum quenches

see a related work by Matthias Punk, Debanjan Chowdhury and Subir Sachdev, Nature Physics 10, 289 (2014)

Kitaev model

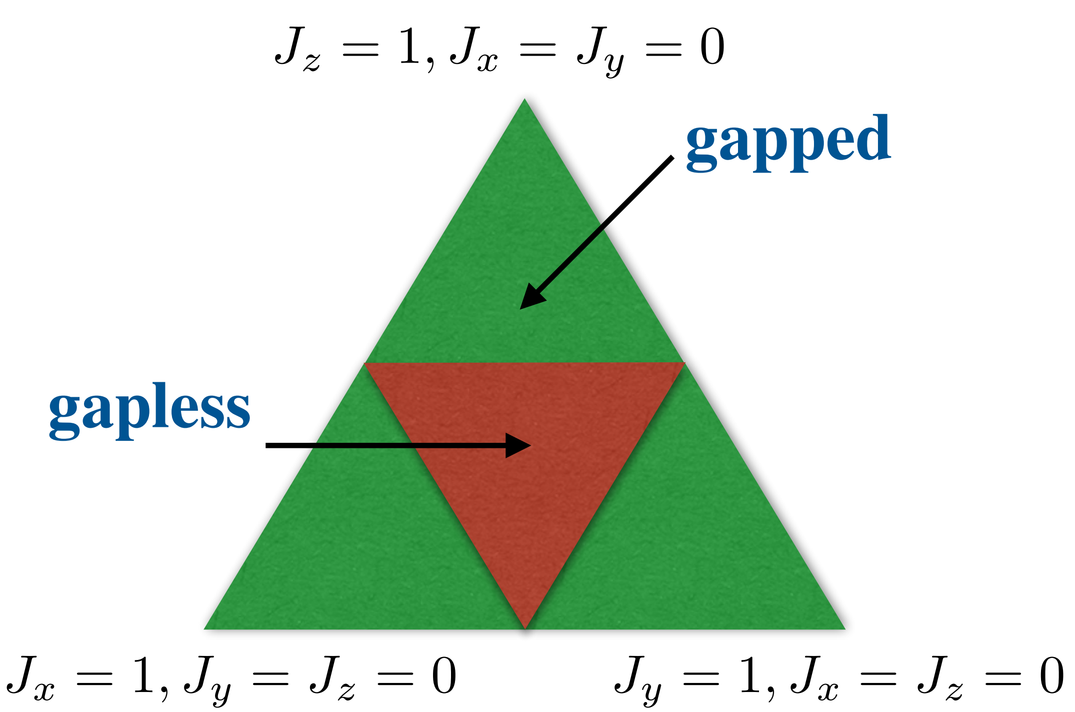
Ising-like Hamiltonian with anisotropic exchange on a honeycomb lattice

$$\hat{H} = -J_x \sum_{\mathrm{x-links}} \hat{\sigma}_j^x \hat{\sigma}_k^x - J_y \sum_{\mathrm{y-links}} \hat{\sigma}_j^y \hat{\sigma}_k^y - J_z \sum_{\mathrm{z-links}} \hat{\sigma}_j^z \hat{\sigma}_k^z$$



A. Kitaev, Ann. Phys. (2006)

Two spin-liquid phases: gapped and gapless

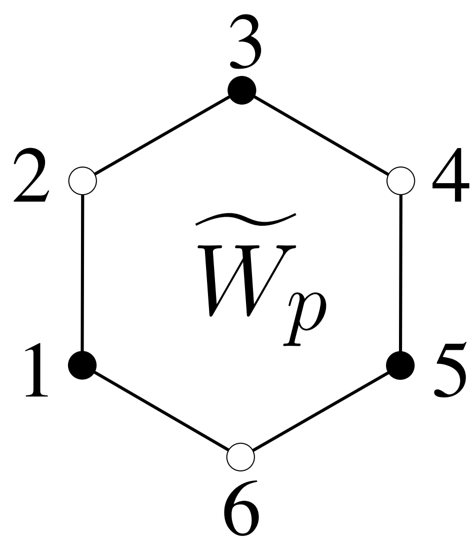


Possible realization in cold atoms and magnetic materials ?

Duan, Demler, Lukin PRL (2003) in cold atoms, Jackeli, Khaliullin PRL (2009, 2010) in Iridates

Kitaev model. Exact solution

Many conserved quantities - local flux operators



$$\tilde{W}_p = \hat{\sigma}_1^x \hat{\sigma}_2^y \hat{\sigma}_3^z \hat{\sigma}_4^x \hat{\sigma}_5^y \hat{\sigma}_6^z$$ **Flux operators**

$[\tilde{W}_p, \hat{H}] = 0$ **and** $[\tilde{W}_p, \tilde{W}_p'] = 0$

$\tilde{W}_p^2 = 1$

The Hilbert space can be separated into sectors $\mathcal{L}_{\{\tilde{W}_p\}}$ **corresponding to eigenvalues** $W_p = \pm 1$

Z_2 - flux sectors

We have *2N* sites and *N* plaquettes, so that Hilbert space dimension within one flux sector is $2^{2N}/2^N \sim 2^N$

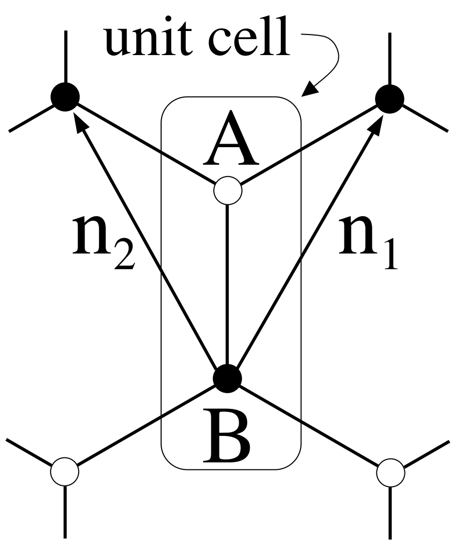
Significant reduction of the Hilbert space dimension

Still need to diagonalize the Hamiltonian in the reduced space

Kitaev model. Exact solution

Introduce Majorana fermions $\hat{c}_{2j-1},\ \hat{c}_{2j}$ living on A, B sublattice

which represent the “real” and “imaginary” part of a complex fermion



$$\hat{c}_{2j} = \hat{a}_j + \hat{a}_j^\dagger, \quad \hat{c}_{2j-1} = i(\hat{a}_j^\dagger - \hat{a}_j)$$

