Nematic orders in a frustrated ferromagnet

Yasir Iqbal
University of Würzburg, Germany

6th Feb, 2017

Julius-Maximilians-
UNIVERSITÄT
WÜRZBURG

ToCoTronics

SFB1170

TP 1

Collaborators

J. Reuther
(FU Berlin)

R. Thomale
(Uni-Würzburg)

B. Kumar
(JNU, Delhi)

P. Ghosh
(JNU, Delhi)

R. Narayanan
(IIT, Madras)

Phases of matter

T

Gases

Liquids

Homogenous and Isotropic

Crystalline solids

Broken symmetries

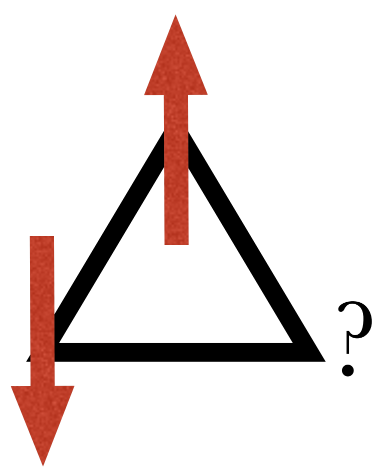
If H(nuc) + H (elec) has the full space translation and rotation group, it is not unreasonable to expect the ground state to retain the full symmetry

^{4}He (low pressure): the ground state wave-function has the fully symmetric

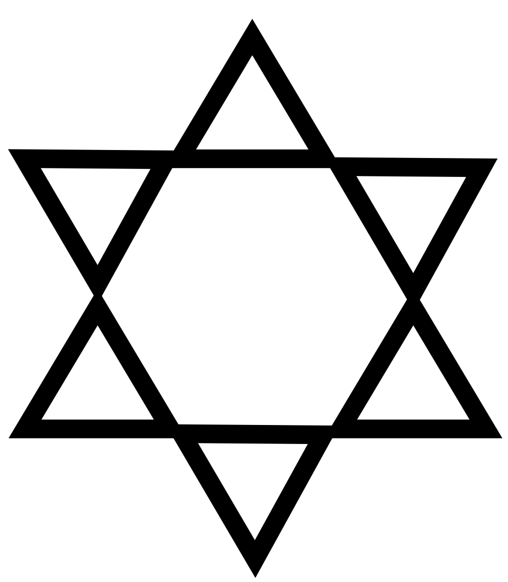
Frustrated Magnetism

Magnetic systems in which either due to geometrical or parametrical reasons, all the interactions in a Hamiltonian can not be simultaneously satisfied

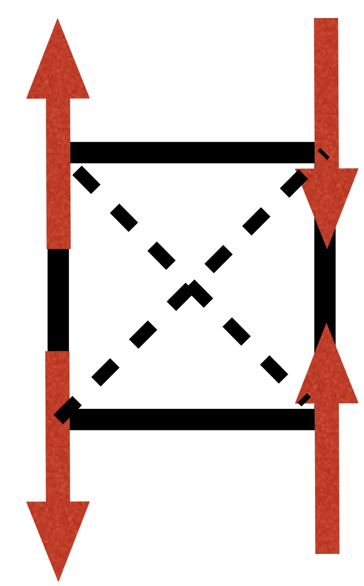
Geometrical frustration



Kagome Lattice



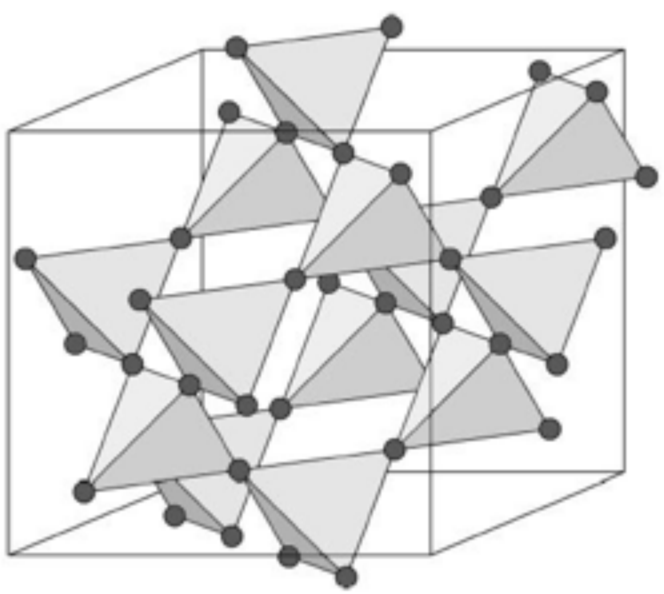
Parametric frustration



Measure of frustration

Degeneracy of the ground-state manifold

Pyrochlore lattice



$$F = (n-1)\frac{Nq}{2}$$

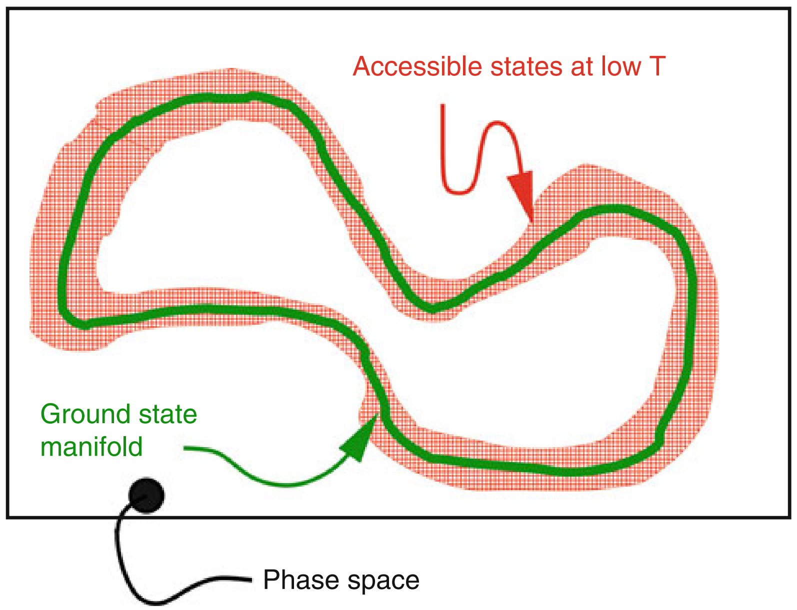
$$C = nN$$

$$n = 3 \text{ and } q = 4$$

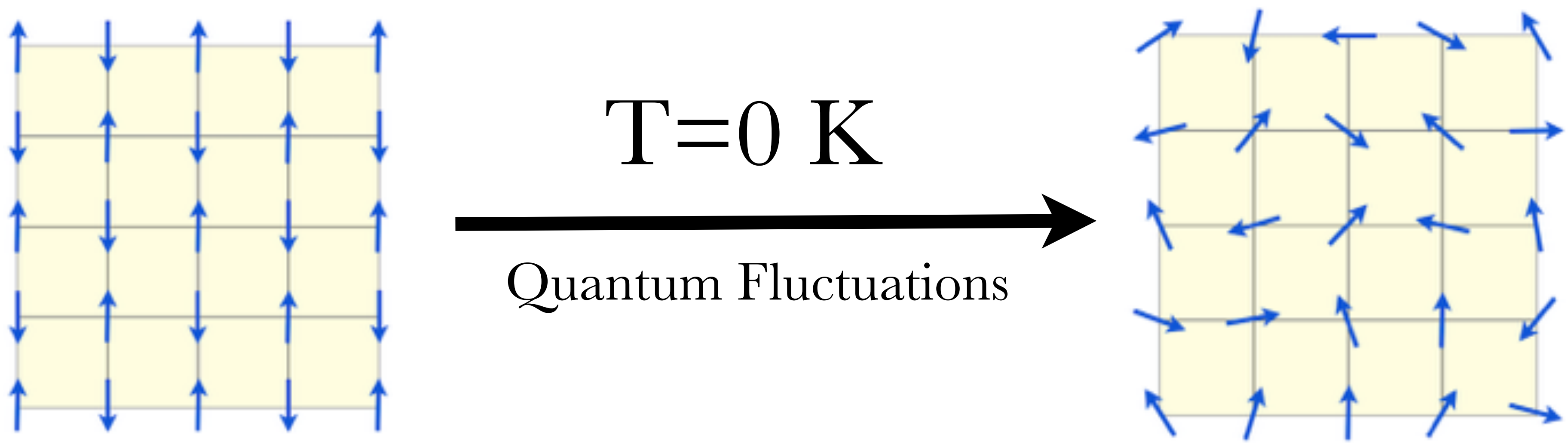
$$F - C = N$$

$$H = J\sum_{\langle ij\rangle} S_i \cdot S_j = \frac{J}{2}\sum_{\alpha} |\mathbf{L}_{\alpha}^2| - \frac{J}{2}\frac{Nq}{2}$$

$$\mathbf{L}_{\alpha} = \sum_{i\in\alpha} S_i$$

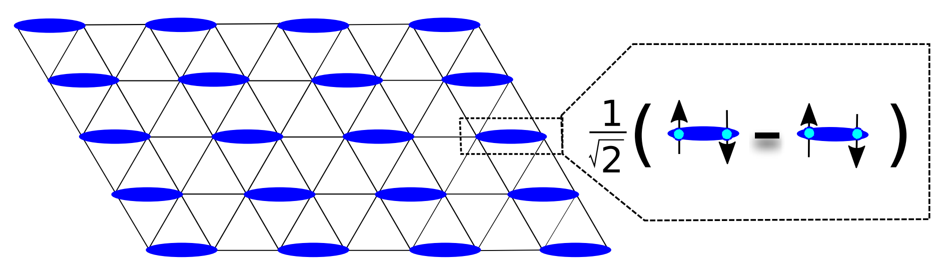


Traditional Recipe for Cooking Spin Liquids



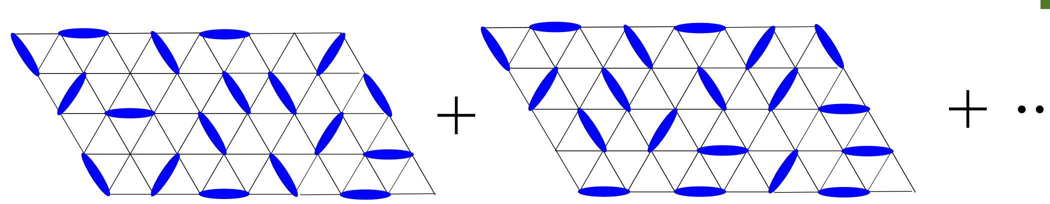
Its a new exciting world!

