Extended degeneracy in the square J_1-J_2-J_3 antiferromagnet

R. Ganesh
Bimla Danu

IMSc Chennai

Gautam Nambiar

IISc, Bangalore & IMSc, Chennai

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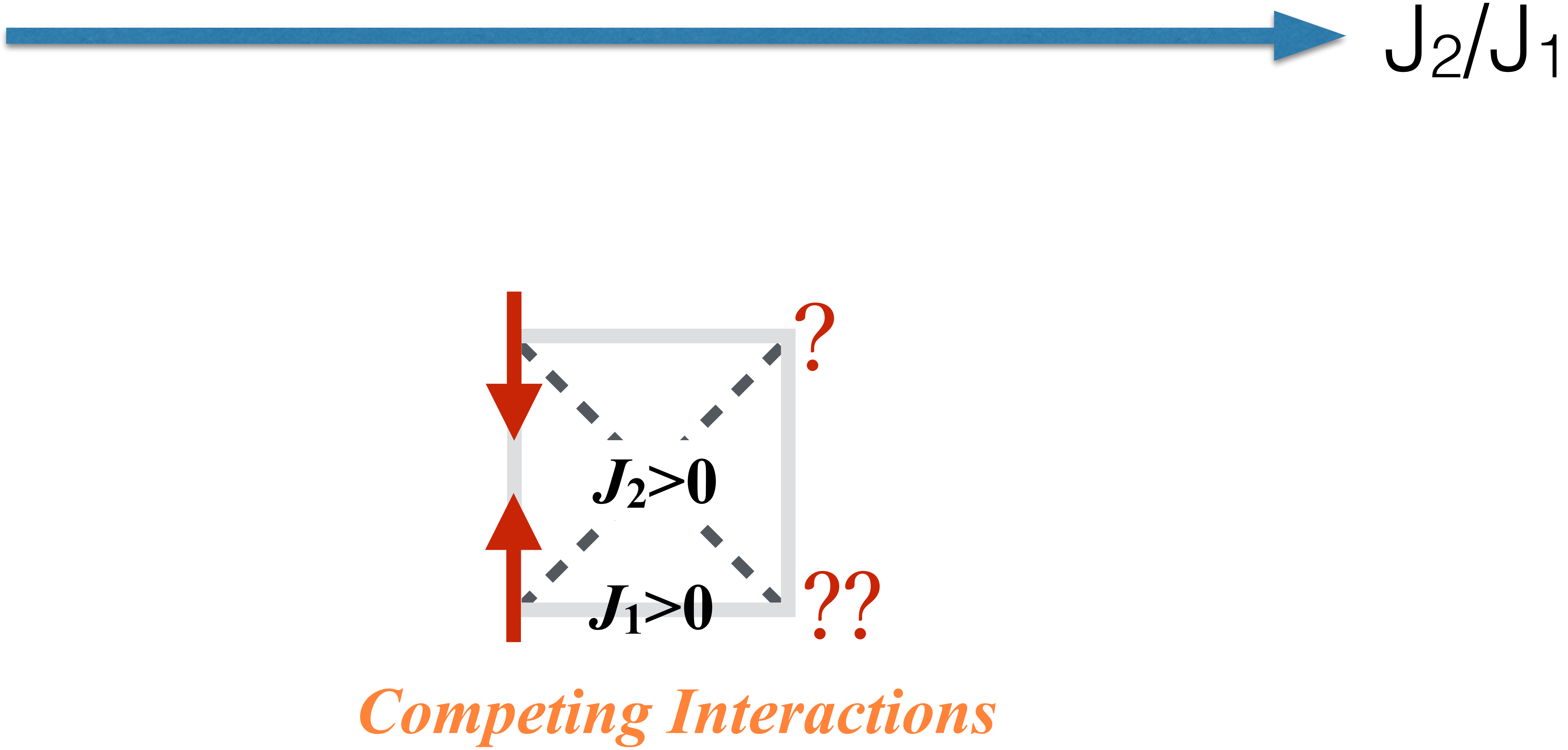
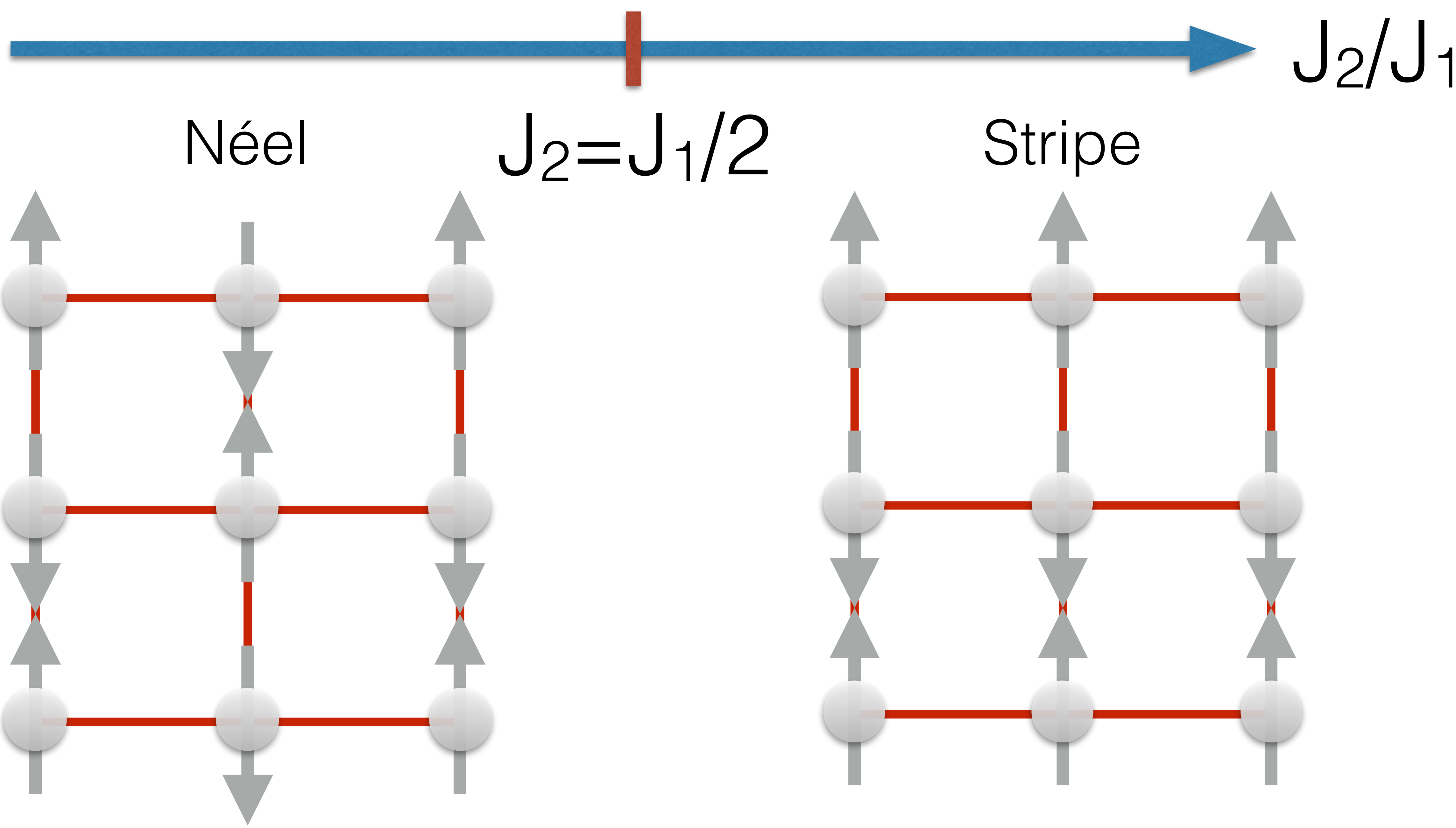
Square J_1-J_2 antiferromagnet



Square J_1-J_2 antiferromagnet

Classical limit



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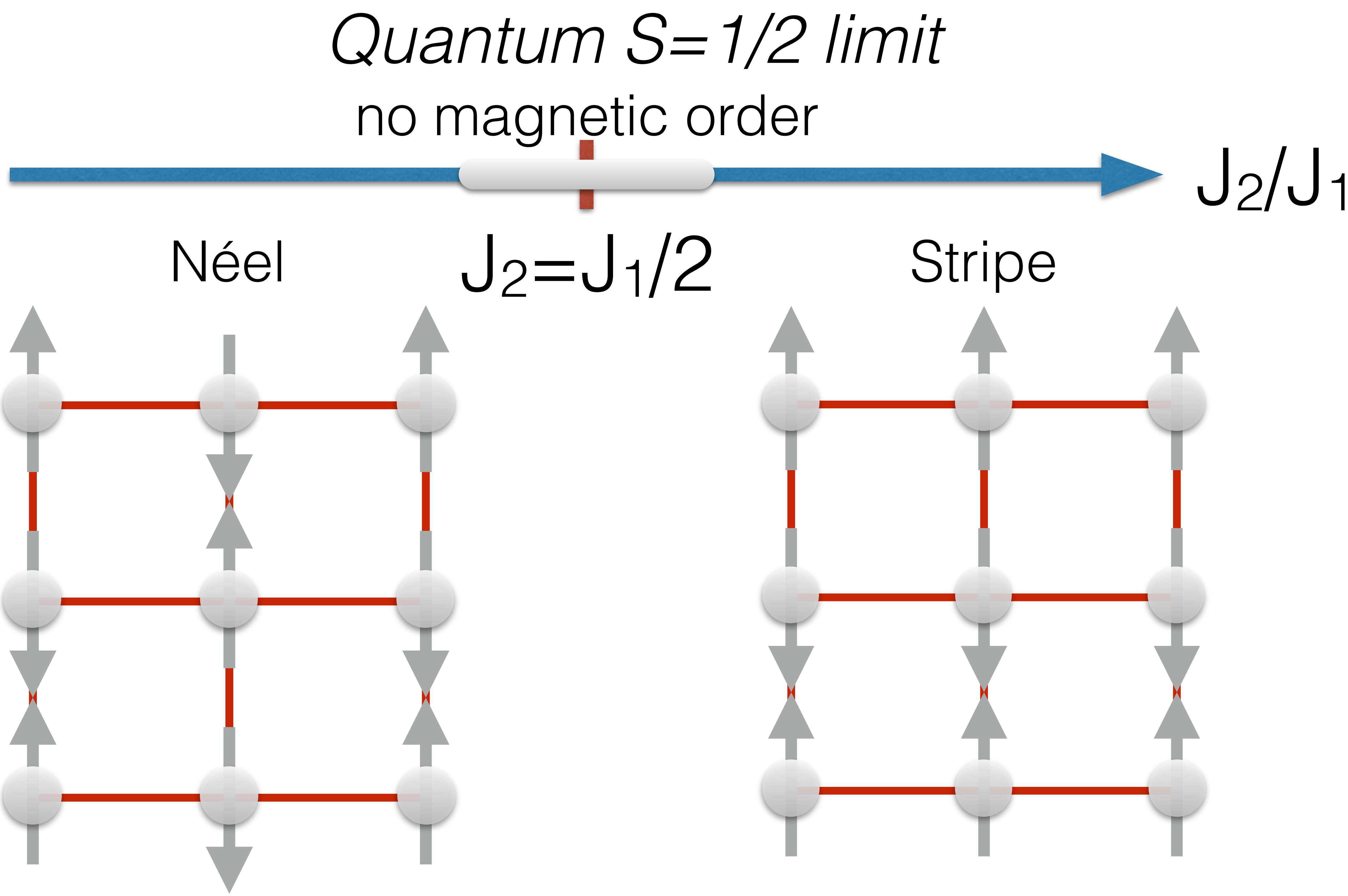
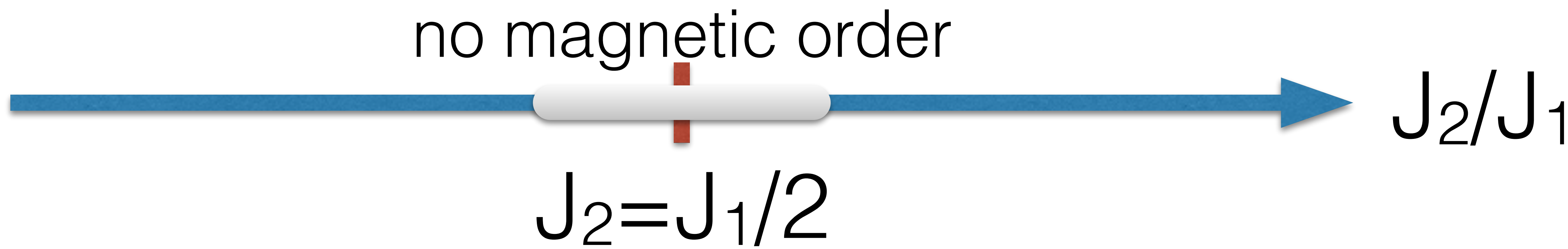


