

# Deconfined quantum criticality

*Science* **303**, 1490 (2004); *Physical Review B* **70**, 144407 (2004),  
**71**, 144508 and **71**, 144509 (2005), cond-mat/0502002

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Krishnendu Sengupta (HRI, India)

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Talk online at <http://sachdev.physics.harvard.edu>



# Outline

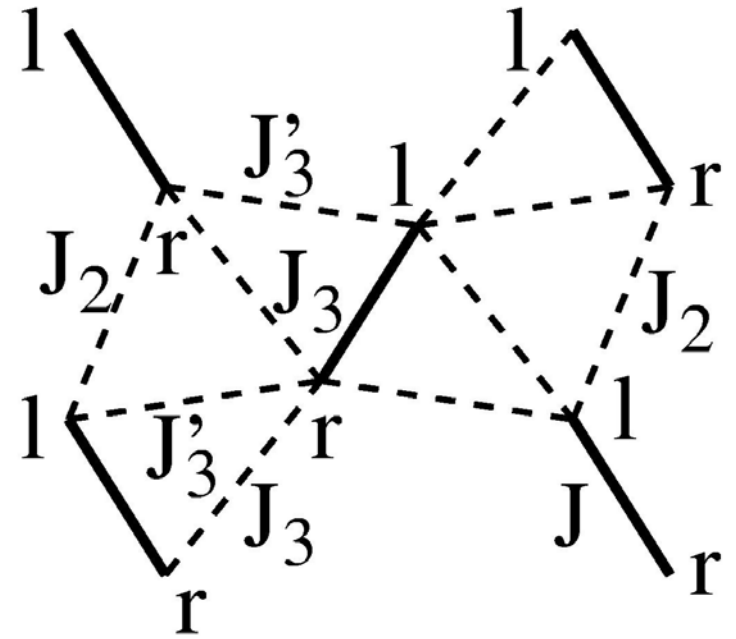
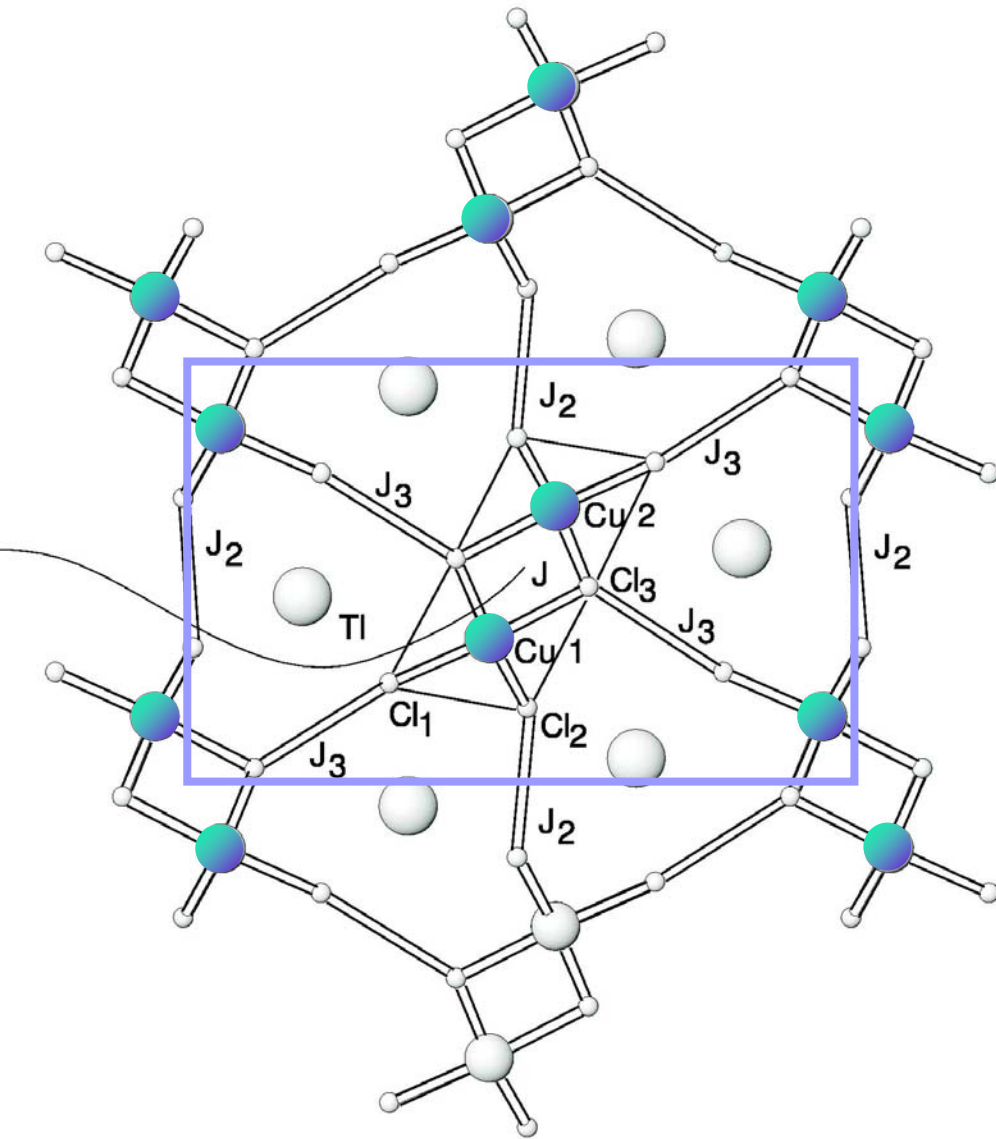
- I. Magnetic quantum phase transitions in “dimerized”  
Mott insulators:  
*Landau-Ginzburg-Wilson (LGW) theory*
  
- II. Magnetic quantum phase transitions of Mott insulators  
on the square lattice
  - A. *Breakdown of LGW theory*
  - B. *Berry phases*
  - C. *Spinor formulation and deconfined criticality*

# I. Magnetic quantum phase transitions in “dimerized” Mott insulators:

*Landau-Ginzburg-Wilson (LGW) theory:*

*Second-order phase transitions described by  
fluctuations of an order parameter  
associated with a broken symmetry*

# TiCuCl<sub>3</sub>



# Coupled Dimer Antiferromagnet

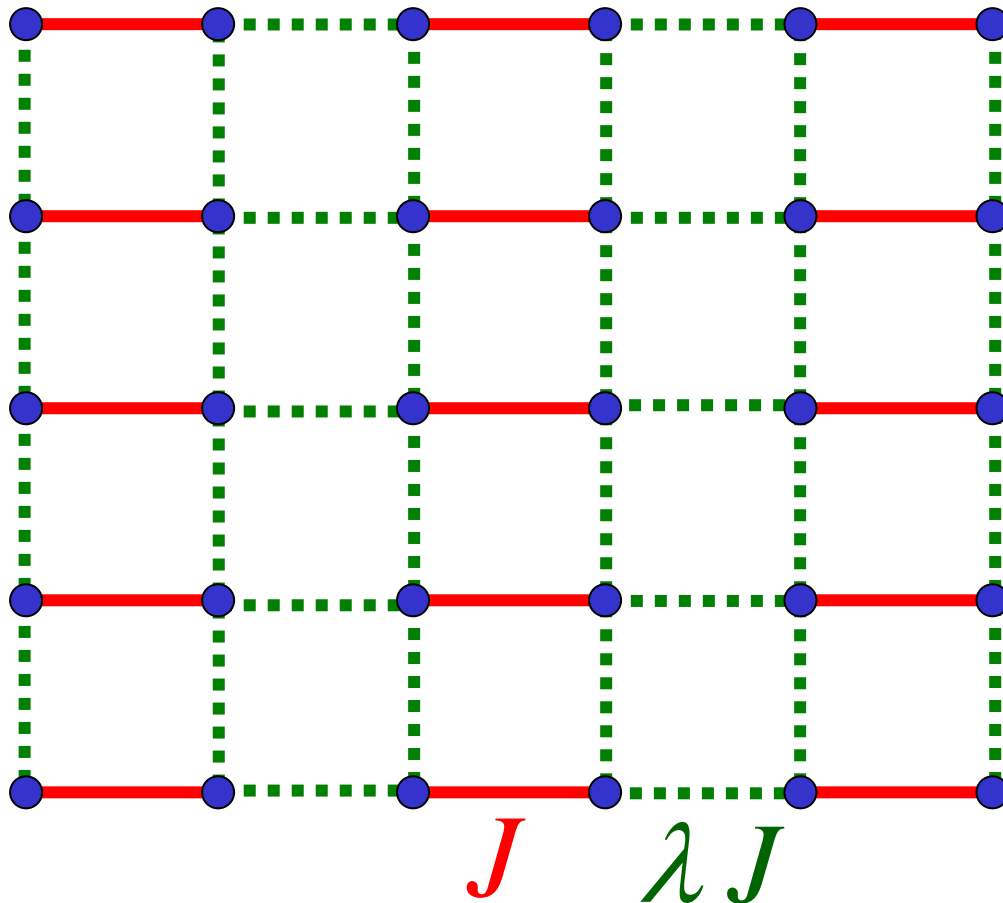
M. P. Gelfand, R. R. P. Singh, and D. A. Huse, *Phys. Rev. B* **40**, 10801-10809 (1989).