Majorana and complex fermions have the following properties

$$\hat{c}_j^2 = 1,\ \hat{c}_j\hat{c}_k = -\hat{c}_k\hat{c}_j,\ j \neq k \qquad \{\hat{a}_j, \hat{a}_k^\dagger\} = \delta_{jk},\ \{\hat{a}_j, \hat{a}_k\} = 0$$

For a complex fermion we can define a vacuum state such that

$$\hat{a}_j|0\rangle = 0$$

(this is not possible for a Majorana fermion, so we use complex fermions in the calculations)

$$\hat{\sigma}_j^\alpha = i\hat{b}_j^\alpha \hat{c}_j$$

spin operators

here we introduced another 3 Majorana fermions per site $\hat{b}_j^\alpha$ which change fluxes

Kitaev model. Exact solution

Now we can write the Kitaev Hamiltonian in terms of Majorana fermions

for example, consider the term

$$-J_x\hat{\sigma}_j^x\sigma_k^x = -J_x i\hat{b}_j^x c_j i\hat{b}_k^x\hat{c}_k = J_x(i\hat{b}_j^x\hat{b}_k^x)i\hat{c}_j\hat{c}_k = iJ_x\hat{u}_{\langle jk\rangle_x}\hat{c}_j\hat{c}_k$$

bond operators $\hat{u}_{\langle jk\rangle_\alpha} = i\hat{b}_j^\alpha\hat{b}_k^\alpha$

the Hamiltonian in terms of fluxes and Majorana fermions

$$\hat{H} = \sum_{j\in A,k\in B,\langle jk\rangle} iJ_{\alpha_{jk}}\hat{u}_{\langle jk\rangle_\alpha}\hat{c}_j\hat{c}_k$$

Bond operators commute with each other and with the Hamiltonian

moreover $\hat{u}^2_{\langle jk\rangle} = 1$ and we can block-diagonalize into sectors $u_{\langle jk\rangle} = \pm 1$

In each flux sector we obtain a quadratic Majorana fermion Hamiltonian

Kitaev model. Exact solution

Introduce two complex fermions by combining Majorana on the links

$$\hat{\chi}_{\mathbf{r}}^{\alpha} = \frac{1}{2}(\hat{b}_j^{\alpha_{jk}} + i\hat{b}_k^{\alpha_{jk}}) \qquad \hat{f}_{\mathbf{r}} = \frac{1}{2}(\hat{c}_{A,\mathbf{r}} + i\hat{c}_{B,\mathbf{r}})$$

The gauge field operators can now be written in terms of bond fermions

$$\hat{u}_{\langle jk \rangle_\alpha} = i\hat{b}_j^{\alpha}\hat{b}_k^{\alpha} = 2\hat{\chi}_{\mathbf{r}}^{\alpha\dagger}\hat{\chi}_{\mathbf{r}}^{\alpha} - 1$$

The eigenstates of the Hamiltonian can be written as a direct product

$$|\Phi\rangle = |\chi\rangle \otimes |f\rangle$$

flux sector   matter sector

In the ground state there is 1 bond fermion on each bond $u_{\langle ij \rangle_\alpha} = 1$

The Hamiltonian is quadratic in terms of matter fermions

Kitaev model. Exact solution

The Hamiltonian can be written in a diagonal form

$$\hat{H}_f = \sum_q |S(\mathbf{q})|(2\hat{a}^\dagger_\mathbf{q}\hat{a}_\mathbf{q} - 1)$$

