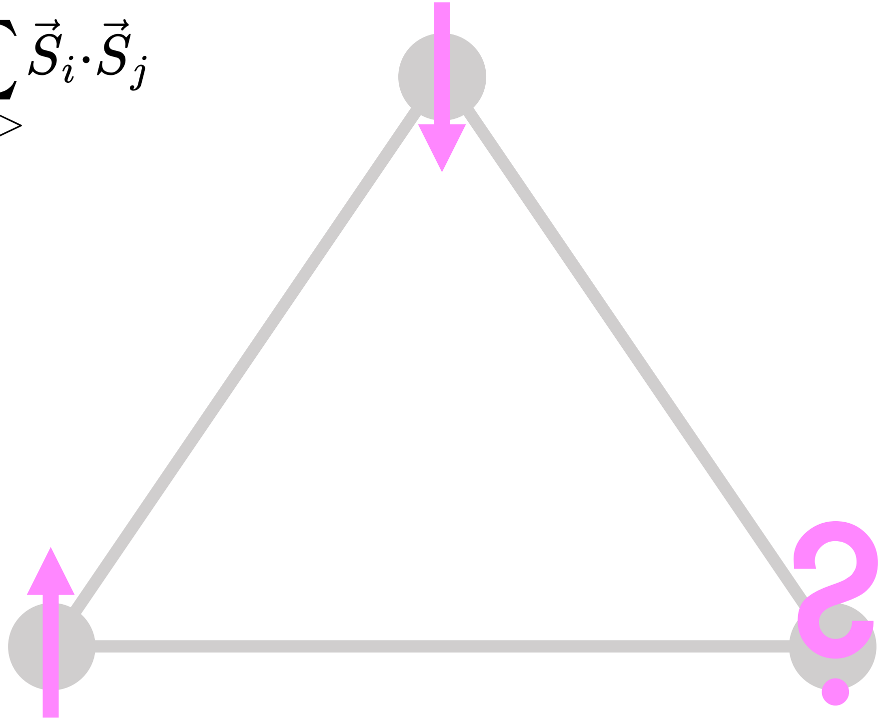
Cluster functional renormalization group approach to Quantum Spin Liquids

Nico Gneist
Institute for Theoretical Physics
University of Cologne
17.12.2019

QSL

Frustration

$$H = -J \sum_{<ij>} \vec{S}_i \cdot \vec{S}_j$$



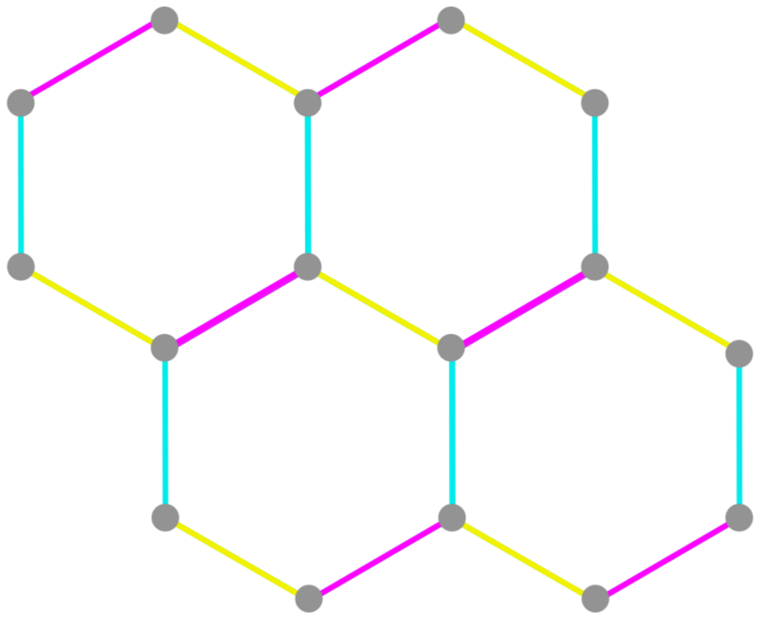
Magnetic frustration prevents magnetic order!

Kitaev model I

$$H = -J_x \sum_{\text{x-bonds}} S_i^x S_j^x - J_y \sum_{\text{y-bonds}} S_i^y S_j^y - J_z \sum_{\text{z-bonds}} S_i^z S_j^z$$

Topological frustration
→ no magnetic ground state

Analytical solution
→ introduces fractionalization



Kitaev model II

$$H = -J_x \sum_{\text{x-bonds}} S_i^x S_j^x - J_y \sum_{\text{y-bonds}} S_i^y S_j^y - J_z \sum_{\text{z-bonds}} S_i^z S_j^z$$

Decompose Spin into 4 Majoranas

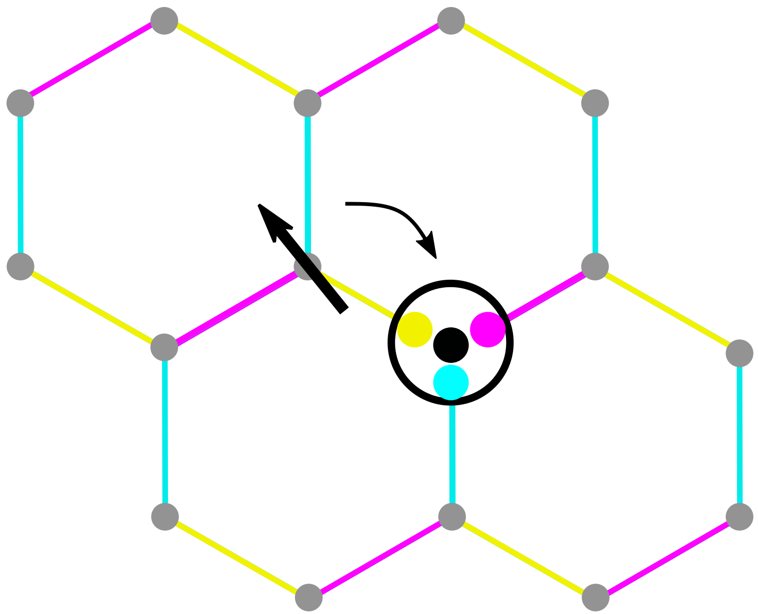
$$S_i^\alpha = i b_i^\alpha c_i \ \ ; \ \ \alpha = x, y, z$$

