Emergence of Mixed Quantum Phases in Spin 1/2 Systems

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Aspet, 13 october 2009.

Collaborators

- Didier Poilblanc (LPT Toulouse)
- Matthieu Mambrini (LPT Toulouse)
- Roderich Moessner (MPI-PKS Dresden)

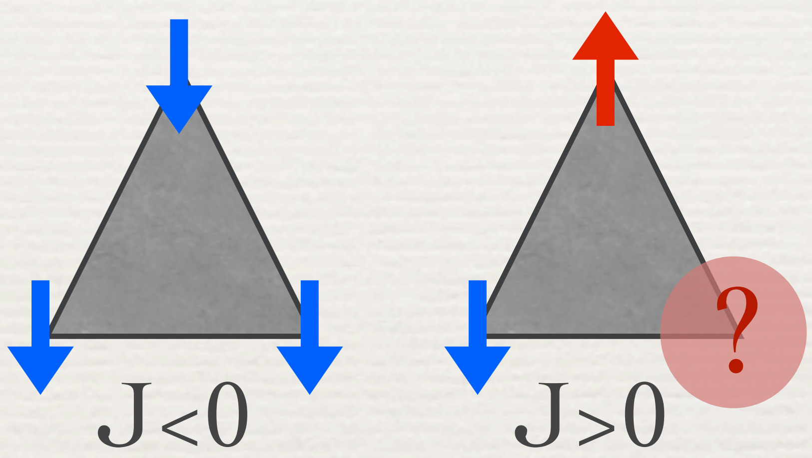
Scope

- Introducing Quantum Spin Liquids
- Rokhsar-Kivelson models: State of the art
- Connection with microscopic Heisenberg magnetism

Physical Motivations

General scheme of frustrated systems

Frustration:



Mott Insulators → Doping → Metals

Cooling

? → High Tc Superconductors

Anderson (87)

No magnetic long range order

Shastry & Sutherland (81)

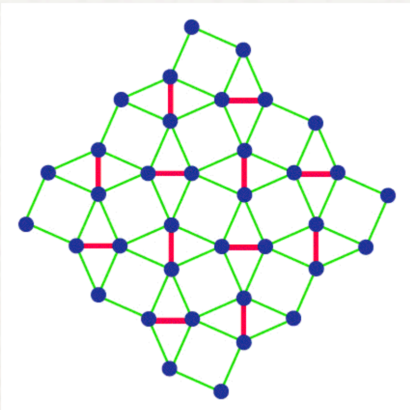
$$\langle \mathbf{S}_i.\mathbf{S}_j \rangle \simeq e^{-\frac{(\mathbf{r}_i - \mathbf{r}_j)}{\xi}}$$

Even at **T=0K**

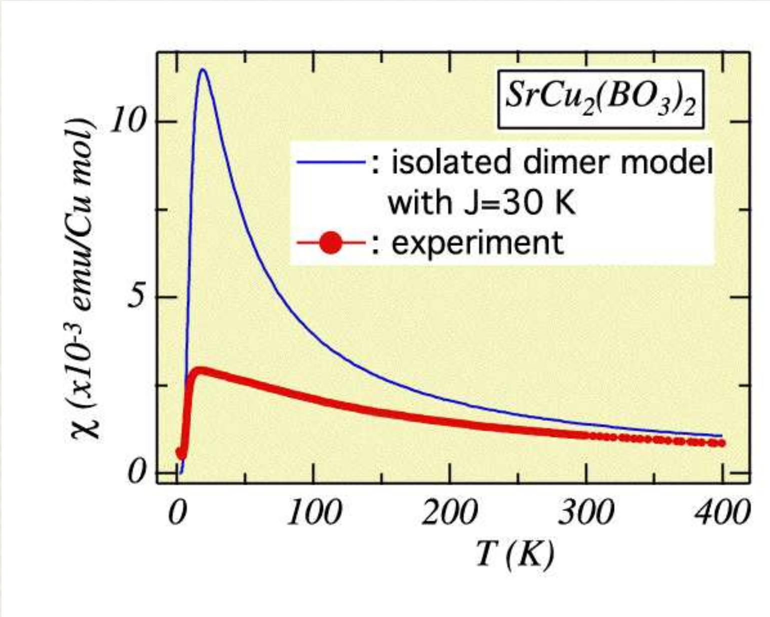
$$\Delta_s = \frac{(\mathbf{r}_i - \mathbf{r}_j)}{\xi / a}$$

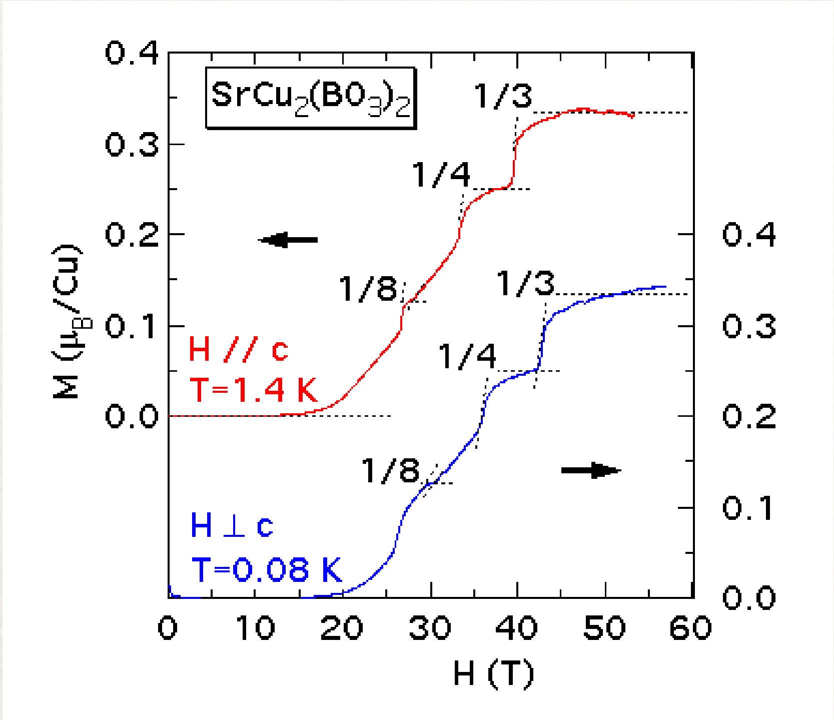
SU(2) is preserved

Some examples: $SrCu_2(BO_3)_2$



Orthogonal dimers





$$\chi(T) \simeq T^{-1/2} e^{-\Delta_s/T}$$

- Bose-condensation of triplets
- Static dimer background
- Exotic phases: SF, SS

Spin gap at low T, singlet GS and new bosonic quantum phases!

Shastry & Sutherland (81), Kageyama *et al.* (2005)

Rokhsar-Kivelson Models

Effective models derived from microscopic systems

- Heisenberg Rokhsar & Kivelson (88), Moessner & Sondhi (01)
- Spin-orbital Vernay, **AR**, Becca, Mila (06)
- Trimerized Kagomé lattice Zhitomirsky (04)

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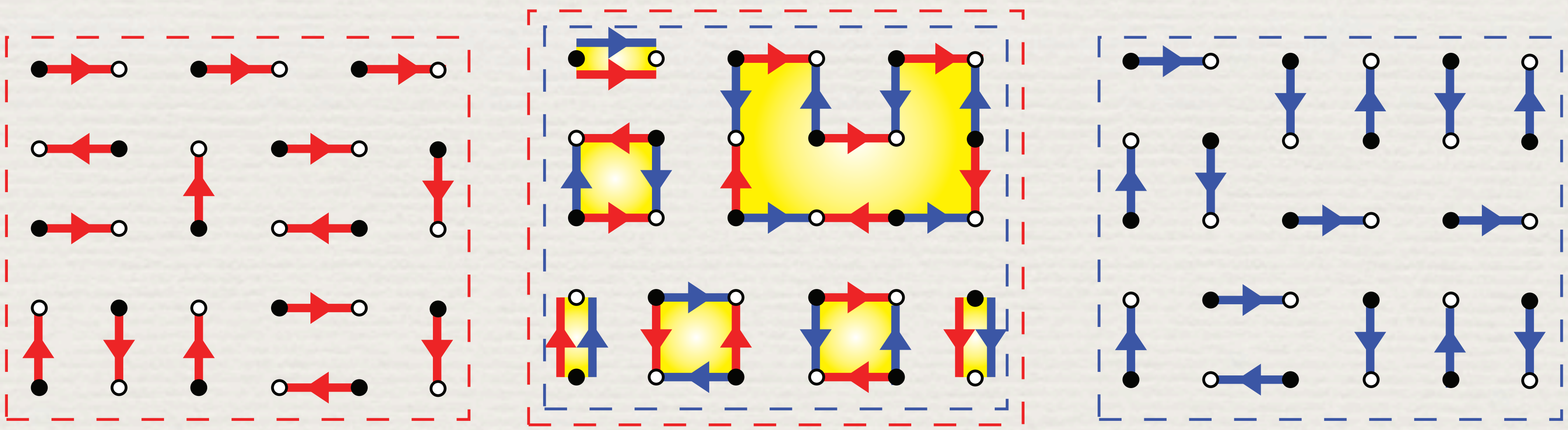
Quantum Dimer Model: projection onto the singlet subspace

$$= \alpha(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$$

$$\alpha = \frac{1}{\sqrt{2}}$$



Truncate at the 4^{th} order:

φ $\quad\langle\varphi|\psi\rangle\quad$ ψ

$$O_{\phi,\psi} = Id + 2\alpha^4 A + 2\alpha^6 B + \cdots$$

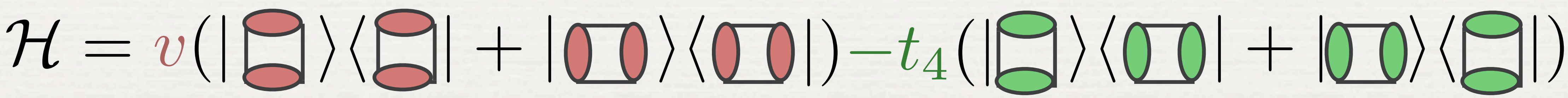
$\Rightarrow$Only loop of length 4!

Sutherland (88)

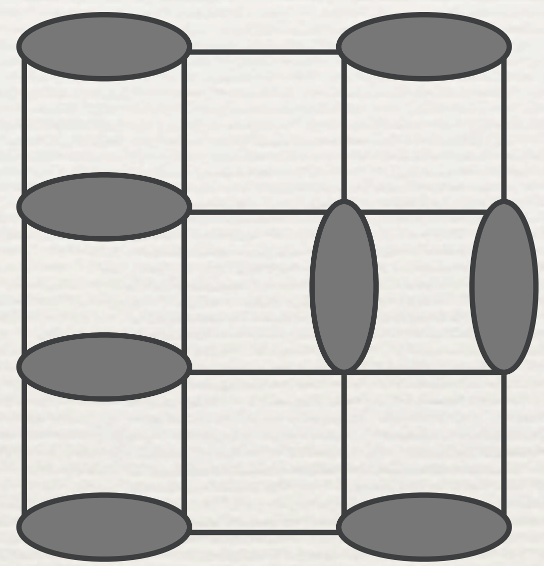
Rokhsar-Kivelson Models

The Quantum Dimer Model

Rokhsar & Kivelson (88)



- v: Potential term
- t4: Kinetic term



Rokhsar-Kivelson Models

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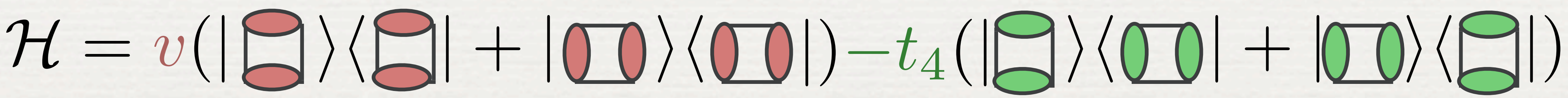