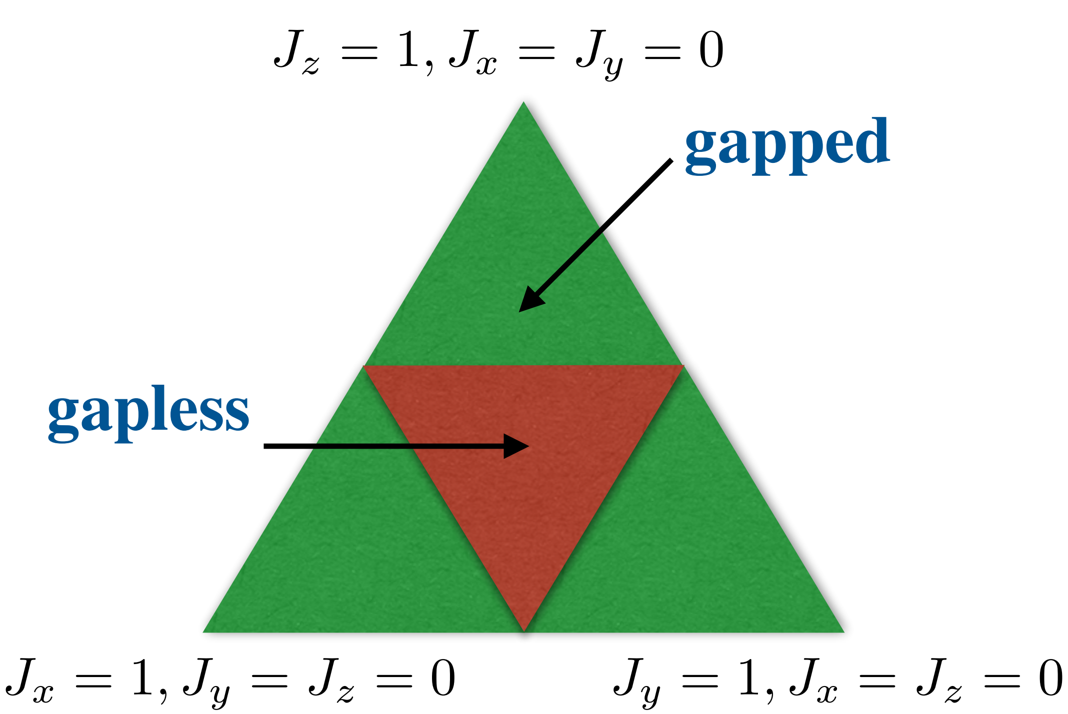
where

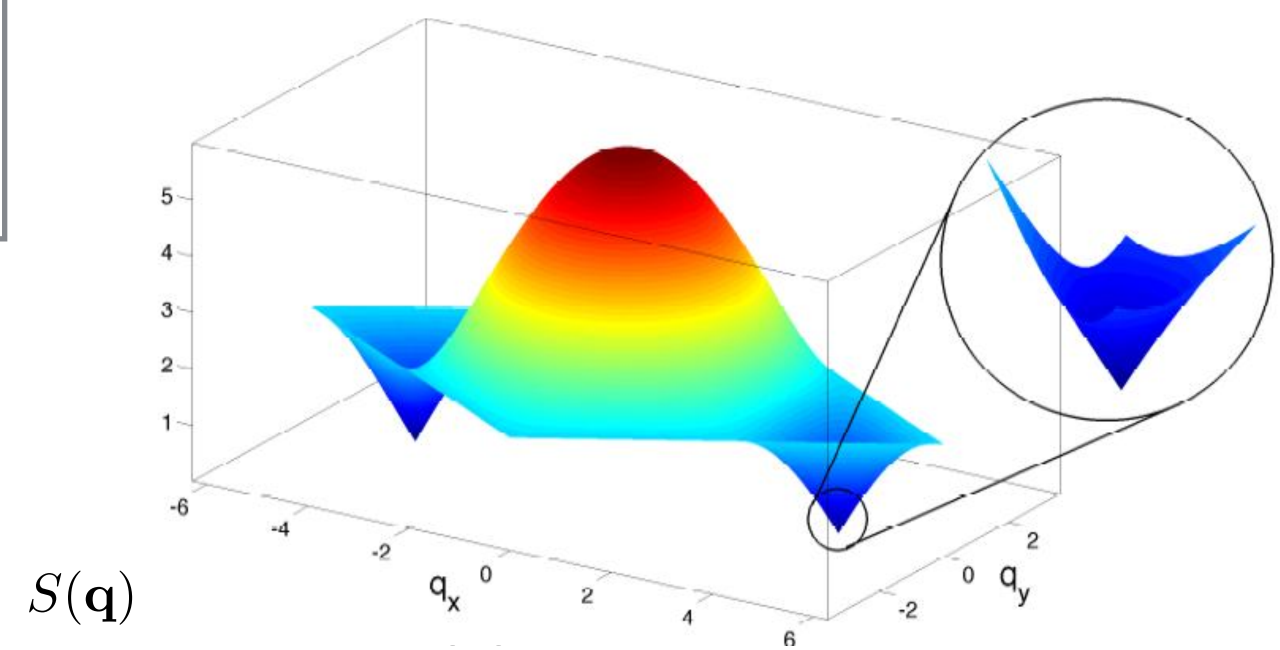
$$S(\mathbf{q}) = J_x e^{i\mathbf{q}\mathbf{n}_1} + J_y e^{i\mathbf{q}\mathbf{n}_2} + J_z$$

in the ground state $\hat{a}_\mathbf{q}|0\rangle = 0$

flux excitations are gapped

matter excitations are gapped or gapless





matter excitation spectrum in the gapless phase

Dynamic structure factor

In an inelastic neutron scattering experiment one measures a Fourier transform of a dynamic spin correlation function

$$S_{ij}^{ab}(t) = \langle 0|\hat{\sigma}_i^a(t)\hat{\sigma}_j^b(0)|0\rangle$$

Our task is to calculate this function

on sublattice A: $\hat{\sigma}_i^\alpha = i\hat{c}_i(\hat{\chi}_{\langle ij\rangle_\alpha} + \hat{\chi}^\dagger_{\langle ij\rangle_\alpha})$

on sublattice B: $\hat{\sigma}_j^\alpha = \hat{c}_j(\hat{\chi}_{\langle ij\rangle_\alpha} - \hat{\chi}^\dagger_{\langle ij\rangle_\alpha})$

$$\langle 0|\hat{\chi}_a^\dagger\hat{\chi}_b|0\rangle = \delta_{ab}$$

Fluxes are static -> N.N. correlations only!

Representation in terms of Majorana fermions

$$S_{ij}^{ab}(t) = -i\langle 0|e^{i\hat{H}_0 t}\hat{c}_i e^{-i(\hat{H}_0+V_a)t}\hat{c}_j|0\rangle\delta_{ab}\delta_{(ij)_{NN}}$$

here $\hat{V}_a = -J_a 2i\hat{c}_i\hat{c}_j$ is a <u>local potential</u>

Note that all correlators beyond nearest neighbour are zero

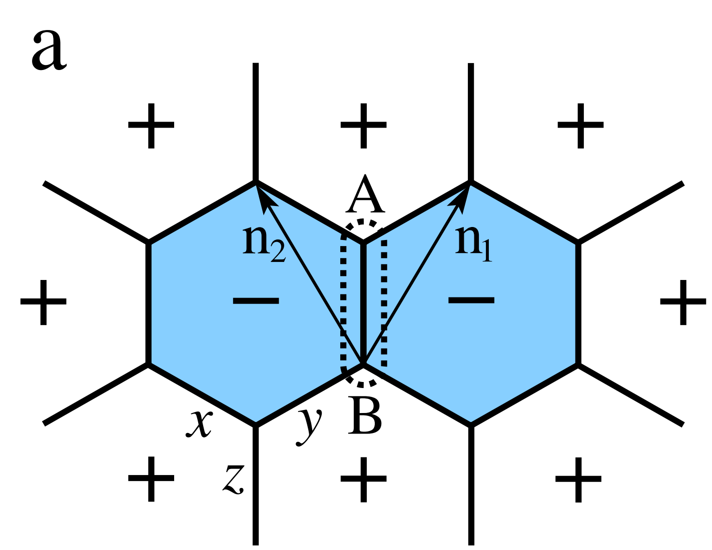
Baskaran et.al, PRL (2007)

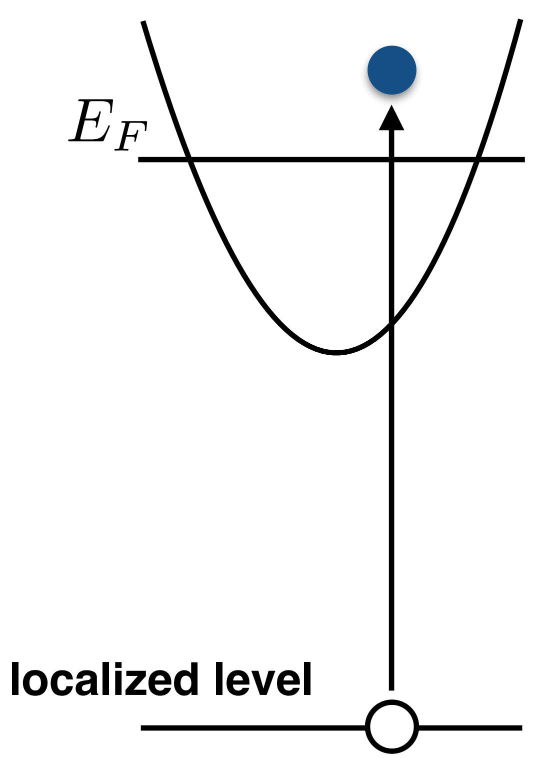
Local quantum quench, X-ray edge problem