Majorana in condensed matter: real and imaginary part of fermion

$$c^\dagger = \frac{1}{2}(\eta + i\xi)$$
$$c = \frac{1}{2}(\eta - i\xi)$$

Enlargement of Hilbert space calls for local constraint

$$D_i = b_i^x b_i^y b_i^z c_i \ \ ; \ \ D_i|\psi\rangle = |\psi\rangle$$



Kitaev model III

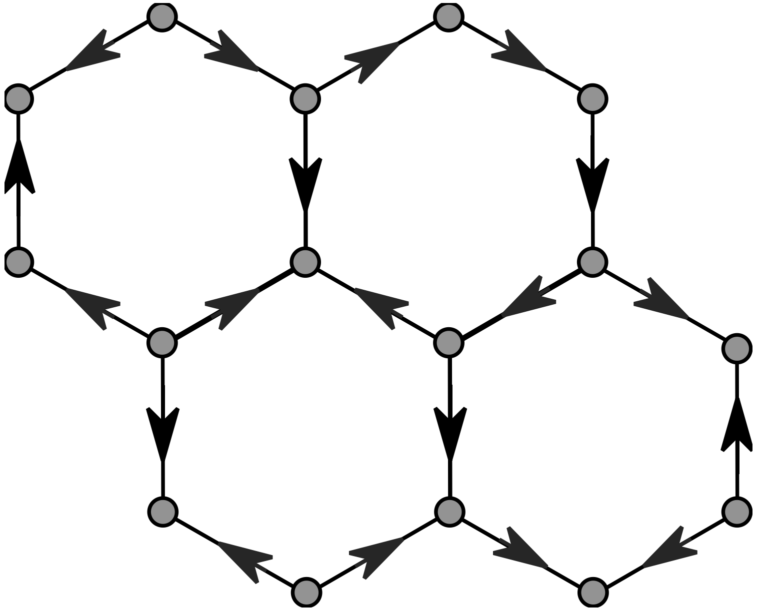
Recombine Majoranas to gauge fields

$$\hat{u}_{ij} = i b_i^{\alpha_{ij}} b_j^{\alpha_{ij}} \quad ; \quad u_{ij} = \pm 1$$

New Hamiltonian

$$H = \frac{i}{2} \sum_{\langle i,j \rangle} J_{ij} \hat{u}_{ij} \, c_i c_j$$

Find useful quantity to diagonalize Hamiltonian in a specific gauge sector



Kitaev model IV

Plaquettes operator:

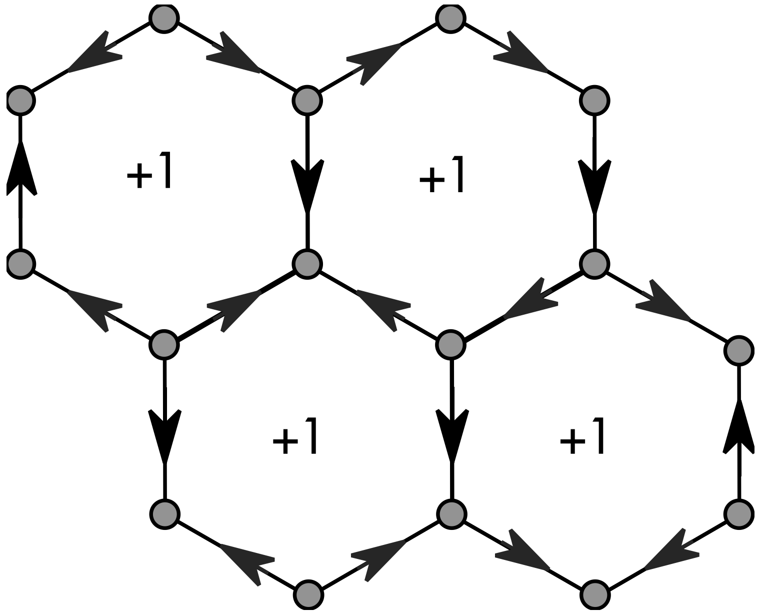
$$W_p = \prod_{\text{i,j of plaquette p}} u_{ij}$$

$$[H, W_p] = 0$$

Lieb theorem:
Ground state is in sector with all plaquettes +1 (or -1)

Solution

$$H = \frac{i}{2} \sum_{<ij>} J_{ij} u_{ij}\, c_i c_j$$



What are we searching for?

1. Spin system with non-magnetic but also non-trivial ground state

2. Fractionalization: new elementary excitations carry only fraction of the quantum number of former excitation

$$H_{\text{Spin}} \propto \sum_{ij} \vec{S}_i \cdot \vec{S}_j$$

Balents/Savary, Wen:
QSL is quadratic in
fractionalized d.o.f

$$H_{\text{QSL}} = \sum_{ij} \left[t_{ij}^{\alpha\beta} \sigma_{ij}^{z} f_{i\alpha}^{\dagger} f_{j\beta} + \Delta_{ij}^{\alpha\beta} \sigma_{ij}^{z} f_{i\alpha}^{\dagger} f_{j\beta}^{\dagger} + \text{h.c.} \right]$$

FRG

FRG I

How to get physics: path integral

$$Z[J] = \int D[\phi] e^{-S[\phi] + \int J\phi}$$

Or:

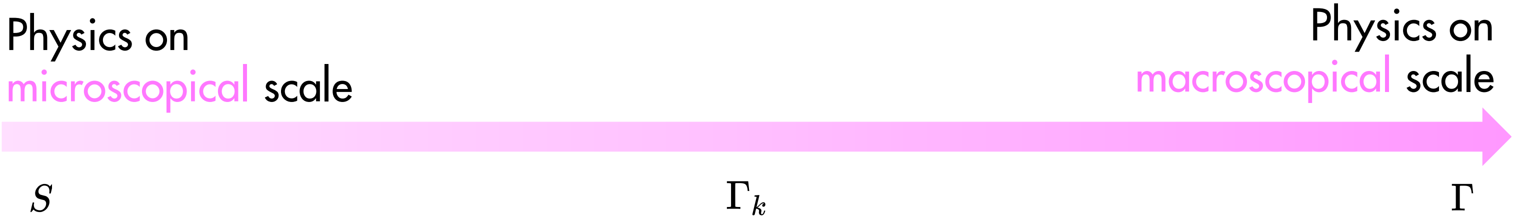
$$\Gamma[\bar{\phi}] = -\ln(Z[J]) + \int J\bar{\phi}$$

S : microscopic action

Γ : effective action (generator of 1PI diagrams)

Solving path integral usually not possible!

FRG II



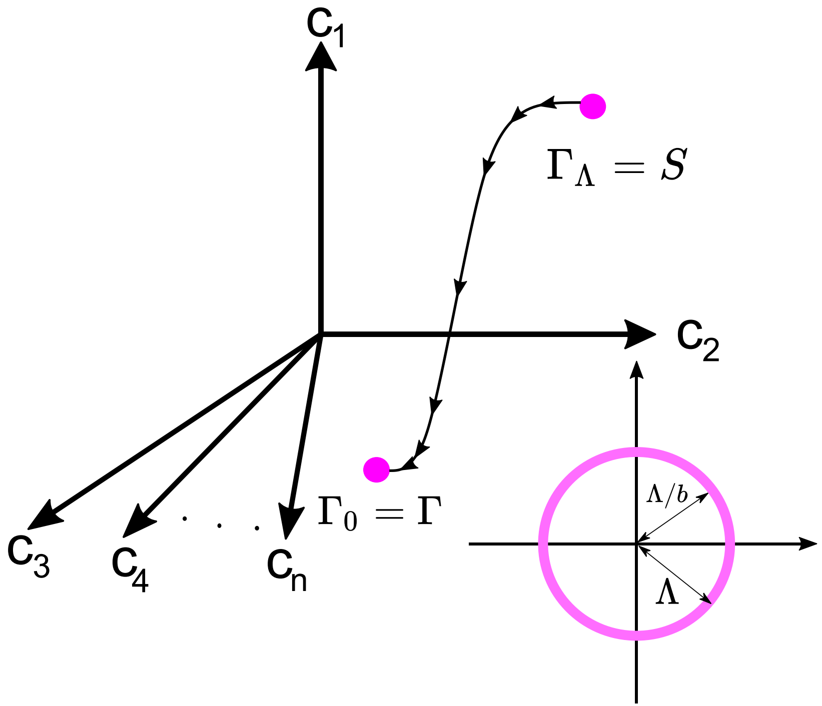
Γ_k : interpolates between scales!