N. Katoh and M. Imada, *J. Phys. Soc. Jpn.* **63**, 4529 (1994).

J. Tworzydło, O. Y. Osman, C. N. A. van Duin, J. Zaanen, *Phys. Rev. B* **59**, 115 (1999).

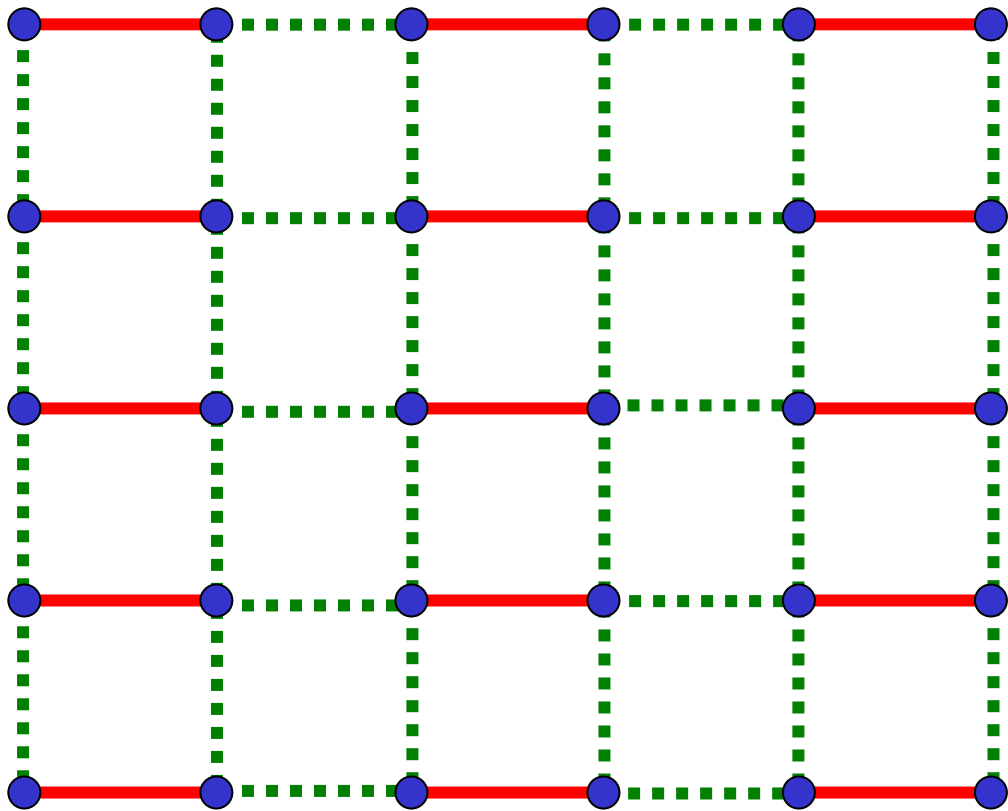
M. Matsumoto, C. Yasuda, S. Todo, and H. Takayama, *Phys. Rev. B* **65**, 014407 (2002).

$S=1/2$  spins on coupled dimers



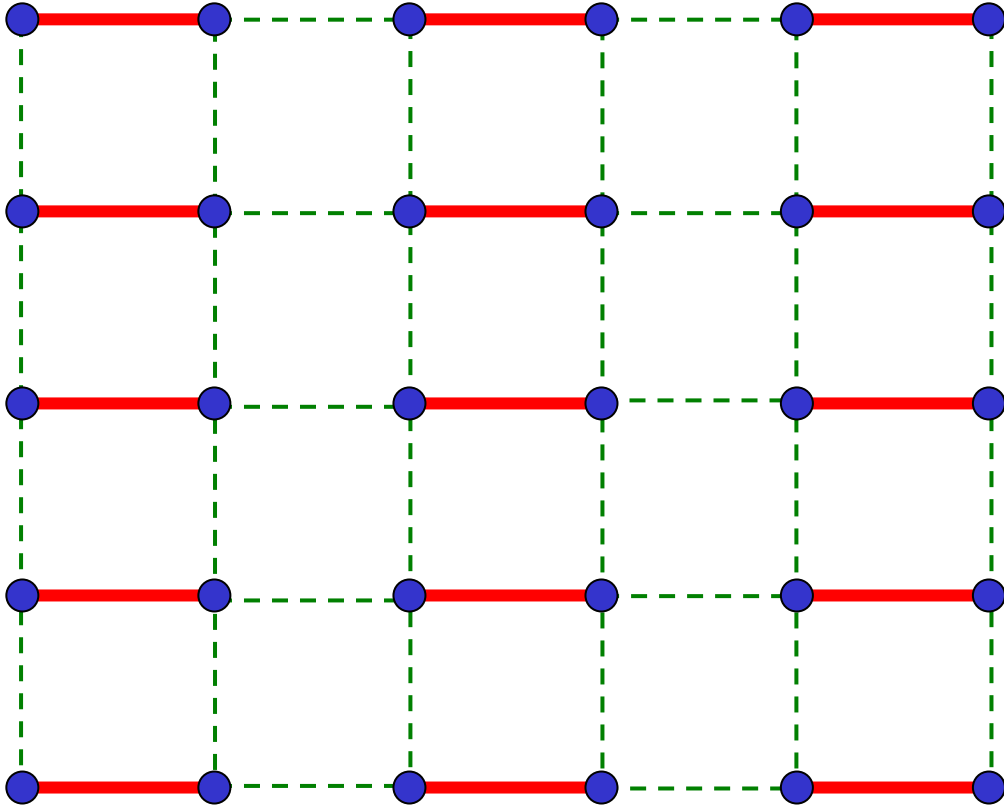
$$H = \sum_{\langle ij \rangle} J_{ij} \vec{S}_i \cdot \vec{S}_j$$