Spin-flip in the INS measurement fractionalizes into two fluxes and a Majorana fermion

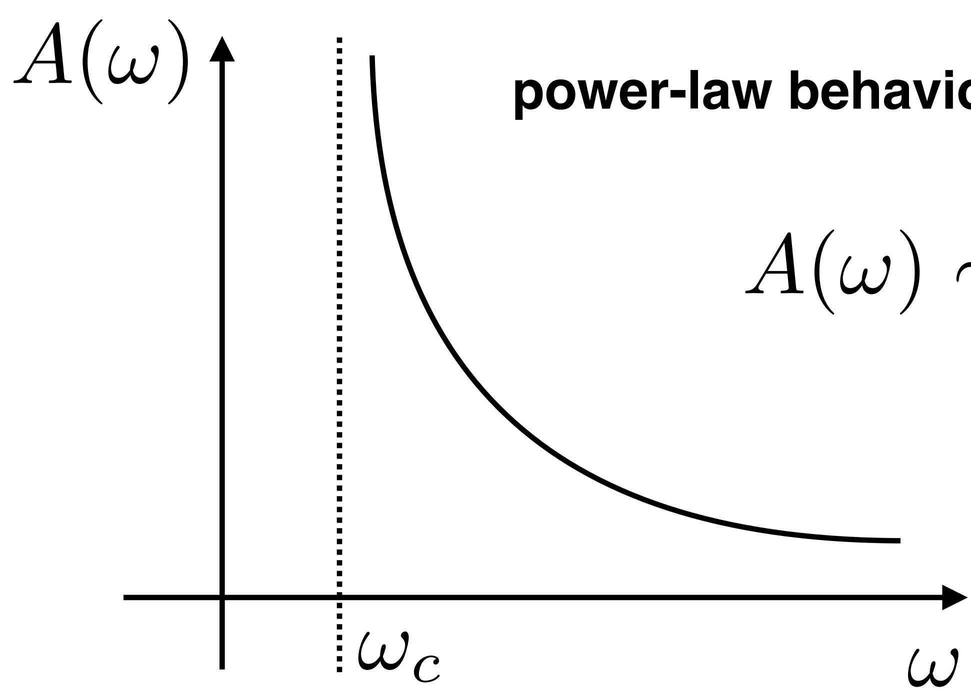
This leads to an abrupt change of a local potential for a Majorana fermion - similar to X-ray edge problem

Singularities in X-ray absorption spectrum





X-ray edge problem



power-law behaviour due to soft excitations

$$A(\omega) \sim (\omega - \omega_c)^{\gamma}$$

Anderson orthogonality catastrophe Phys. Rev. Lett. 18, 1049 (1967)

Lehmann representation

Qualitative features of the dynamic response can be read-off from the Lehmann representation

$$S_{ij}^{ab}(\omega) = -i \sum_{\lambda} \langle M_0|\hat{c}_i|\lambda\rangle\langle\lambda|\hat{c}_j|M_0\rangle \times \delta(\omega - (E_\lambda - E_0))\delta_{ij}\delta_{ab}$$

states with two extra fluxes

Response is gapped due to the flux-gap $\Delta = E_{\lambda_0} - E_0$

$J_x = J_y = J_z,\ \Delta \sim 0.26J$

Above the flux gap the response reflects the nature of the matter fermion ground state

$\hat{H}$ conserves fermion parity $\langle M_0|\hat{c}_i|\lambda\rangle$ changes parity

There are two possibilities depending on the parity of the ground state !

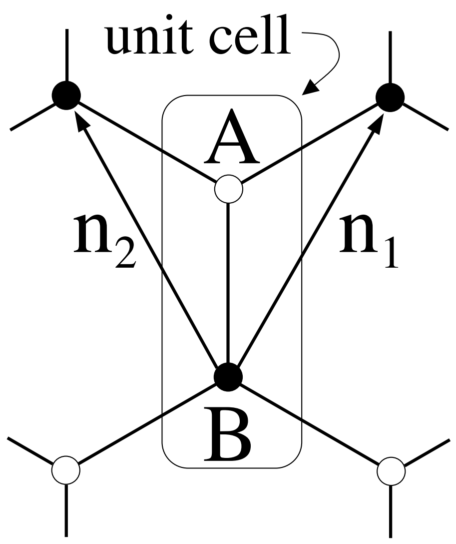
Dynamical phase diagram

(I) If the ground states with and without flux have **different parity**
the first contribution to the response starts with $\langle M_0|\hat{c}_i|\lambda_0\rangle$

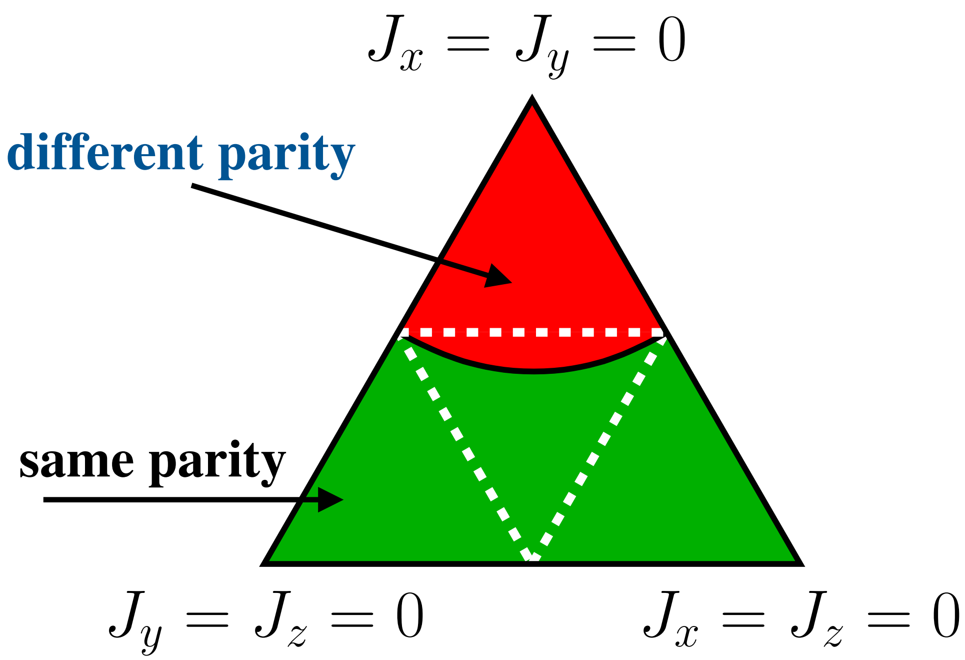
$$S^{(0)}(\omega) \sim \delta(\omega - \Delta)$$ **+ two-particle response**