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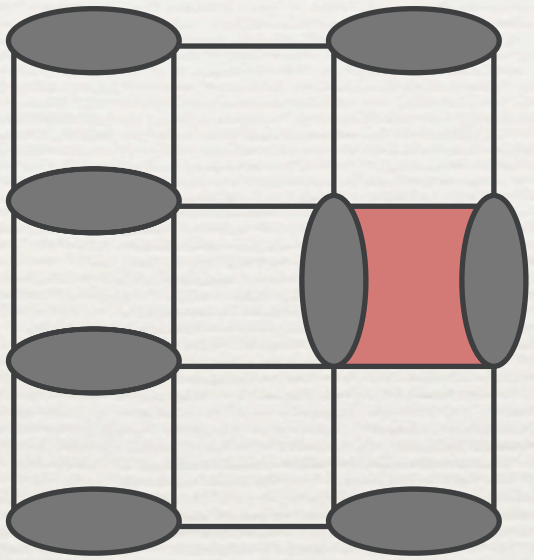

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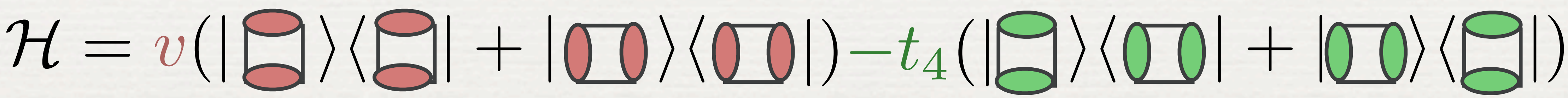

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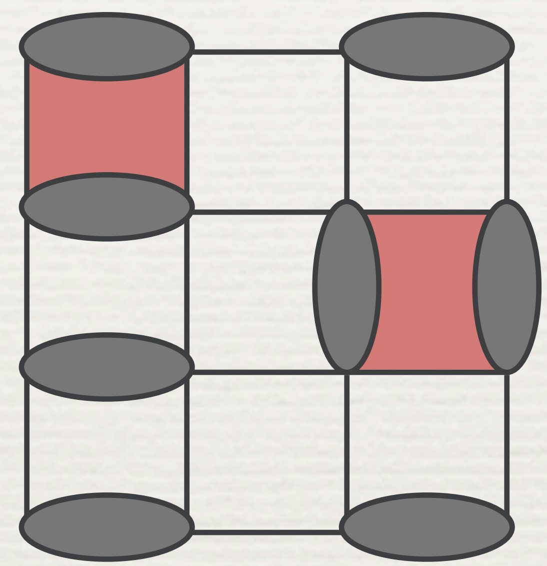

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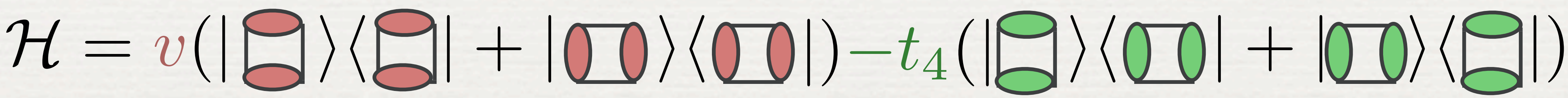

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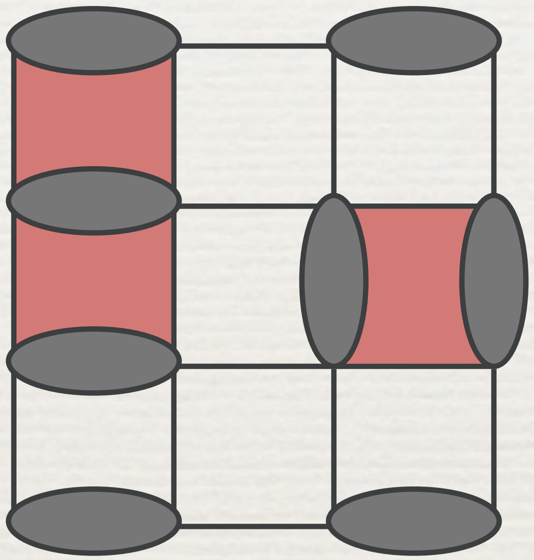
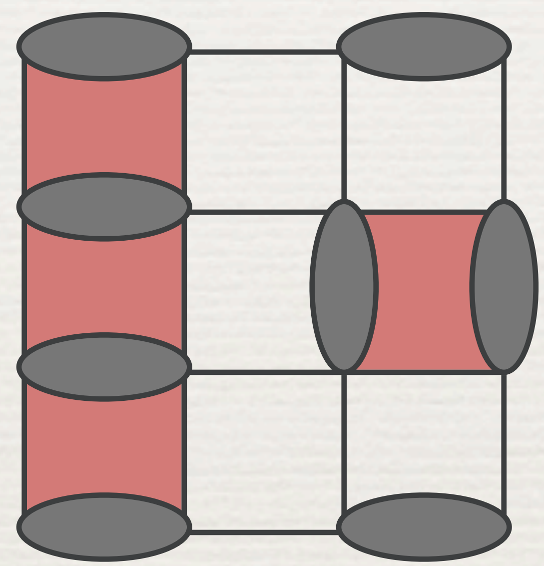


Rokhsar-Kivelson Models

The Quantum Dimer Model

Rokhsar & Kivelson (88)

$$\mathcal{H} = v(|\ \rangle\langle\ | + |\ \rangle\langle\ |) - t_4(|\ \rangle\langle\ | + |\ \rangle\langle\ |)$$



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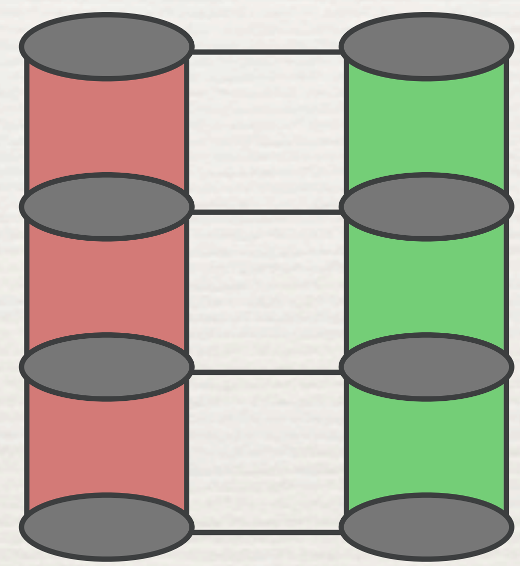

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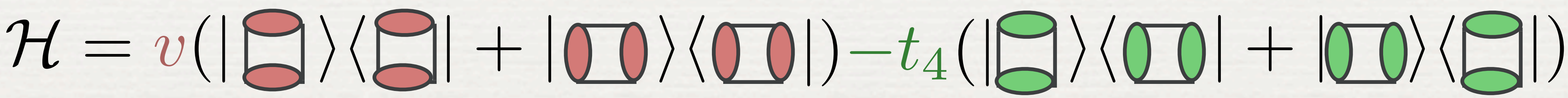

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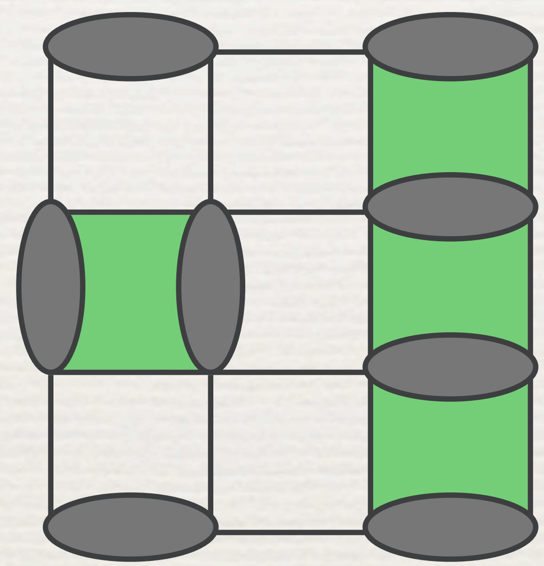

$\Rightarrow$ Competition

Rokhsar-Kivelson Models

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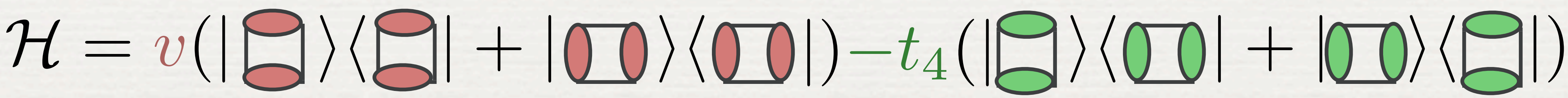

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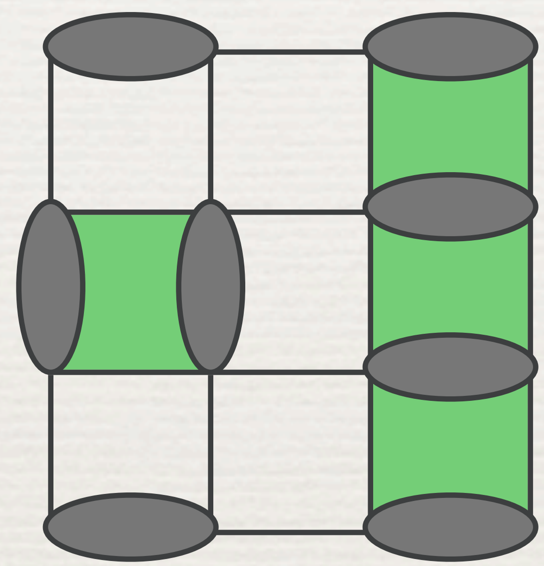
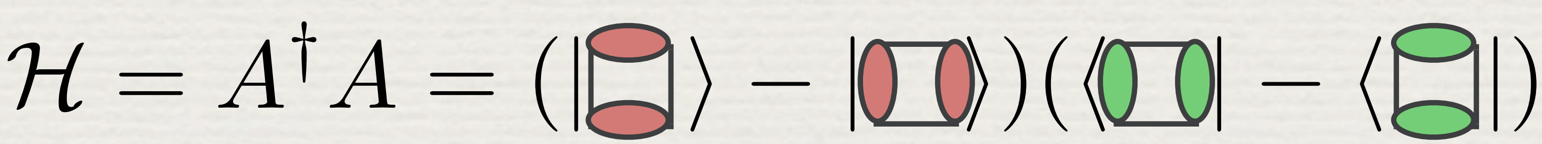


$\Rightarrow$ Competition

t4=v $\Longrightarrow$ RK point: Factorization of the Hamiltonian!



$$\text{GS:} \quad A|\Psi\rangle = 0 \;\; \Rightarrow \;\; |\Psi\rangle = \frac{1}{\sqrt{N}} \sum |c\rangle \;\; \Rightarrow \;\; \text{RVB liquid}$$

Anderson (73)

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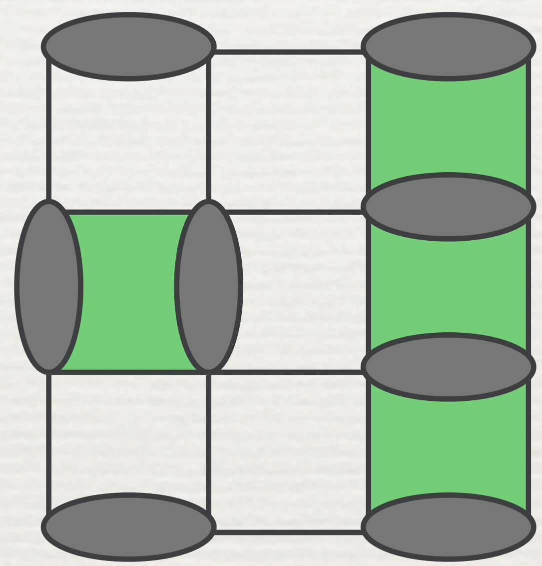

$\Rightarrow$ Competition

t4=v $\Rightarrow$ RK point: Factorization of the Hamiltonian!

$$\mathcal{H} = A^\dagger A = (|\;\rangle - |\;\rangle)(\langle\;| - \langle\;|)$$