$$0 \leq \lambda \leq 1$$



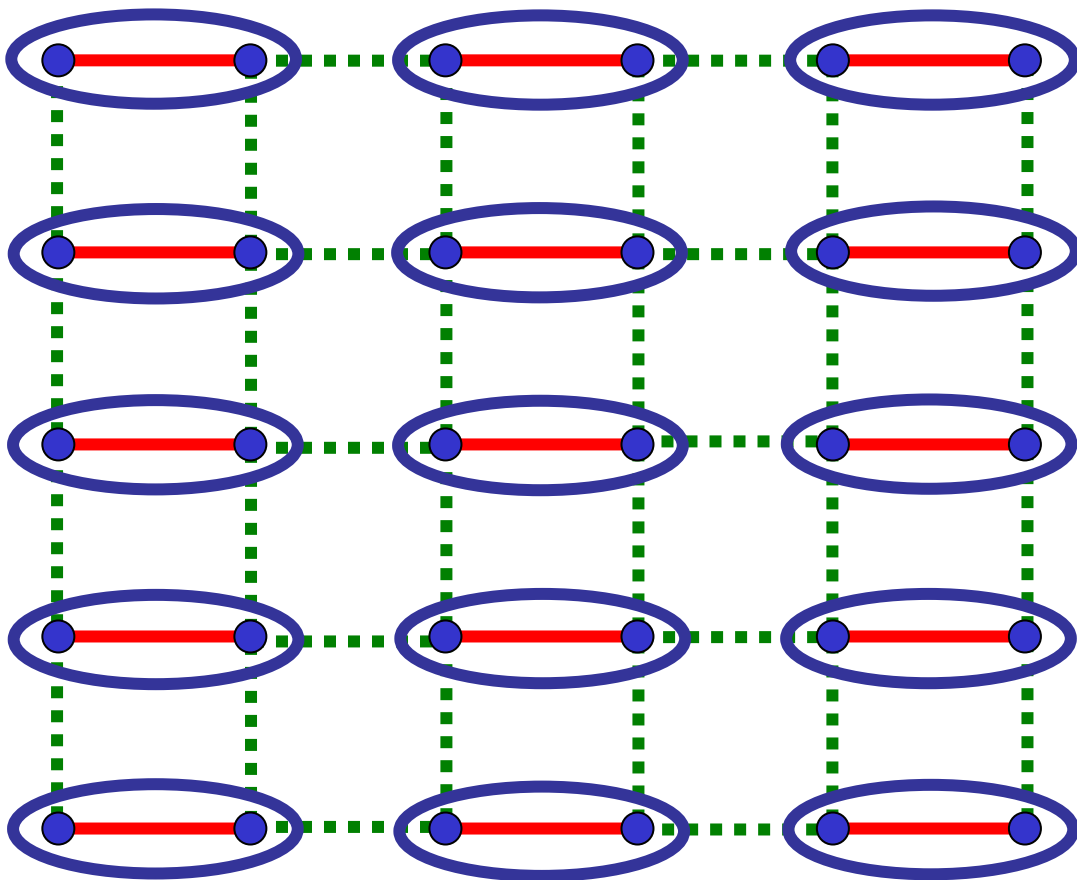
$\lambda$  close to 0

Weakly coupled dimers



$\lambda$  close to 0

Weakly coupled dimers



Paramagnetic ground state

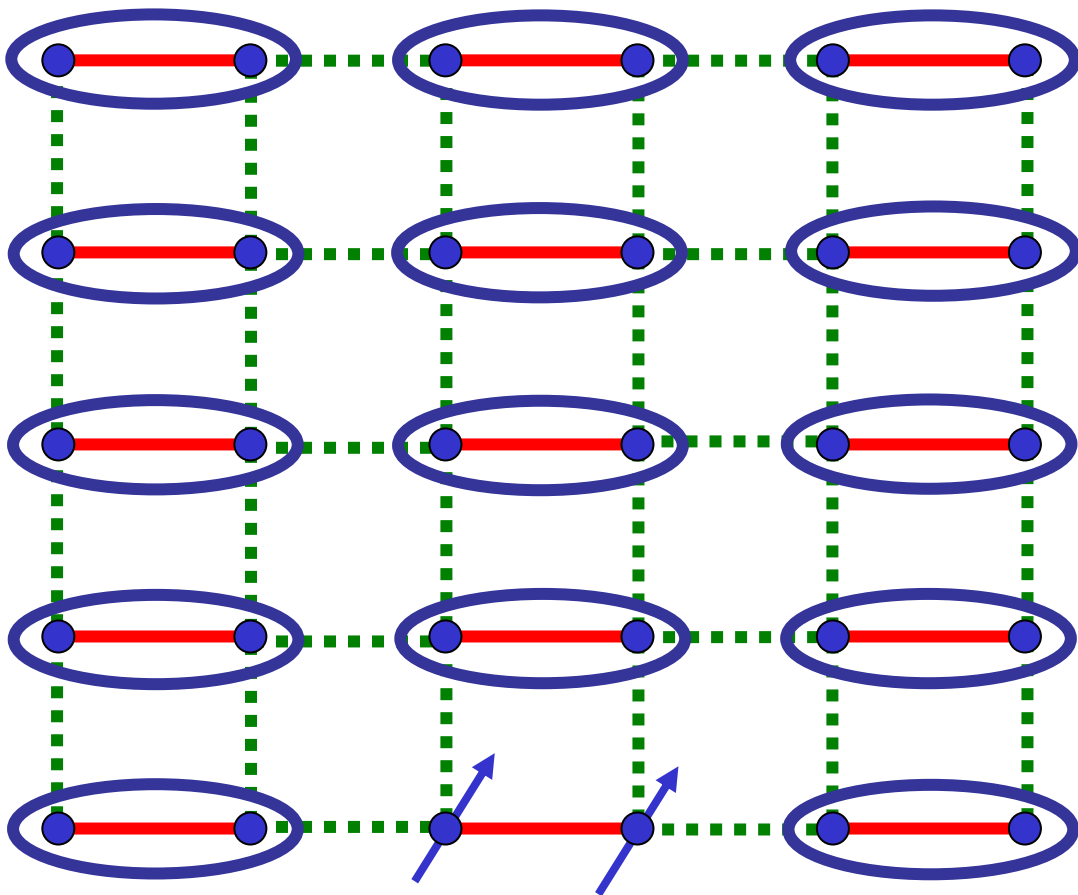
$$\text{dimer} = \frac{1}{\sqrt{2}} (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$$

$$\langle \vec{S}_i \rangle = 0$$



$\lambda$  close to 0

Weakly coupled dimers

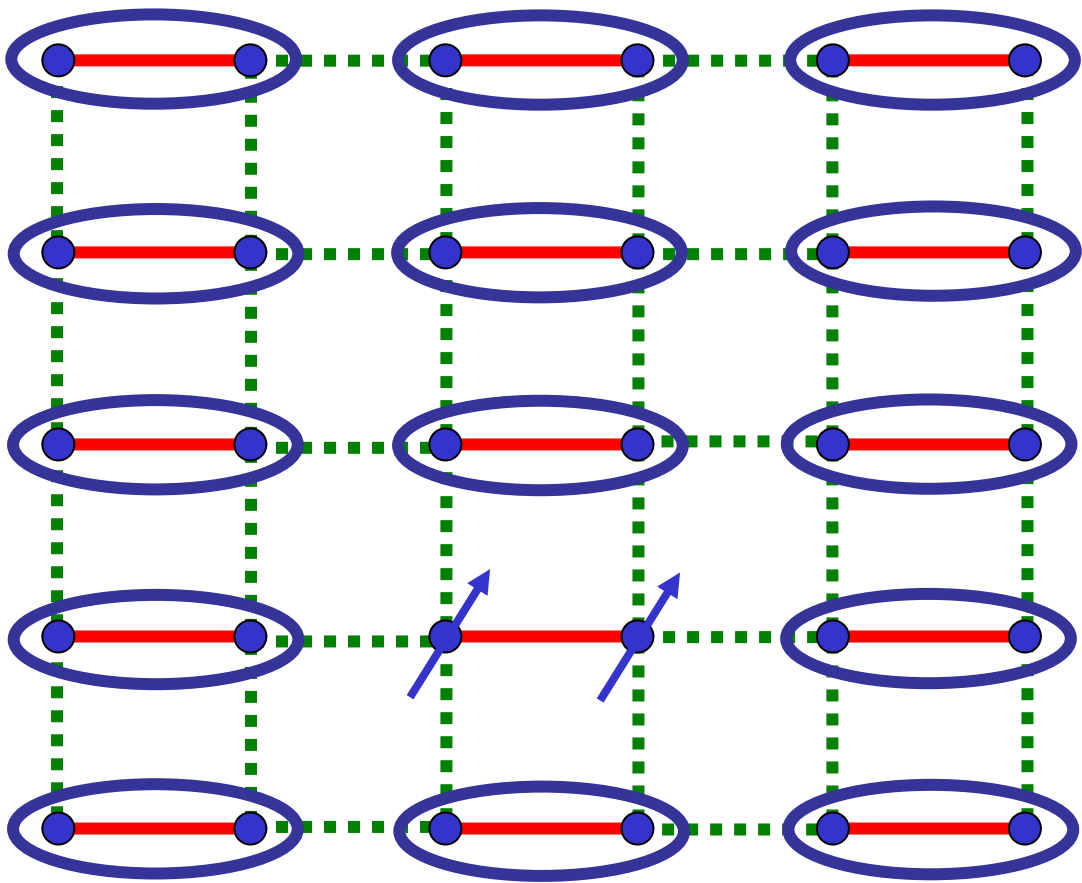


$$\text{Dimer} = \frac{1}{\sqrt{2}} (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$$