(II) If the ground states $|M_0\rangle$ and $|\lambda_0\rangle$ have the **same parity**
the first contribution to the response starts with $\langle M_0|\hat{c}_i|\lambda_0 \text{ and } 1 \text{ exc.}\rangle$

single particle response, no delta-function



qualitatively, deep in the gapped phase
the flipped flux binds one fermion on the
A-B bond -> change of parity



new dynamical phase diagram !

Single-particle response

$$S_{ij}^{ab}(\omega) = -i \sum_{\lambda} \langle M_0 | \hat{c}_i | \lambda \rangle \langle \lambda | \hat{c}_j | M_0 \rangle \times \delta(\omega - (E_\lambda - E_0)) \delta_{ij} \delta_{ab}$$

we are interested in the response in the green region of the phase diagram

note that $|M_0\rangle$ **is the vacuum of** $\hat{a}$ **operators**

the Hamiltonian $\hat{H} = \hat{H}_0 + \hat{V}_a$ **is quadratic, diag. via Bogoliubov transf.**

$$\hat{b}_\lambda = \sum_{\mathbf{q}} X^*_{\lambda \mathbf{q}} \hat{a}_{\mathbf{q}} + Y^*_{\lambda \mathbf{q}} \hat{a}^\dagger_{\mathbf{q}}$$

single particle states are given by $|\lambda\rangle = \hat{b}^\dagger_\lambda |\lambda_0\rangle$

two-flux ground state $|\lambda_0\rangle = [X^\dagger X]^{\frac{1}{4}} e^{-\frac{1}{2} \hat{\mathbf{a}}^\dagger X^{*-1} Y^* \hat{\mathbf{a}}^\dagger}$

for example the overlap between two g.s. $|\langle \lambda_0 | M_0 \rangle| = \sqrt{|\mathrm{det} X|}$

expansion of the exponent terminates - exact 1 quasi-particle contribution

Mapping to X-ray edge problem

Let us look at the expression

$$S^{zz}_{A0B0} = -i\langle M_0 | e^{i\hat{H}_0 t} \hat{c}_{A0} e^{-i(\hat{H}_0 + \hat{V}_z)t} \hat{c}_{B0} | M_0 \rangle$$

this can be written as

$$S^{zz}_{ij} = -i\langle M_0 | \hat{c}_i(t) \hat{S}(t,0) \hat{c}_j(0) | M_0 \rangle$$

here

$$\hat{c}_i(t) = e^{i\hat{H}_0 t} \hat{c}_i e^{-i\hat{H}_0 t} \qquad \hat{V}_z(t) = -2iJ_z \hat{c}_i(t) \hat{c}_j(t)$$

and the S-matrix

$$\hat{S}(t,0) = e^{i\hat{H}_0 t} e^{-i(\hat{H}_0 + \hat{V}_z)t} = \mathrm{Texp}\{-i \int_0^t dt' \hat{V}_z(t')\}$$

now transform to complex fermions

Mapping to X-ray edge problem

A general form in terms of complex fermions is

$$\sim \langle M_0|(\hat{f}(t) \pm f_0^\dagger(t))\mathrm{Texp}\{-i\int_0^t dt'\hat{V}_z(t')\}(\hat{f}(0) \pm f_0^\dagger(0))|M_0\rangle$$

here $\hat{V}_z(t) = -4J_z[\hat{f}_0^\dagger(t)\hat{f}_0(t) - 1/2]$ is a local (on-site) potential

which is switched-on at time t=0

now we can use Wick theorem

note that one would expect anomalous terms in the expansion

however these terms vanish, e.g. $F_0 = -i\langle M_0|\mathrm{T}[\hat{f}(t)\hat{f}(t')]|M_0\rangle = 0$

$$S^{zz}(t) = i[G(t,0) \pm G(0,t)]$$

$$G(t,0) = -i\langle \mathrm{T}\hat{f}(t)\hat{f}^\dagger(t)e^{-i\int_0^t dt'\hat{V}_z(t')}|M_0\rangle$$