$$\Gamma_{k\to\Lambda} = S \qquad \Gamma_{k\to 0} = \Gamma$$

$$\partial_k \Gamma_k = \frac{1}{2}\mathrm{STr}\left\{\partial_k R_k \left[\Gamma_k^{(2)} + R_k\right]^{-1}\right\}$$

(Wetterich, 1989)

Shell-integration corresponds to solving the flow equation



Pseudofermion ansatz

Reminder:
we want an effective description in fractionalized dofs!

$$H_{\text{Spin}} \propto \sum_{ij} \vec{S}_i \cdot \vec{S}_j \quad \overset{?}{\Longrightarrow} \quad H_{\text{QSL}} = \sum_{ij} \left[t_{ij}^{\alpha\beta} \sigma_{ij}^z f_{i\alpha}^\dagger f_{j\beta} + \Delta_{ij}^{\alpha\beta} \sigma_{ij}^z f_{i\alpha}^\dagger f_{j\beta}^\dagger + \text{h.c.} \right]$$

„Allow“ system directly to have fractionalized degrees of freedom:
use Abrikosov fermions directly for microscopic action and then use FRG

$$\vec{S}_i^{\alpha} = \frac{1}{2} f_{i\mu}^\dagger T_{\mu\nu} f_{i\nu}$$

$$H_{\text{Spin}} \to H_{\text{Fermions}} \quad \overset{\text{FRG}}{\Longrightarrow} \quad H_{\text{QSL}}$$

Does this sound familar?

Yes!

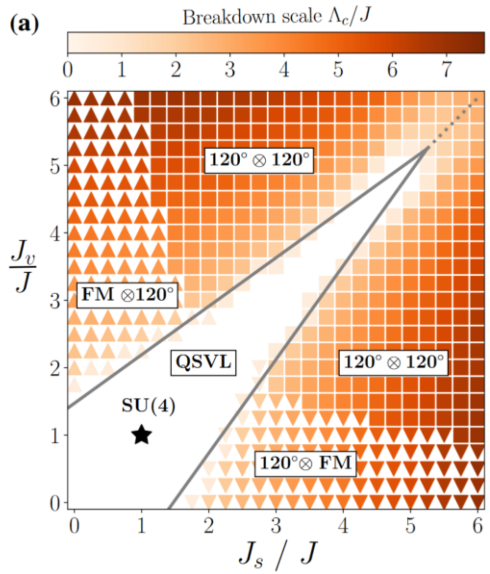
PF-FRG, a FRG method base on the same decomposition already exists!

Works well for determining phase boundaries

Applicable for large variety of spin systems

Works in 2D & 3D

Now: which QSL in the specified area?



SU(N) MODEL

SU(N) Heisenberg model

i. Decompose SU(N)-spin into fermions

$$H = -\frac{J}{N}\sum_{<ij>} \vec{S}_i \cdot \vec{S}_j \qquad \vec{S}_i^{\alpha} = \frac{1}{2} f^{\dagger}_{i\mu} T_{\mu\nu} f_{i\nu}$$

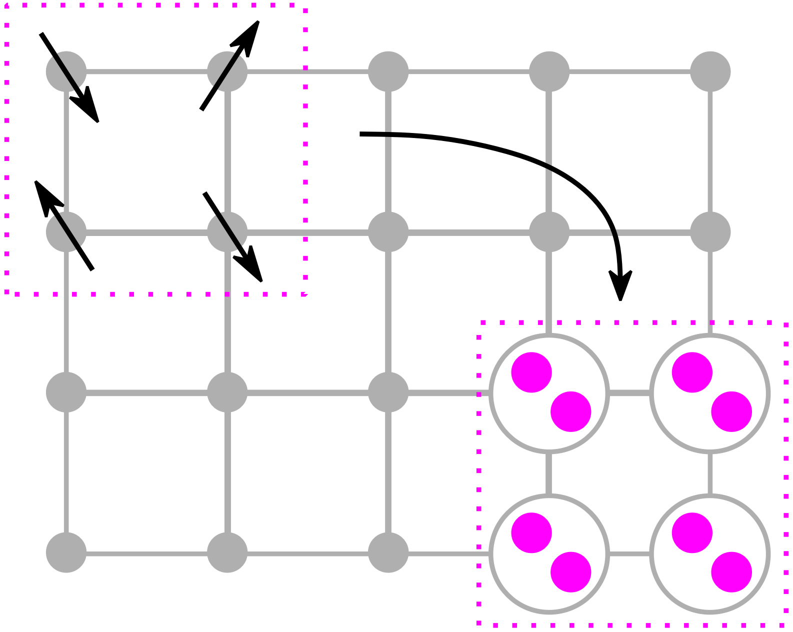
$$\to S[f] = \int_{\tau} \left\{ \sum_i f^{\dagger}_{i\alpha} \dot{f}_{i\alpha} - \frac{J}{N} \sum_{<ij>} f^{\dagger}_{i\alpha} f_{j\alpha} f^{\dagger}_{j\beta} f_{i\beta} \right\}$$

ii. Impose constraint

$$|\uparrow\rangle, |\downarrow\rangle \to |\cancel{0}\rangle, |\downarrow\rangle, |\uparrow\rangle, |\cancel{\uparrow\downarrow}\rangle$$

iii. Decouple via Hubbard-Stratonovich

$$Q_{ij} \propto f^{\dagger}_{j\alpha} f_{i\alpha}$$



Treat model in large N at first!

QSL Phases ($N \to \infty$)

iv.In large N, constraint not necessary
Ansatz: (Arovas, Auerbach 1988)

$$Q_{ij} = Qe^{i\theta}$$

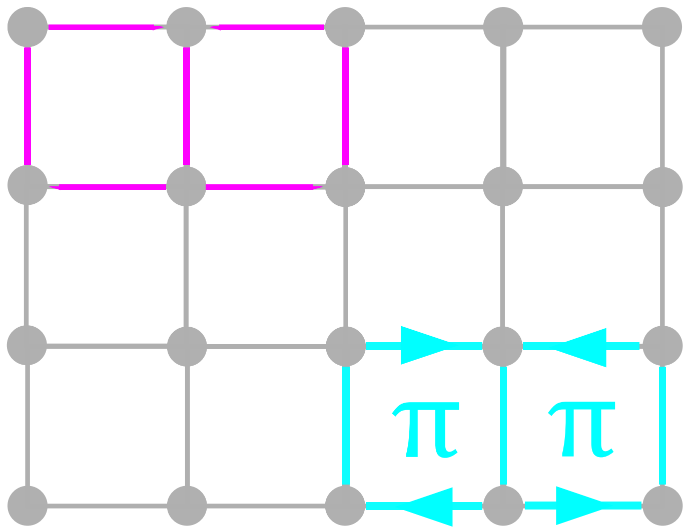
v. Two QSL phases in large N

BZA:

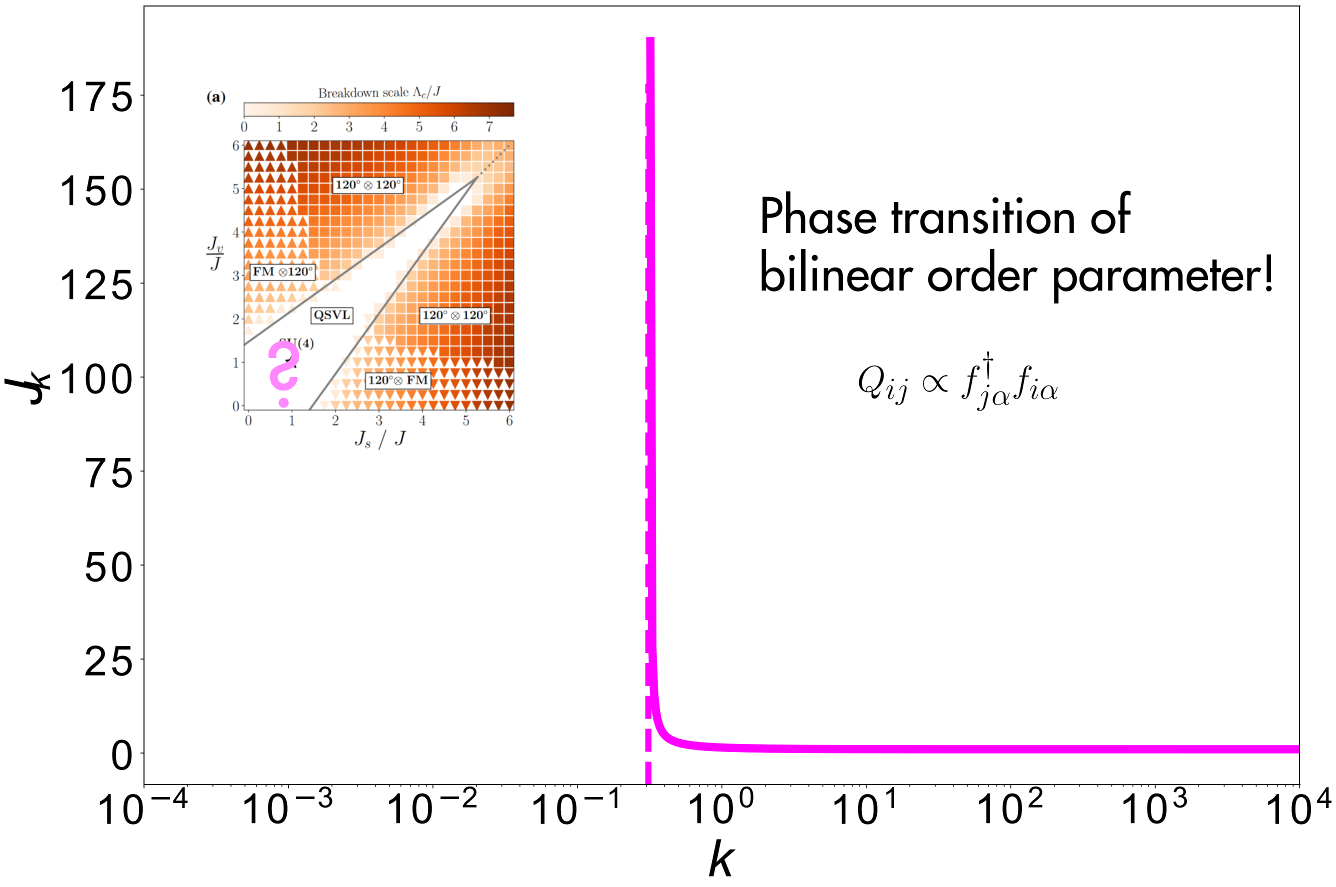
$$Q_{ij} = Q \quad \text{on all links}$$

π-Flux:

$$Q_{ij} = Qe^{\pm i\pi/2} \text{ on x-bonds}$$



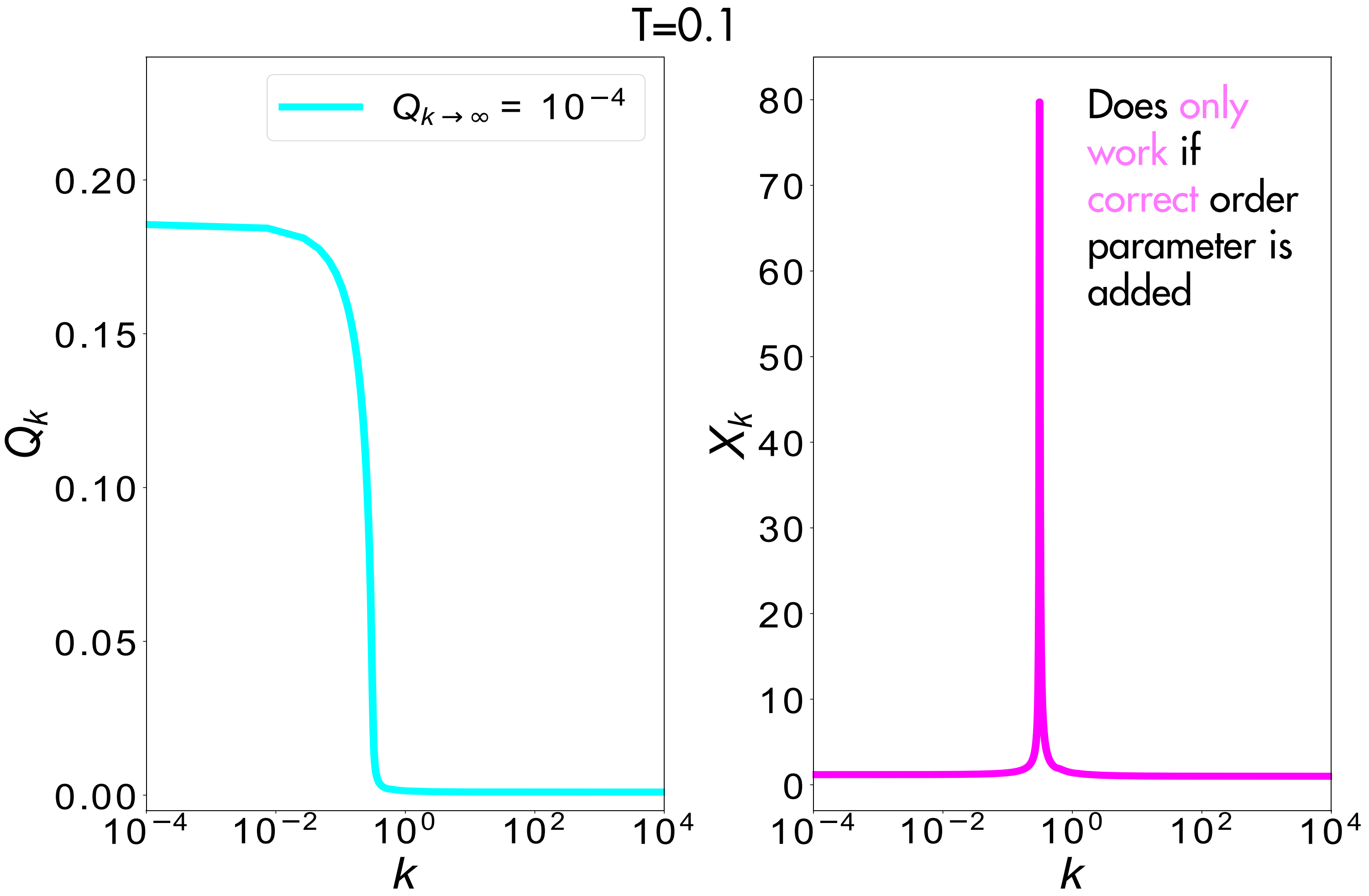
Basic implementation ($N \to \infty$)