Excitation:  
 $S=1$  quasiparticle

$\lambda$  close to 0

Weakly coupled dimers

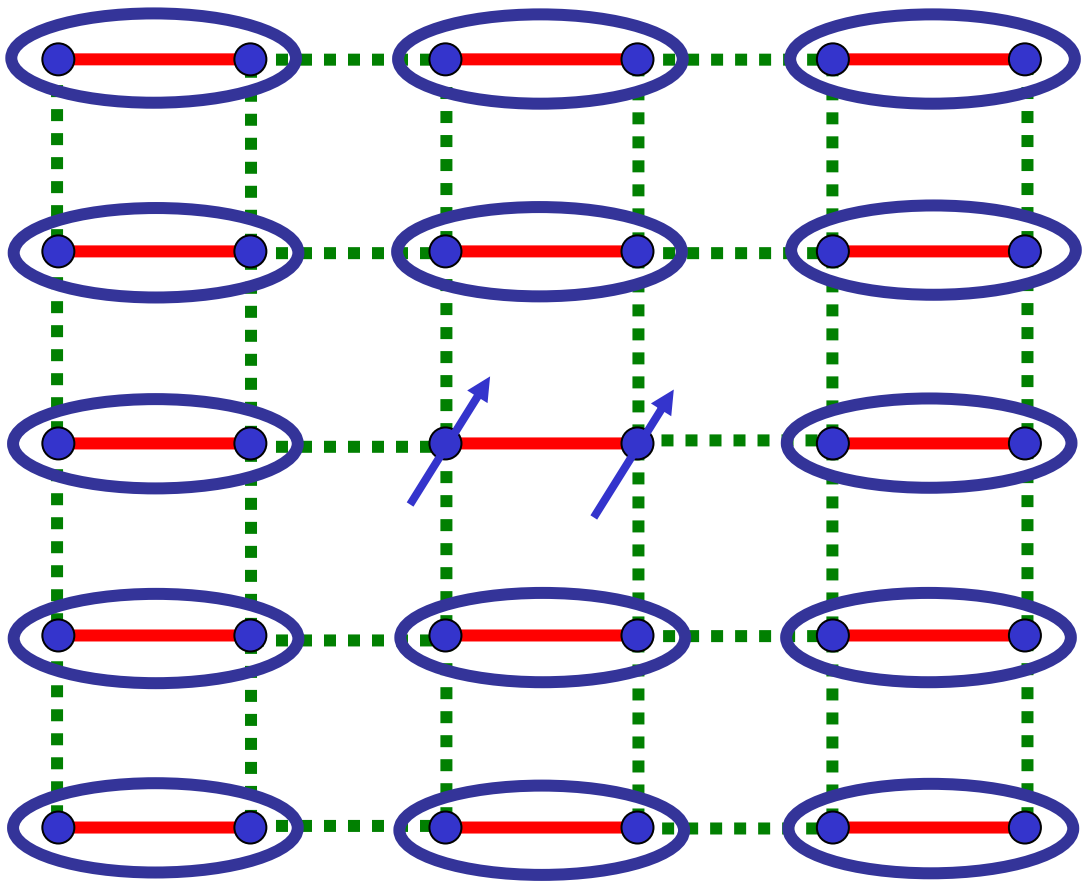


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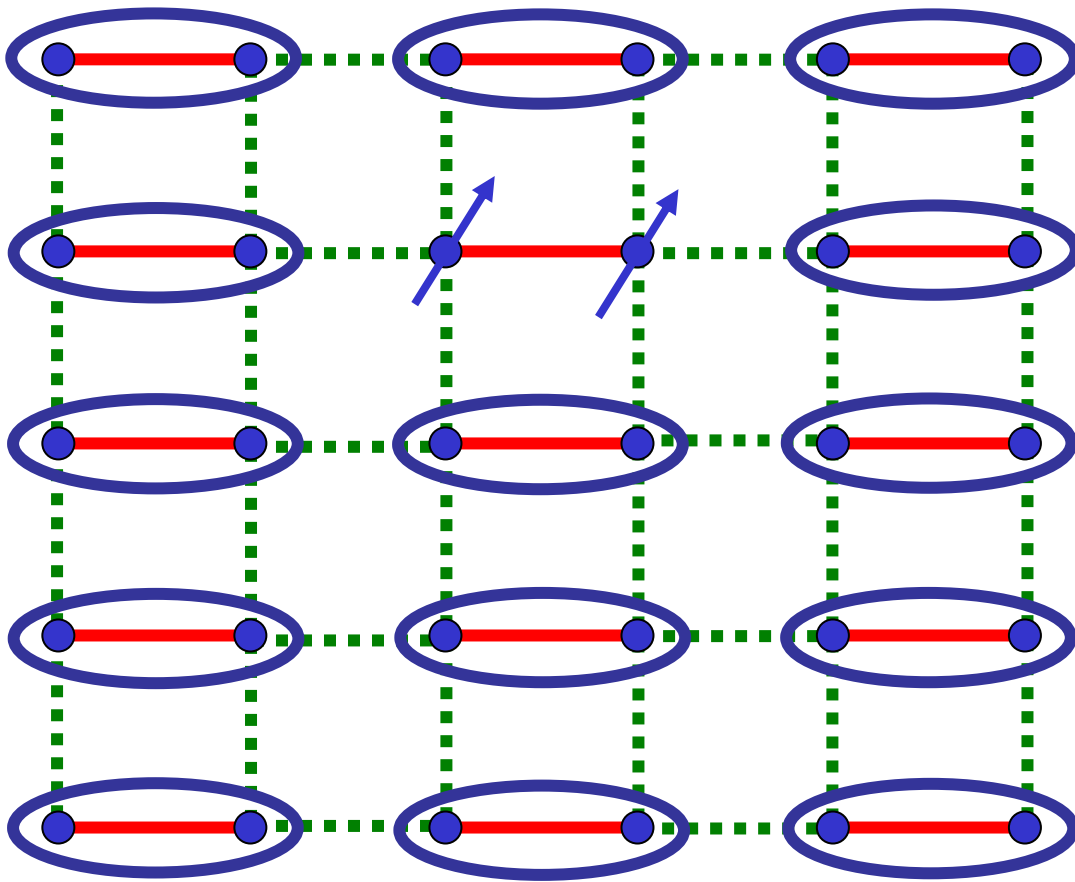