similar Green functions appear in the X-ray edge problem calculations

Mapping to X-ray edge problem

Expansion of the GF separates into connected and disconnected contributions

connected diagrams can be obtained from disconnected ones

need to solve a singular a singular integral equation

$$G_c(t,0) = G_0(t,0) - 4J_z \int_0^t dt' G_0(t,t') G_c(t',0)$$

Exact solution by Nozieres De Dominicis in the case $G_0(t) \sim \frac{1}{t}$

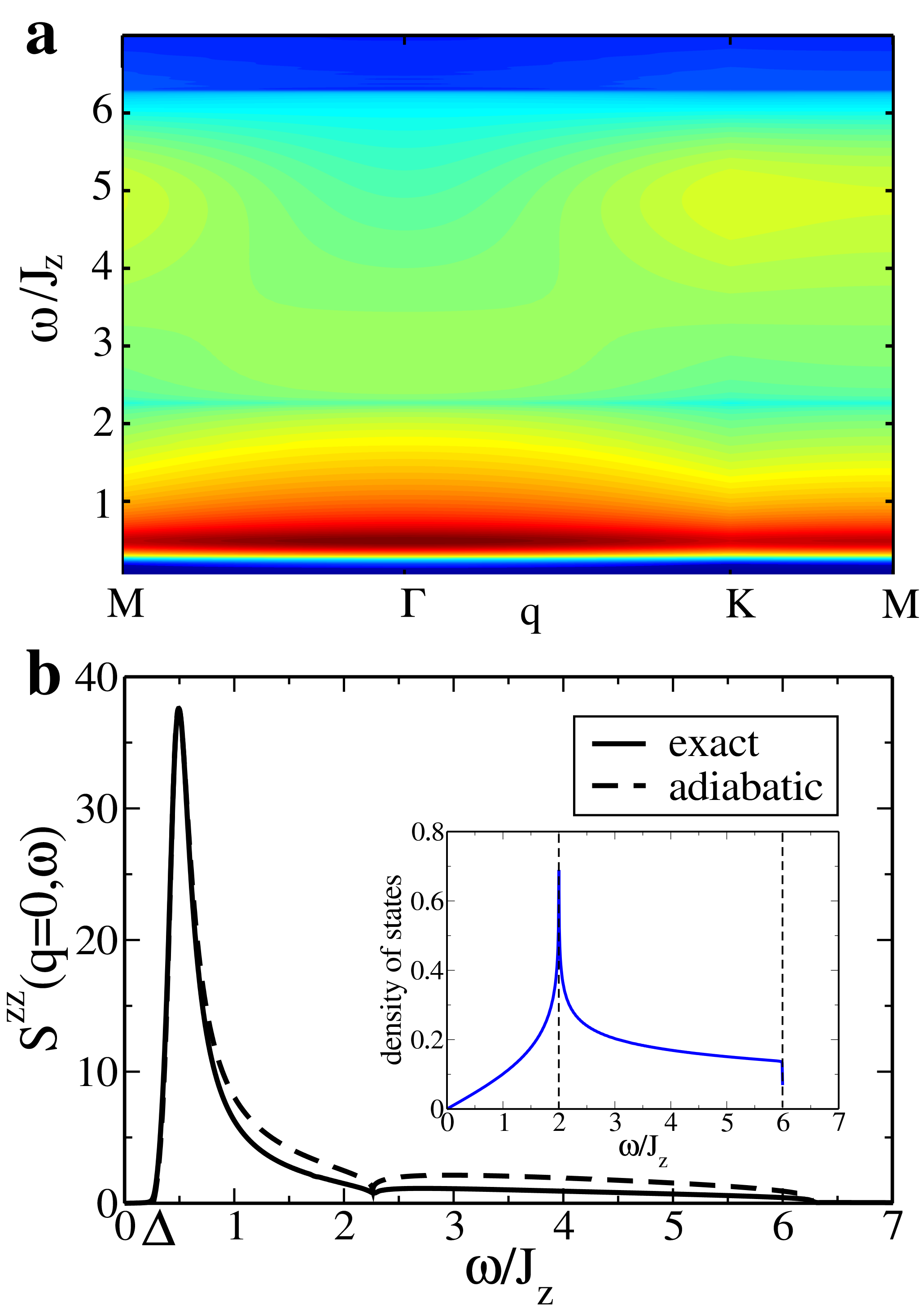
in our calculation (Kitaev model) the behaviour of the bare GF is complicated, and the asymptotics is of different form $G_0(t) \sim \frac{1}{t^2}$

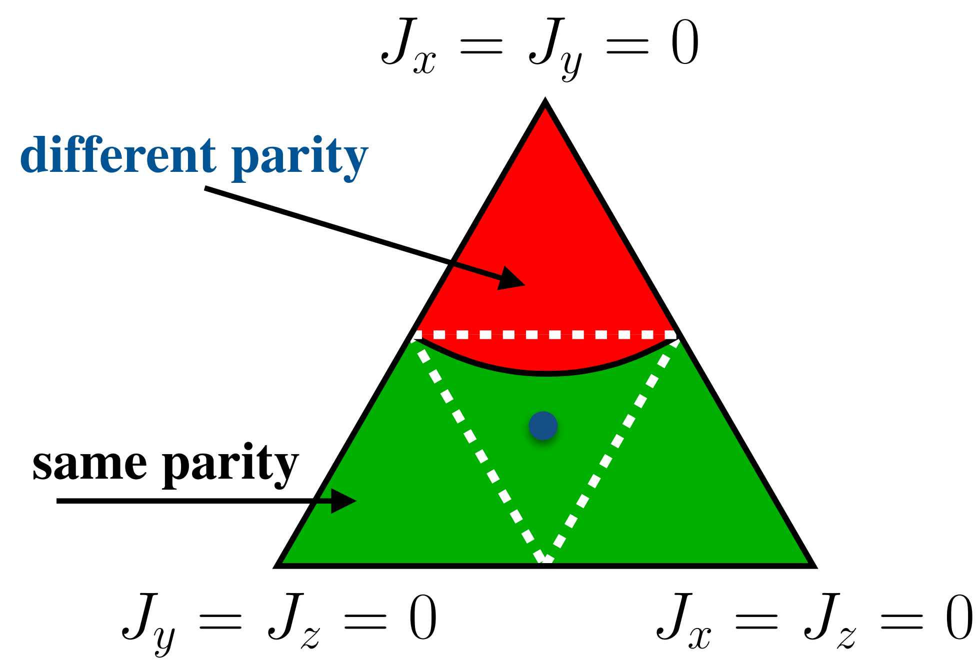
ND solution is not applicable, need to use general methods from the theory of singular integral equations, see a classic book by Mushkeleshvili

A simplified approach (with a potential switched on and off adiabatically) provides a good approximation in our case (compared to the X-ray edge)

Dynamic structure factor (green phase)