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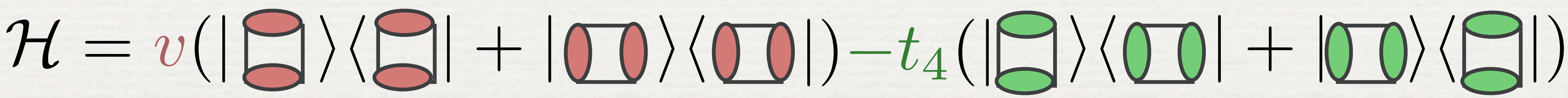
Anderson (73)

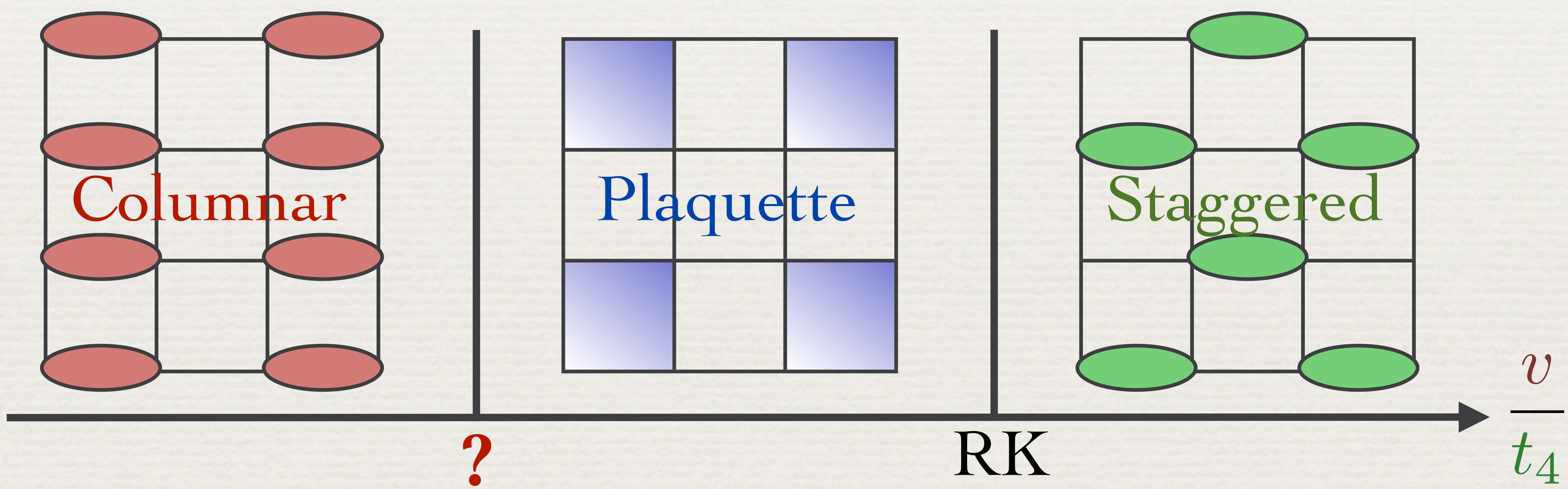
RK Models: Quantum GS coincides with the classical equilibrium

Rokhsar-Kivelson Models

In a more general ground

Rokhsar & Kivelson (88)





- Rich phase diagram: Exotic phases, non-conventional behavior

Rokhsar-Kivelson Models

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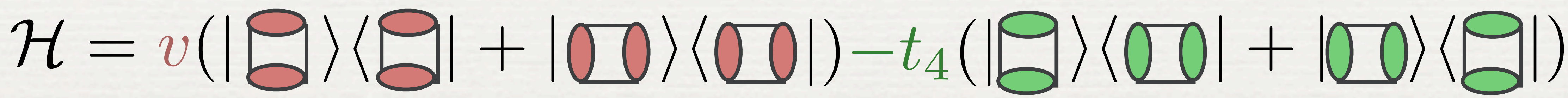
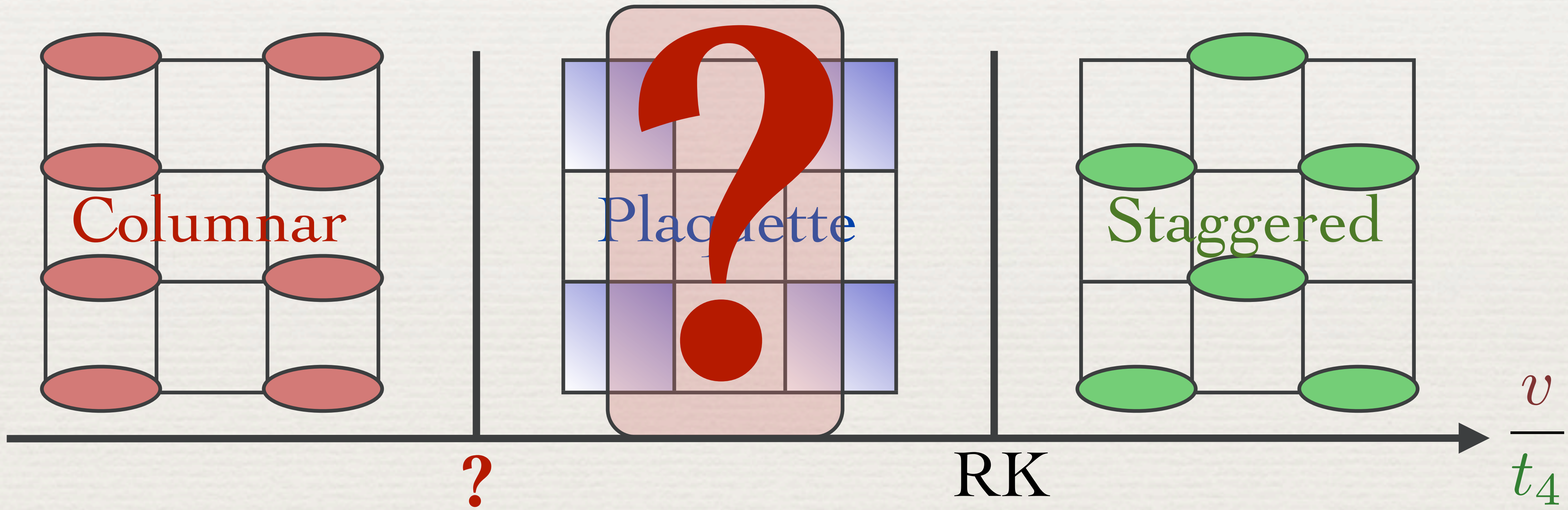


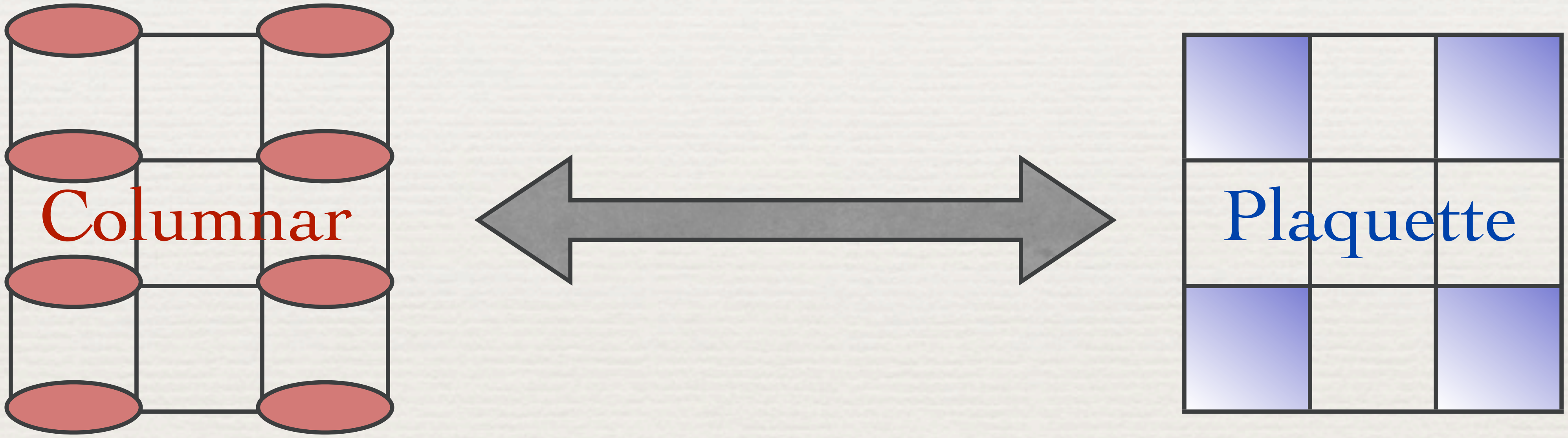


- Rich phase diagram: Exotic phases, non-conventional behavior
- After 20 years, still not a clear answer for the ground state!

Long time conflicting results

For several systems, same studies give ≠ results

- Square QDM: Plaquette-Columnar transition point?
- Square Heisenberg AF: Nature of the gapped phase?



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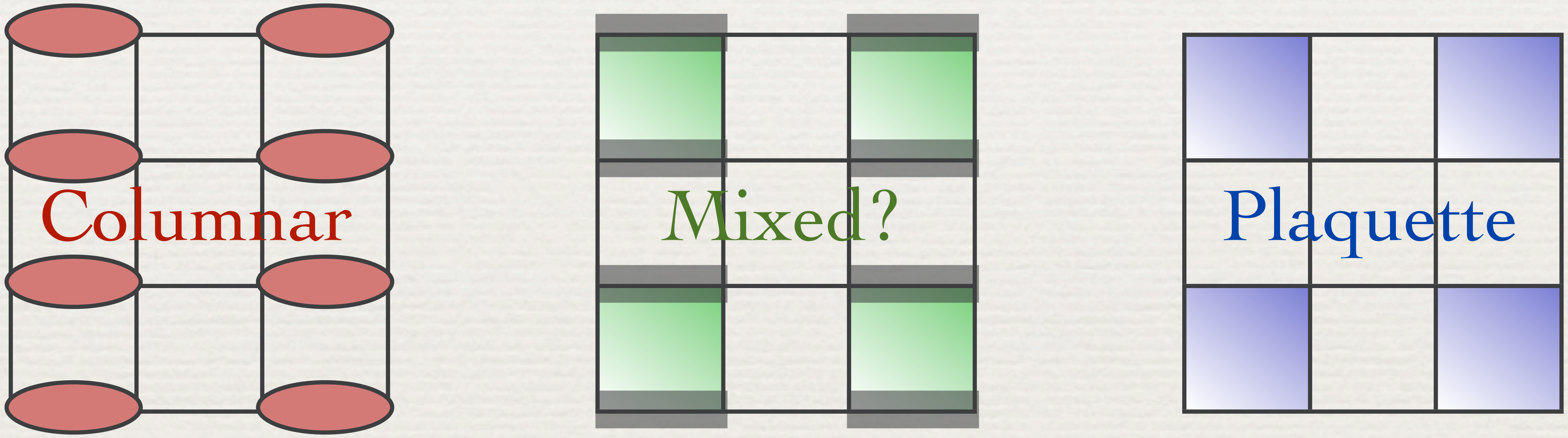


Break both translations and $\pi/2$ rotations

- Effective field theory in term of Height Models
- Microscopic realization on Heisenberg systems

Height representation of the QDM

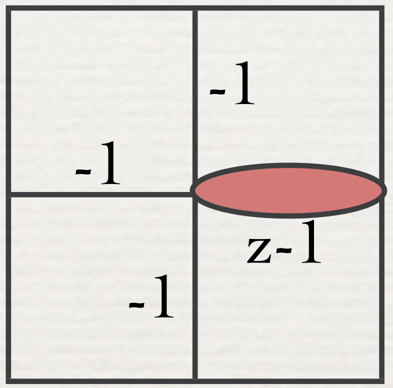
From RK (classical) to quantum case

Henley (03)