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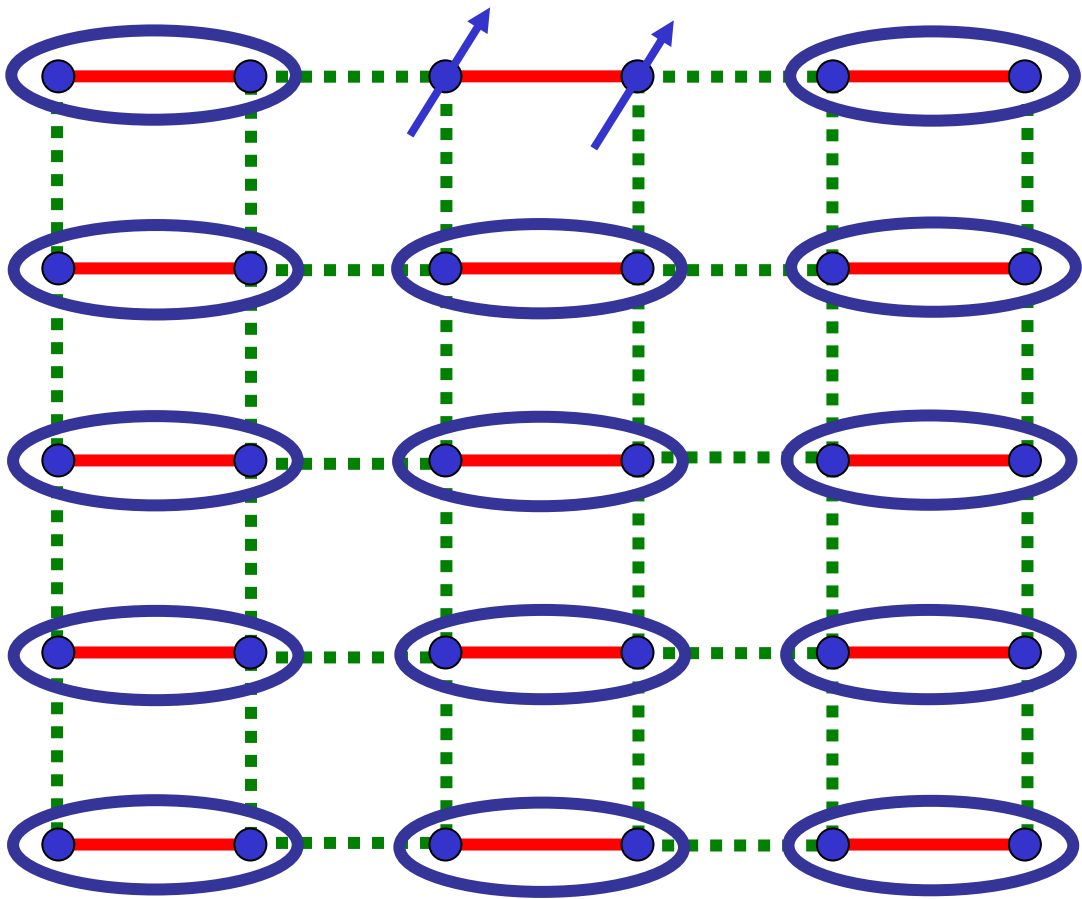


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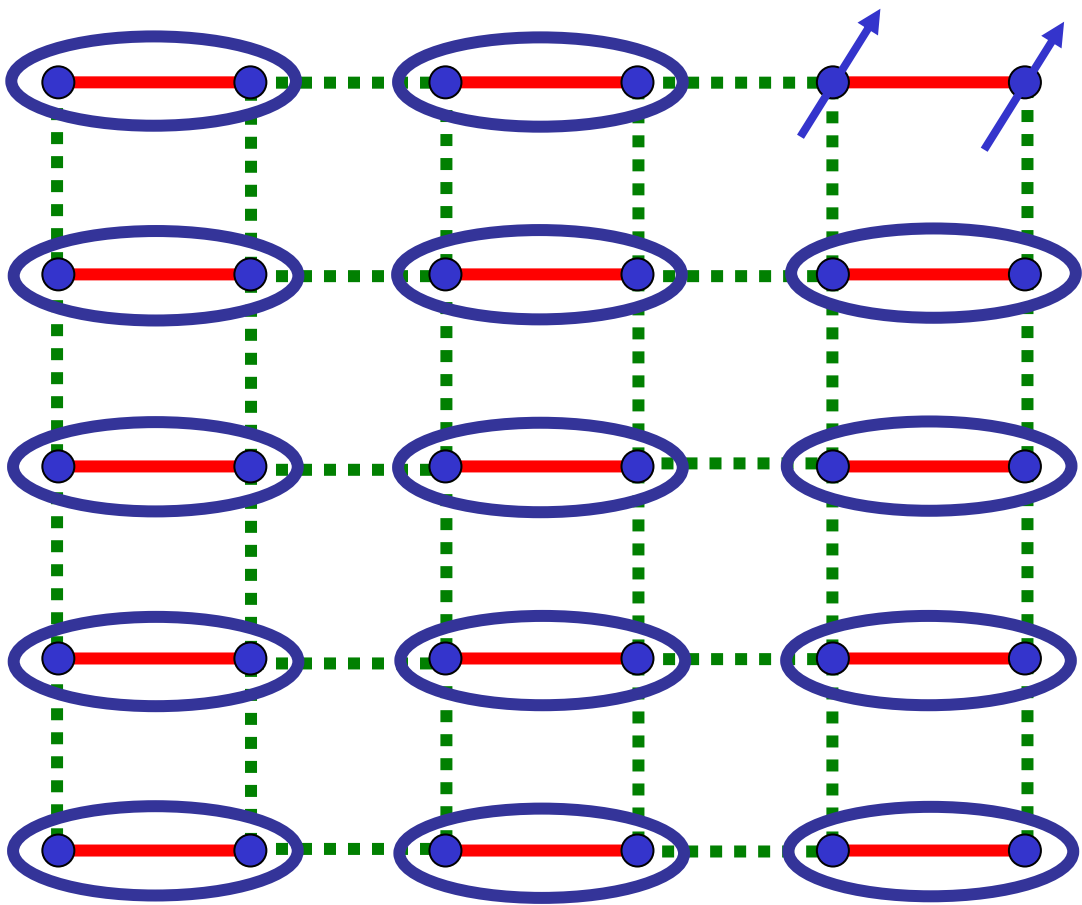


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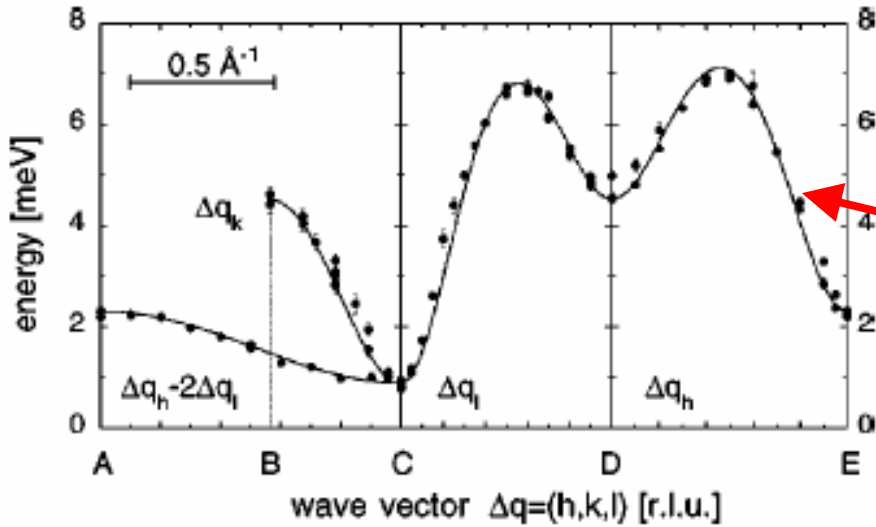
Excitation:  
 $S=1$  quasiparticle

Energy dispersion away from  
antiferromagnetic wavevector

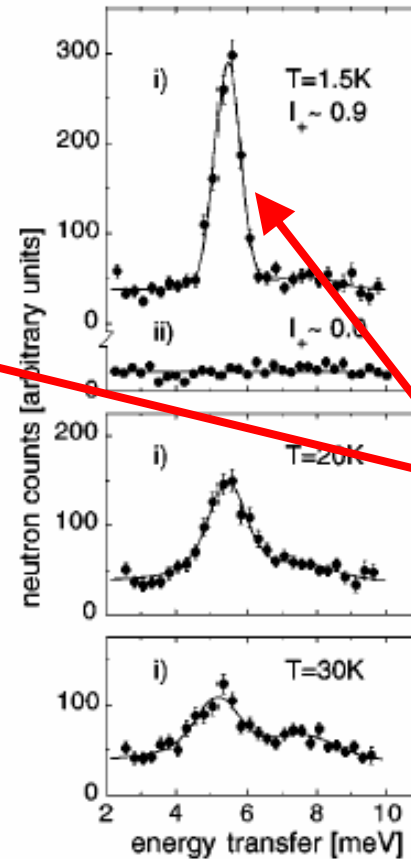
$$\varepsilon_p = \Delta + \frac{c_x^2 p_x^2 + c_y^2 p_y^2}{2\Delta}$$