Quantum orders

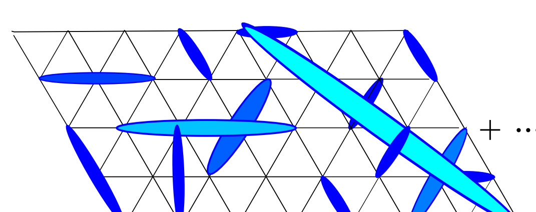


Long Range Entanglement

Resonating Valence-bond (Baskaran, Zou, & Anderson, 1987)



Projective Symmetry Groups (Wen, 1991, 2002)



A "Modern" recipe for cooking spin liquids

Frustrate ferromagnetic order using competing AF interactions

↓

The resulting paramagnetic state in a FM environment has an *enhanced* propensity for resonating triplet bonds, and weakened propensity for resonating singlet bonds

↓

This scenario opens up the possibility of stabilising an exotic variant of a quantum paramagnet, dubbed a *spin nematic*

Spin Nematic

Characterised by an absence of dipolar magnetic order, $\langle \hat{\mathbf{S}}_i \rangle = 0$

It still breaks *SU*(2) spin rotation symmetry due to a non-zero quadrupolar order parameter of the form

$$\mathcal{O}_{ij}^{\mu\nu} = \langle \hat{S}_i^{\mu} \hat{S}_j^{\nu} \rangle - \frac{\delta_{\mu\nu}}{3} \langle \hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_j \rangle \ (\text{with } \mu,\, \nu = x, y, z)$$

Time-reversal symmetry is preserved

It can be viewed as a quantum spin analog of the nematic state in liquid crystals.

Andreev & Grishchuk '84

Chandra, Coleman & Larkin ' 90

Gorkov & Sokol ' 90

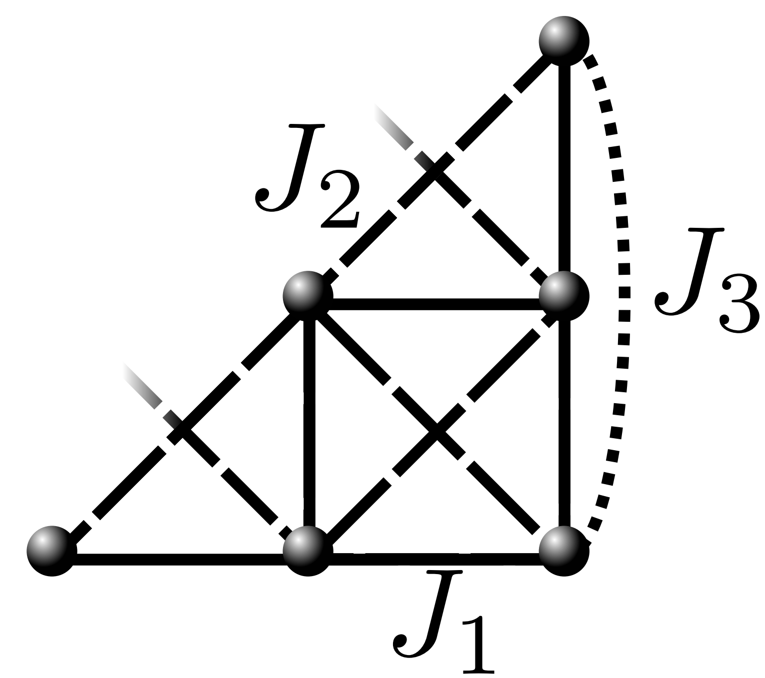
Nematic orders in a frustrated ferromagnet

Phys. Rev. B **94**, 224403 (2016), Iqbal *et al.*

A simple frustrated 2D system with competing AF and FM interactions on the square lattice

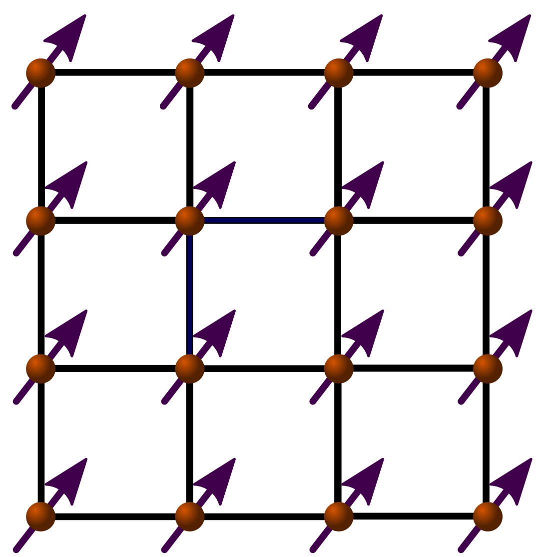
$$\hat{\mathcal{H}} = J_1 \sum_{\langle i,j \rangle} \hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_j + J_2 \sum_{\langle\langle i,j \rangle\rangle} \hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_j + J_3 \sum_{\langle\langle\langle i,j \rangle\rangle\rangle} \hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_j$$

$$J_1 \leqslant 0 \text{ (FM) and } J_2, J_3 \geqslant 0 \text{ (AF)}$$



Classical Orders

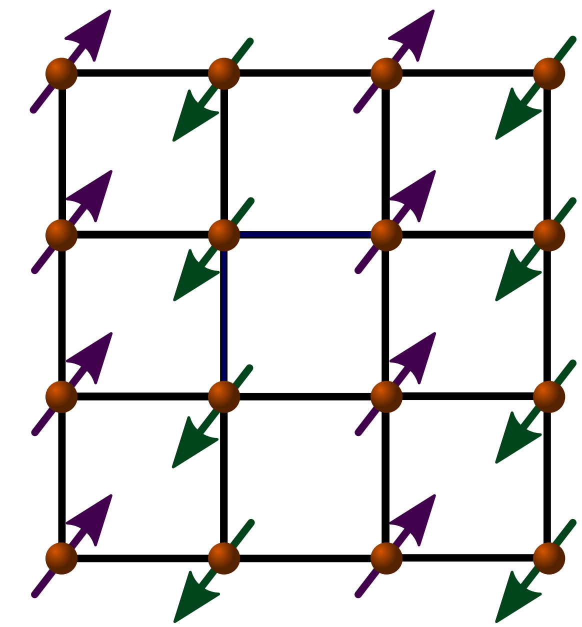
FM



J_1-J_2 limit

$J_2/|J_1| = \frac{1}{2}$

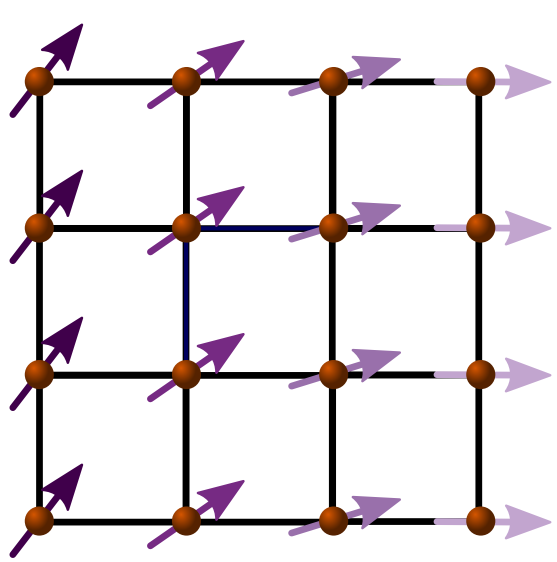
Stripe AF $(\pi, 0)$



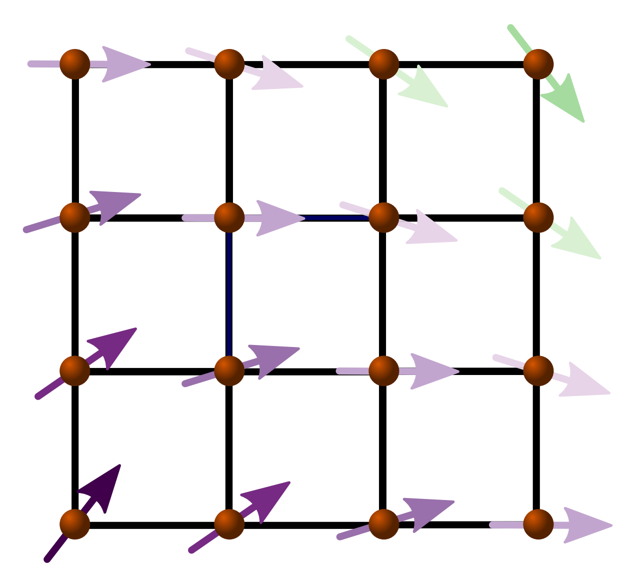
$+J_3$

Incommensurate orders

1D spiral (q,0)