Square J_1-J_2 antiferromagnet

Quantum S=1/2 limit



Columnar VBS	ED	Kotov et al, PRB 1999
Staggered VBS	RG of coupled chains	Metavitsiadis et al, PRB 2014
Plaquette singlet order	ED and QMC	Capriotti and Sorella, PRL 2000
Gapped spin liquid	DMRG	Jiang et al, PRB 2012
Gapless spin liquid	variational wavefunction	Hu et al, PRB 2013

Square J_1-J_2 antiferromagnet

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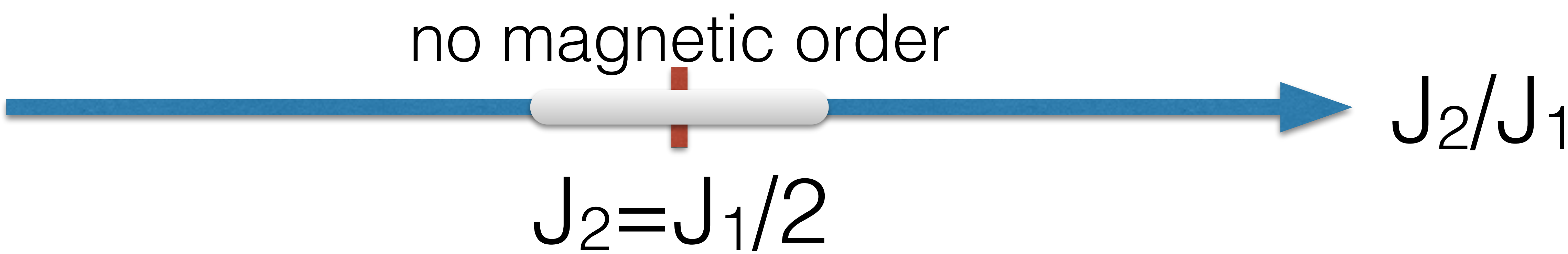

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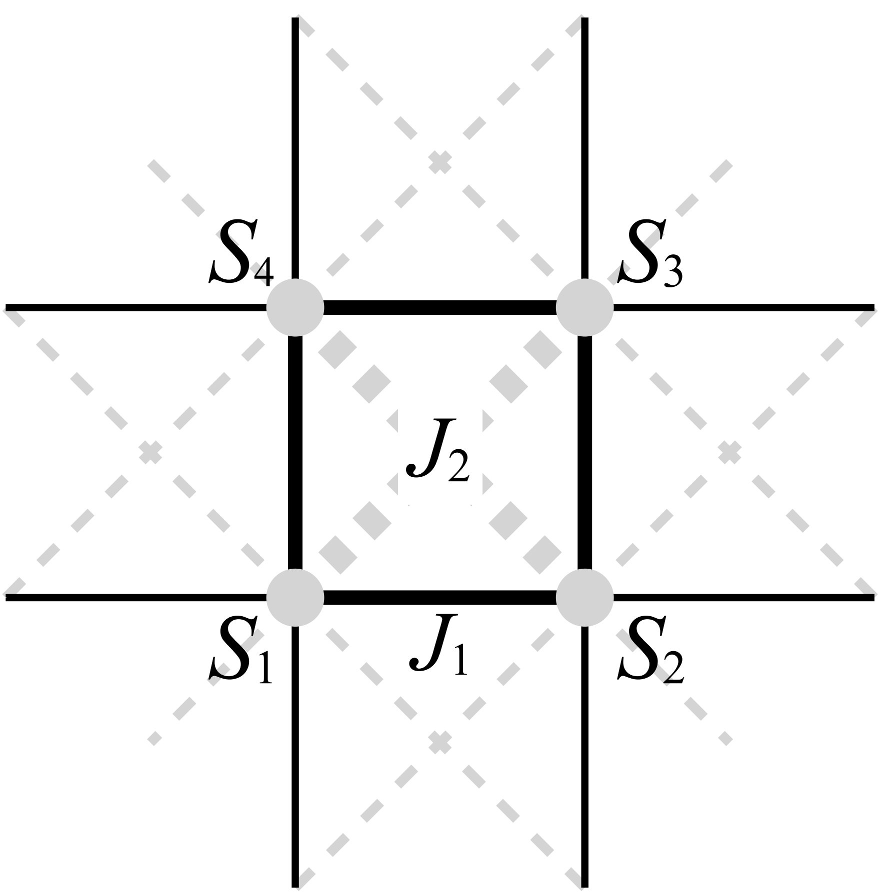
Need new physical ideas to make progress!

Classical degeneracy

Origin of quantum disordered phase:
extended classical degeneracy at $J_2=J_1/2$

$$H_{J_2=J_1/2} = \sum_{\boxtimes} H_{\boxtimes} = \sum_{\boxtimes} \frac{J_1}{4}(\mathbf{S}_1+\mathbf{S}_2+\mathbf{S}_3+\mathbf{S}_4)^2$$

Chandra, Coleman and Larkin, PRL 1990



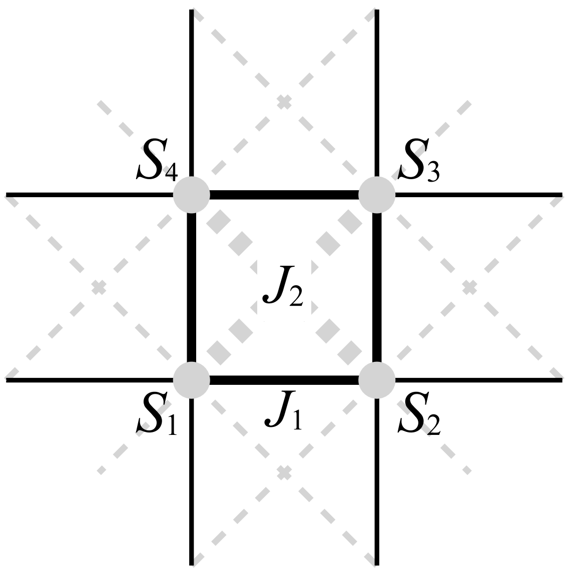
Energy is the sum of positive terms
⇒ ground state should satisfy

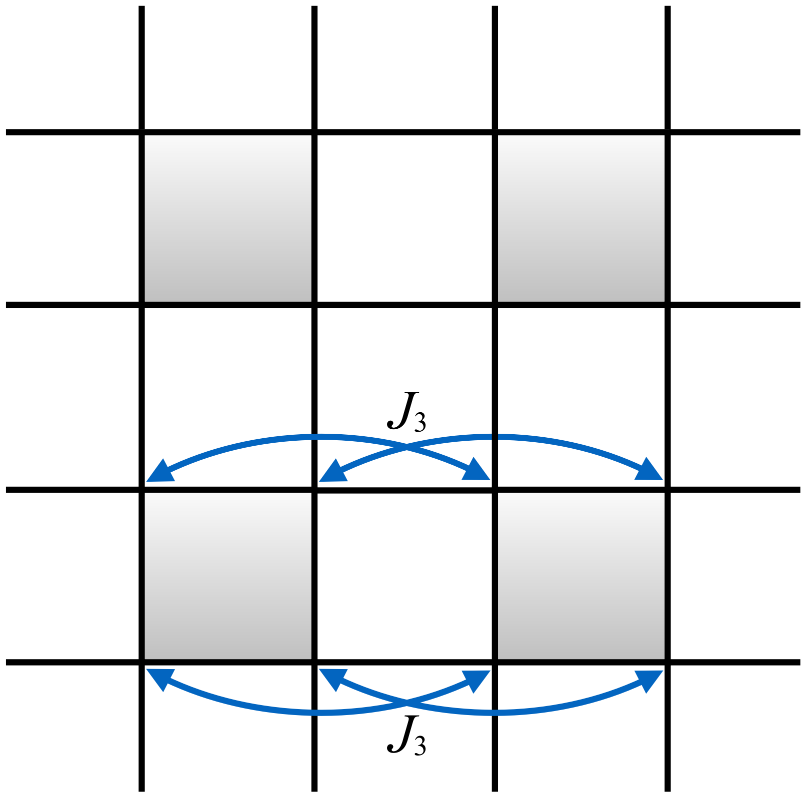
$$\mathbf{S}_1+\mathbf{S}_2+\mathbf{S}_3+\mathbf{S}_4=0$$

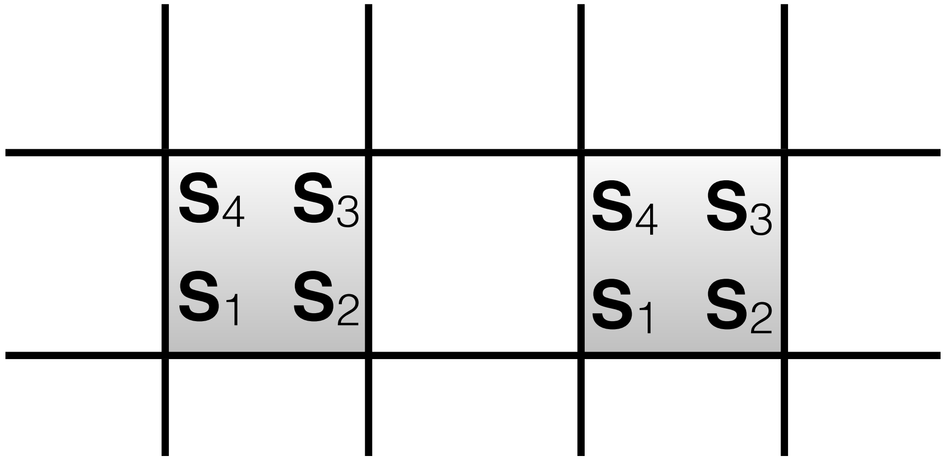
on every square
⇒ infinite degeneracy!