$\Delta \rightarrow$  spin gap

# TiCuCl<sub>3</sub>



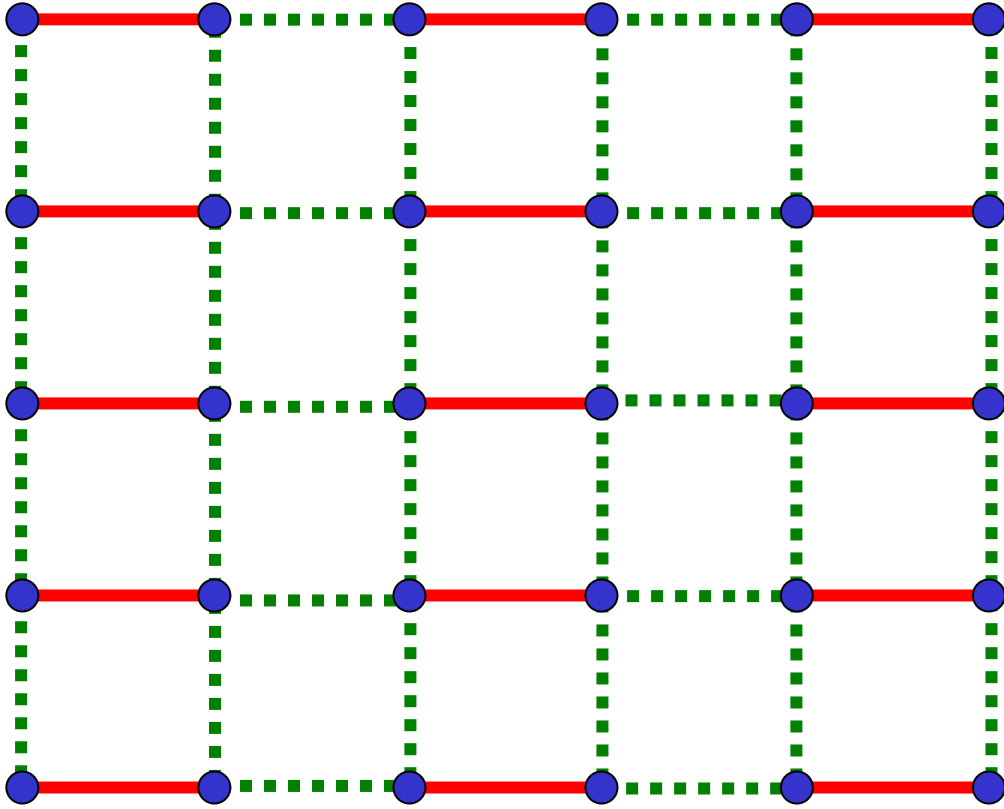
N. Cavadini, G. Heigold, W. Henggeler, A. Furrer, H.-U. Güdel, K. Krämer and H. Mutka, *Phys. Rev. B* 63 172414 (2001).



S=1  
quasi-  
particle

FIG. 1. Measured neutron profiles in the  $a^*c^*$  plane of TiCuCl<sub>3</sub> for  $i=(1.35,0,0)$ ,  $ii=(0,0,3.15)$  [r.l.u.]. The spectrum at  $T=1.5$  K

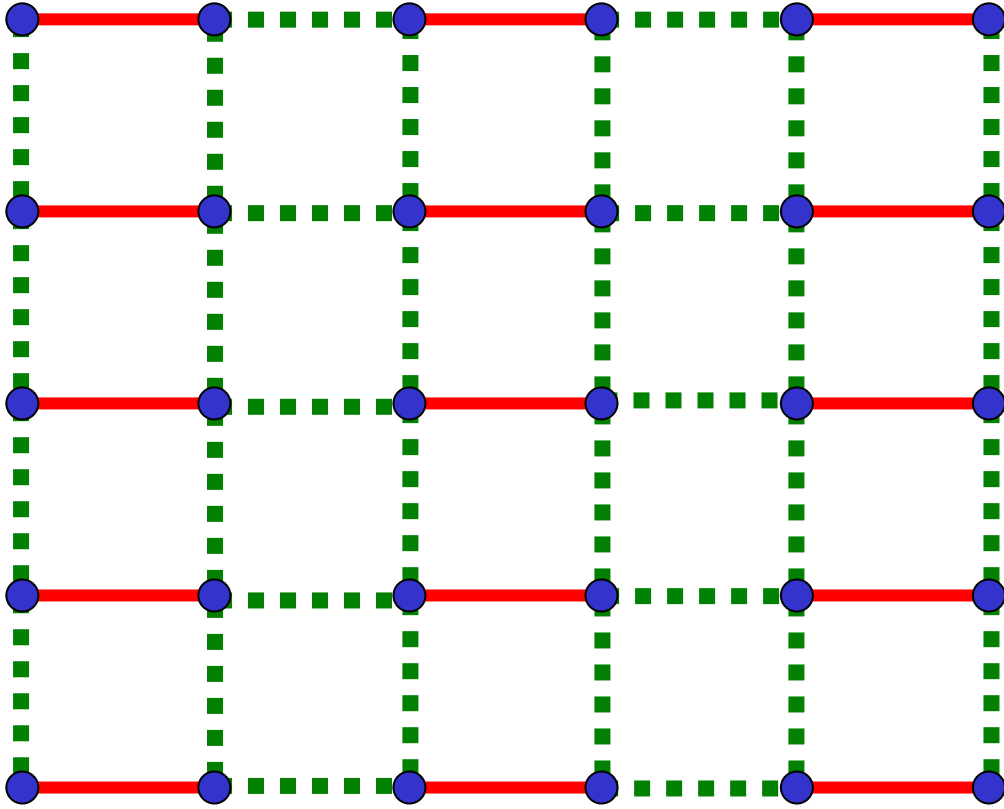
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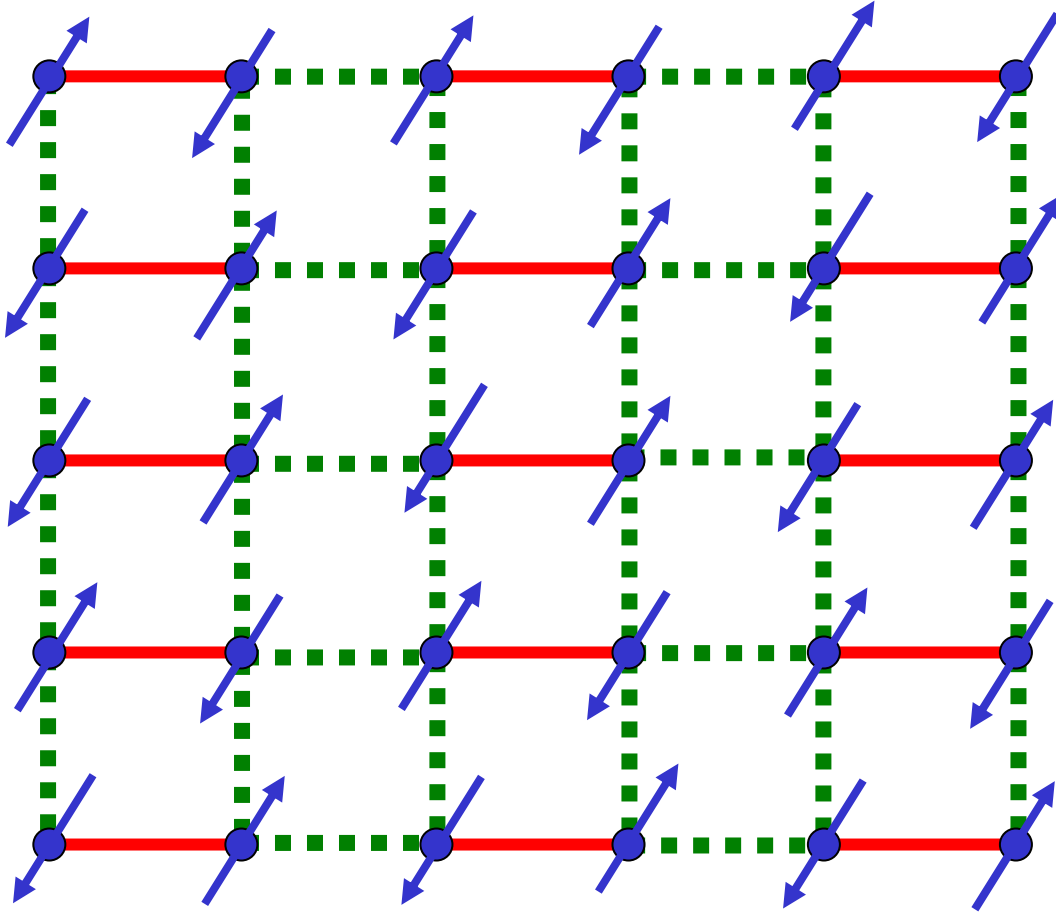
$\lambda$  close to 1