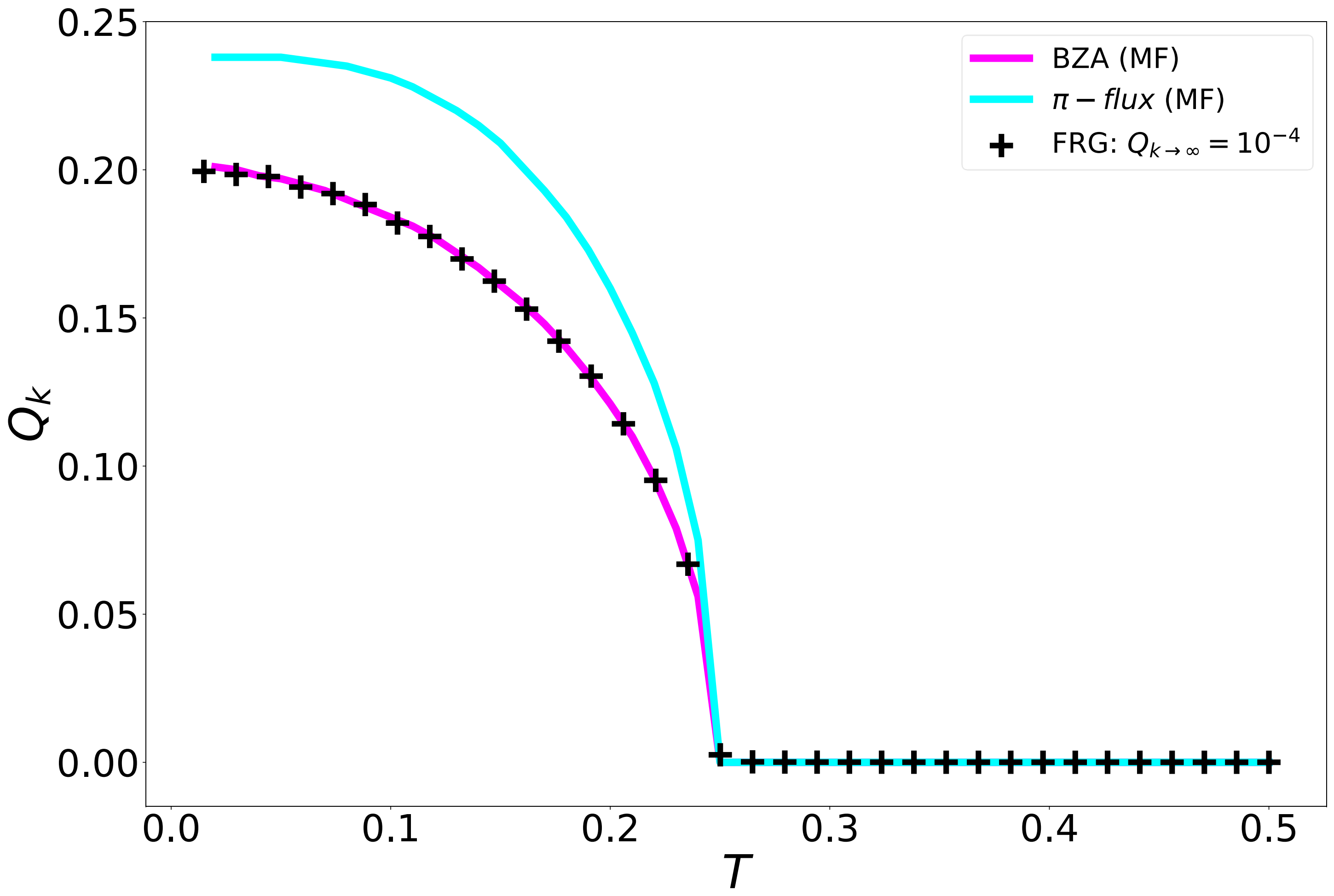
Phase transition of
bilinear order parameter!

$$Q_{ij} \propto f^{\dagger}_{j\alpha} f_{i\alpha}$$

Flow into broken phase ($N \to \infty$)



BZA ($N \to \infty$)



Why BZA? (N $\to \infty$)

Recap order parameter:

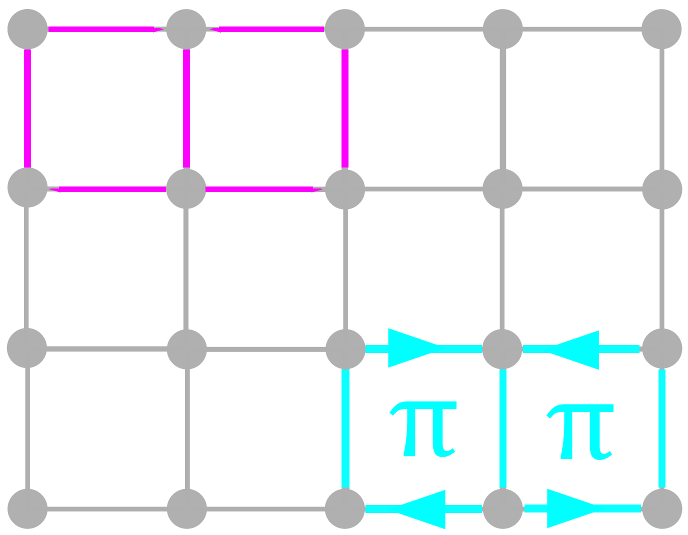
$$\Gamma_{\text{esb}} = \int_\tau \left\{ Q_k \sum_{<ij>} f^\dagger_{i\alpha} f_{j\alpha} + f^\dagger_{j\alpha} f_{i\alpha} \right\}$$

Order parameter is fixed on each bond!

π-flux requires non-uniform bond values, e.g.

$$Q_{ij} = Qe^{\pm i\pi/2} \text{ on x-bonds}$$

Introduce anisotropic order parameters by clustering



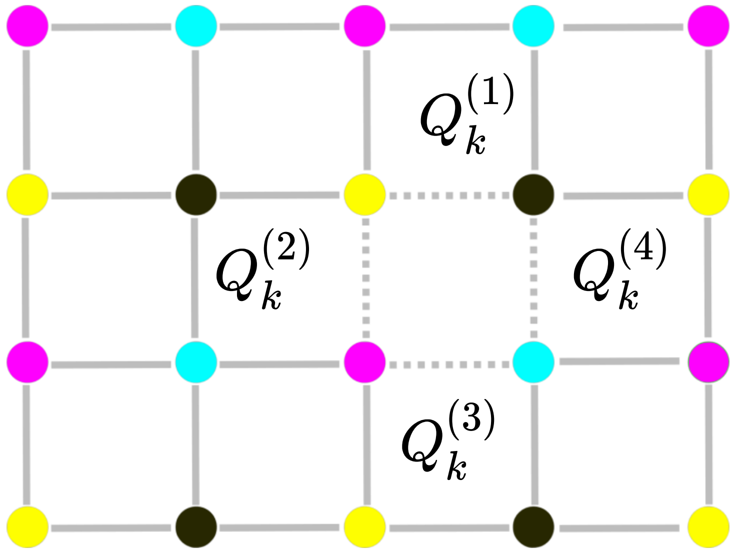
Clustering

4 Sublattices: ABCD, eg. $f_{i\alpha} \to f_{i\alpha}^{A}$

Example of new order parameter:

$$\int_\tau \sum_{\langle ij \rangle} \left\{ Q_k^{(3)} f_{i\alpha}^{\dagger,B} f_{j\alpha}^{C} + Q_k^{*(3)} f_{j\alpha}^{\dagger,C} f_{i\alpha}^{B} \right\}$$