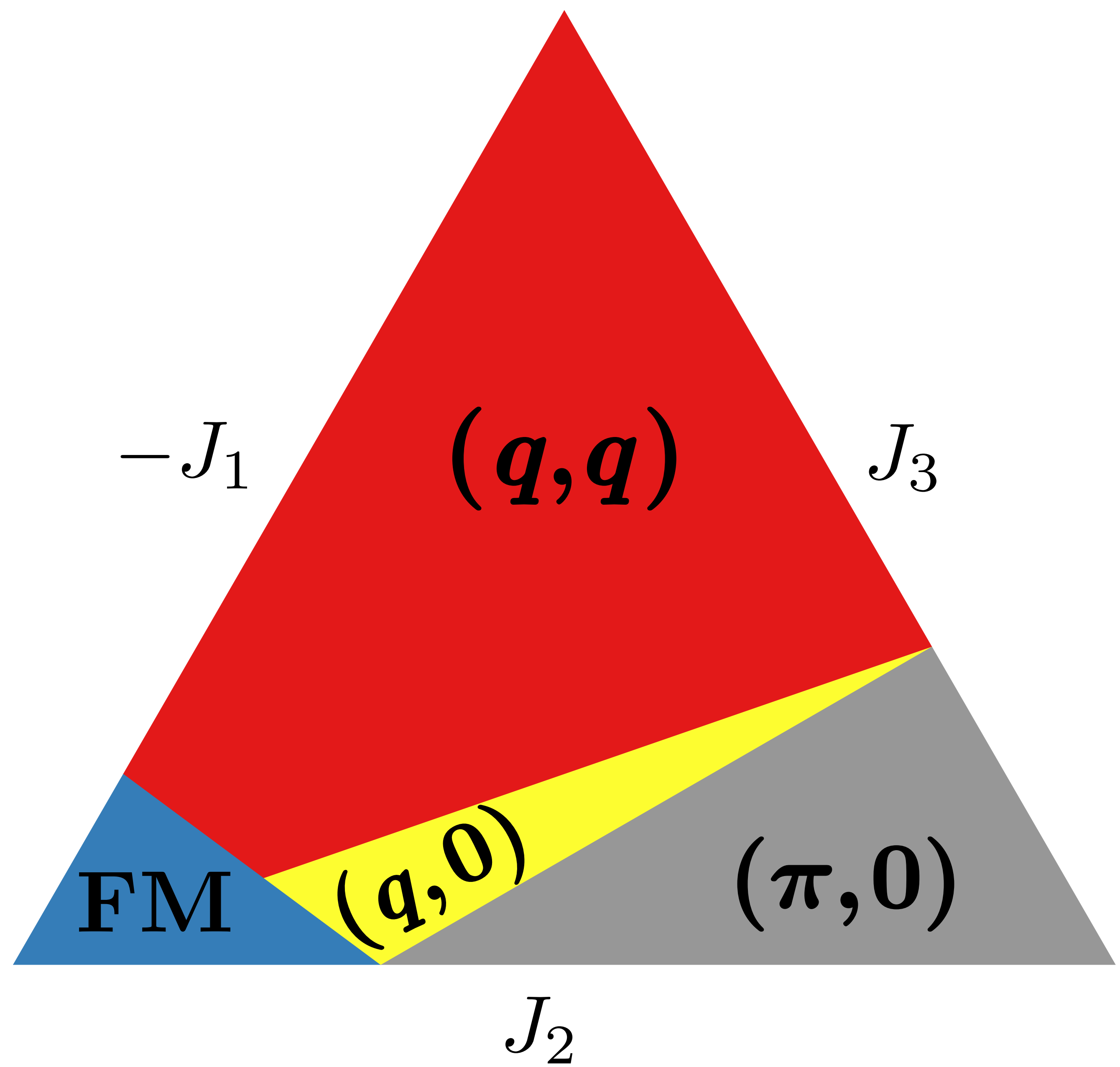


2D spiral (q,q)



Rastelli, Reatto & Tassi ' 86

Classical Phase Diagram



$$|J_1| + J_2 + J_3 = 1$$

What is the effect of quantum fluctuations?

Pseudo-fermion Functional RG

A new and powerful method developed to deal with spin models featuring two-body spin interactions

$$H = \sum_{ij} \sum_{\mu=x,y,z} J_{ij}^{\mu} S_i^{\mu} S_j^{\mu}$$

Recently extended to treat off-diagonal antisymmetric interactions (Dzyaloshinskii-Moriya) [Hering & Reuther' 16]

Pseudo-fermions: Cut the physical spin operator into two halves

This is achieved by rewriting the physical spin operator at each site *i* in terms of fermionic operators for spinons

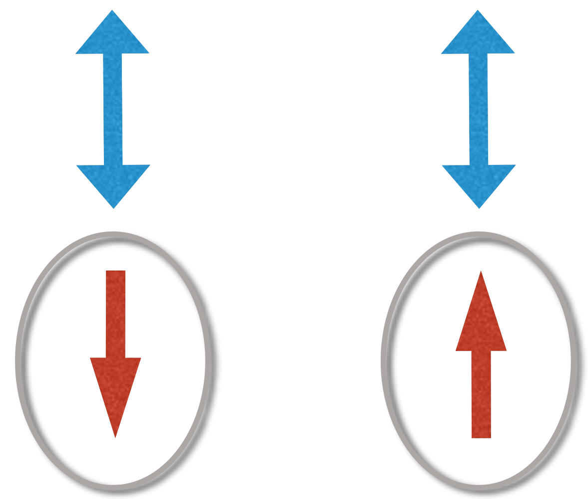
$$\hat{\mathbf{S}}_i = \frac{1}{2} \sum_{\alpha,\beta} \hat{c}_{i,\alpha}^{\dagger} \boldsymbol{\sigma}_{\alpha\beta} \hat{c}_{i,\beta} \qquad \alpha, \beta = \uparrow \text{ or } \downarrow$$

Abrikosov' 1965

Hilbert Space Enlargement: Constraint problem

Enlarged basis for a a given site *i* is spanned by the following states

$$|n_{i,\uparrow} n_{i,\downarrow}\rangle : \quad \cancel{|0,0\rangle} \quad |0,1\rangle \quad |1,0\rangle \quad \cancel{|1,1\rangle}$$



$$c^\dagger_{i,\uparrow} c_{i,\uparrow} + c^\dagger_{i,\downarrow} c_{i,\downarrow} = 1 \qquad \text{needs to be fulfilled}$$

- Exact fulfilment of the constraint using *Fedotov-Popov* method.

(V. N. Popov and S. A. Fedotov, Sov. Phys. JETP 67, 535 (1988))

$$\textit{imaginary} \text{ chemical potenial } \mu_{i,\uparrow} = \mu_{i,\downarrow} = \frac{i\pi}{2\beta}$$

- Average fulfilment of the constraint, i.e., $\langle c^\dagger_{i,\uparrow} c_{i,\uparrow} + c^\dagger_{i,\downarrow} c_{i,\downarrow}\rangle = 1$

$$\mu_{i,\uparrow} = \mu_{i,\downarrow} = 0$$

Fermionic Hamiltonian

$$H = \sum_{ij} \sum_{\mu} J_{ij}^{\mu} \mathbf{S}_i^{\mu} \mathbf{S}_j^{\mu} \rightarrow \frac{1}{4} \sum_{ij} \sum_{\mu} J_{ij}^{\mu} (c_i^{\dagger} \sigma^{\mu} c_i)(c_j^{\dagger} \sigma^{\mu} c_j)$$

Standard procedure: Mean-field decoupling

$$\langle S_i^{\mu} \rangle = \frac{1}{2} \langle c_i^{\dagger} \sigma^{\mu} c_i \rangle \qquad \langle c_{i,\alpha}^{\dagger} c_{j,\alpha} \rangle \qquad \langle c_{i,\uparrow}^{\dagger} c_{j,\downarrow}^{\dagger} \rangle$$

Spin mean-field | Hopping | Pairing

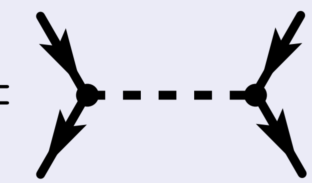
Quantum paramagnets
(RVB Ansätze)
Wen' 2002

How to treat the spin Hamiltonian in its full complexity?

Diagrammatics

Exploiting Feynman diagrammatics in the fermionic language

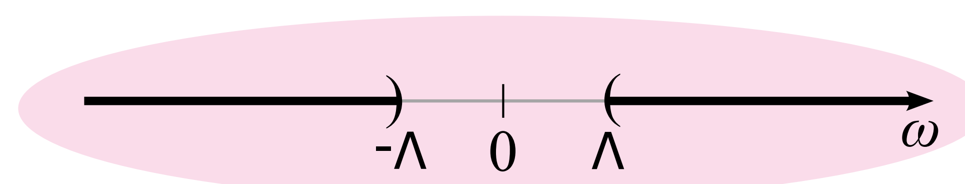
Propagator: $G_0(i\omega) = \frac{1}{i\omega} =$ 

Interaction vertex: $\Gamma_0 =$  $\sim J$

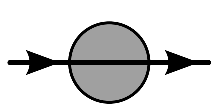
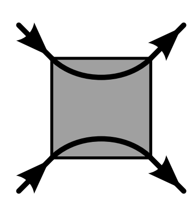
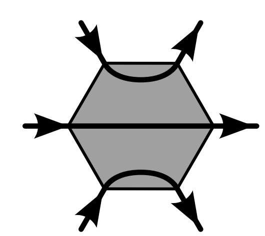
Summing up terms order by order is not the way to go, since the Hamiltonian at hand, does not have any *small* parameter built in it.