- Gauss Law: $\nabla.\mathbf{E} = 0$
- Realized by chosing a good gauge ϕ

$$\sum \phi = 0$$

- Defining the height variable h: $\mathbf{E} = \nabla \times h$



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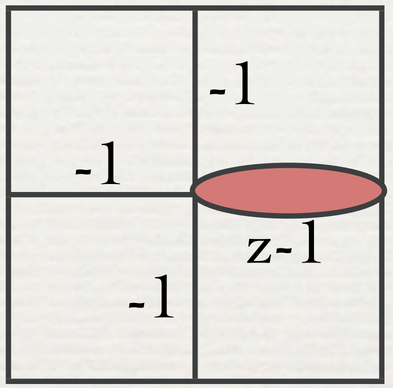

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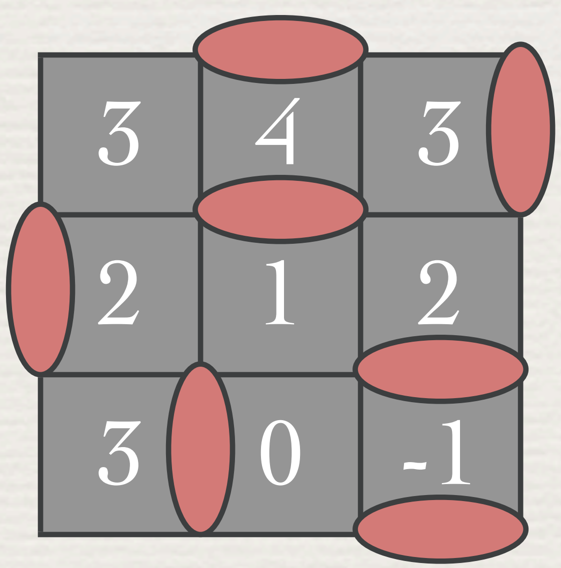

1 to 1 mapping between dimers and heights

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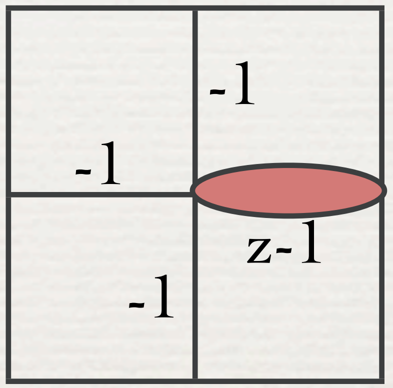

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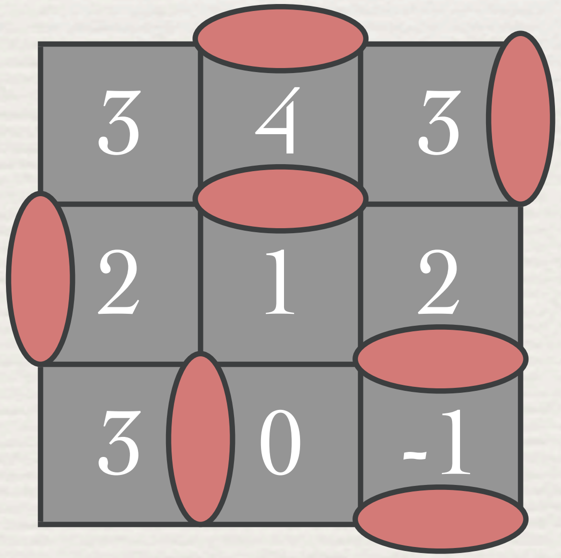

1 to 1 mapping between dimers and heights

- Columnar: <h> = half integer
- Plaquette: <h> = integer

Fluctuating 2D brane ⇒ effective field theory

Height representation of the QDM

Coarse-graining of the h variable

One can obtain a d=2+1 effective field theory:

$$S = \int d\tau d^2x \left[(\partial_\tau h(r))^2 + \rho(\nabla h(r))^2 + \lambda \cos(2\pi h(r)) + \mu \cos(4\pi h(r))\right]$$

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Dynamical energy

Locking potential that considers roughness

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New quartic term in the expansion

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Dynamical energy

Locking potential that considers roughness

New quartic term in the expansion

Searching for uniform configuration h = cste

- Only the mean value is relevant to distinguich the phases
- Competition between two simple terms:

$$S \simeq \lambda \cos(2\pi < h >) + \mu \cos(4\pi < h >) = 0$$

Height representation of the QDM

$$S \simeq \lambda \cos(2\pi < h >) + \mu \cos(4\pi < h >) = 0$$

First case: μ=0 (old case)

- λ>0: <h> = half integer — Columnar
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- λ=0: <h> = ∀ — Continuous deg.

Height representation of the QDM

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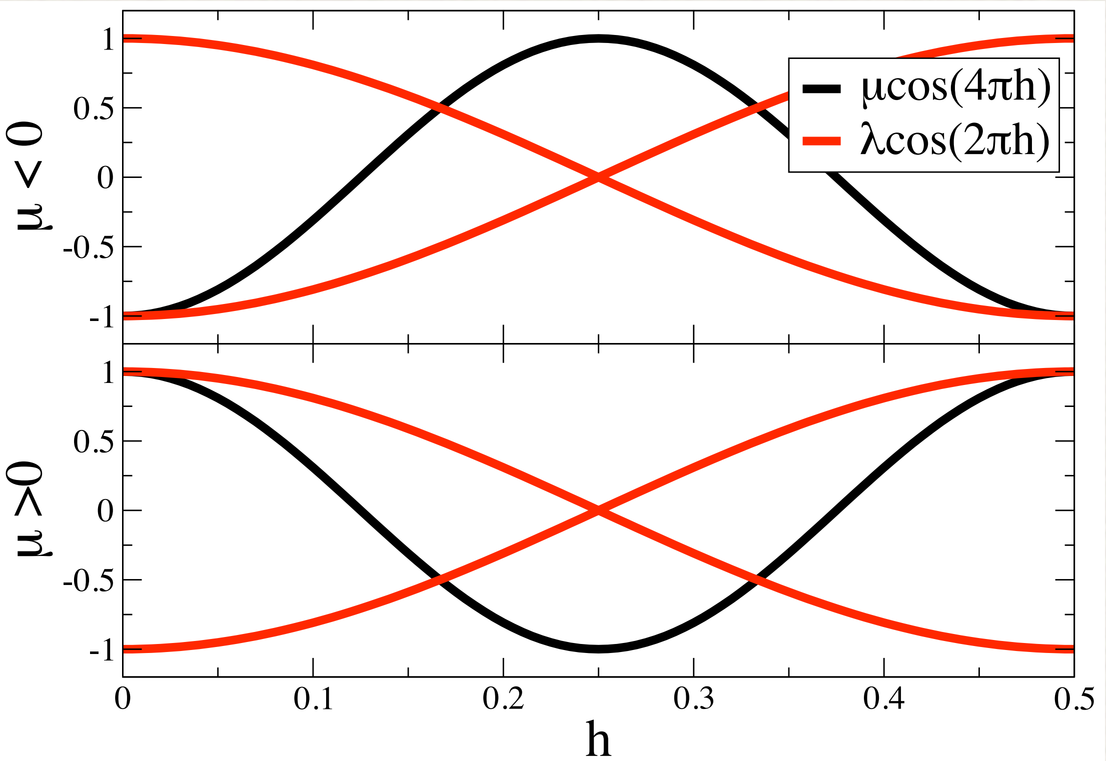
Second case: μ≠0



- μ<0: lift of the continuous deg.

  1st order transition scenario

- μ>0:Competition!

$$2\pi h = \begin{cases} 0, & \text{if } \lambda < -4\mu \\ \pi, & \text{if } \lambda > 4\mu \\ \arccos(-\lambda/4\mu), & \text{if } |\lambda| < 4\mu \end{cases}$$

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Mixed phase!

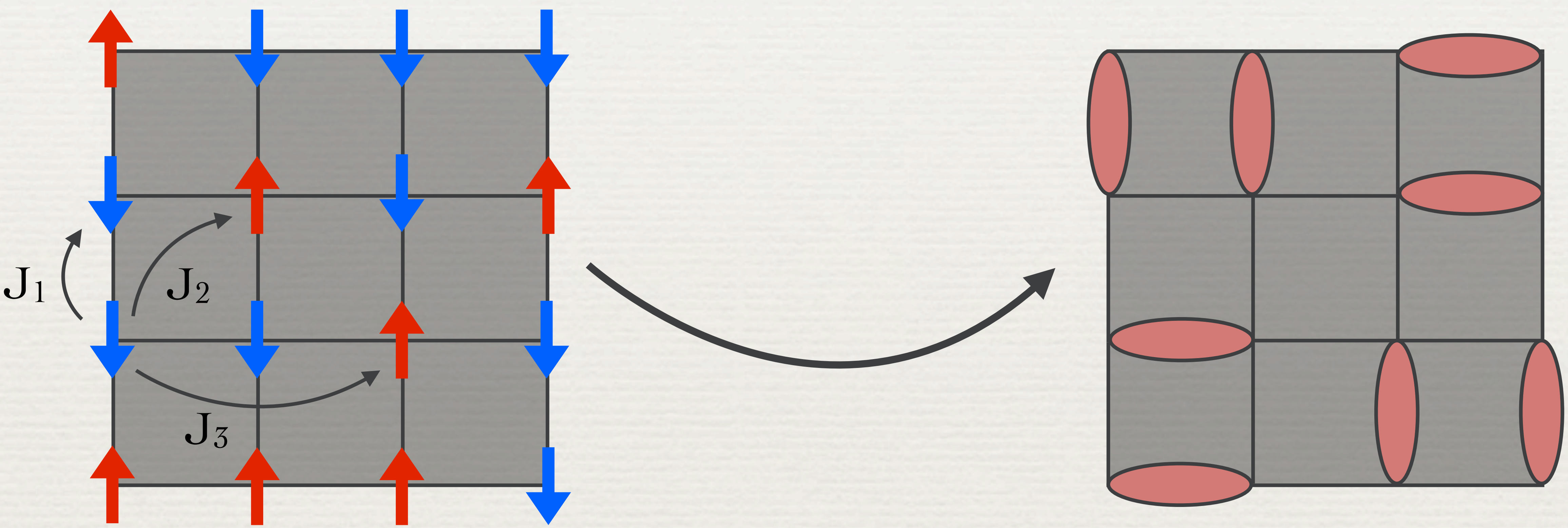
- Continuous extrapolation
- 2nd order phase transition

AR, D. Poilblanc & R. Moessner PRL (08)

Mixed phase in Heisenberg systems

A Generalized QDM for the square Heisenberg AF

Attempting to characterize spin-1/2 systems with RK models



Only for specific values of J_1 -J_2 -J_3

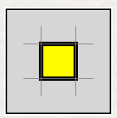
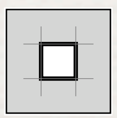
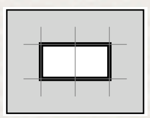
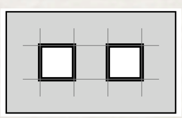
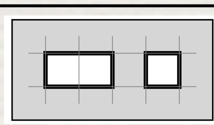
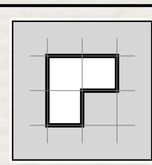
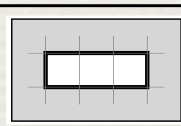
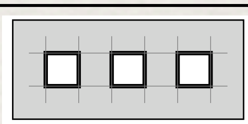
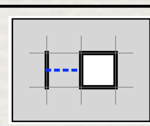
$$\mathcal{H} = J_1 \sum_{nn} \mathbf{S}_i.\mathbf{S}_j + J_2 \sum_{nnn} \mathbf{S}_i.\mathbf{S}_j + J_3 \sum_{nnnn} \mathbf{S}_i.\mathbf{S}_j$$

When the true GS is made of dimer coverings

Mambrini *et al.* (05)