Weakly dimerized square lattice



$\lambda$  close to 1

Weakly dimerized square lattice



Excitations:  
2 spin waves (*magnons*)

$$\varepsilon_p = \sqrt{c_x^2 p_x^2 + c_y^2 p_y^2}$$

Ground state has long-range spin density wave  
(Néel) order at wavevector  $\mathbf{K} = (\pi, \pi)$

$$\langle \vec{\phi} \rangle \neq 0$$

spin density wave order parameter:  $\vec{\phi} = \eta_i \frac{\vec{S}_i}{S}$  ;  $\eta_i = \pm 1$  on two sublattices



## Neutron Diffraction Study of the Pressure-Induced Magnetic Ordering in the Spin Gap System TiCuCl<sub>3</sub>

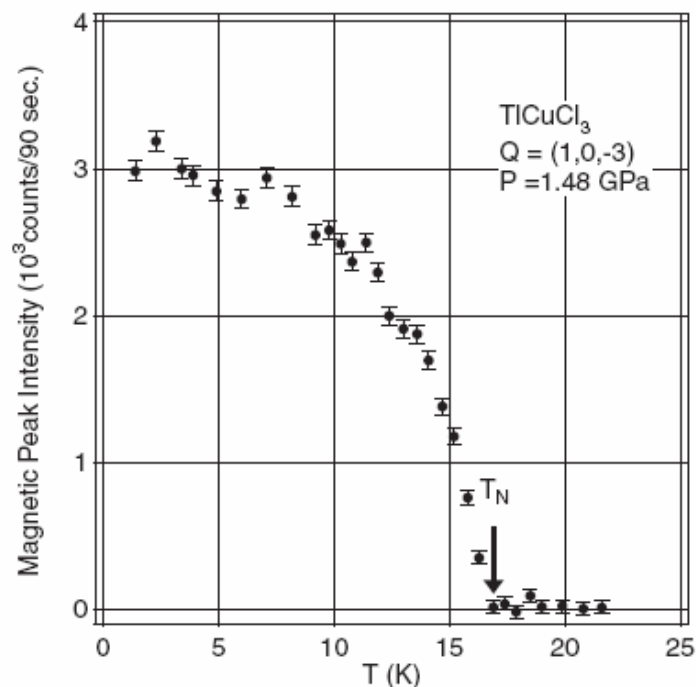
Akira OOSAWA\*, Masashi FUJISAWA<sup>1</sup>, Toyotaka OSAKABE, Kazuhisa KAKURAI and Hidekazu TANAKA<sup>2</sup>

*Advanced Science Research Center, Japan Atomic Energy Research Institute, Tokai, Ibaraki 319-1195*

<sup>1</sup>*Department of Physics, Tokyo Institute of Technology, Oh-okayama, Meguro-ku, Tokyo 152-8551*

<sup>2</sup>*Research Center for Low Temperature Physics, Tokyo Institute of Technology, Oh-okayama, Meguro-ku, Tokyo 152-8551*

(Received February 3, 2003)



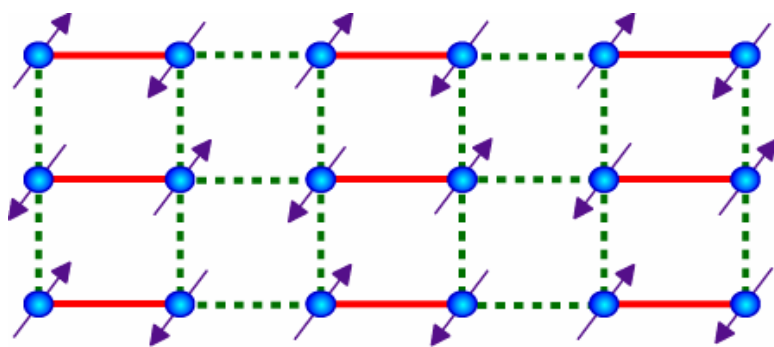
*J. Phys. Soc. Jpn* **72**, 1026 (2003)

Fig. 3. Temperature dependence of the magnetic Bragg peak intensity for  $Q = (1, 0, -3)$  reflection measured at  $P = 1.48$  GPa in TiCuCl<sub>3</sub>.

$T=0$

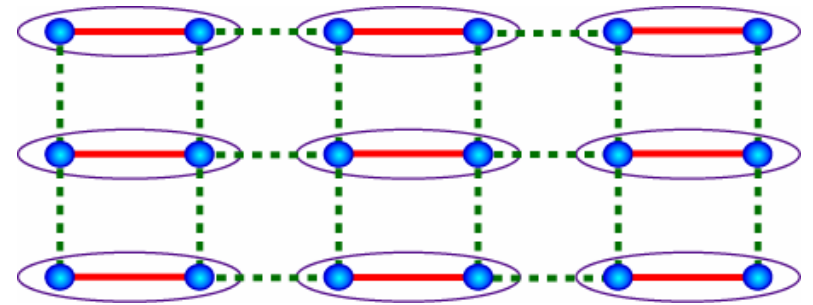
$$\lambda_c = 0.52337(3)$$

M. Matsumoto, C. Yasuda, S. Todo, and H. Takayama,  
*Phys. Rev. B* **65**, 014407 (2002)



Néel state

$$\langle \vec{\phi} \rangle \neq 0$$



Quantum paramagnet

$$\langle \vec{\phi} \rangle = 0$$

$\lambda$

1

$\lambda_c$

Pressure in  $\text{TlCuCl}_3$

The method of bond operators (S. Sachdev and R.N. Bhatt, *Phys. Rev. B* **41**, 9323 (1990)) provides a quantitative description of spin excitations in  $\text{TlCuCl}_3$  across the quantum phase transition (M. Matsumoto, B. Normand, T.M. Rice, and M. Sigrist, *Phys. Rev. Lett.* **89**, 077203 (2002))

# LGW theory for quantum criticality

Landau-Ginzburg-Wilson theory: write down an effective action for the antiferromagnetic order parameter  $\vec{\varphi}$  by expanding in powers of  $\vec{\varphi}$  and its spatial and temporal derivatives, while preserving all symmetries of the microscopic Hamiltonian

$$S_{\varphi} = \int d^2x d\tau \left[ \frac{1}{2} \left( (\nabla_x \vec{\varphi})^2 + c^2 (\partial_{\tau} \vec{\varphi})^2 + (\lambda_c - \lambda) \vec{\varphi}^2 \right) + \frac{u}{4!} (\vec{\varphi}^2)^2 \right]$$

S. Chakravarty, B.I. Halperin, and D.R. Nelson, *Phys. Rev. B* **39**, 2344 (1989)

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For  $\lambda < \lambda_c$ , oscillations of  $\vec{\varphi}$  about  $\vec{\varphi} = 0$  constitute the *triplon* excitation