Introduce an infra-red frequency cutoff in the propagator:

$$G_0(i\omega) = \frac{1}{i\omega} \longrightarrow G_0^\Lambda(i\omega) = \frac{\Theta(|\omega|-\Lambda)}{i\omega}$$

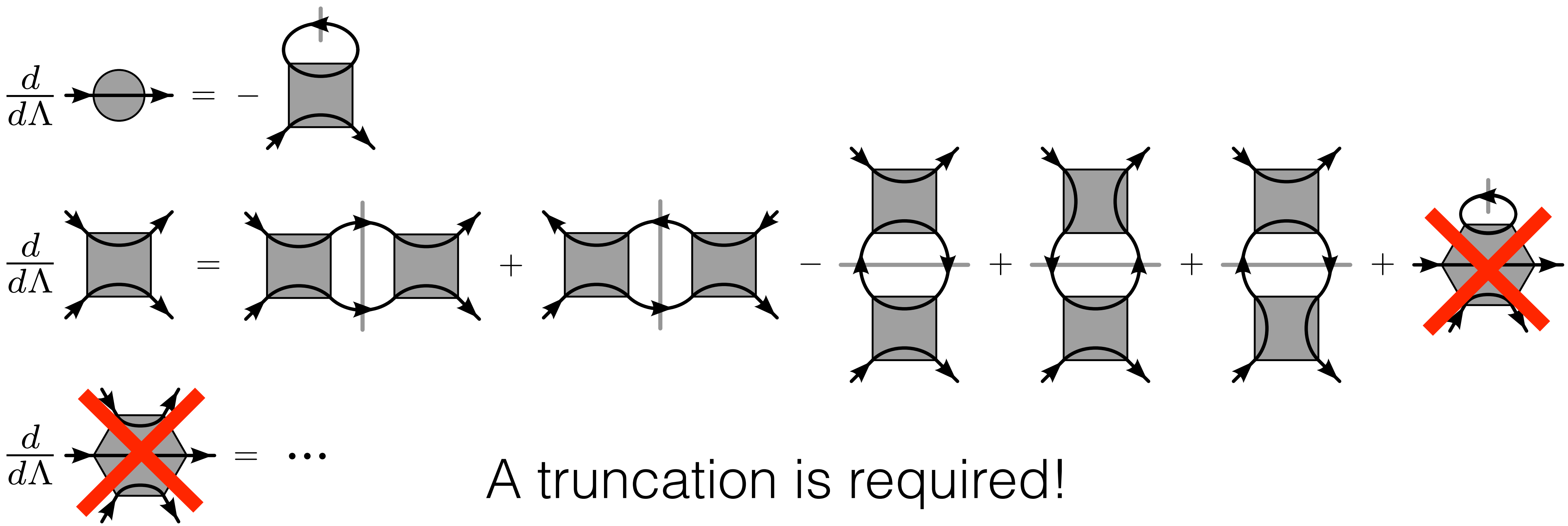


Then:

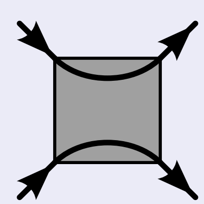
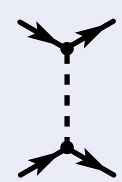
$\Sigma =$  $\longrightarrow \Sigma^\Lambda$, $\Gamma =$  $\longrightarrow \Gamma^\Lambda$, $\Gamma_3 =$  $\longrightarrow \Gamma_3^\Lambda$

m-particle vertex functions

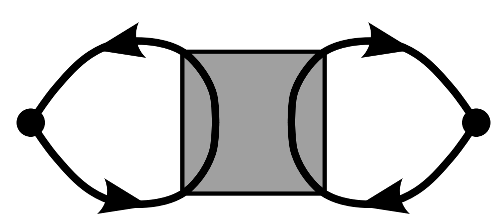
FRG formulates differential equations for the *m*-particle vertex functions



A truncation is required!

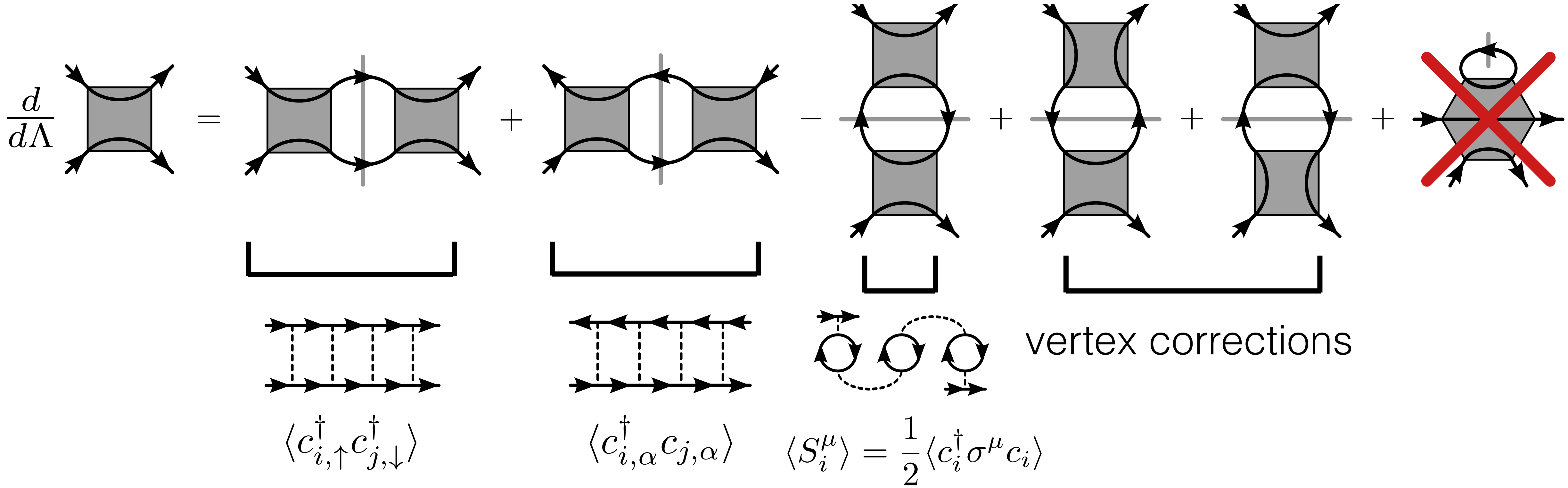
Flow starts with  $\xrightarrow{\Lambda\to\infty}$  $\sim J$ and ends at $\Lambda = 0$.

Spin-susceptibility is calculated from the two-particle vertex

$\chi^{\Lambda}(\mathbf{k}) =$ 

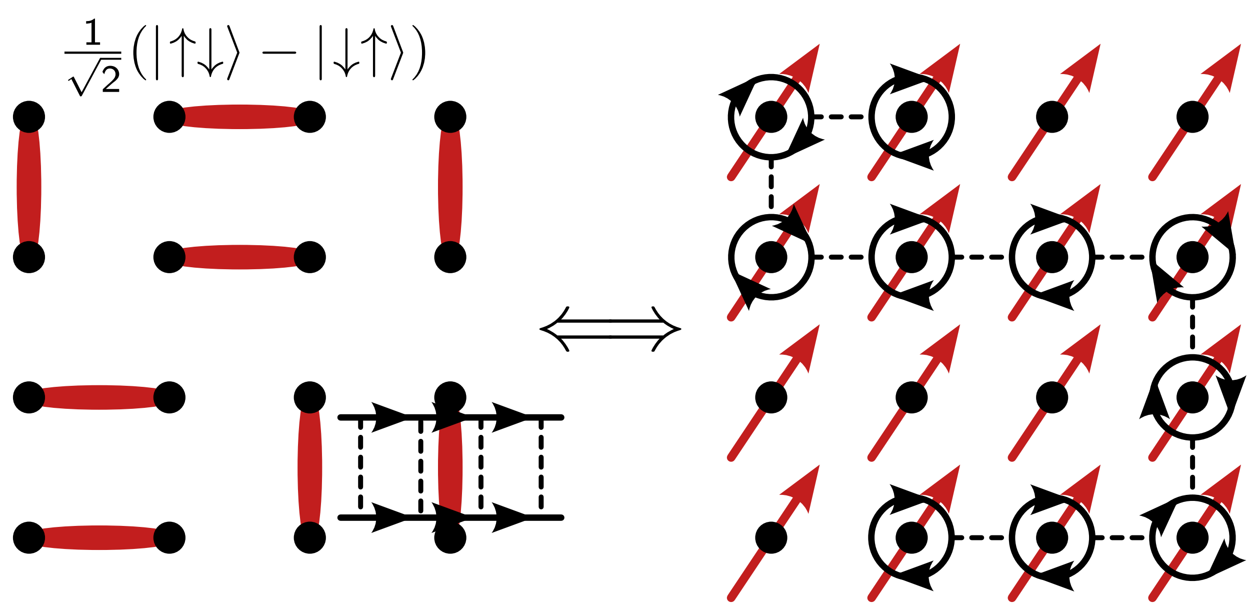
Ladder and bubble diagrams

FRG sums up diagrammatic contributions in infinite order in J



Ladder diagrams

RVB states (Dimer states and spin liquids)