Mixed phase in Heisenberg systems

New systematic procedure for deriving effective models

Processes	$\mathcal{O}$	$\mathcal{H}$	$\mathcal{H}^{\text{eff}} = \mathcal{O}^{-1/2}\mathcal{H}\mathcal{O}^{-1/2}$
Id	1	0	0
	$\emptyset$	$\emptyset$	$2(J_1 - J_2)\alpha^4$
	α^2	$2(-J_1 + J_2)\alpha^2$	$-2\,(J_1 - J_2)\,\alpha^2\left(1 + \alpha^4\right)$
	α^4	$2(-2J_1 + 2J_2 + J_3)\alpha^4$	$2\,(-J_1 + J_2 + J_3)\,\alpha^4$
	α^4	$4(-J_1 + J_2)\alpha^4$	0
	α^6	$2(-3J_1 + 3J_2 + J_3)\alpha^6$	0
	α^6	$2(-3J_1 + 3J_2 + 2J_3)\alpha^6$	$2\,(-J_1 + J_2 + J_3)\,\alpha^6$
	α^6	$2(-3J_1 + 3J_2 + 2J_3)\alpha^6$	$(-J_1 + J_2 + 2J_3)\,\alpha^6$
	α^6	$2(-J_1 + J_2)\alpha^6$	0
	$\emptyset$	$\emptyset$	$(J_1 - J_2 - J_3)\,\alpha^6$

We reorganize the overlap expansion in term of same prefactors

Mixed phase in Heisenberg systems

New systematic procedure for deriving effective models

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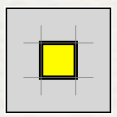
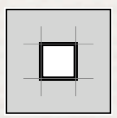
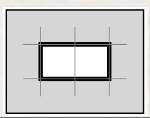
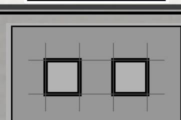
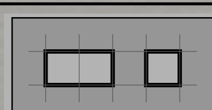
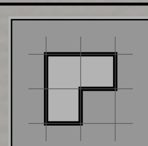
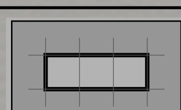
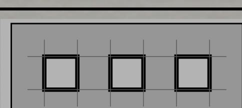
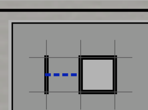
Id	1	0	0
	$\emptyset$	$\emptyset$	$2(J_1 - J_2)\alpha^4$
	α^2	$2(-J_1 + J_2)\alpha^2$	$-2\left(J_1 - J_2\right)\alpha^2\left(1 + \alpha^4\right)$
	α^4	$2(-2J_1 + 2J_2 + J_3)\alpha^4$	$2\left(-J_1 + J_2 + J_3\right)\alpha^4$
	α^4	$4(-J_1 + J_2)\alpha^4$	0
	α^6	$2(-3J_1 + 3J_2 + J_3)\alpha^6$	0
	α^6	$2(-3J_1 + 3J_2 + 2J_3)\alpha^6$	$2\left(-J_1 + J_2 + J_3\right)\alpha^6$
	α^6	$2(-3J_1 + 3J_2 + 2J_3)\alpha^6$	$\left(-J_1 + J_2 + 2J_3\right)\alpha^6$
	α^6	$2(-J_1 + J_2)\alpha^6$	0
	$\emptyset$	$\emptyset$	$\left(J_1 - J_2 - J_3\right)\alpha^6$

Negligible

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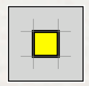
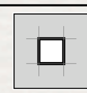
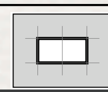
	$\emptyset$	$\emptyset$	$2(J_1 - J_2)\alpha^4$
	α^2	$2(-J_1 + J_2)\alpha^2$	$-2\,(J_1 - J_2)\,\alpha^2\,(1+\alpha^4)$
	α^4	$2(-2J_1 + 2J_2 + J_3)\alpha^4$	$2\,(-J_1 + J_2 + J_3)\,\alpha^4$
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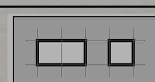
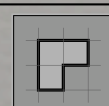
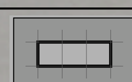
	α^6	$2(-3J_1 + 3J_2 + J_3)\alpha^6$	0
	α^6	$2(-3J_1 + 3J_2 + 2J_3)\alpha^6$	$(-J_1 + J_2 + J_3)\,\alpha^6$
	α^6	$2(-3J_1 + 3J_2 + 2J_3)\alpha^6$	$(-J_1 + J_2 + 2J_3)\,\alpha^6$
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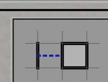
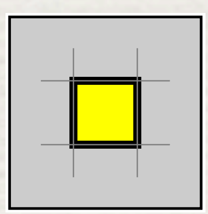
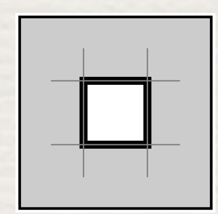
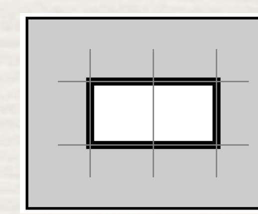
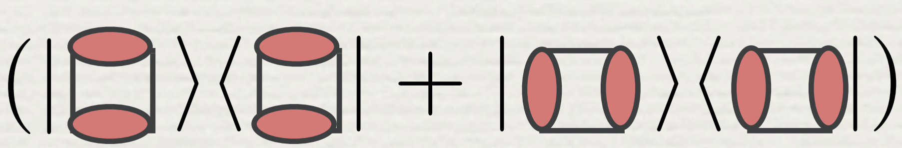
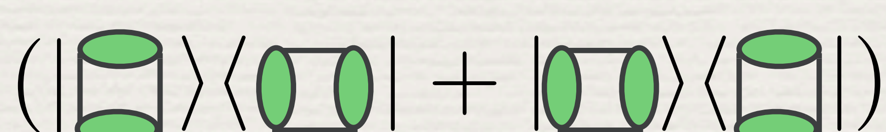
	$\emptyset$	$\emptyset$	$(J_1 - J_2 - J_3)\,\alpha^6$

Negligible

$$\mathcal{H} = \underbrace{\cos(\phi)\sin(\theta)}_{v}$$  $$+ \underbrace{\cos(\phi)\cos(\theta)}_{t_4}$$  $$+ \underbrace{\sin(\phi)}_{t_6}$$ 





Mixed phase in Heisenberg systems

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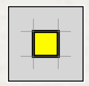
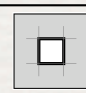
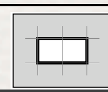
	$\emptyset$	$\emptyset$	$2(J_1 - J_2)\alpha^4$
	α^2	$2(-J_1 + J_2)\alpha^2$	$-2\,(J_1 - J_2)\,\alpha^2\,(1 + \alpha^4)$
	α^4	$2(-2J_1 + 2J_2 + J_3)\alpha^4$	$2\,(-J_1 + J_2 + J_3)\,\alpha^4$
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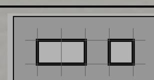
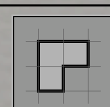
	α^6	$2(-3J_1 + 3J_2 + J_3)\alpha^6$	0
	α^6	$2(-3J_1 + 3J_2 + 2J_3)\alpha^6$	$(-J_1 + J_2 + J_3)\,\alpha^6$
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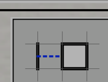	$\emptyset$	$\emptyset$	$(J_1 - J_2 - J_3)\,\alpha^6$

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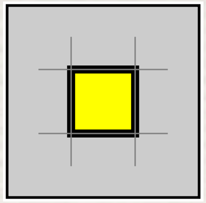
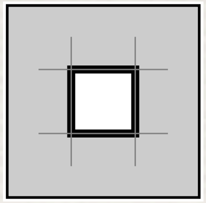
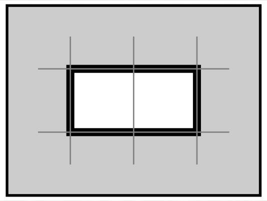
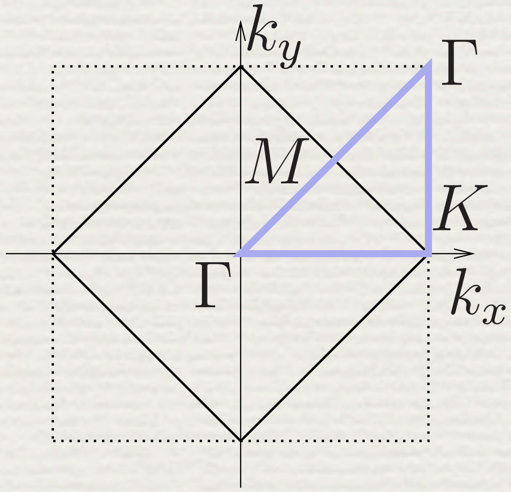
$$\mathcal{H} = \underbrace{\cos(\phi)\sin(\theta)}_{v}$$  $$+ \underbrace{\cos(\phi)\cos(\theta)}_{t_4}$$  $$+ \underbrace{\sin(\phi)}_{t_6}$$ 

Kinetic competition between loop-4 and loop-6

Mixed phase in Heisenberg systems

Symmetry classification of the expected phases

	Γ, A_1	Γ, B_1	M, A_1	K, A_1	K, B_1	M, A_1*
Columnar	X	X	X			
Plaquette	X		X	X		
Mixed	X	X	X	X	X	X



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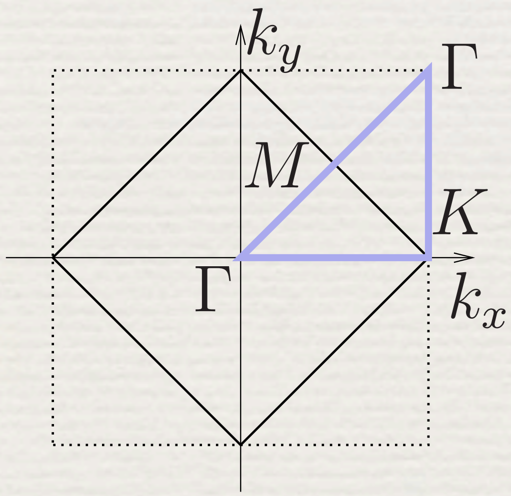

- One has to access the correct symmetry sectors
- P+ operator
- P- operator

$$P_\pm = d_i d_j \pm d_k d_l$$

$$d_i = \begin{cases} 1 \text{ if a dimer} \\ 0 \text{ if not} \end{cases}$$

$$\boxed{\begin{array}{ccc} & j & \\ k & & l \\ & i & \end{array}}$$

Mixed phase in Heisenberg systems

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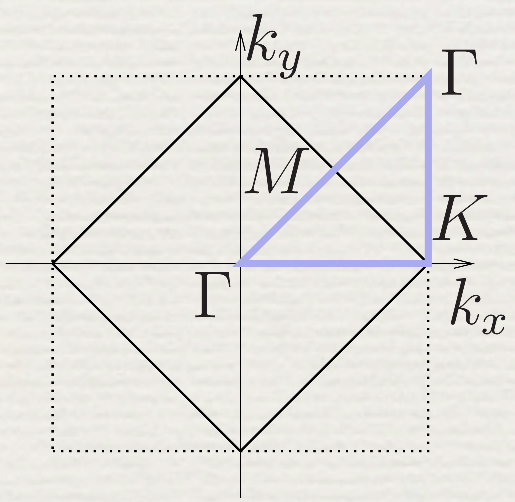