$$J_x = J_y = J_z = 1$$



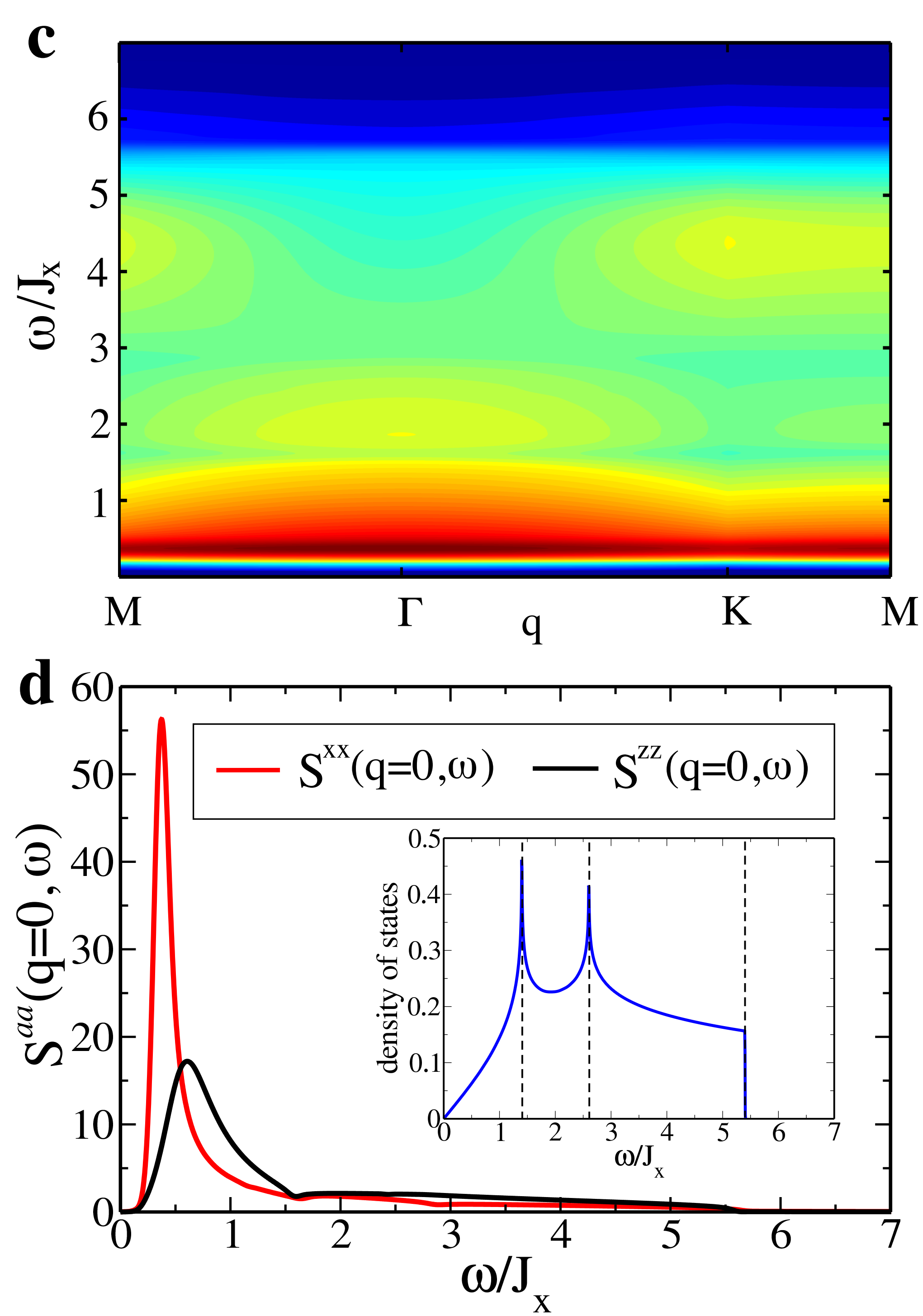


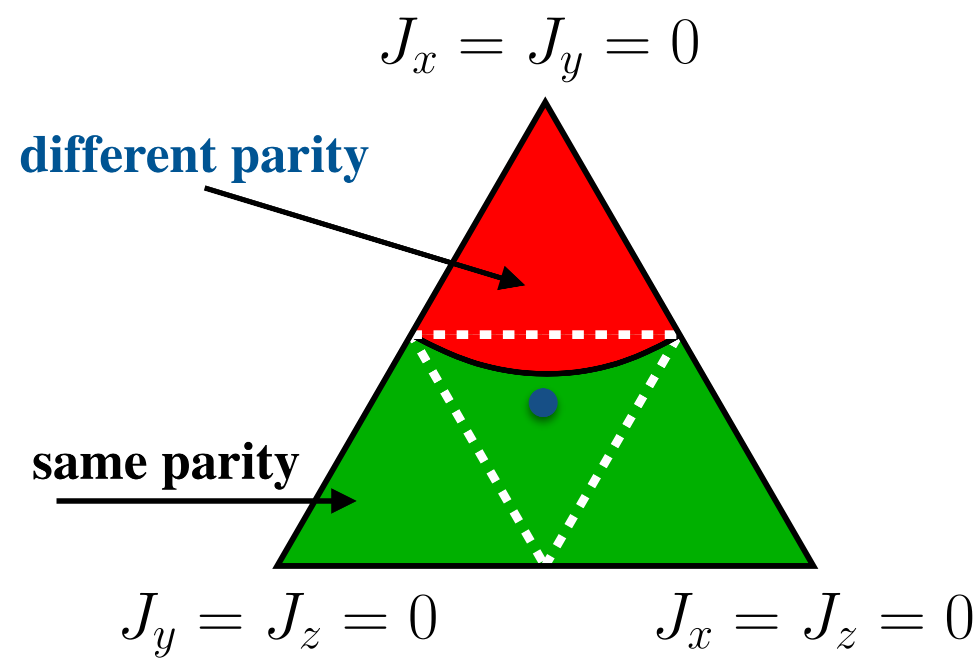
- Response is gapped - gap for gauge-flux
- Broad features
- Van-Hove singularities
- Band edge of matter fermions

many-particle contributions approx. 2.5%

Dynamic structure factor (green phase)