RPA Bubble diagrams

Magnetic order

Competition between Ladder and bubble diagrams

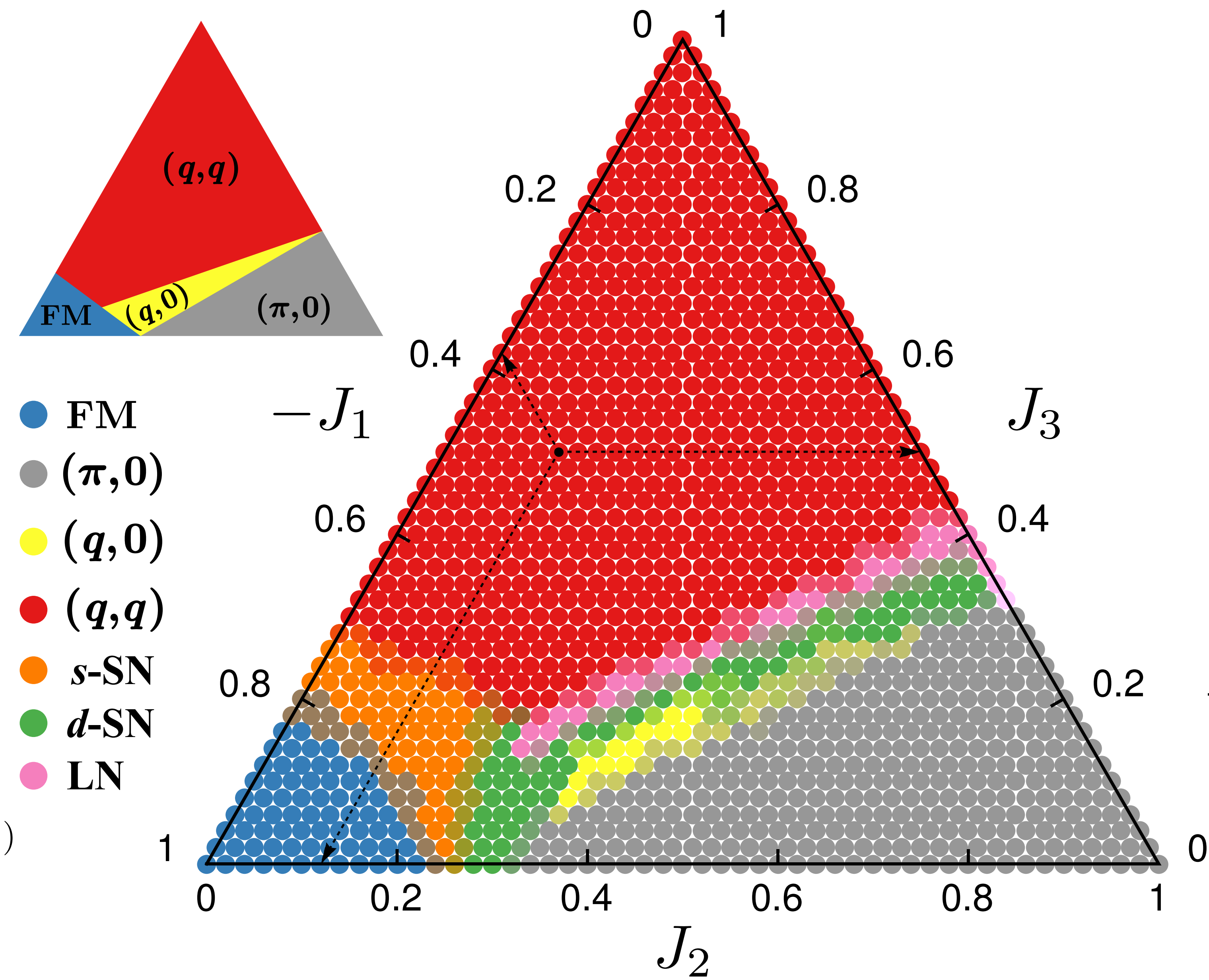
- ladder diagrams are the leading contributions in a $\frac{1}{N}$ expansion
  $\Longrightarrow$ quantum paramagnet states
- RPA bubble diagrams are the leading contributions in a $\frac{1}{S}$ expansion
  $\Longrightarrow$ magnetic order
- neglecting three-particle vertices are sub-leading in $\frac{1}{N}$ and $\frac{1}{S}$

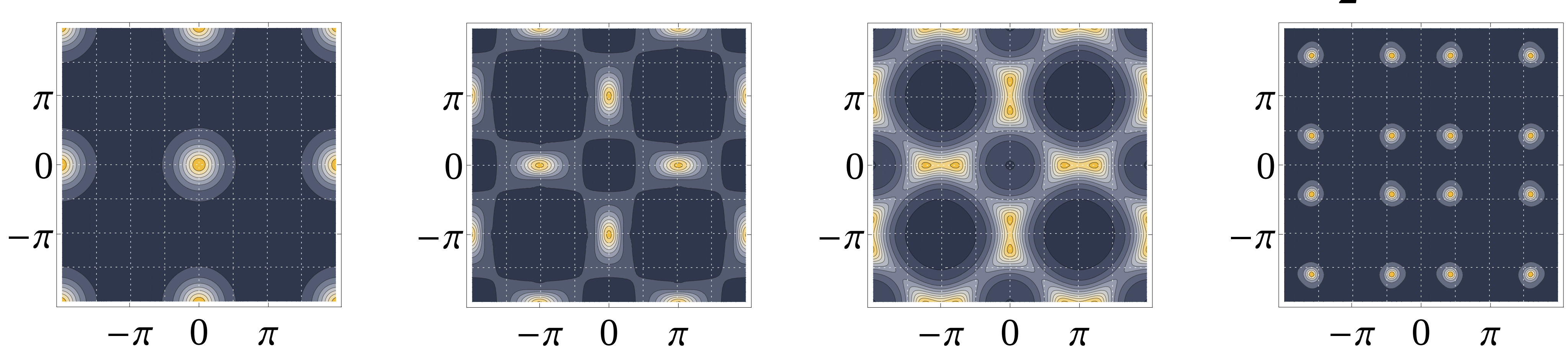
Hence, deep inside ordered and disordered phases, this proves to be accurate, however, phase boundaries which feature competition between ordering and disordering tendencies are subject to uncertainty

The FRG equations are solved with the full frequency dependence of the vertex functions. The typical system sizes we treat are ~1000-sites in 2d and ~4000-sites in 3d.

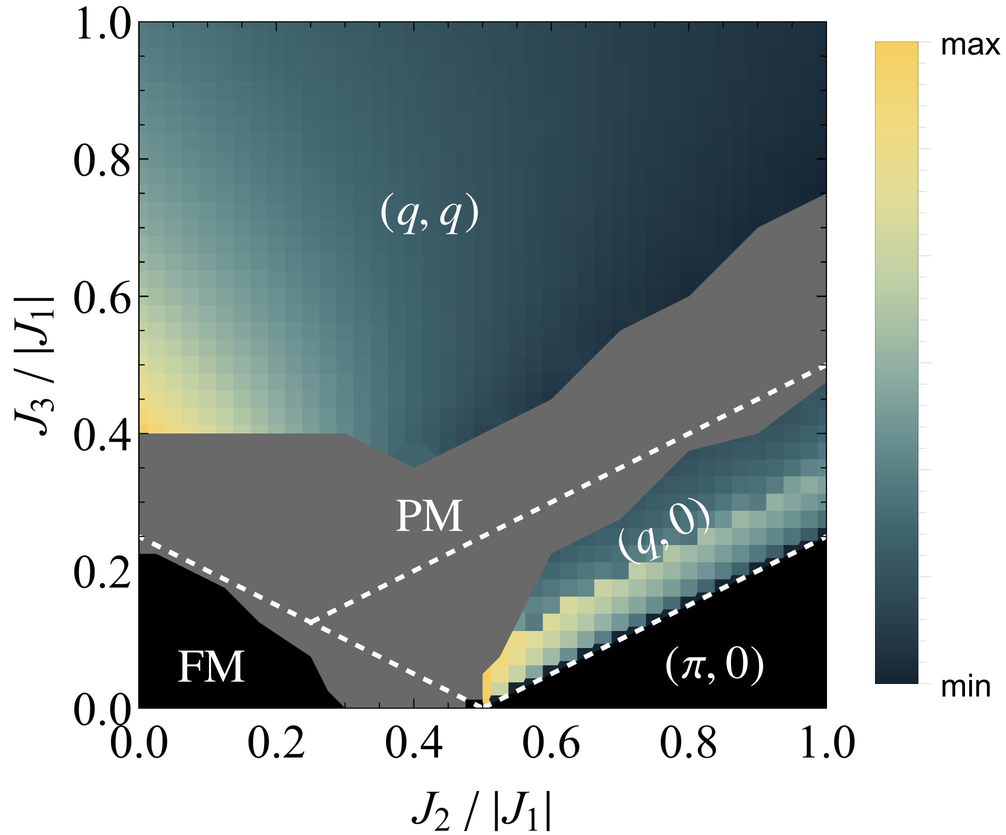
Quantum Phase Diagram: Magnetic Orders

* Diminished extent of FM phase
* Quantum fluctuations extend the domain of stability of the stripe AF
* Quantum effects drastically shrink the domain of 1D spiral (q,0) order to a small pocket
* The 2D spiral (q,q) order prevails over large regions of the phase diagram
* Throughout the domain of both spiral orders we do not observe a discontinuous jump of the spiral wave-vector to $q \to \frac{\pi}{2}$, thus pointing to the absence of commensurate orders at $\mathbf{Q} = (\pm\frac{\pi}{2}, 0)$ and $(\pm\frac{\pi}{2}, \pm\frac{\pi}{2})$