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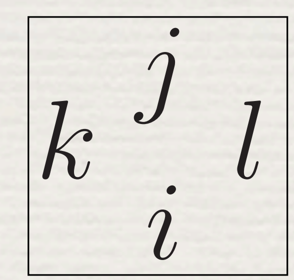
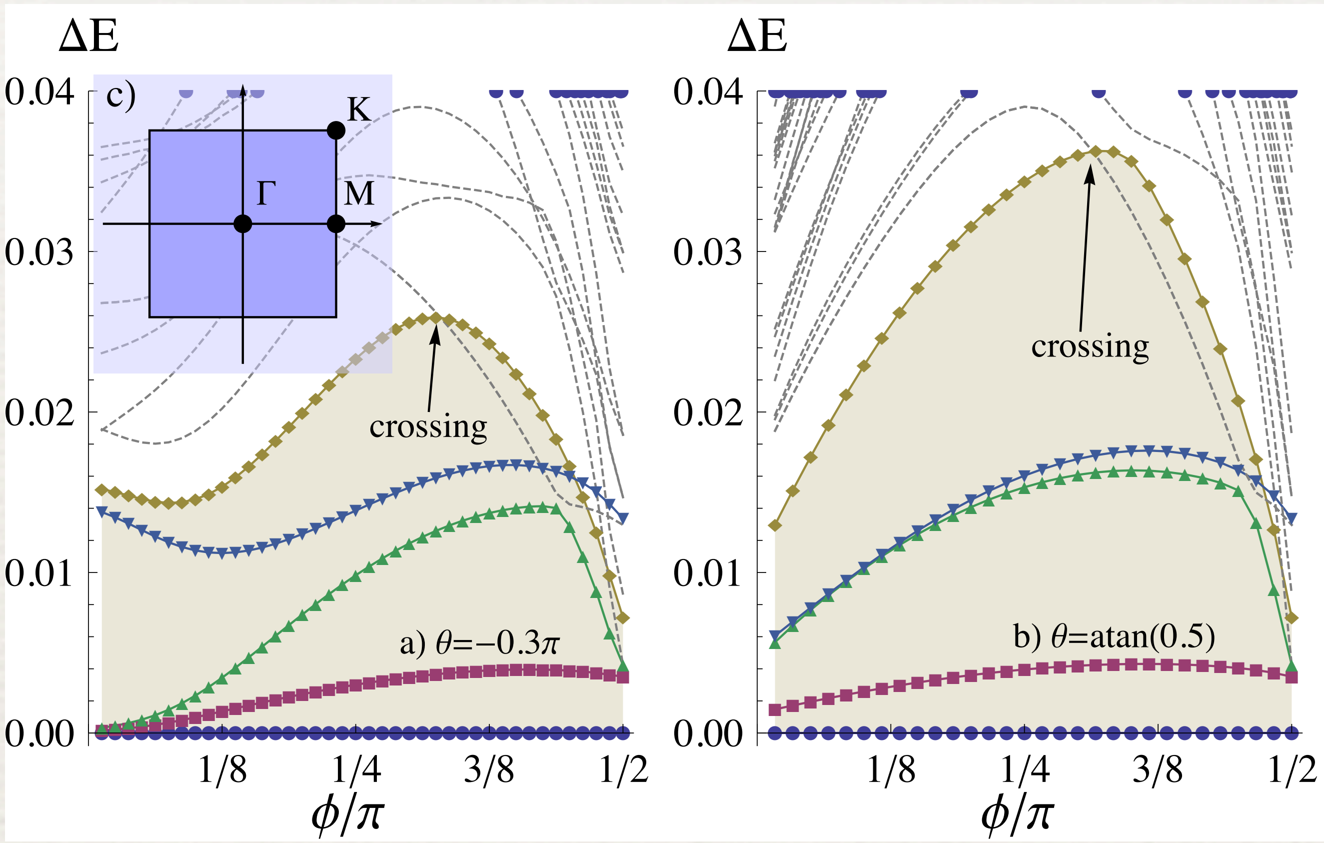


Numerical computation of the energy and the structure factors

- Exact Diagonalizations
- Green Function Quantum Monte-Carlo

Mixed phase in Heisenberg systems

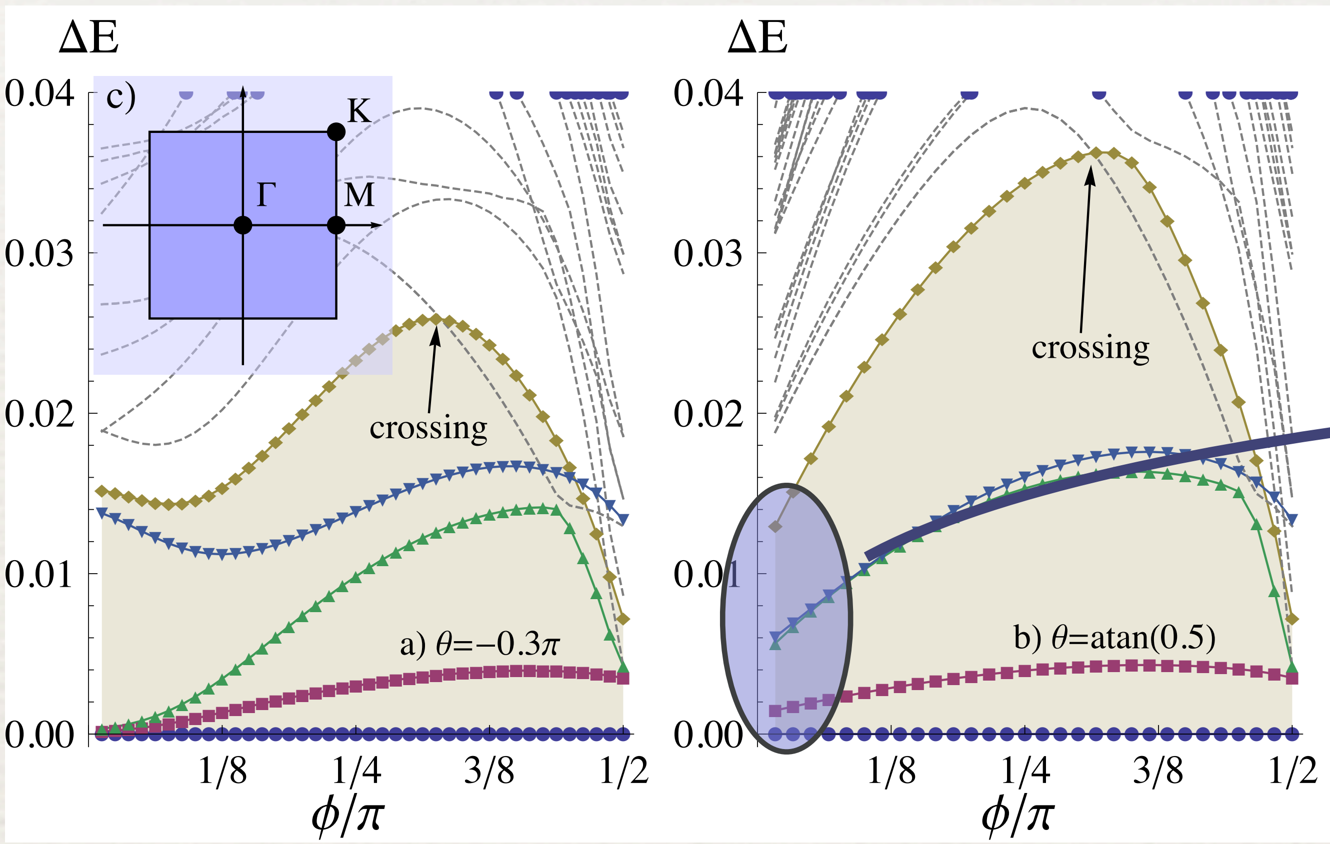
Eigen energy spectra by exact diagonalizations



- Rather large cluster size
- All symmetry sector available
- The whole range of parameter accessible

Mixed phase in Heisenberg systems

Eigen energy spectra by exact diagonalizations



Set of states compatible with the mixed phase

- Rather large cluster size
- All symmetry sector available
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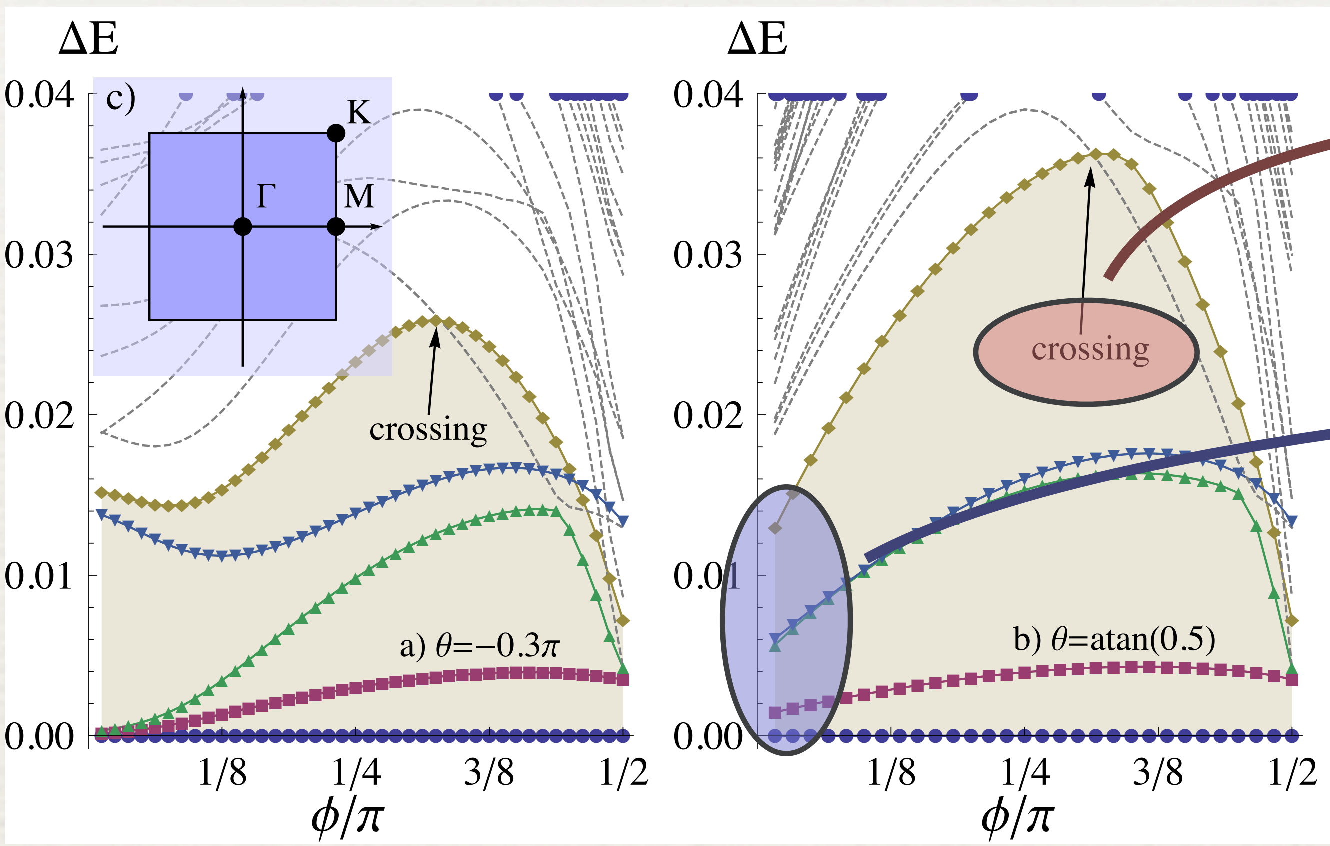
Mixed phase in Heisenberg systems

Eigen energy spectra by exact diagonalizations



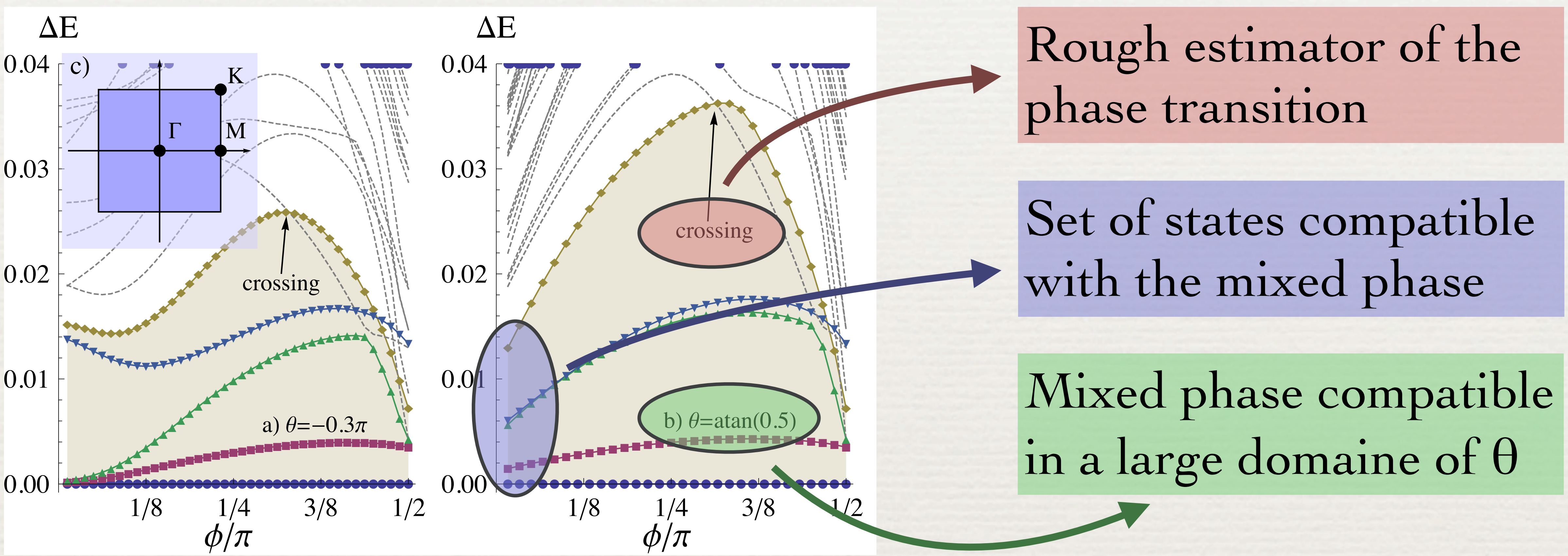
Rough estimator of the phase transition

Set of states compatible with the mixed phase

- Rather large cluster size
- All symmetry sector available
- The whole range of parameter accessible