high frustration — allows several competing phases

Tuning knob to reduce degeneracy: ferromagnetic J_3







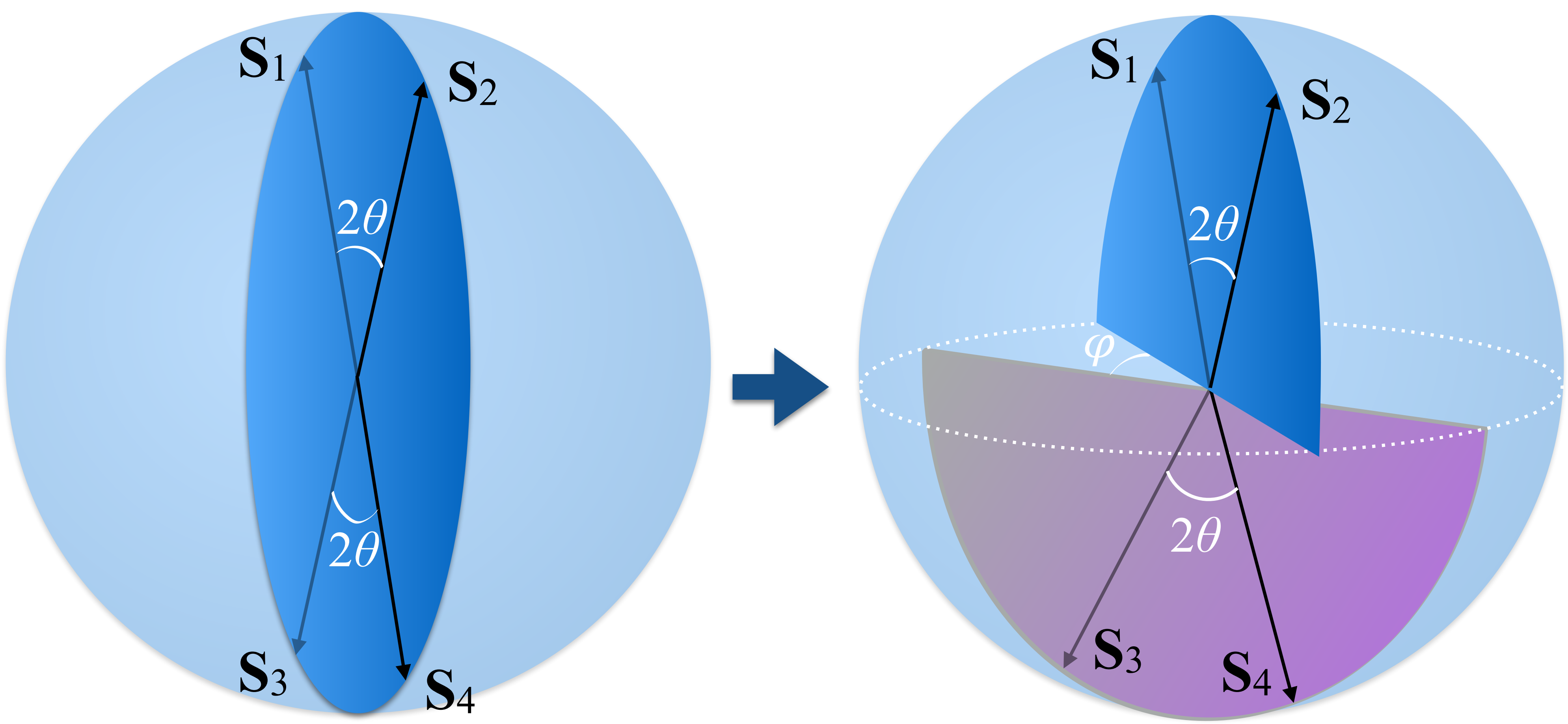
$J_3<0 \Rightarrow$ shaded squares must have the same configuration

- four site magnetic unit cell
- shaded square must satisfy zero-sum condition
- unshaded squares automatically satisfy zero-sum condition
- free parameters: (θ,φ) for just one shaded square

Zero-sum condition on a single square

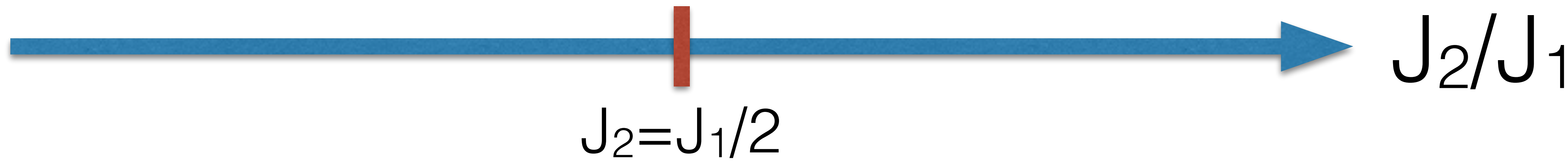
Four spins with the constraint $\mathbf{S}_1 + \mathbf{S}_2 + \mathbf{S}_3 + \mathbf{S}_4 = 0$

⇒ two free parameters upto a global rotation: $\theta \in [0,\pi]$ and $\varphi \in [0,2\pi)$

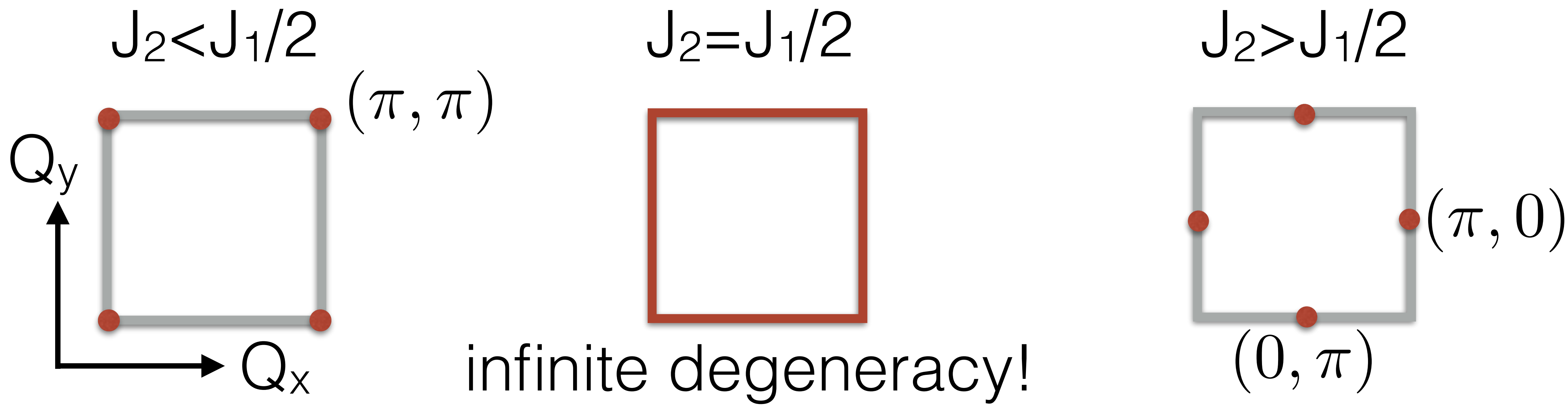


(θ,φ) define an emergent vector order parameter!

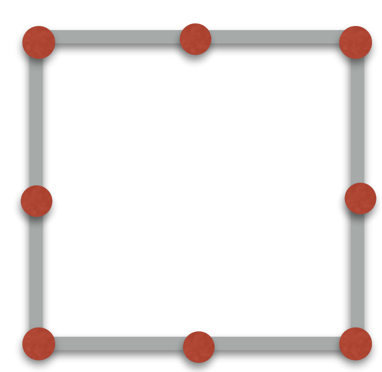
Square J_1-J_2 classical AFM



Spiral ansatz: $\mathbf{S}_i = S\,\{\cos(\mathbf{Q}\cdot\mathbf{r}_i)\hat{x} + \sin(\mathbf{Q}\cdot\mathbf{r}_i)\hat{y}\}$

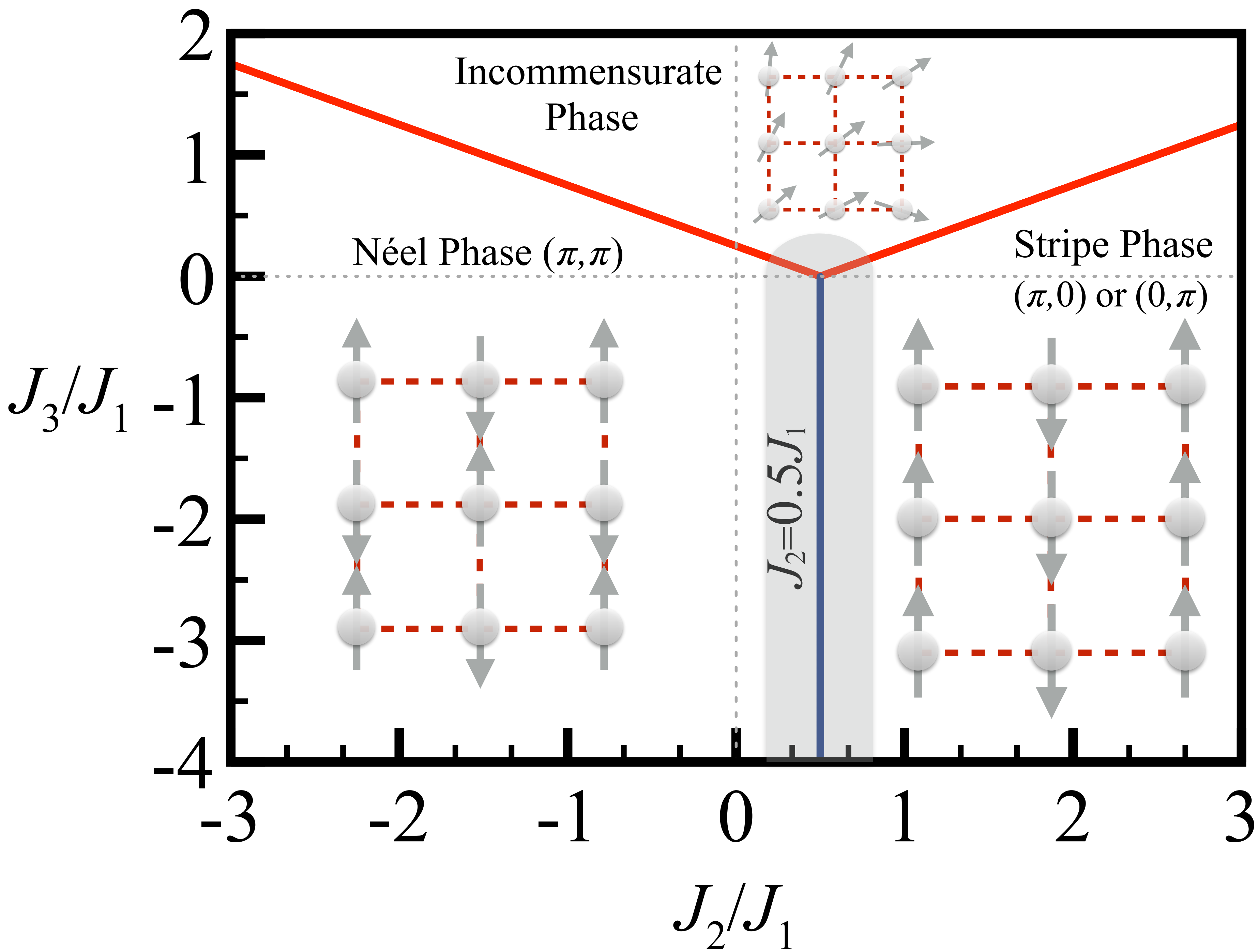


Selected spirals with $J_3 < 0$



J1-J2-J3 classical phase diagram

Spiral ansatz: $\mathbf{S}_i = S\left\{\cos(\mathbf{Q}\cdot\mathbf{r}_i)\hat{x} + \sin(\mathbf{Q}\cdot\mathbf{r}_i)\hat{y}\right\}$