Same for $Q^{(*),1,2,4}$ and $J^{1,2,3,4}$



Complete Clustering Ansatz (N $\to \infty$)

$$\Gamma_k = \int_\tau \Big\{ f^\dagger_{i\alpha} \dot{f}_{i\alpha}$$

$$- \frac{J^{(1)}_k}{N} \sum_{\langle ij \rangle} f^{\dagger,A}_{j\alpha} f^C_{i\alpha} f^{\dagger,C}_{j\beta} f^A_{i\beta} - \frac{J^{(2)}_k}{N} \sum_{\langle ij \rangle} f^{\dagger,A}_{j\alpha} f^D_{i\alpha} f^{\dagger,D}_{j\beta} f^A_{i\beta}$$

$$- \frac{J^{(3)}_k}{N} \sum_{\langle ij \rangle} f^{\dagger,B}_{j\alpha} f^C_{i\alpha} f^{\dagger,C}_{j\beta} f^B_{i\beta} - \frac{J^{(4)}_k}{N} \sum_{\langle ij \rangle} f^{\dagger,B}_{j\alpha} f^D_{i\alpha} f^{\dagger,D}_{j\beta} f^B_{i\beta}$$

INITIAL INTERACTION

$$+Q^1_k \sum_{\langle ij \rangle} f^{\dagger,A}_{i\alpha} f^C_{j\alpha} + Q^2_k \sum_{\langle ij \rangle} f^{\dagger,A}_{i\alpha} f^D_{j\alpha}$$

$$+Q^3_k \sum_{\langle ij \rangle} f^{\dagger,B}_{i\alpha} f^C_{j\alpha} + Q^4_k \sum_{\langle ij \rangle} f^{\dagger,B}_{i\alpha} f^D_{j\alpha}$$