Mixed phase in Heisenberg systems

Eigen energy spectra by exact diagonalizations



Need to go beyond the size effects
Green Function Quantum Monte Carlo

- Thermodynamic limit by finite size scaling
- Computation of the structure factor

Mixed phase in Heisenberg systems

Structure factor in different symmetry sectors

$$M_{\pm} = \frac{1}{L}\sqrt{\frac{\langle\Psi_0|P_{\pm}(-q)P_{\pm}(q)|\Psi_0\rangle}{\langle\Psi_0|\Psi_0\rangle}}$$

- Large sizes, 16x16 sites
- M+: Plaquette order
- M-: Columnar order

Mixed phase in Heisenberg systems

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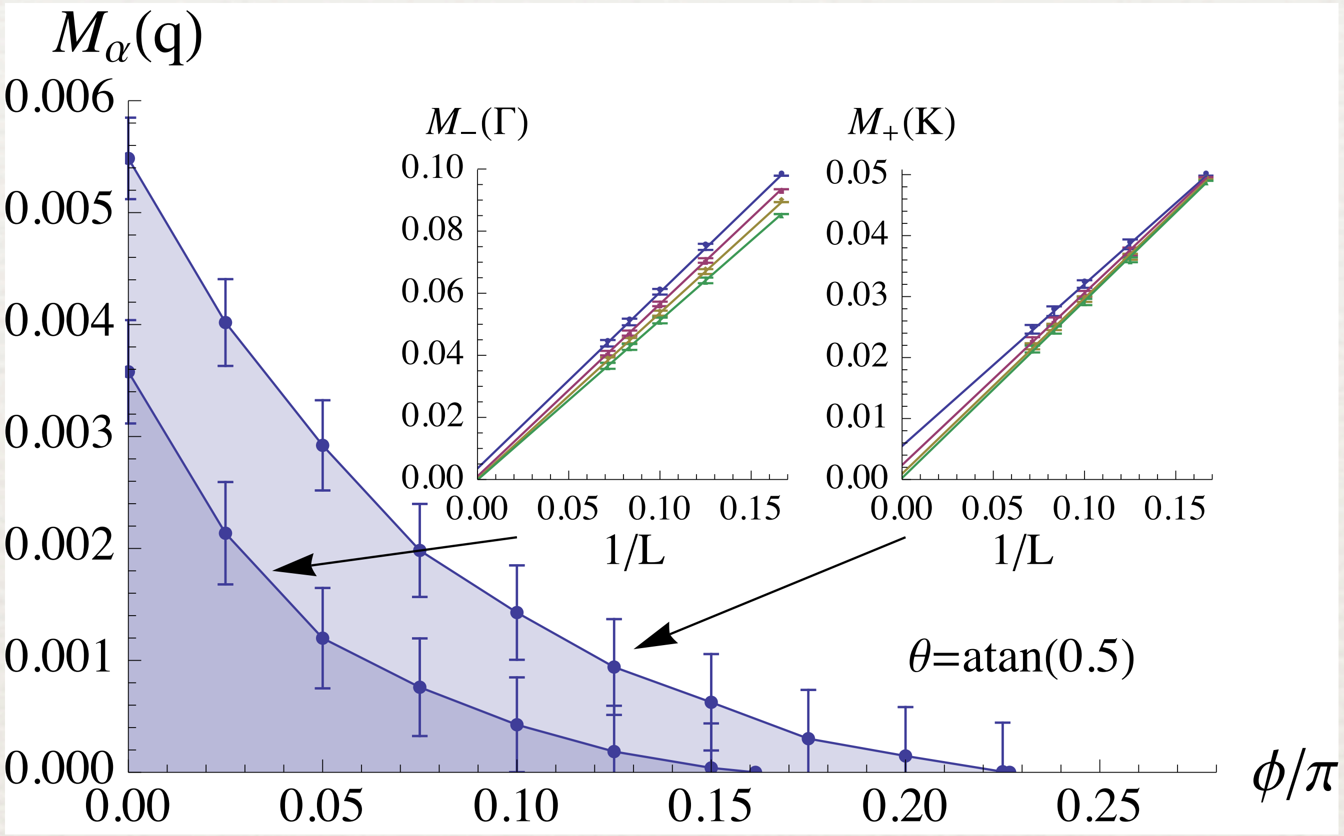


- In a large domain, both M+ and M- are non zero

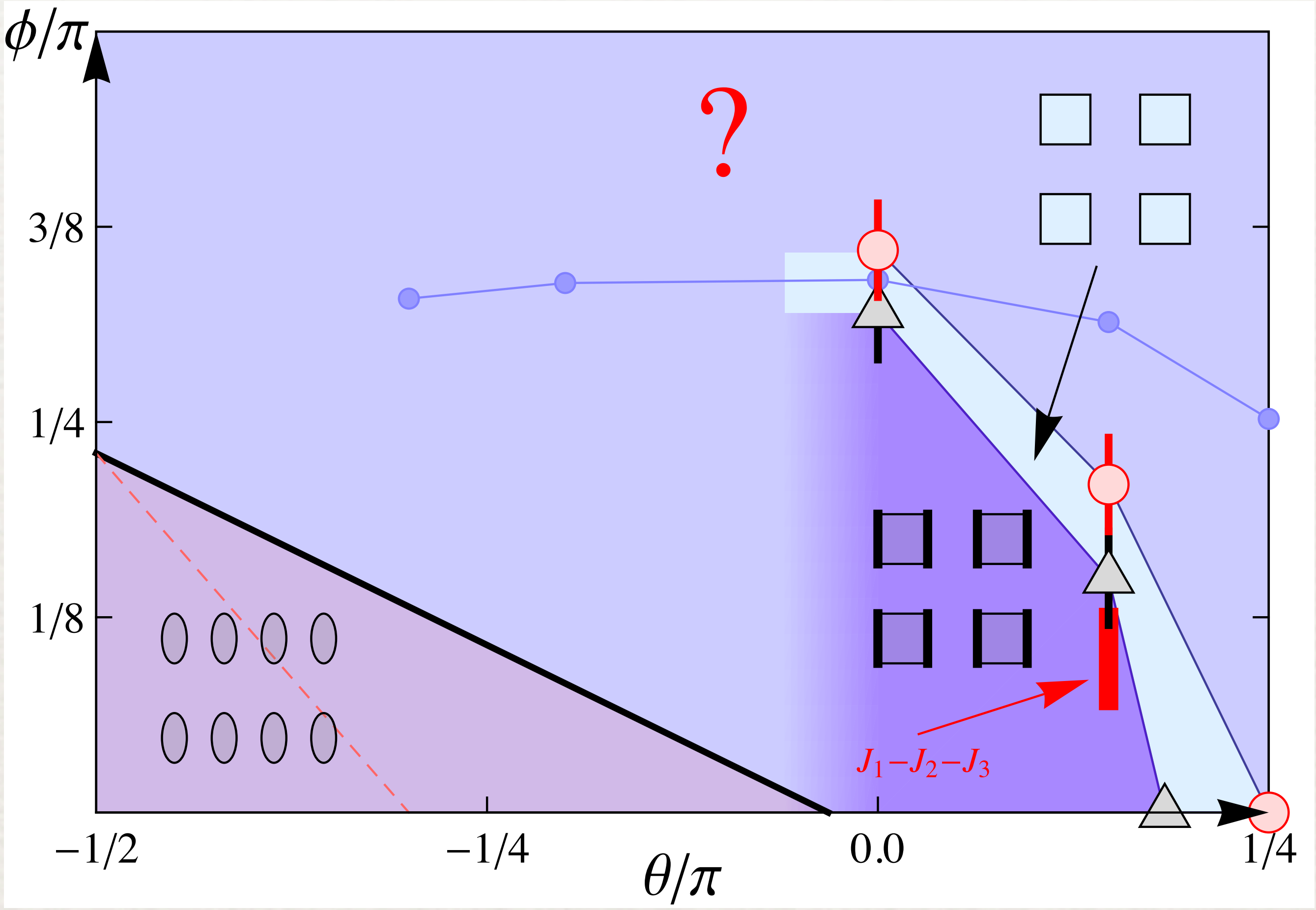
  Mixed phase driven by kinetic competition

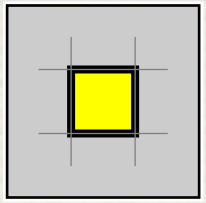
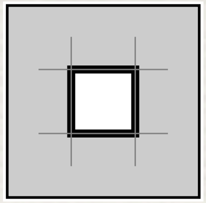
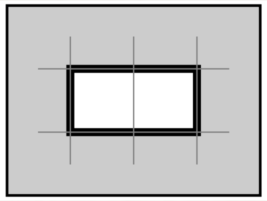
- Tiny region where M+=0 and M- non zero

  A pure plaquette phase is also present

Mixed phase in Heisenberg systems

Phase diagram at the thermodynamic limit



$$\mathcal{H} = \underbrace{\cos(\phi)\sin(\theta)}_{v}$$  $$+ \underbrace{\cos(\phi)\cos(\theta)}_{t_4}$$  $$+ \underbrace{\sin(\phi)}_{t_6}$$ 