Shifts in Spiral wave-vectors

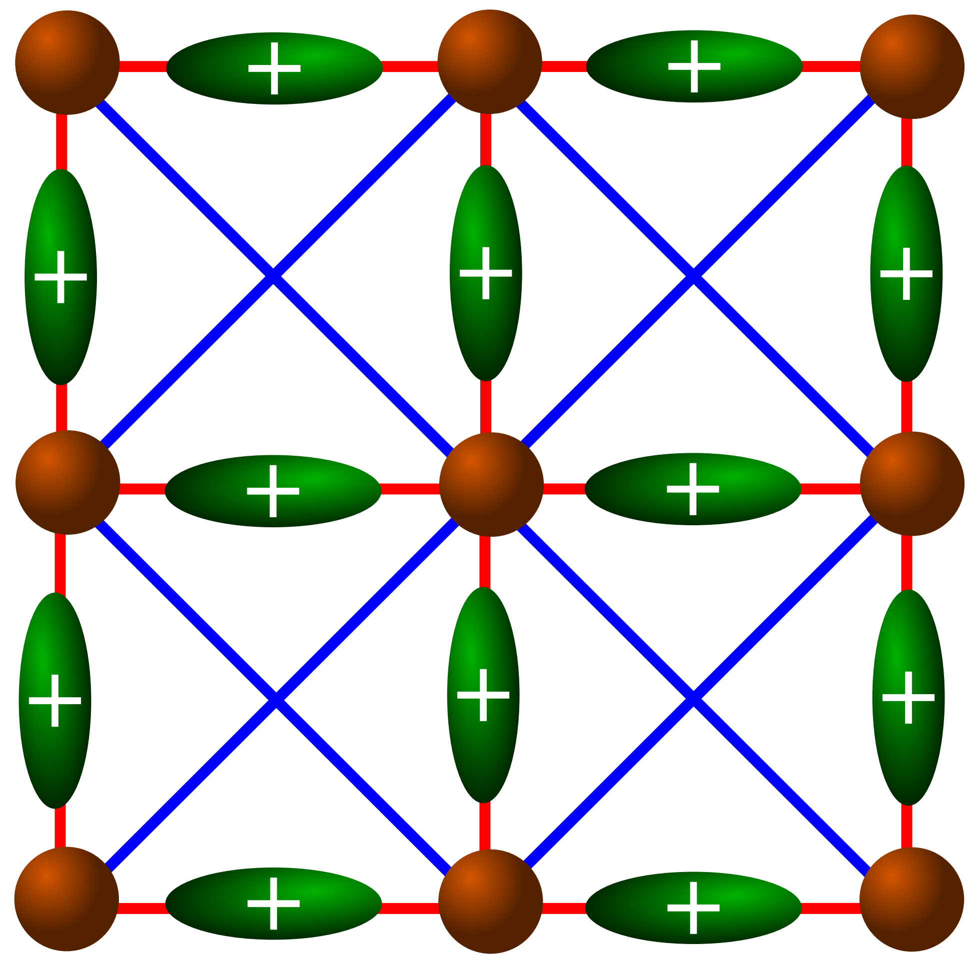


Deviation $\delta\mathbf{Q} = \mathbf{Q} - \mathbf{Q}_{\rm cl}$ of the ordering wave vector $\mathbf{Q}$ from its classical value $\mathbf{Q}_{\rm cl}$ as a function of $J_2/|J_1|$ and $J_3/|J_1|$. The shifts in the black regions are identically zero, and the gray region denotes the PM phase. The classical boundaries are marked with white dashed lines.

- Throughout the HM ordered phases it is found that quantum fluctuations always *increase* the magnitude of the wave vectors leading to more antiferromagnetic types of order
- In the (q,q) HM phase, the shift $\delta\mathbf{Q}$ has a maximal value of $\delta\mathbf{Q} \approx 37\%$ and decreases monotonically with increasing $J_2/|J_1|$ and $J_3/|J_1|$
- Similarly, shifts of $\approx 100\%$ are found in portions of the classical $(q,0)$ HM phase that is turned into stripy AF order by quantum fluctuations, thus leading to the appearance of a ridge-like feature of $\delta\mathbf{Q}$ in the vicinity of the quantum phase boundary

Identifying the nature of Paramagnetic phase

● ***s*-SN**

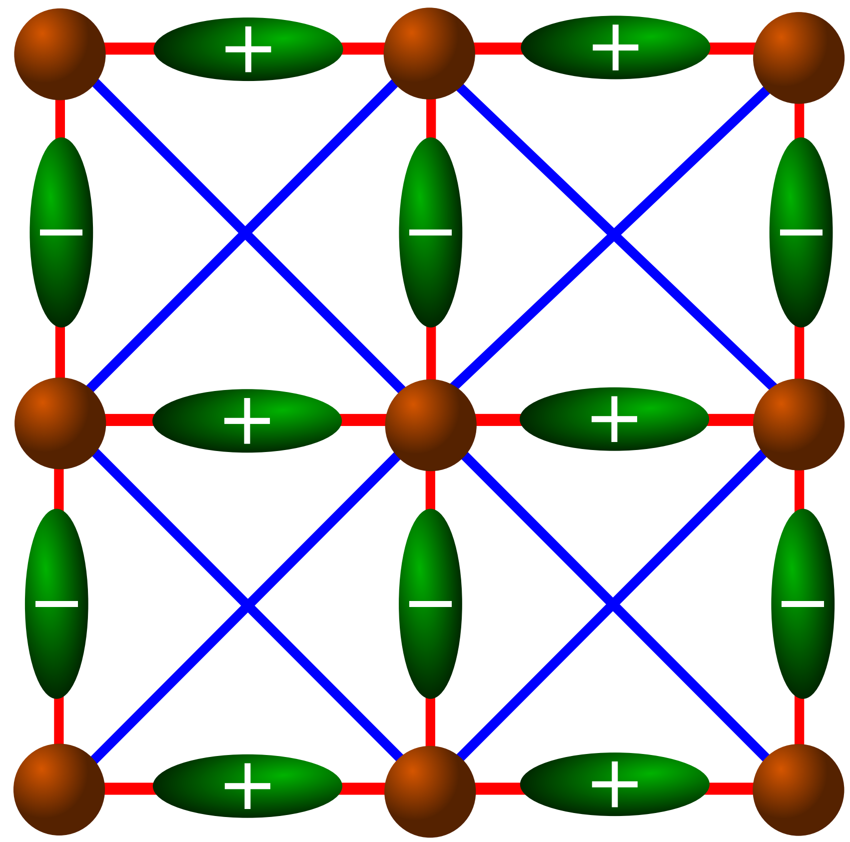


$$\mathcal{O}_{s\text{-SN}} = \mathcal{O}^{zz}_{i,i+\hat{x}} - \mathcal{O}^{xx}_{i,i+\hat{x}} = \mathcal{O}^{zz}_{i,i+\hat{y}} - \mathcal{O}^{xx}_{i,i+\hat{y}}$$

$$\hat{\mathcal{H}}_{s\text{-SN}} = \delta \sum_i (\hat{S}^z_i \hat{S}^z_{i+\hat{x}} - \hat{S}^x_i \hat{S}^x_{i+\hat{x}} - \hat{S}^y_i \hat{S}^y_{i+\hat{x}}) + (\hat{x} \to \hat{y})$$