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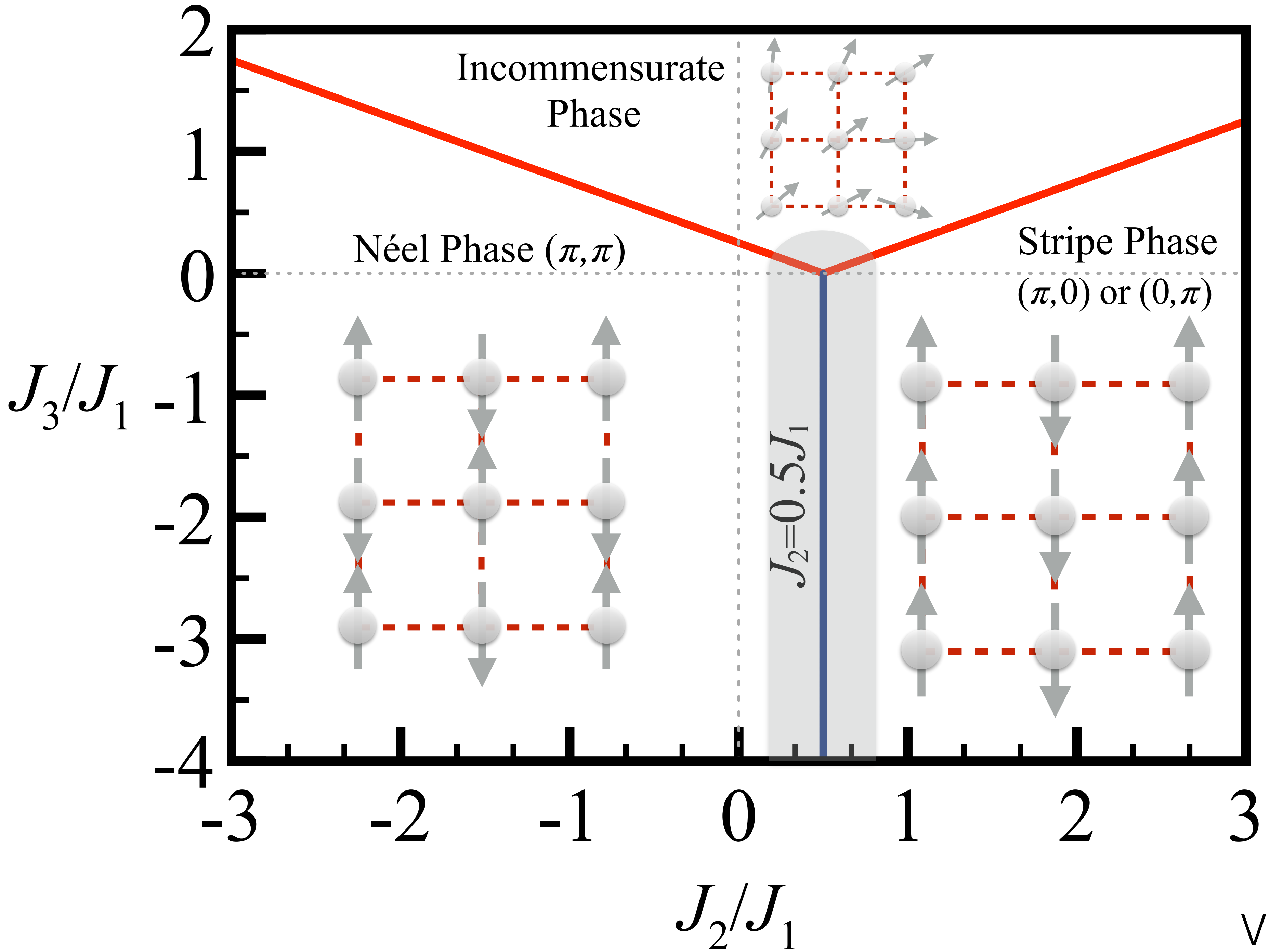
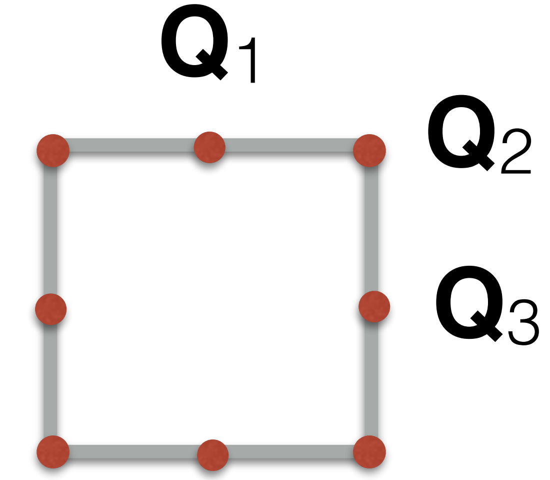


Selected Q's along line of interest



Three Q vectors satisfy 2Q ≡ 0

⇒ spirals can coexist

Villain, J. Phys. France 1977

$J_2 = J_1/2$; $J_3 < 0$ line

Coexisting spirals:

$$\mathbf{S}_i = S\{\cos(\mathbf{Q}_1.\mathbf{r}_i)\hat{u} + \cos(\mathbf{Q}_2.\mathbf{r}_i)\hat{v} + \cos(\mathbf{Q}_3.\mathbf{r}_i)\hat{w}\}$$

Uniform spin length at every site ⇒

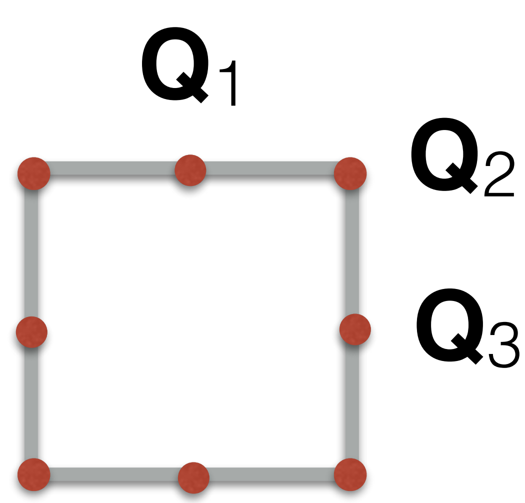
$$|\hat{u}|^2 + |\hat{v}|^2 + |\hat{w}|^2 = 1$$

$$\hat{u}\cdot\hat{v} = \hat{v}\cdot\hat{w} = \hat{w}\cdot\hat{u} = 0$$

This reduces to a four site magnetic unit cell with

$$\mathbf{S}_1 + \mathbf{S}_2 + \mathbf{S}_3 + \mathbf{S}_4 = 0$$

Selected spirals with $J_3 < 0$



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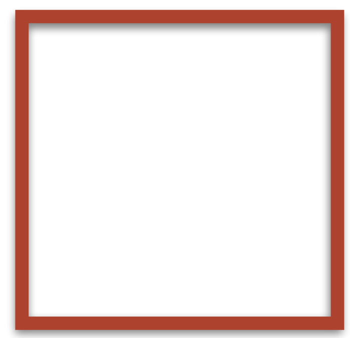
Villain, J. Phys. France 1977

$J_2 = J_1/2$; $J_3 = 0$ g.s. degeneracy

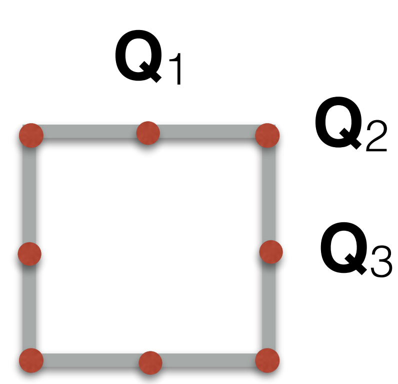
Spiral ansatz: $\mathbf{S}_i = S\left\{\cos(\mathbf{Q}\cdot\mathbf{r}_i)\hat{x} + \sin(\mathbf{Q}\cdot\mathbf{r}_i)\hat{y}\right\}$