Mixed phase in Heisenberg systems

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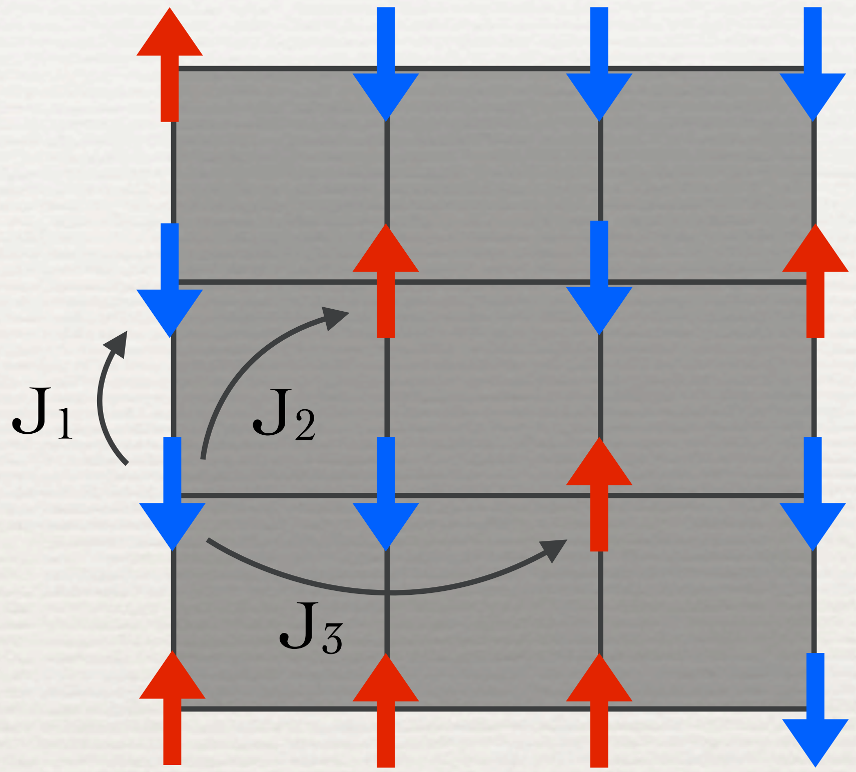
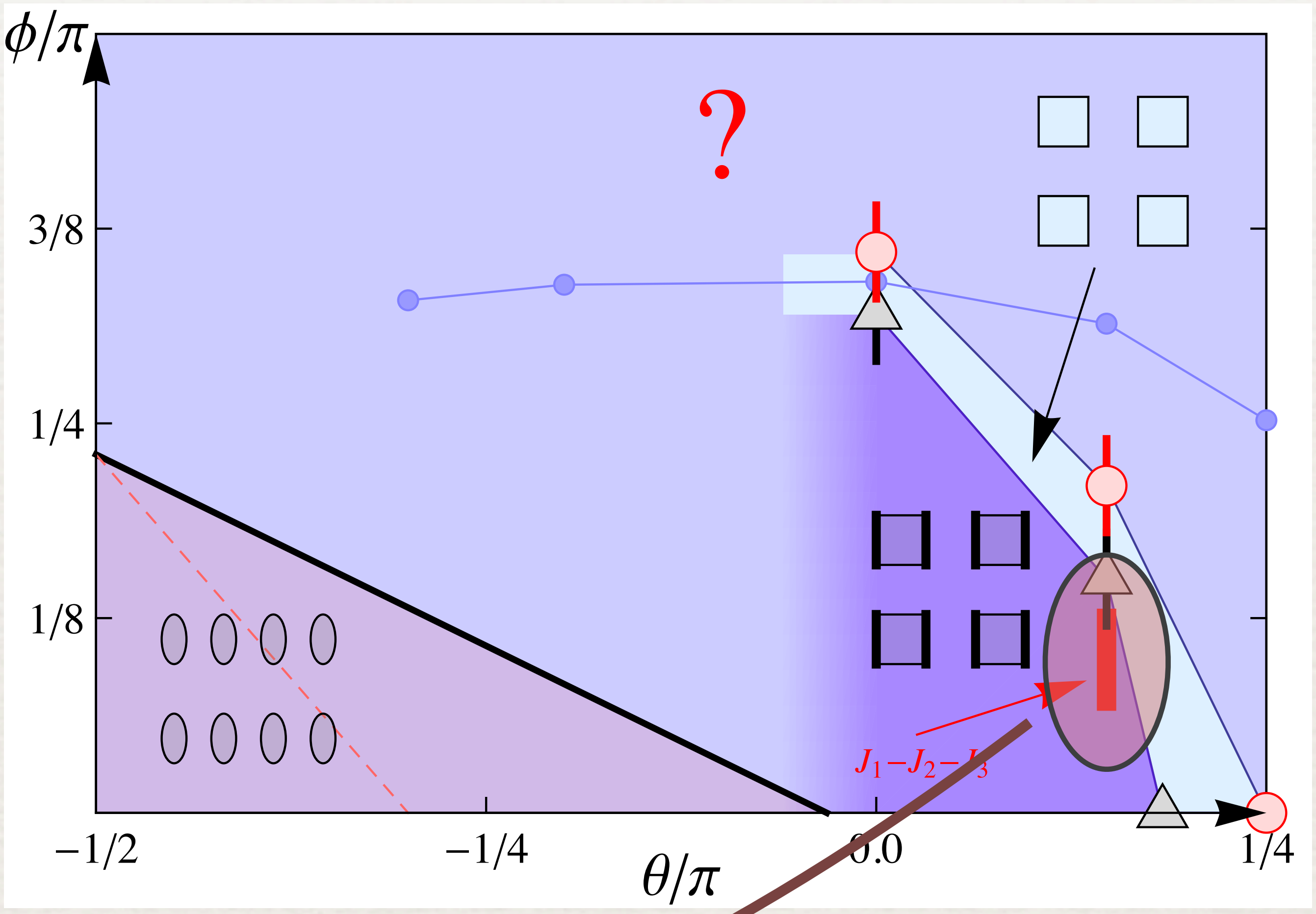
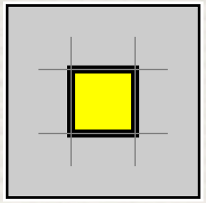
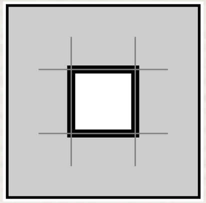
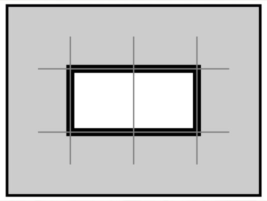


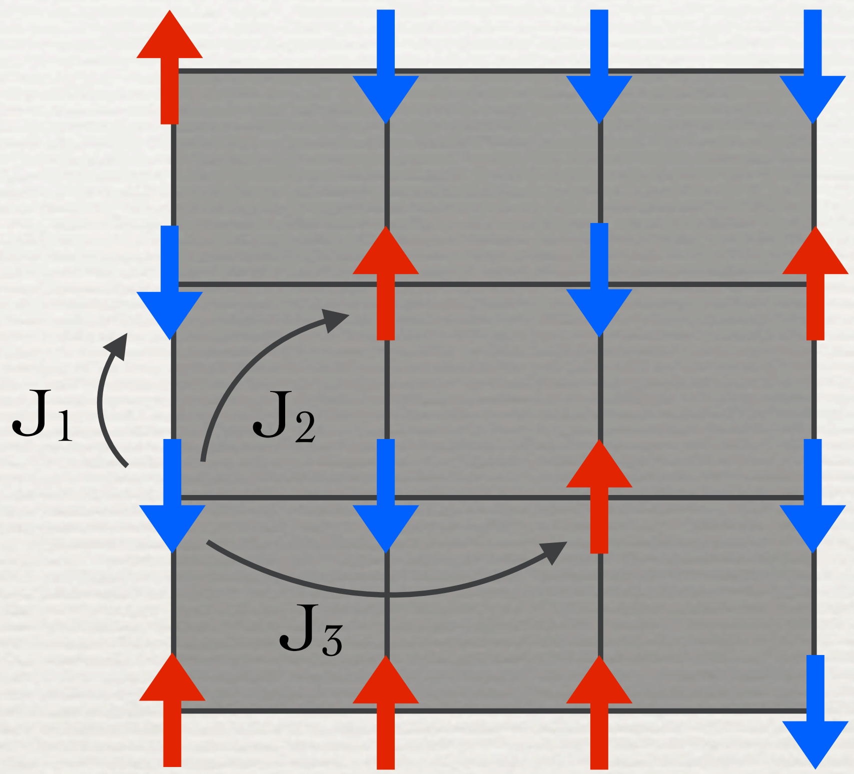


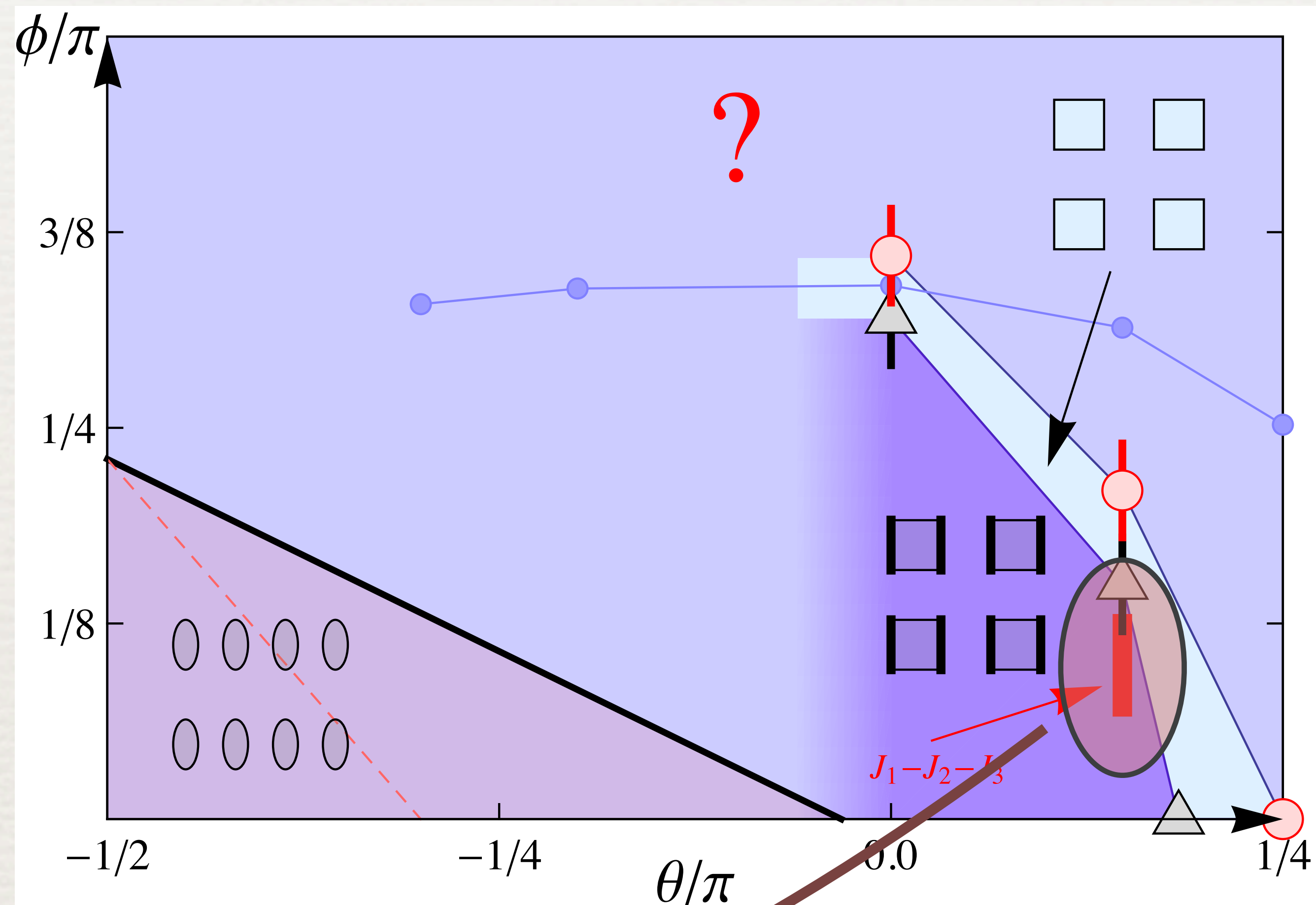
$$\mathcal{H} = J_1 \sum_{nn} \mathbf{S}_i.\mathbf{S}_j + J_2 \sum_{nnn} \mathbf{S}_i.\mathbf{S}_j$$

$$\mathcal{H} = \underbrace{\cos(\phi)\sin(\theta)}_{v}$$  $$+ \underbrace{\cos(\phi)\cos(\theta)}_{t_4}$$  $$+ \underbrace{\sin(\phi)}_{t_6}$$ 

Mixed phase in Heisenberg systems

Phase diagram at the thermodynamic limit





$$\mathcal{H} = J_1 \sum_{nn} \mathbf{S}_i.\mathbf{S}_j + J_2 \sum_{nnn} \mathbf{S}_i.\mathbf{S}_j$$

The microscopic singlet line lies in the mixed phase domain

First time that a mixed phase is observed in a microscopic spin-1/2 system

AR, M. Mambrini & D. Poilblanc, arXiv:0905.2039, to appear in PRB

Summary and Concluding Remarks

1- New kind of quantum spin liquid state has been evidenced

2- Rokhsar-Kivelson models: best candidates for these studies

3- New way of deriving effective constraint model

4- Application to an old conflicting system gives new insights

$\Rightarrow$ As in the QDM, the mixed phase scenario reconciliates previous conflicting results

Outlook

Find such phases in other systems: Kagomé AFM?