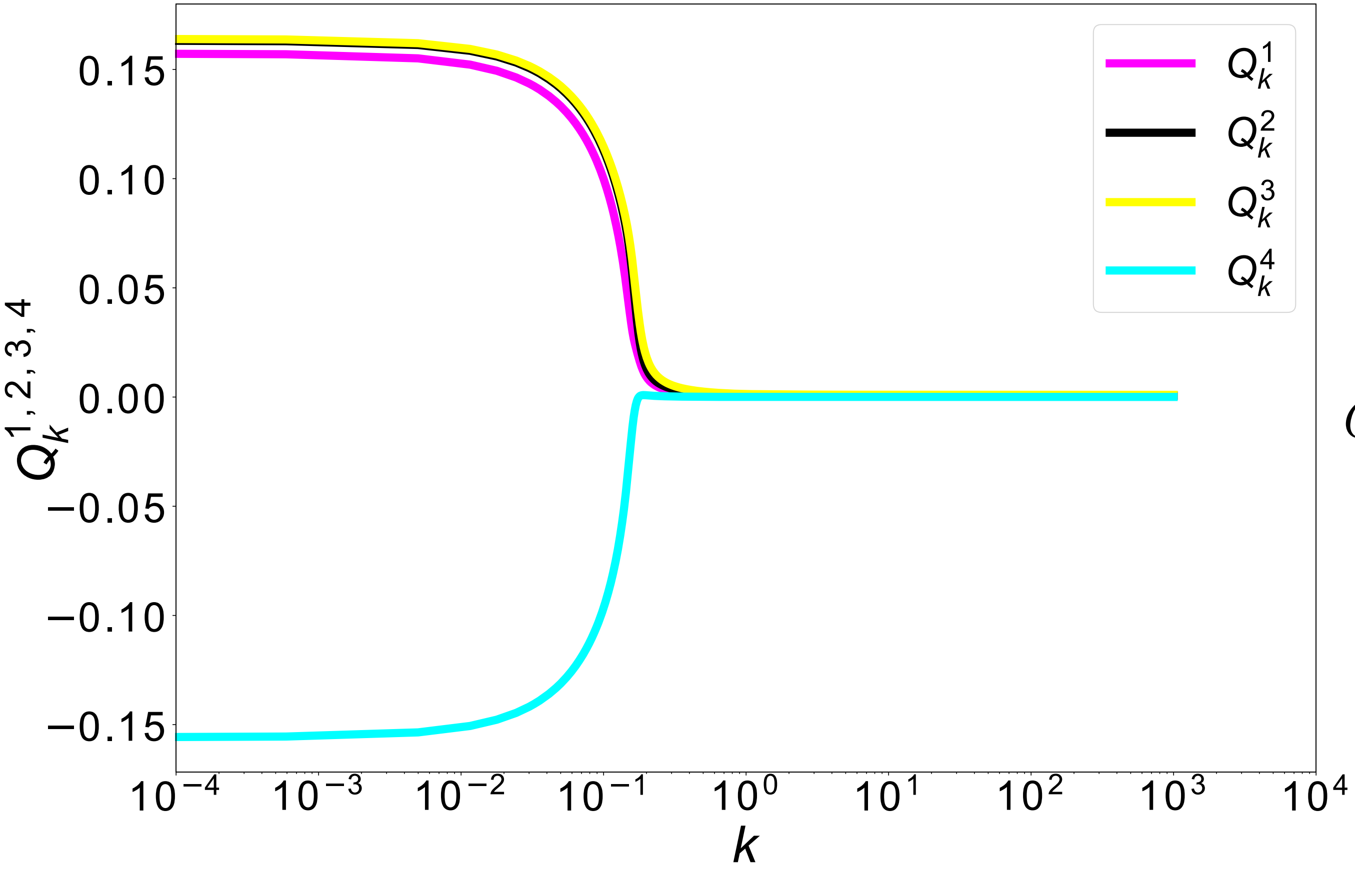
$$+ \text{h.c. order parameters}$$

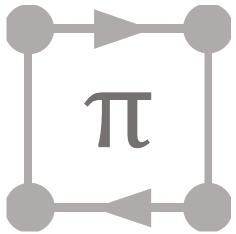
SYMMETRY BREAKING TERM

$$+ \text{32 new generated couplings}$$

GENERATED INTERACTIONS

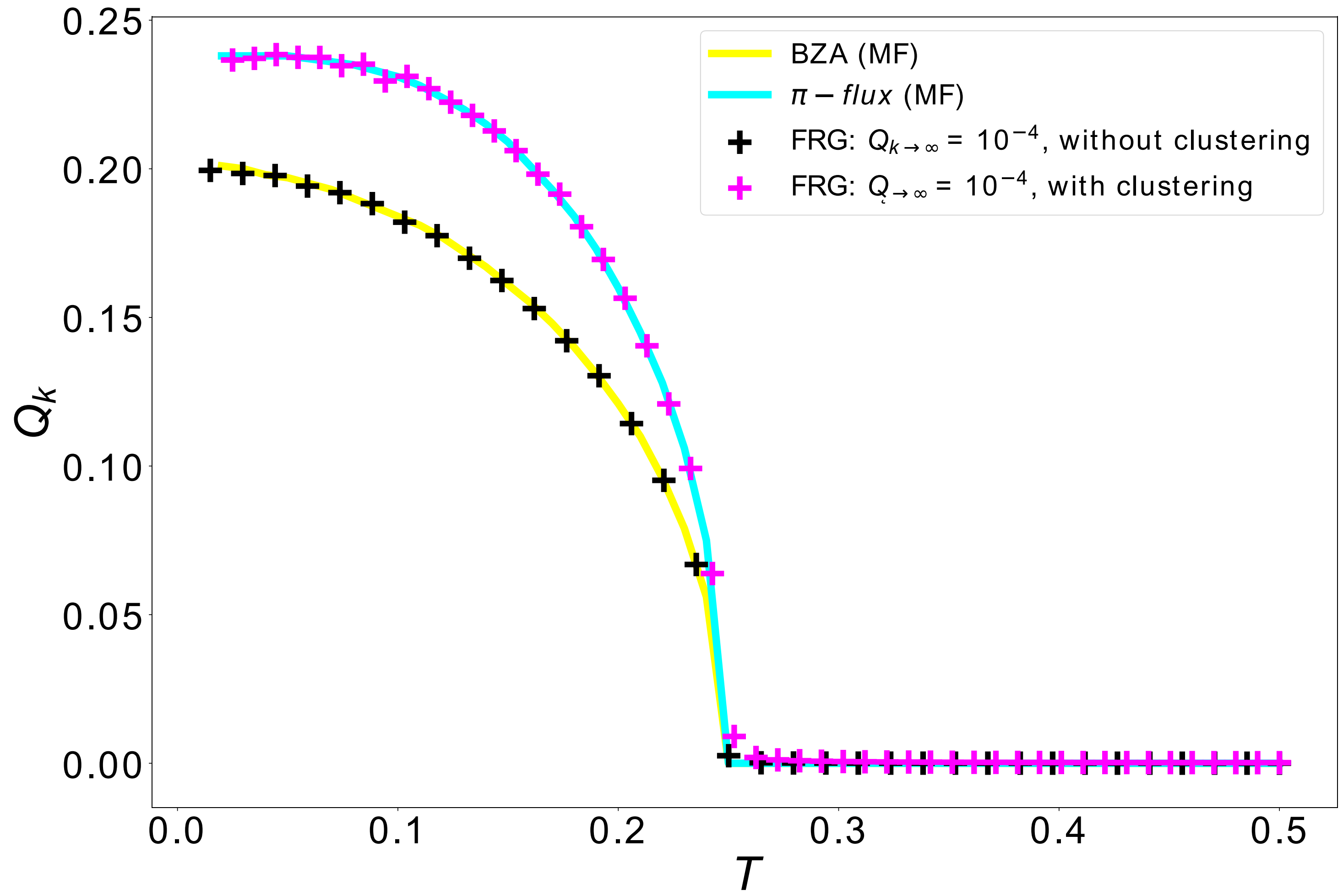
π - flux ($N \to \infty$)





$$Q_{ij} = Qe^{i\theta}$$

Total result ($N \to \infty$)