$$J_x = J_y, J_z = 0.70 J_x$$

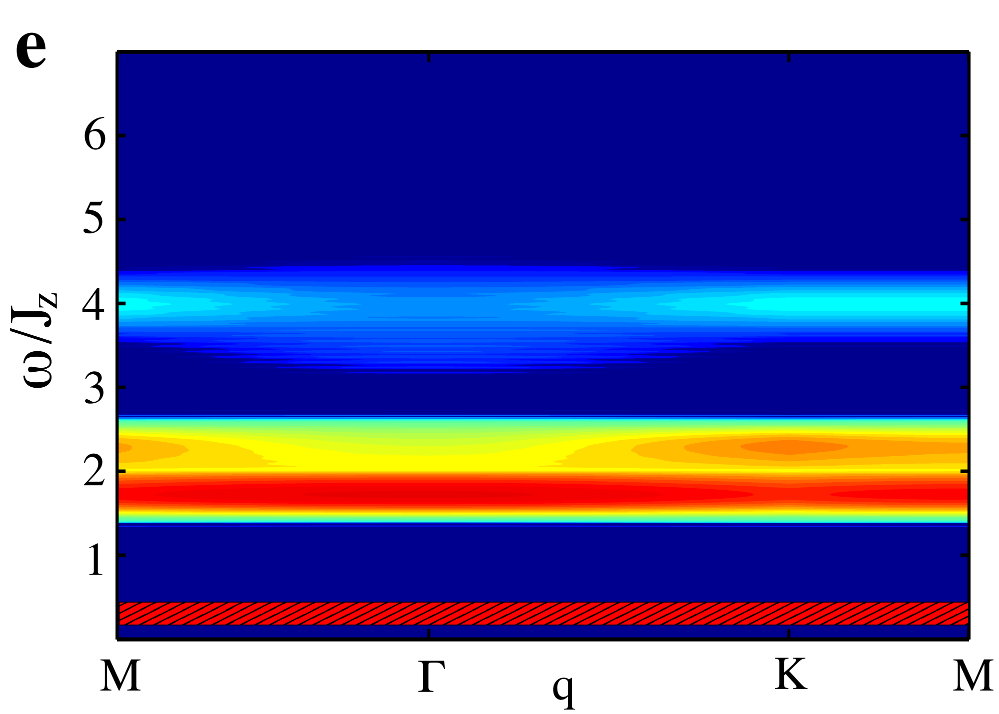


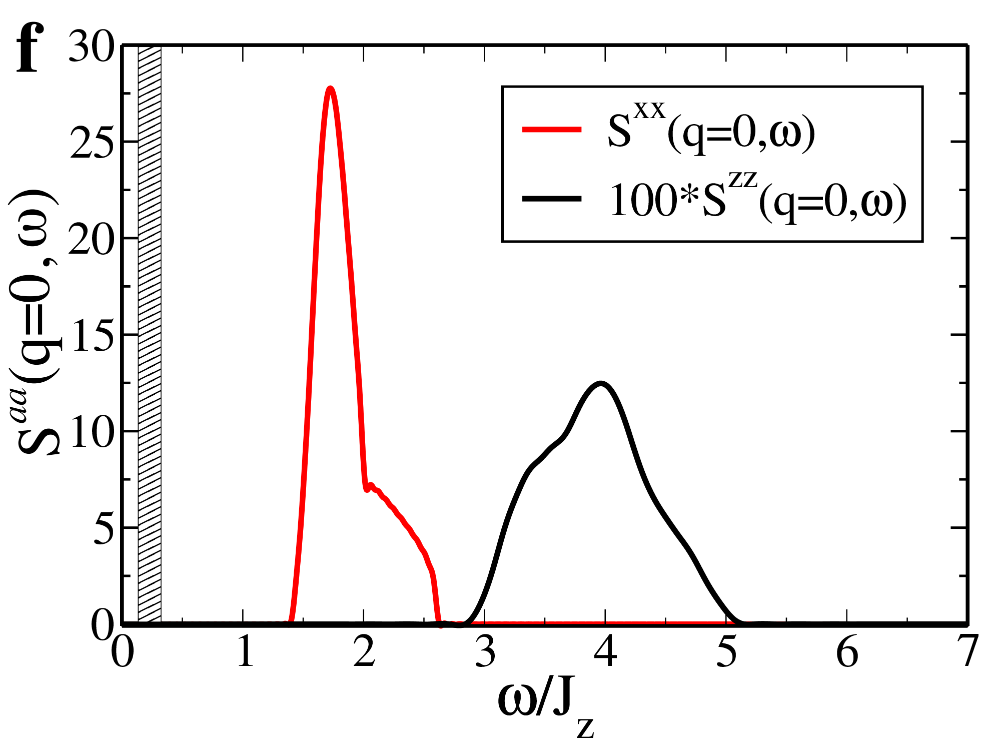


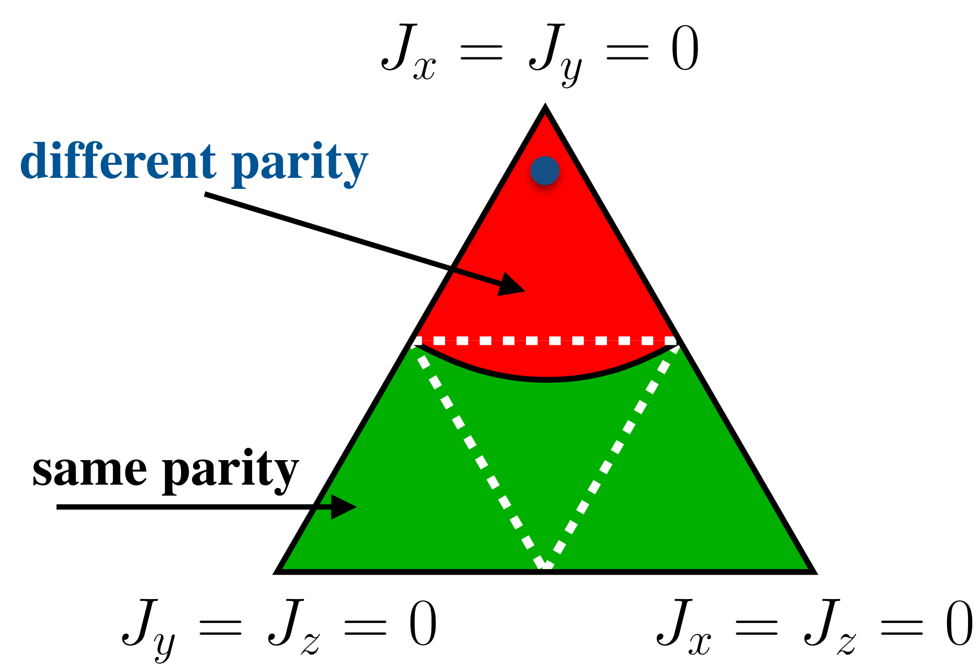
- Response is gapped - gap for gauge-flux
- Broad features
- Van-Hove singularities
- Band edge of matter fermions
- Anisotropic response

Dynamic structure factor (red phase)

$$J_x = J_y, J_z = 0.15 J_x$$







- Response is gapped - gap for gauge-flux
- Delta-function response above the flux gap
- Broad features
- Van-Hove singularities
- Band edge of matter fermions
- Anisotropic response

Sharp features in the response

Summary

- **Emergent quasiparticles show up as characteristic features in the dynamic structure factor**

  flux gap and the features of Majorana fermion spectrum

- **New dynamical phase diagram**

- **Sharp features in the response despite short-range correlations**

- **Response in the presence of magnetic field, disorder, Heisenberg pert.**

Raman response: J. Knolle, Gia-Wei Chern, D. L. Kovrizhin, R. Moessner, N. B. Perkins, arXiv:1406.3944