Selected **Q** values 

g.s. manifold composed of two sectors

Xiong and Wen 2013

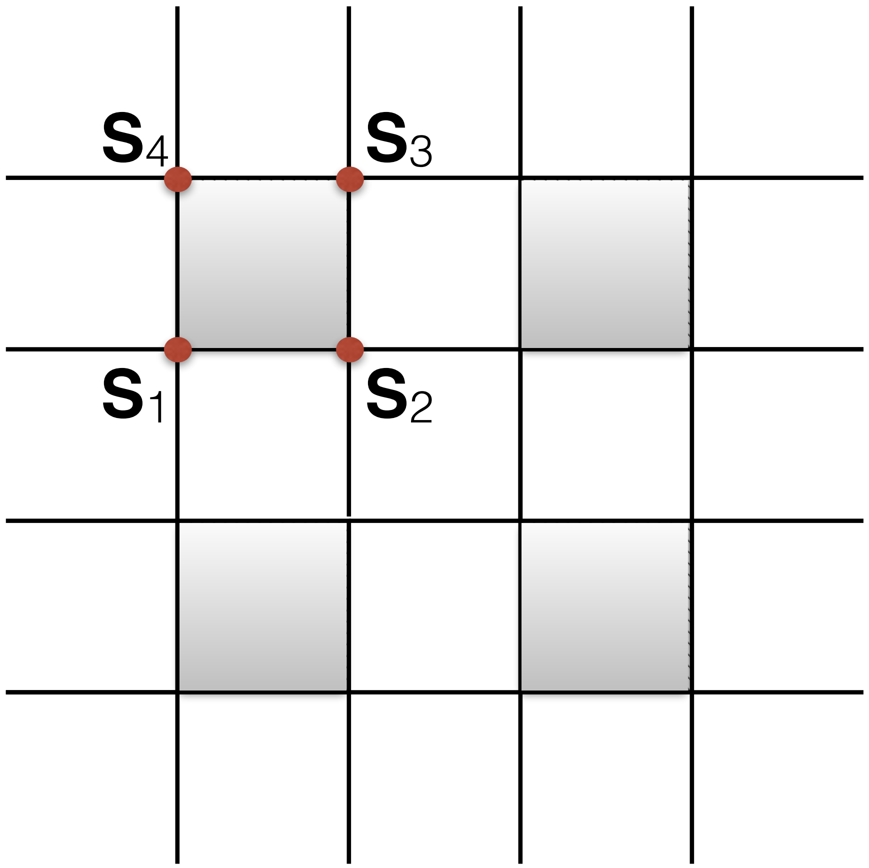
single spiral states with any Q on the BZ boundary



coexistence states with **Q**$_1$, **Q**$_2$ and **Q**$_3$

- ferromagnetic J3 picks this sector

$J_2 = J_1/2$; $J_3 < 0$ line



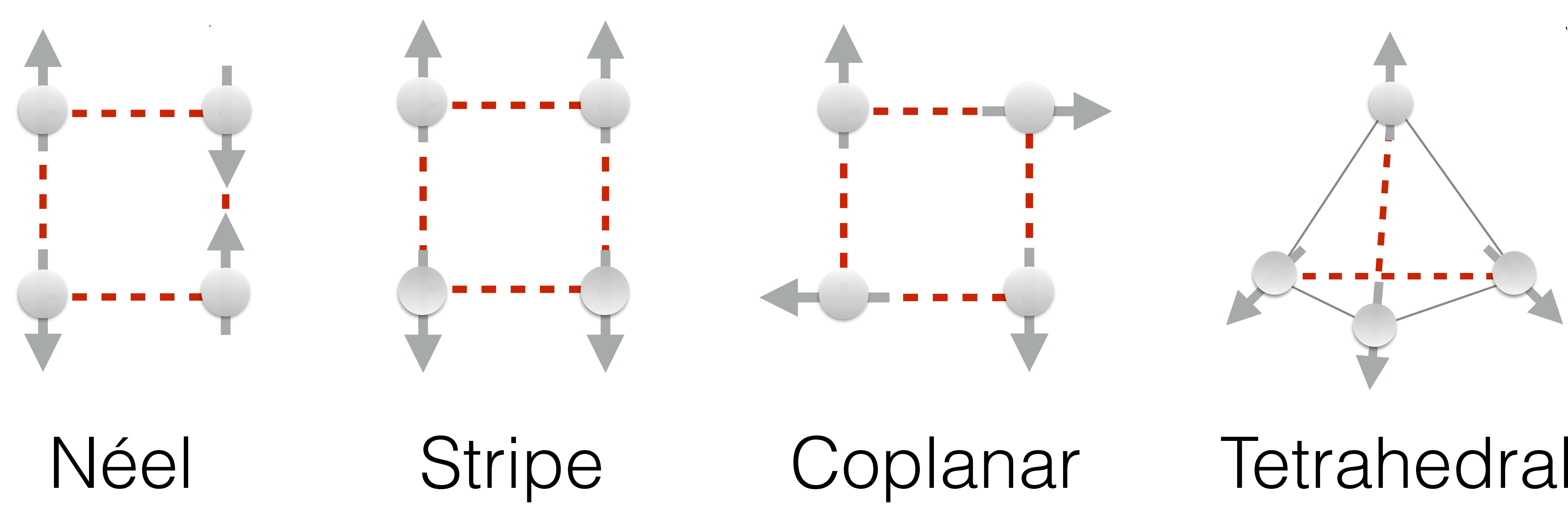
Classical ground state manifold:
four site magnetic unit cell with the condition

$$\mathbf{S}_1 + \mathbf{S}_2 + \mathbf{S}_3 + \mathbf{S}_4 = 0$$

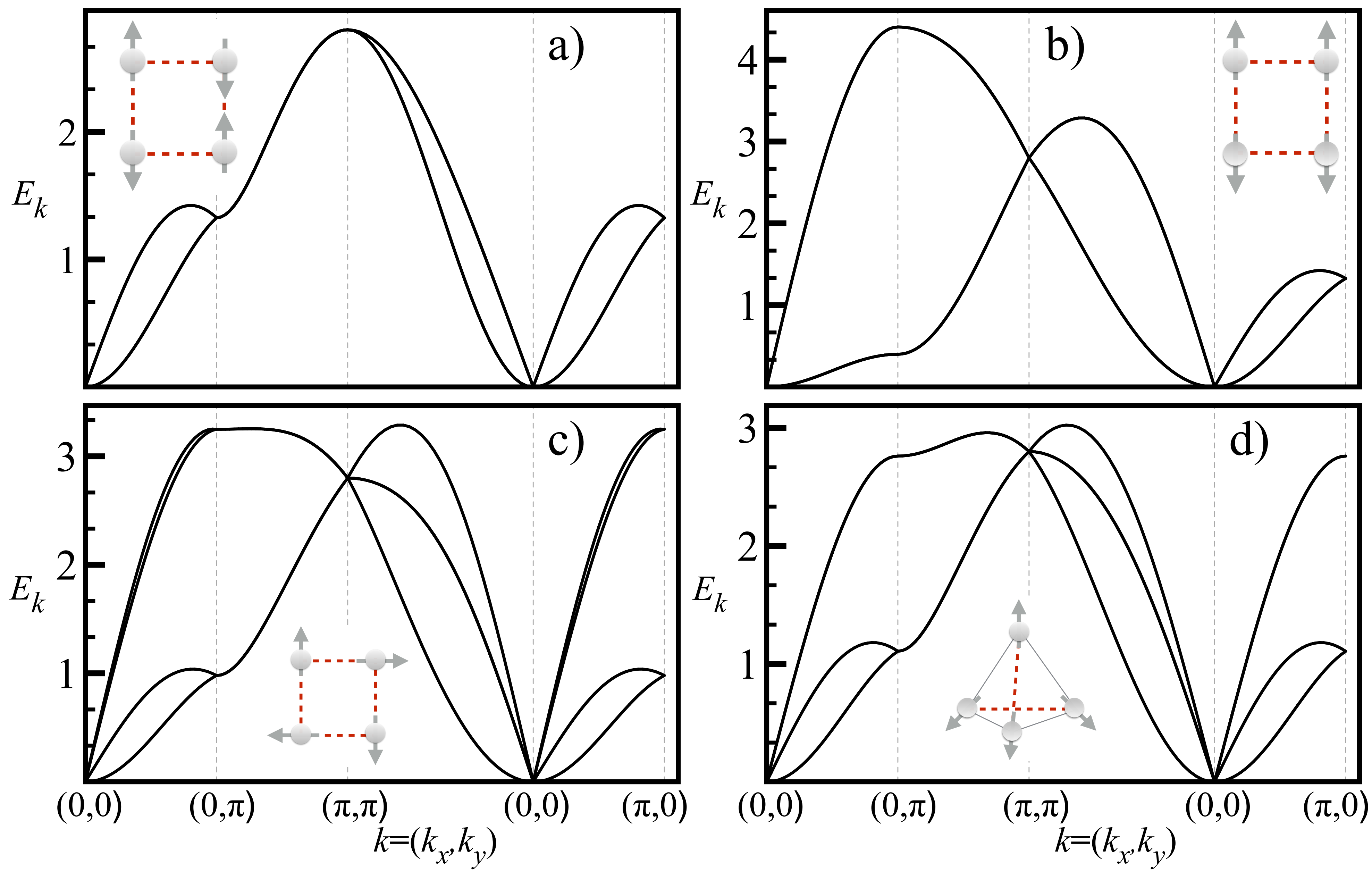
⇒ two parameter family of states

parametrised by (θ,φ)

Some (symmetric) ground states from the manifold:



Spin wave fluctuations

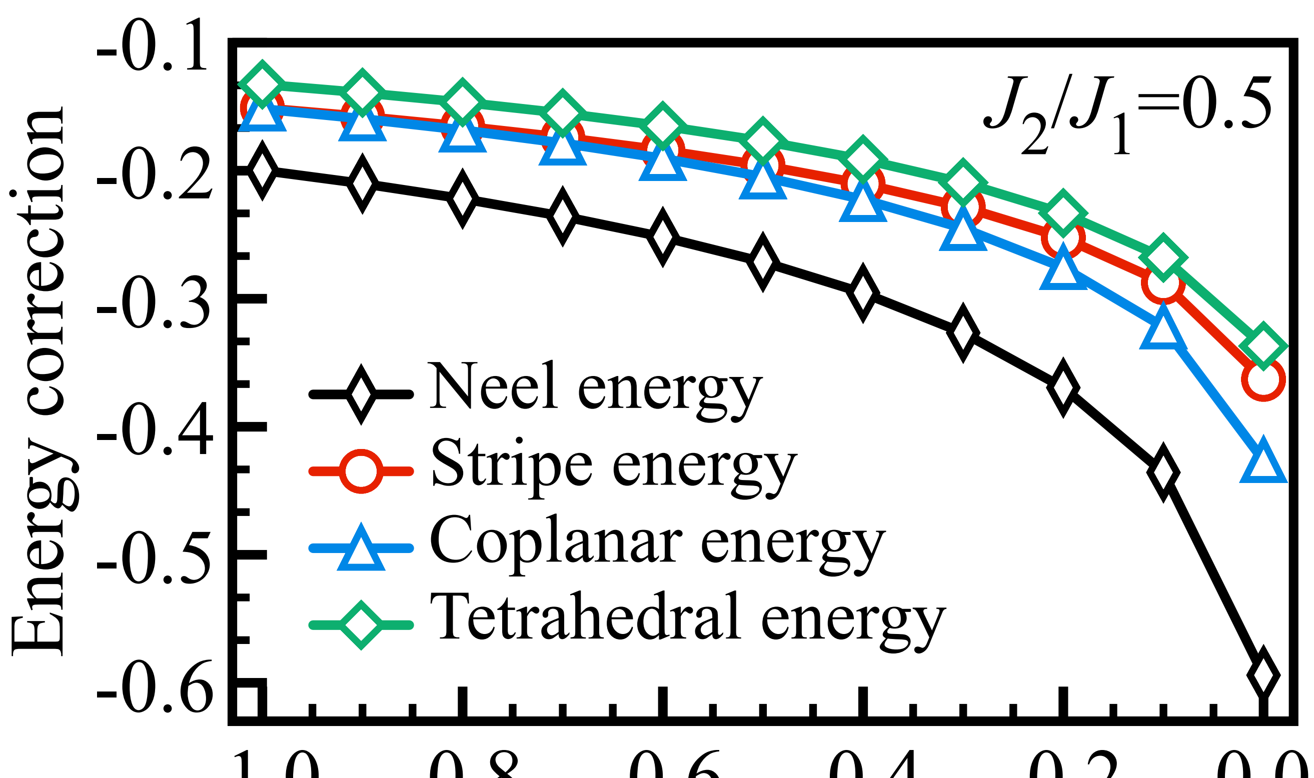


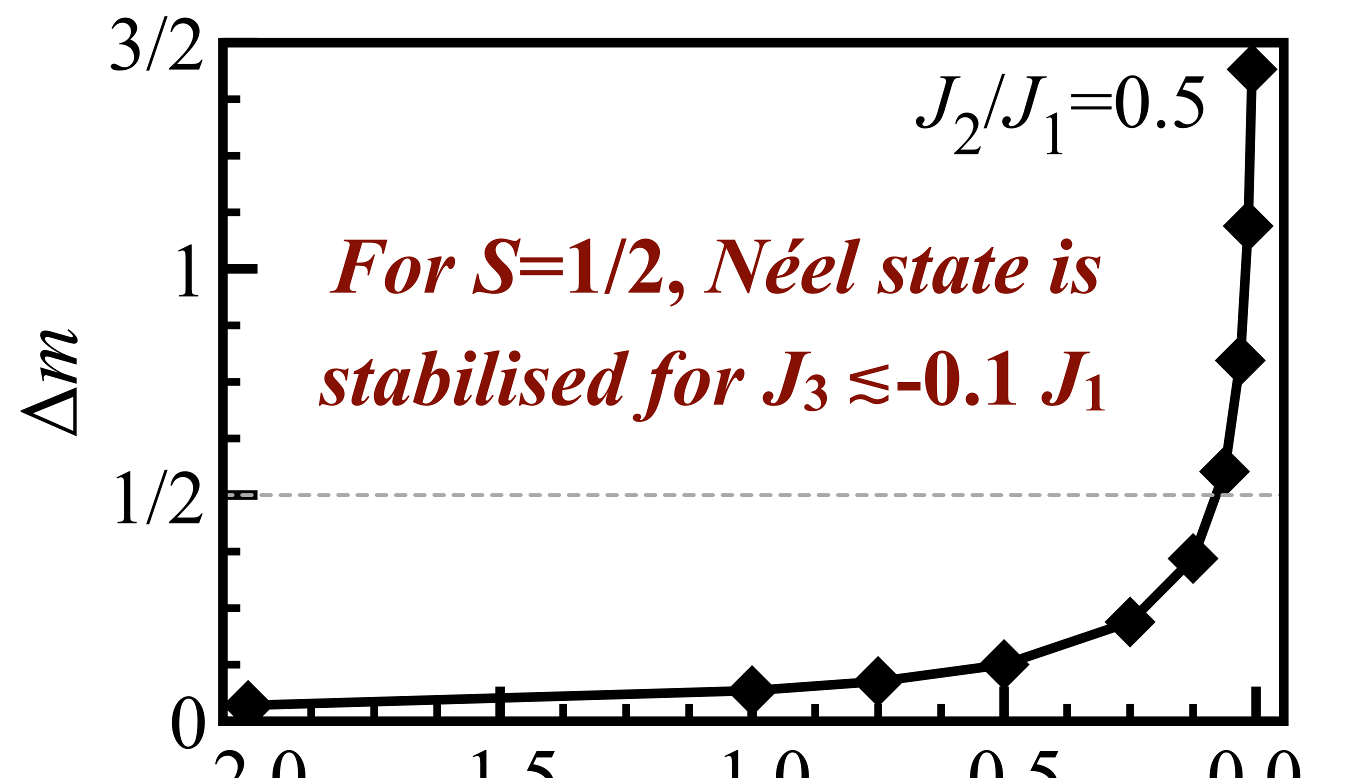
Two kinds of Goldstone modes occur in every g.s.:
linear ($\varepsilon_{\mathbf{k}} \sim k$) - characteristic of anti-ferromagnetism
quadratic ($\varepsilon_{\mathbf{k}} \sim k^2$) - characteristic of ferromagnetism

Quantum g.s. selection by spin waves

Holstein Primakov spin wave theory for spin-S: $E_{state} = S^2 E_{classical} + S \underbrace{\sum_{\mathbf{k}} \sum_j \epsilon_{j,\mathbf{k}}}$

zero point energy of spin waves (1/S correction) - breaks degeneracy





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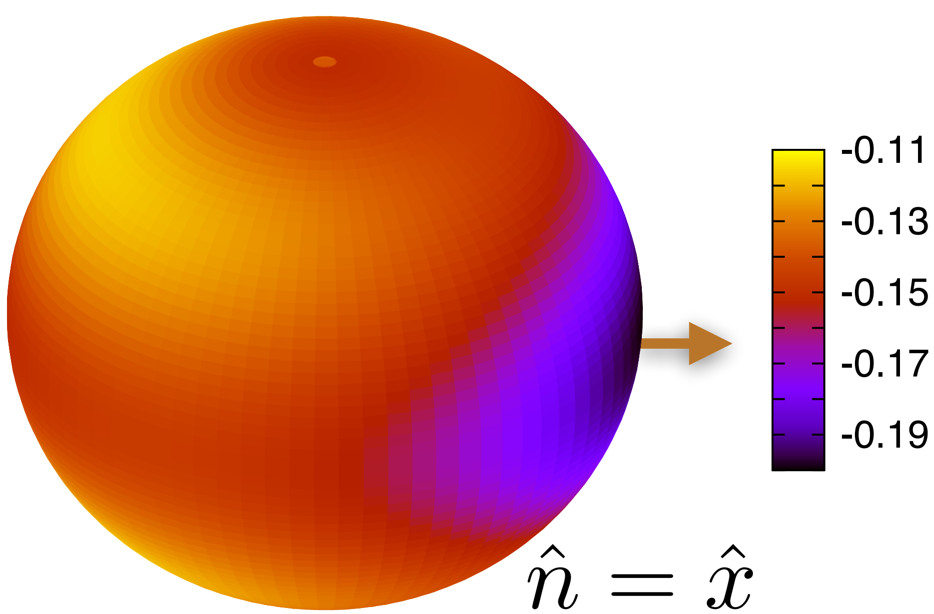
Zero point energy vs. (θ,φ)