Identifying the nature of Paramagnetic phase

d-SN

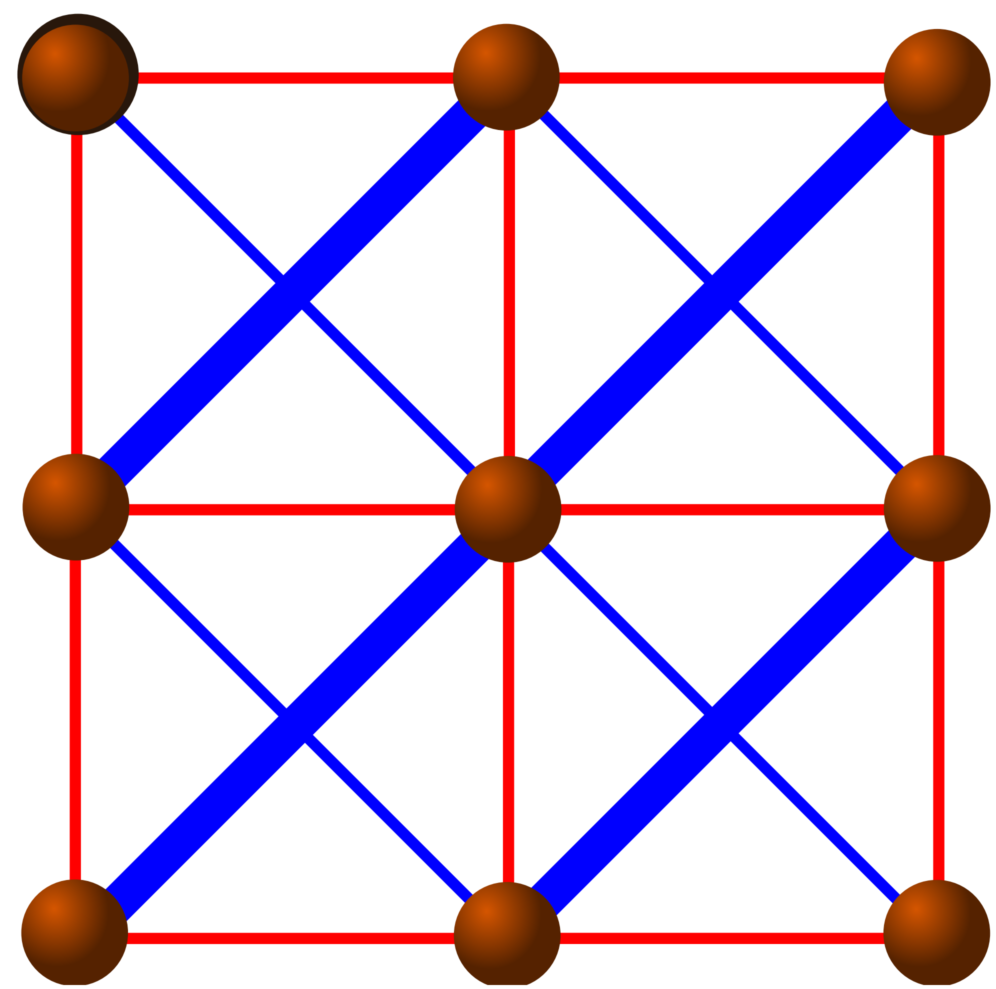


$$\mathcal{O}_{d\text{-SN}} = \mathcal{O}^{zz}_{i,i+\hat{x}} - \mathcal{O}^{xx}_{i,i+\hat{x}} = -(\mathcal{O}^{zz}_{i,i+\hat{y}} - \mathcal{O}^{xx}_{i,i+\hat{y}})$$

$$\hat{\mathcal{H}}_{d\text{-SN}} = \delta \sum_i (\hat{S}^z_i \hat{S}^z_{i+\hat{x}} - \hat{S}^x_i \hat{S}^x_{i+\hat{x}} - \hat{S}^y_i \hat{S}^y_{i+\hat{x}}) - (\hat{x} \to \hat{y})$$

Identifying the nature of Paramagnetic phase

- **LN**



$$\mathcal{O}_{\mathrm{LN}} = \langle \hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_{i+\hat{x}+\hat{y}} \rangle - \langle \hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_{i+\hat{x}-\hat{y}} \rangle$$

$$\hat{\mathcal{H}}_{\mathrm{LN}} = \delta \sum_i (\hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_{i+\hat{x}+\hat{y}} - \hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_{i+\hat{x}-\hat{y}})$$

Nematic response functions

Static (imaginary time-integrated) spin correlator

$$C_{ij}^{\mu\nu} = \int_0^\infty d\tau \langle \hat{S}_i^\mu(\tau) \hat{S}_j^\nu(0) \rangle, \text{ with } \hat{S}_i^\mu(\tau) = e^{\tau \hat{\mathcal{H}}} \hat{S}_i^\mu e^{-\tau \hat{\mathcal{H}}}.$$

$$d\text{-SN: } C_+ = \frac{1}{2}(C_{i,i+\hat{x}}^{zz} + C_{i,i+\hat{y}}^{xx}) \,, \; C_- = \frac{1}{2}(C_{i,i+\hat{y}}^{zz} + C_{i,i+\hat{x}}^{xx}),$$

$$s\text{-SN: } C_+ = C_{i,j}^{zz} \,, \; C_- = C_{i,j}^{xx} \,,$$

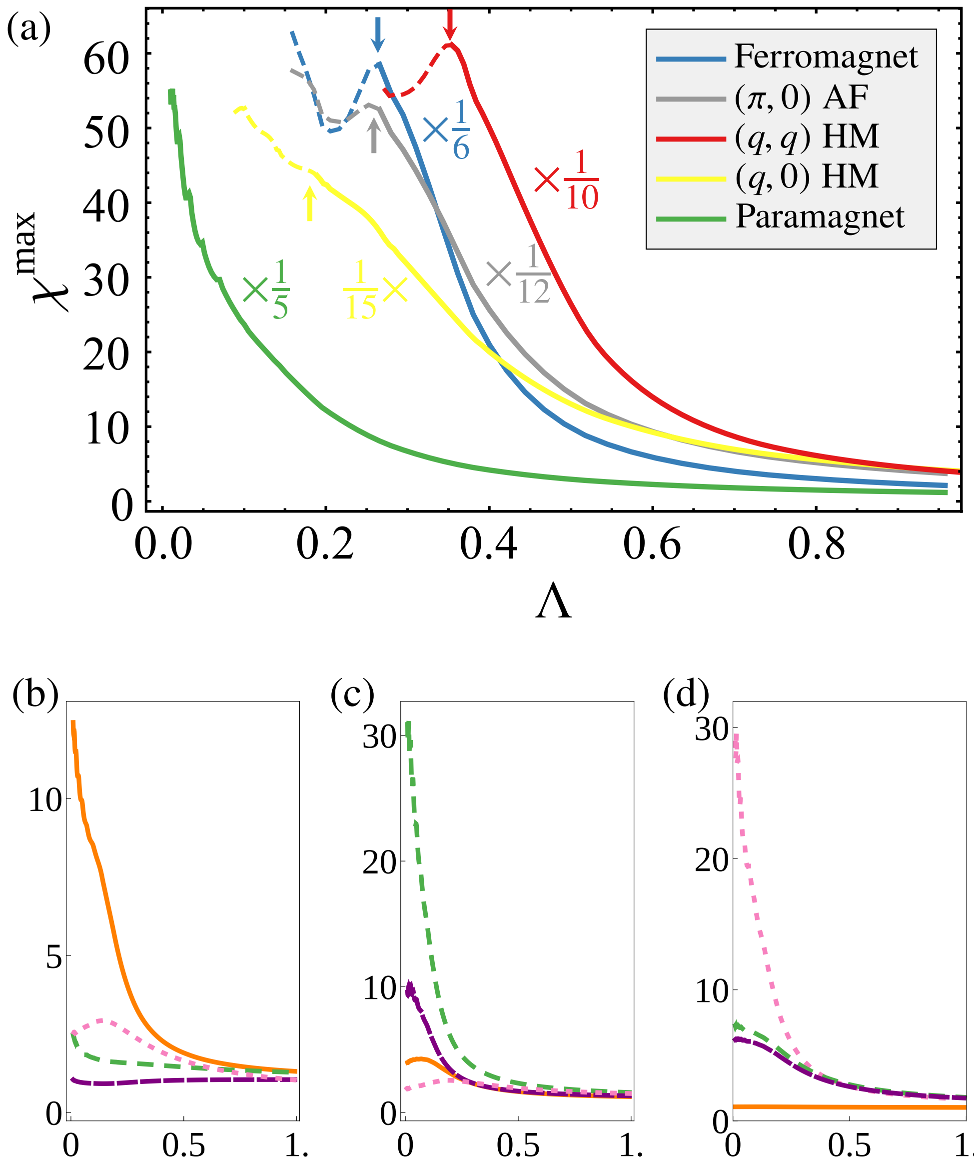
$$\text{LN : } C_+ = C_{i,i+\hat{x}+\hat{y}}^{\mu\mu} \,, \; C_- = C_{i,i+\hat{x}-\hat{y}}^{\mu\mu} \,,$$

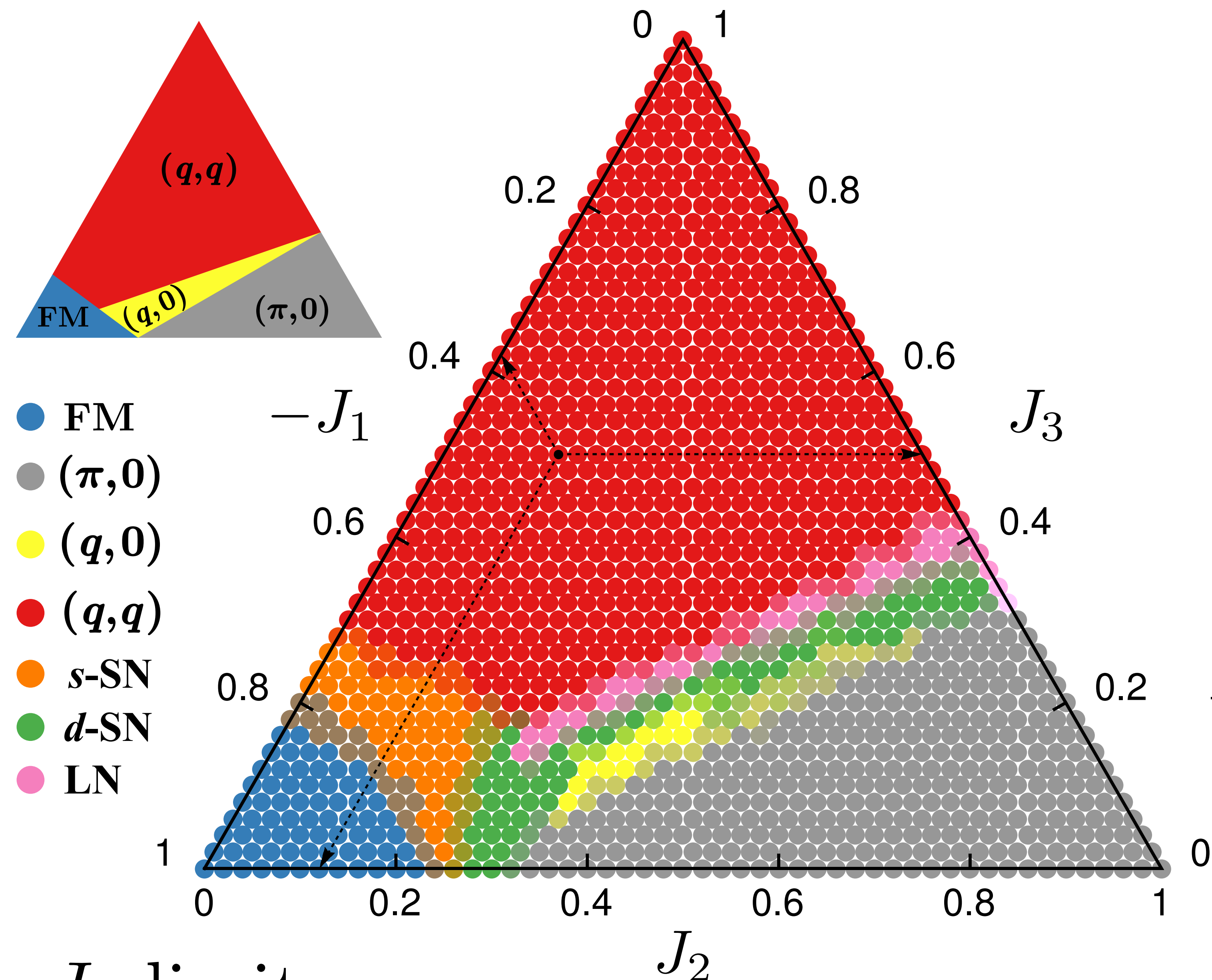
$$\kappa_{\text{nem}} = \frac{J}{\delta} \frac{C_+^\Lambda - C_-^\Lambda}{C_+^\Lambda + C_-^\Lambda}$$