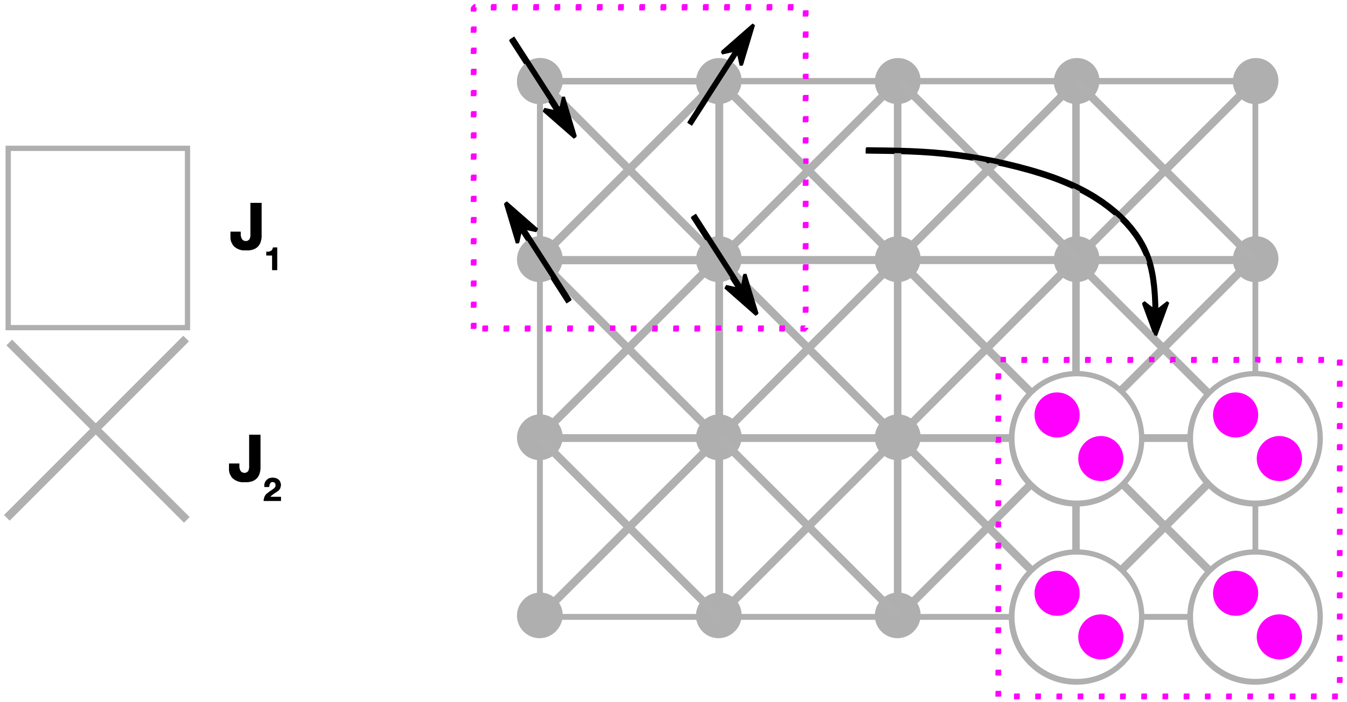


$J_1 - J_2$

MODEL

$J_1 - J_2$ model

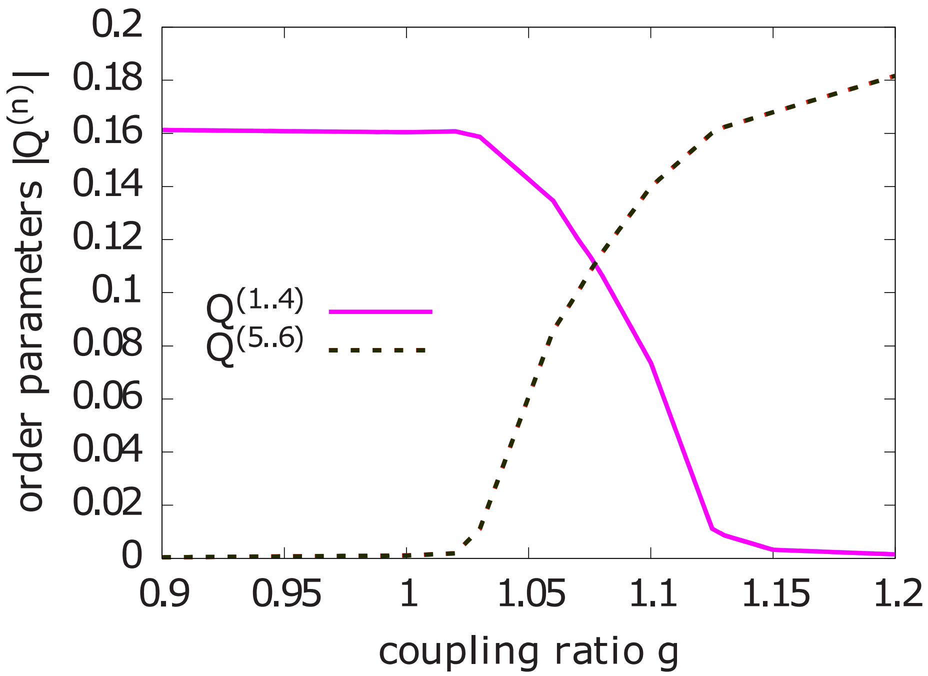
$$H = -\frac{J_1}{N}\sum_{\langle ij\rangle}\vec{S}_i\cdot\vec{S}_j - \frac{J_2}{N}\sum_{\langle\langle ij\rangle\rangle}\vec{S}_i\cdot\vec{S}_j$$



$J_1 - J_2$ model ($N \to \infty$)

Implementation: completely analogous to former model, „just" with a few more couplings

Result: BZA and Pi-Flux phase existing also in the new model in large N

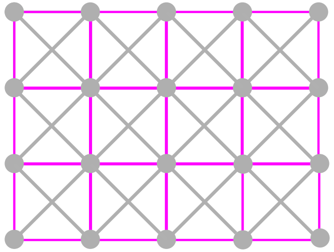


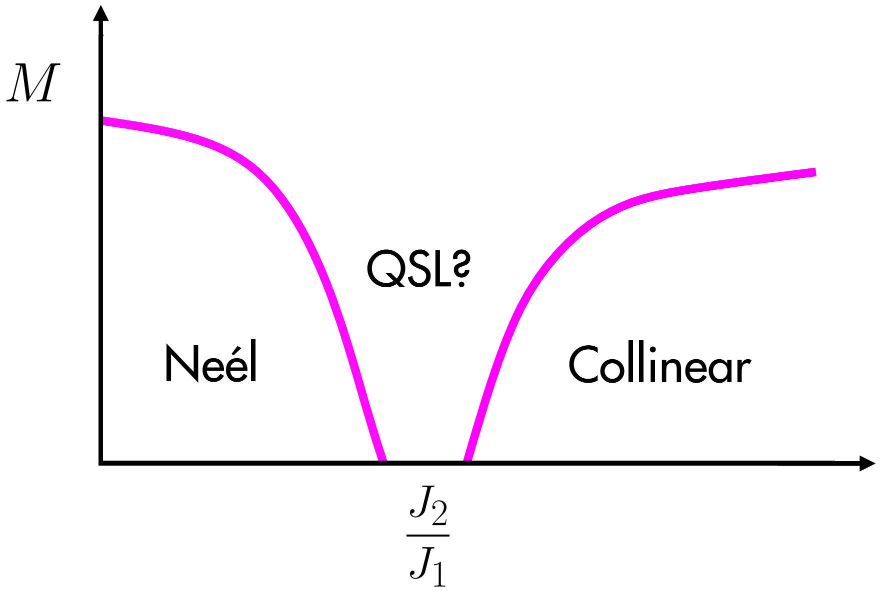
$$g = \frac{J_2}{J_1}$$

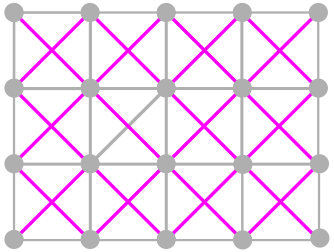
Question: What happens N=2?

$J_1 - J_2$ model (N = 2)

Question: What happens at N=2?







Difficulty:

implement constraint!

Constraint (N=2)

Problem: constraint not negligible!

Spins → Fermions

$$|\uparrow\rangle, |\downarrow\rangle \rightarrow |\not{0}\rangle, |\downarrow\rangle, |\uparrow\rangle, |\not{\uparrow\downarrow}\rangle$$

$$\sum_{\alpha} f_{i\alpha}^{\dagger} f_{i\alpha} = \frac{N}{2} \quad , \forall i$$

Solution: Popov-Fedotov chemical potential

$$\mu_{\mathrm{PF}} = i\frac{\pi T}{2}$$

$$\Gamma_{PF} = \int_{\tau} \sum_{i} \mu_{PF,k} f_{i\alpha}^{\dagger} f_{i\alpha}$$

→ Filters unphysical states on level of the partition function

Result (N=2)

Implement Cluster FRG for model while…

…using bilinear QSL order parameters…
…using clustering to enable Pi-Flux phase…
…using chemical potential to impose constraint…

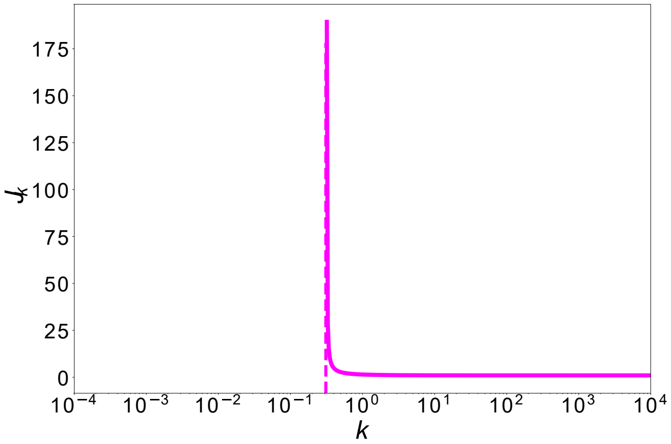
Result:

No magnetic order

No bilinear order parameter can regularize the divergence

There is no (bilinear) spin liquid in this model!

Suggestion: Non-blinear order (plaquette?)



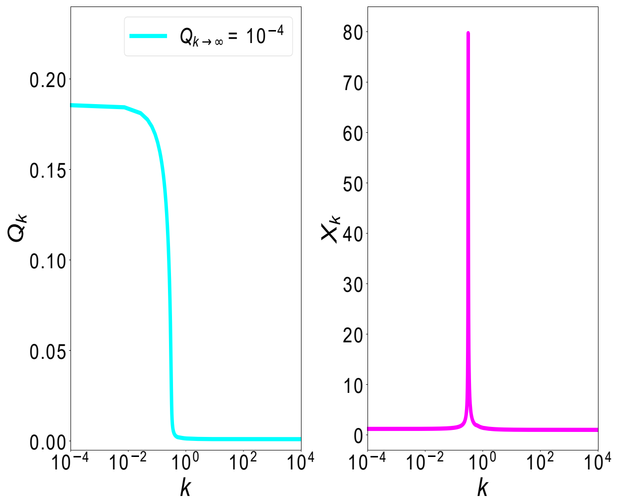
Conclusion & Outlook

Development of novel approach to identify spin liquids

Approach is unbiased

Succesfully benchmarked at a known result

First result: no spin liquid in the J_1 -J_2 model



Under construction: implement method for Kitaev model with complex fermions