$\hat{n} = \hat{x}$

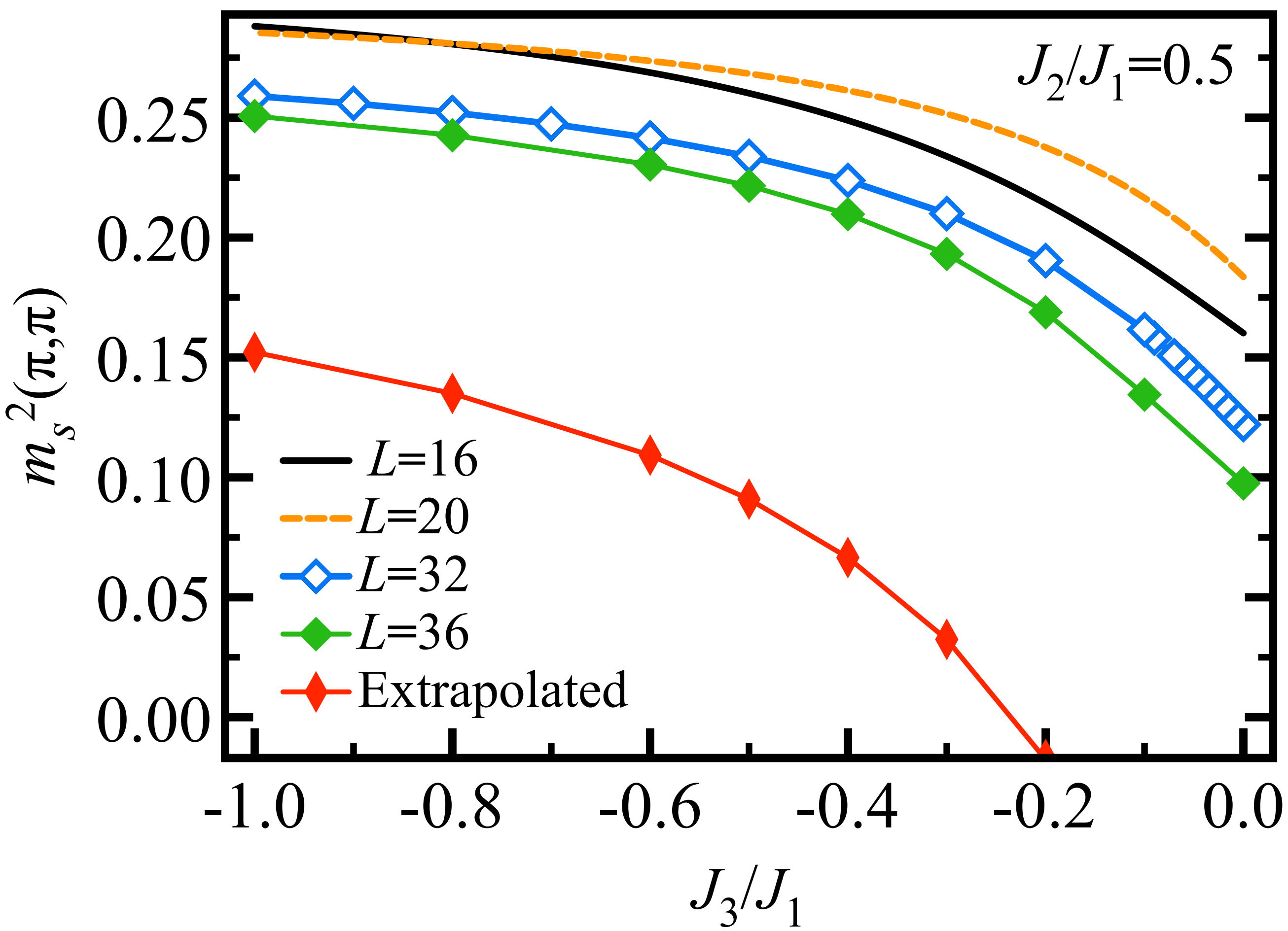
$\mathbf{Q}=(\pi,\pi)$

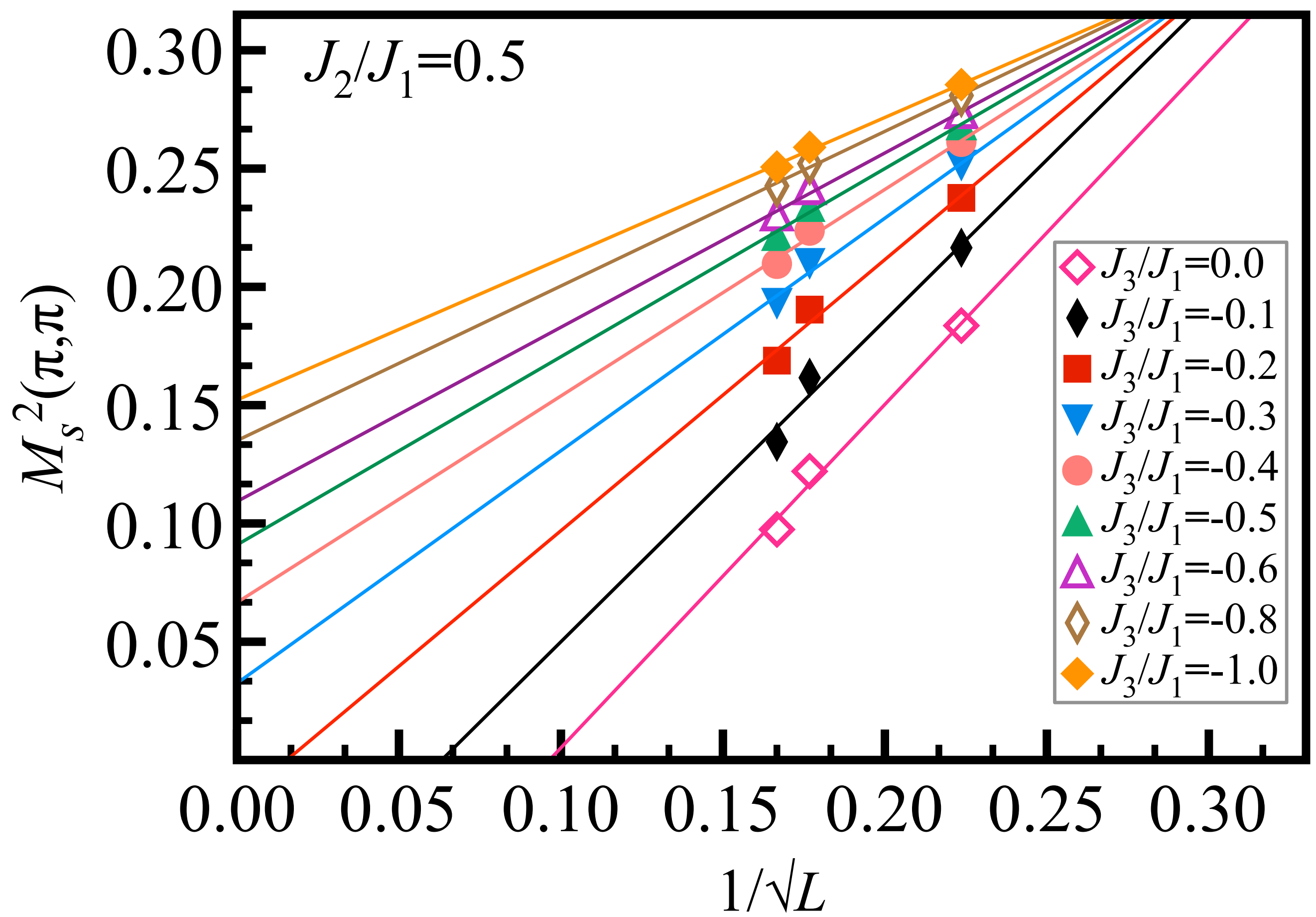
Zero point energy is minimum for Néel state,

$\{\theta,\varphi\} = \{\pi/2, 0\}$

$\Rightarrow$ quantum fluctuations ‘select’ Néel order

Exact diagonalisation for S=1/2



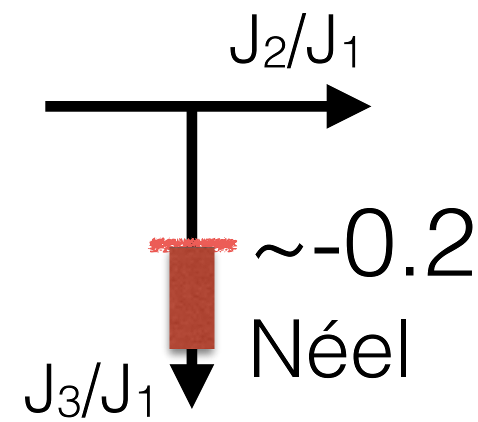


Néel moment in the ground state

$$m_s^2(\mathbf{Q}) = \frac{\mathbf{1}}{\mathbf{L^2}} \sum_{\mathbf{i,j}} \langle \mathbf{S_i.S_j} \rangle \mathbf{e}^{\mathbf{iQ.(r_i - r_j)}}$$

Extrapolated to the thermodynamic limit

$$M_s^2(\mathbf{Q}) = \mathbf{m_s^2}(\mathbf{Q}) + \frac{const}{\sqrt{\mathbf{L}}}$$



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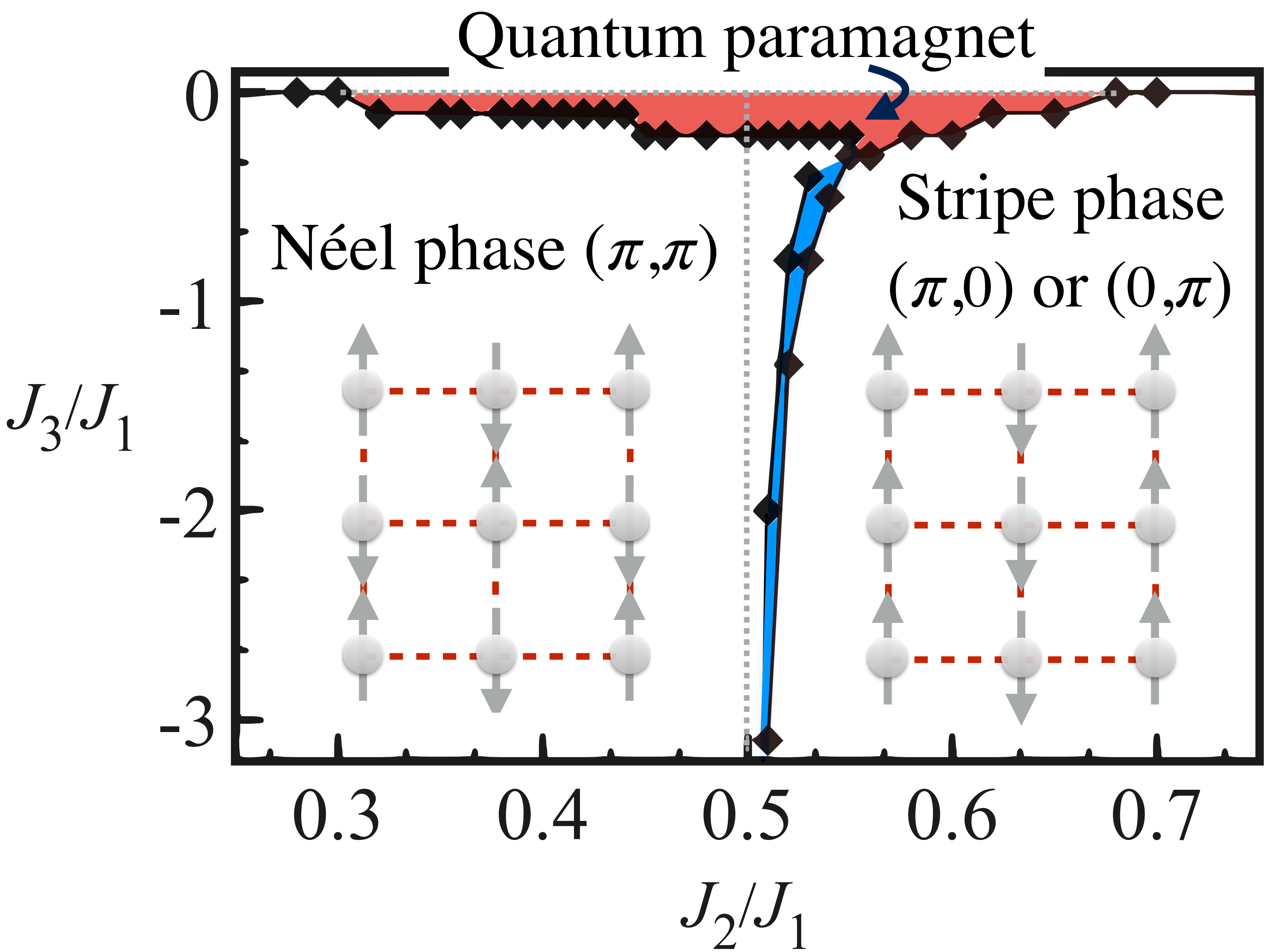
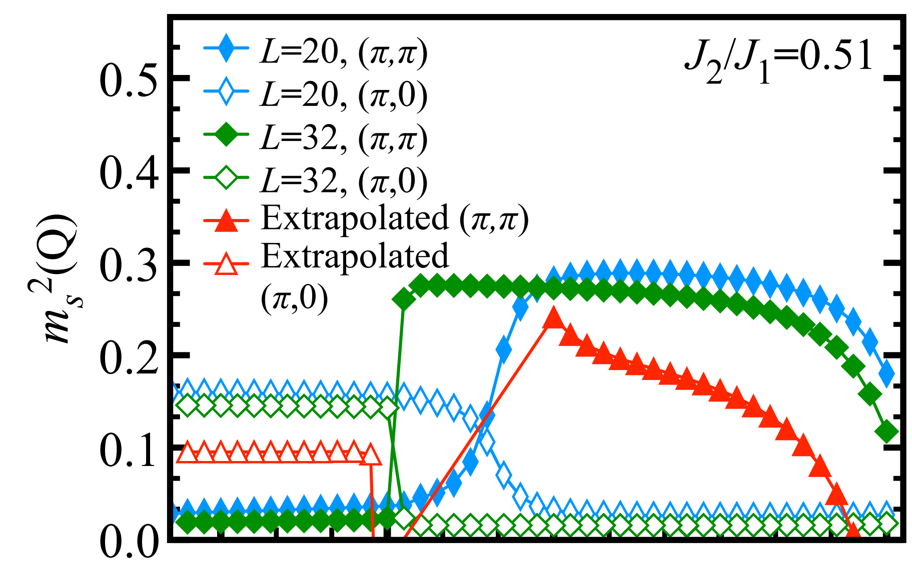
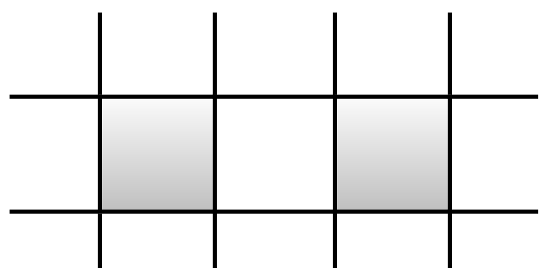