enhancement $\kappa_{\text{nem}} > 1$

rejection $\kappa_{\text{nem}} < 1$

Intertwined Nematic Orders





J_1-J_2 limit

Shannon, Momoi, Sindzingre ' 2006

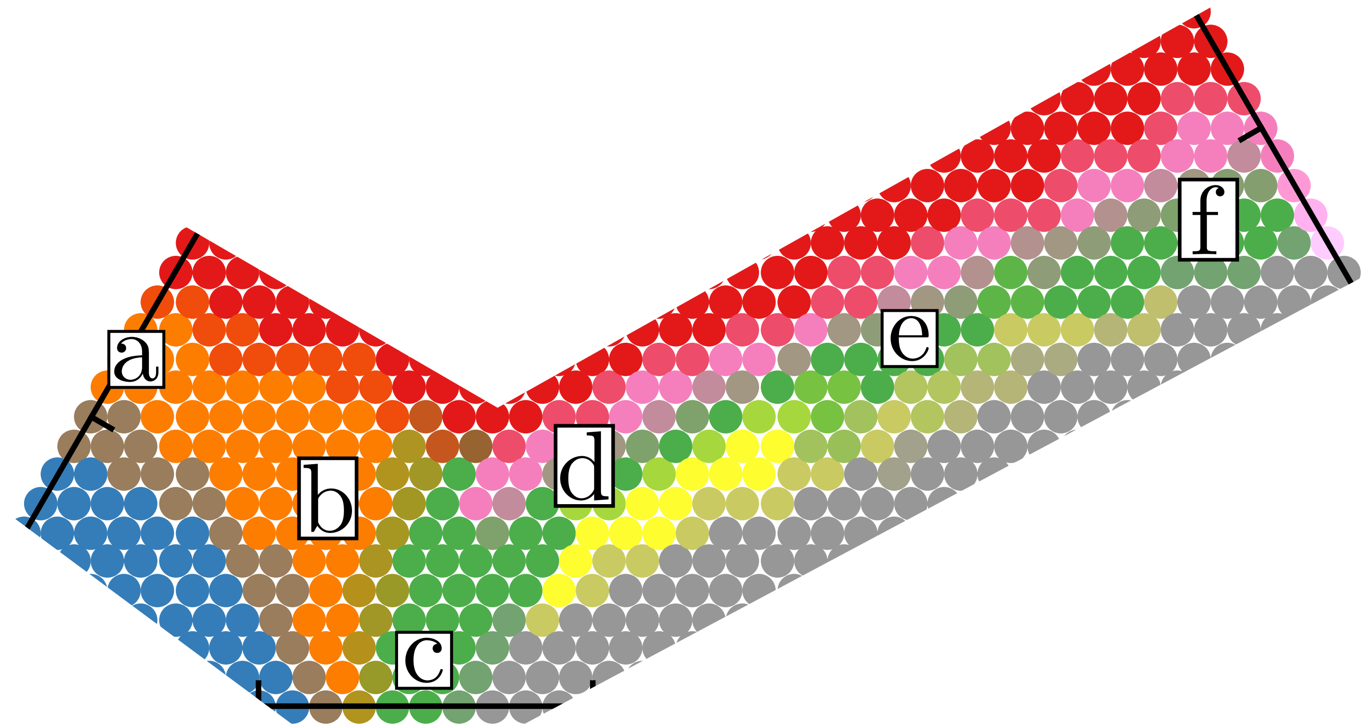
Sindzingre *et al.* ' 2009

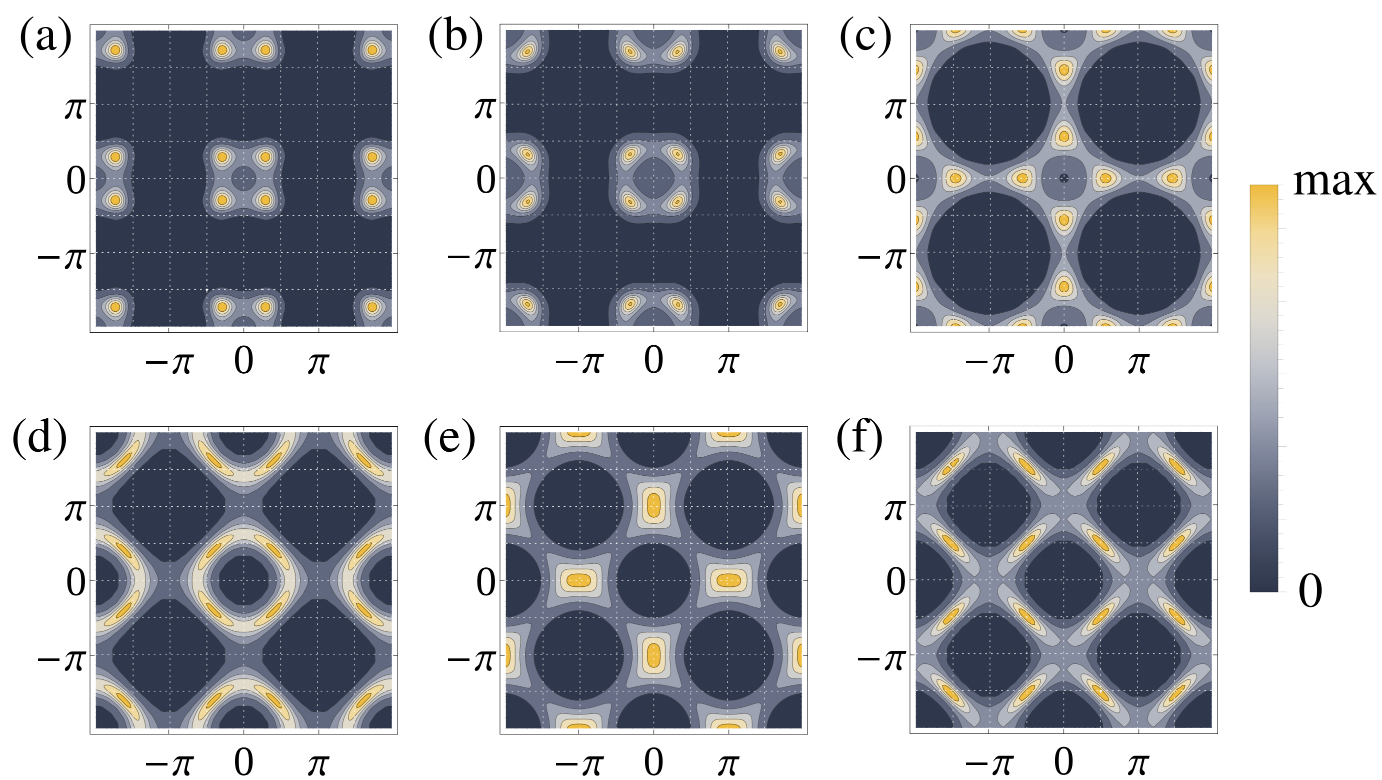
Richter *et al.* ' 2010

Shindou, Yunoki, Momoi ' 2011

* Previous ED studies were inconclusive on the issue of the existence of a Paramagnetic phase
* High-order coupled cluster method found no evidence for a Paramagnetic phase
* Variational Monte Carlo study employing projected BCS wave-functions found an extended Paramagnetic phase

Susceptibility Profiles of Paramagnetic phases





CONCLUSIONS

- Pseudo-fermion Functional Renormalisation group method provides a powerful method to study two and three-dimensional spin models with arbitrary two-body interactions.
- Nematic order and valence-bond crystal order formation can be investigated.
- Finite-temperature correlation profiles are straightforwardly computed. Quantities such as Néel temperature can be accurately estimated, in light of the correspondence between the RG cutoff parameter and temperature.
- The method has a very efficient scaling with increasing system size, enabling one to simulate very large system sizes ~20x20x20 sites thus enabling one to obtain reliable estimates in the thermodynamic limit.


Thank you !
Greetings from the fair city of Würzburg