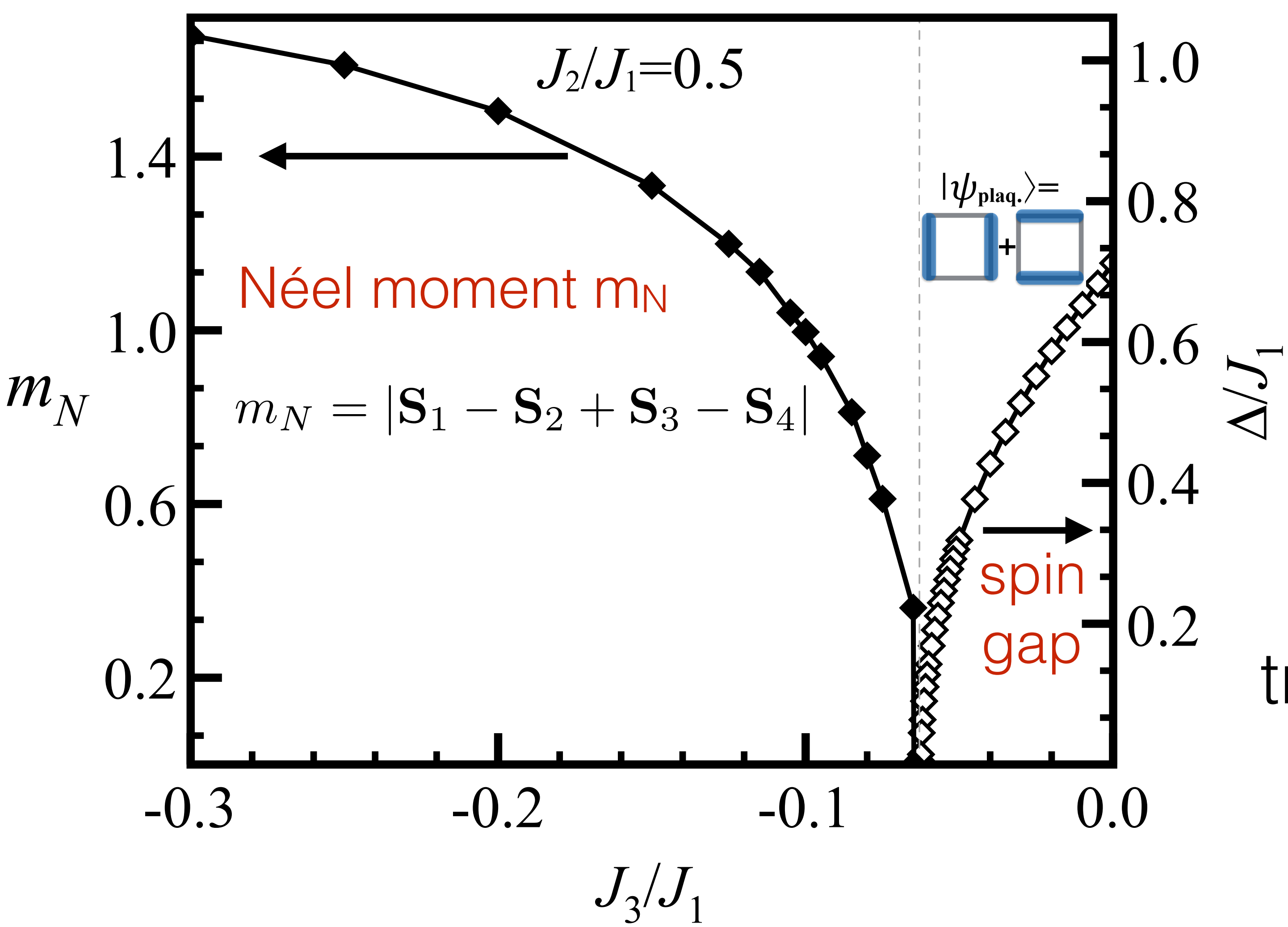
Quantum fluctuations strongly prefer Néel order
⇒ Néel order eats into classical stripe region

Plaquette factorised ansatz

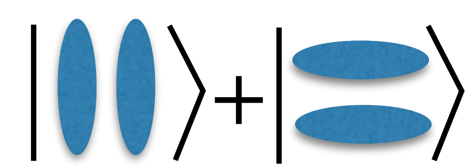
Classically, magnetic unit cell has four sites
⇒ suggests plaquette-factorisable quantum wavefunction for S=1/2 case



$$|\Psi_{var}\rangle \equiv \prod_{plaq.} |\Psi_{plaq.}\rangle$$



Variational solution:

$|\Psi_{plaq.}\rangle \sim$ 

for $J_3 \gtrsim$ -0.06 J_1

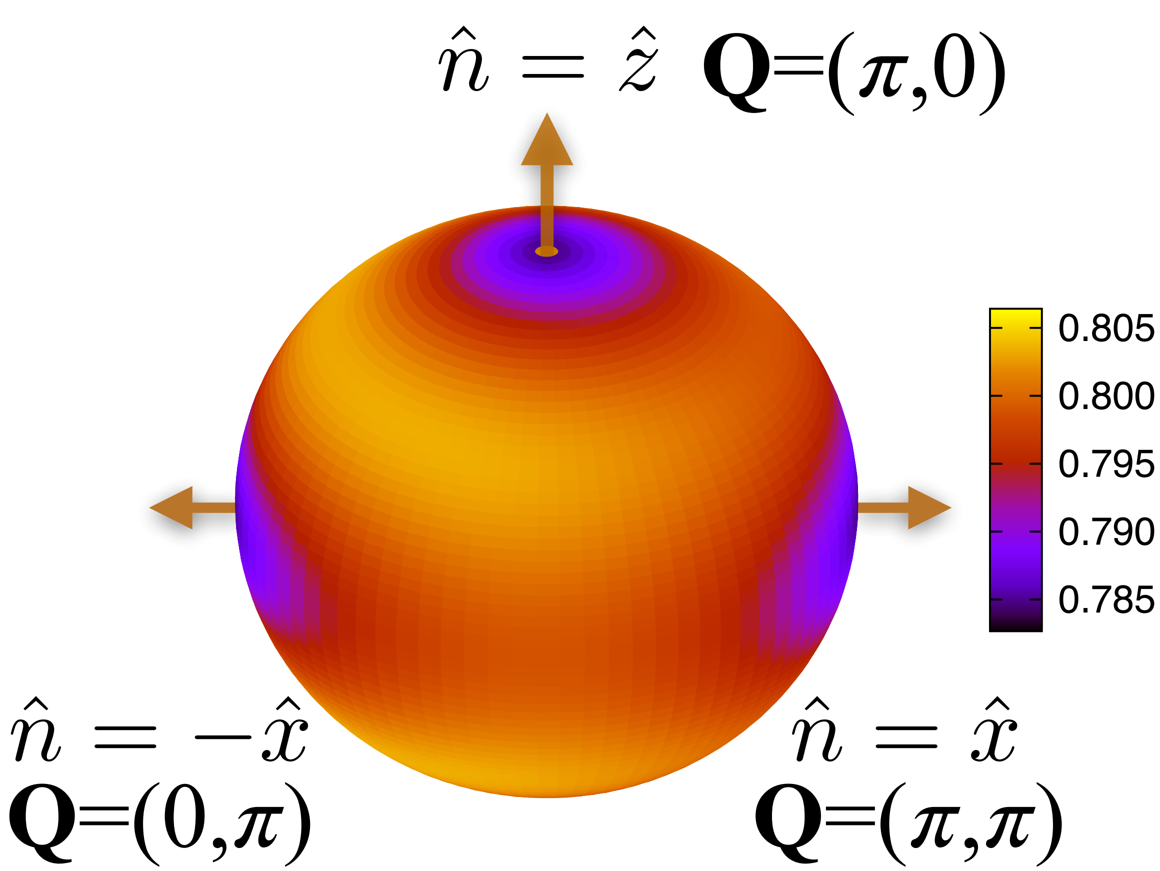
We find a triplon condensation transition at $J_3 \sim$ -0.06 J_1 leading to Néel order

Thermal g.s. selection by spin waves - purely classical model

Free energy due to spin wave excitations at low temperatures:

$$F = k_B T \sum_{\mathbf{k}} \sum_i \ln(\epsilon_{i,\mathbf{k}})$$

Free energy vs. (θ,φ)



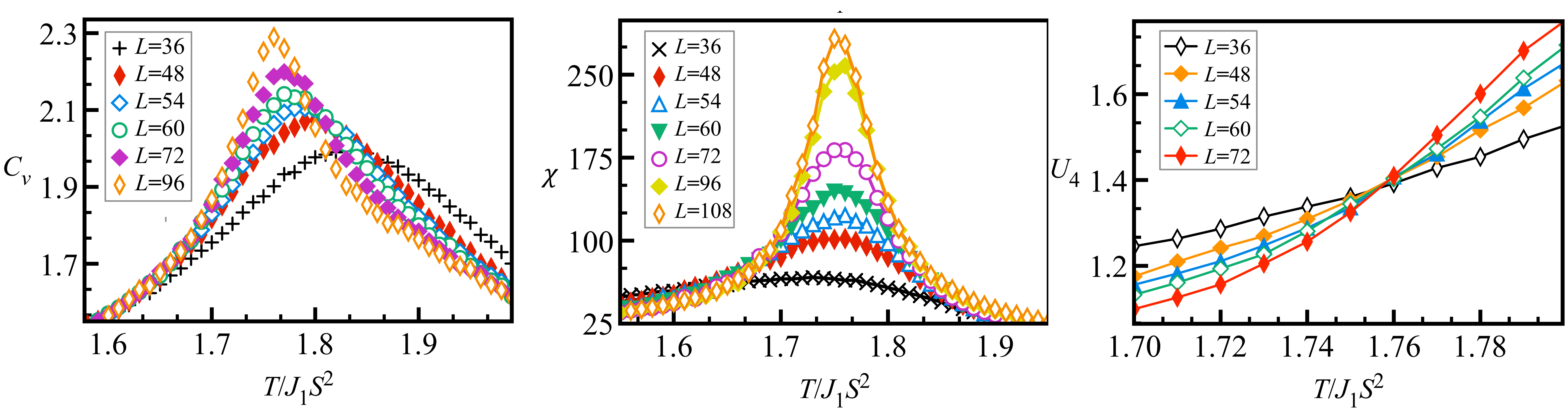
Three degenerate minima:
Néel, horizontal stripe and vertical stripe

⇒ system will pick one of three

⇒ $\mathbb{Z}_3$ symmetry breaking

Classical Monte Carlo results

- At any non-zero temperature, rotational symmetry is restored - in accordance with Mermin-Wagner theorem
- Discrete $\mathbb{Z}_3$ symmetry breaking persists upto some T_c
- Phase transition seen in classical Monte Carlo
- Critical exponents of 3-state Potts model universality class



$\alpha/\nu \approx 0.402(0.4)$ $\beta/\nu \approx 0.132(0.1333)$ $\gamma/\nu \approx 1.561(1.7333)$

Summary

- Quantum disordered phase in square J_1-J_2 AFM arises from infinite degeneracy in classical limit
- Ferromagnetic J_3 partially lifts this degeneracy ~ coexisting spirals or equivalently four-site magnetic unit cell
- With J_3 coupling, quantum disordered term gives rise to Néel order, as seen from
    - spin wave theory
    - exact diagonlisation
    - plaquette factorised variational ansatz
- Quantum disordered phase in J_1-J_2 model must be driven by classical degeneracy of single-spiral states — suggests square J_1-J_2 XY model has the same disordered g.s.
- Classical model at finite temperatures: $\mathbb{Z}_3$ symmetry breaking with a phase transition in the 3-state Potts model class