A.V. Chubukov, S. Sachdev, and J. Ye, *Phys. Rev. B* **49**, 11919 (1994)

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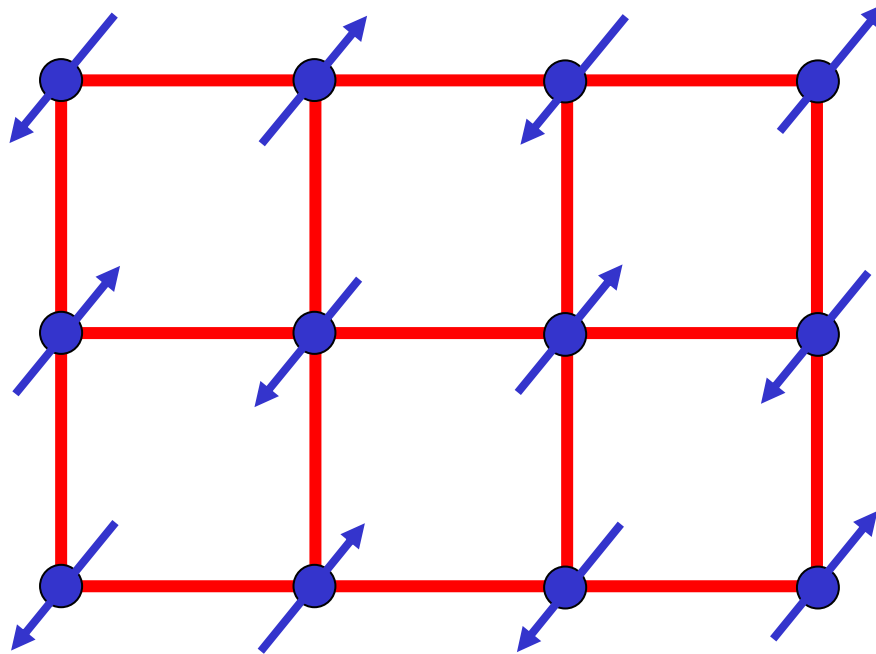
## II. Magnetic quantum phase transitions of Mott insulators on the square lattice:

### *A. Breakdown of LGW theory*



## Square lattice antiferromagnet

$$H = \sum_{\langle ij \rangle} J_{ij} \vec{S}_i \cdot \vec{S}_j \quad ; \quad \vec{S}_i \Rightarrow \text{spin operator with } S=1/2$$



Ground state has long-range Néel order

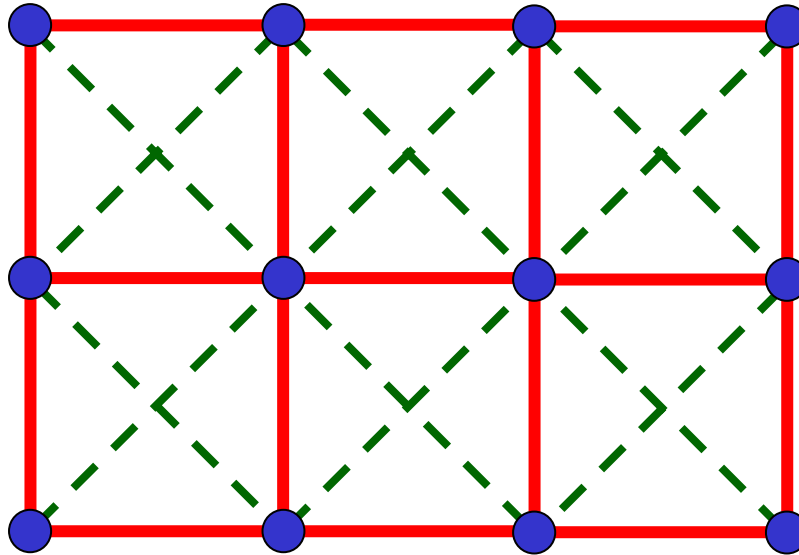
Order parameter  $\vec{\phi} = \eta_i \vec{S}_i$

$\eta_i = \pm 1$  on two sublattices

$$\langle \vec{\phi} \rangle \neq 0$$

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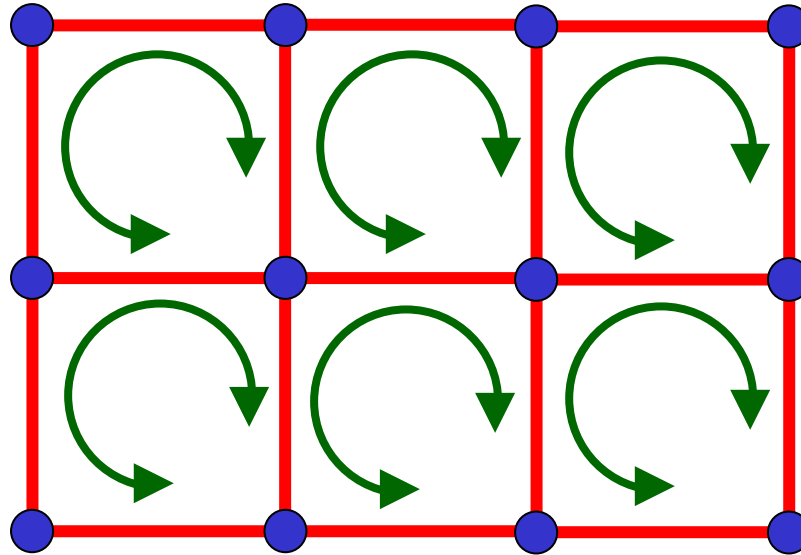


Destroy Neel order by perturbations which preserve full square lattice symmetry *e.g.* second-neighbor or ring exchange.

What is the state with  $\langle \vec{\phi} \rangle = 0$  ?

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## LGW theory for quantum criticality

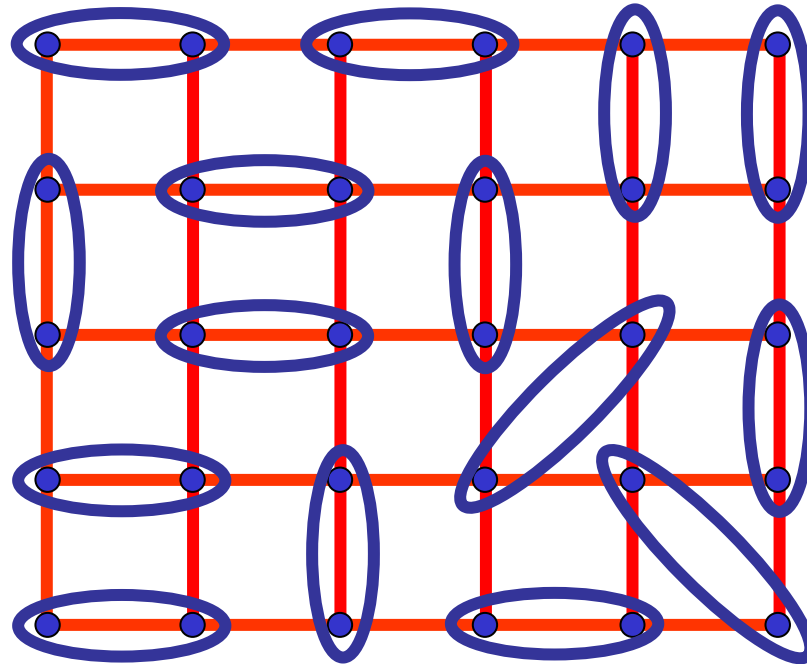
Landau-Ginzburg-Wilson theory: write down an effective action for the antiferromagnetic order parameter  $\vec{\varphi}$  by expanding in powers of  $\vec{\varphi}$  and its spatial and temporal derivatives, while preserving all symmetries of the microscopic Hamiltonian

$$S_{\varphi} = \int d^2x d\tau \left[ \frac{1}{2} \left( (\nabla_x \vec{\varphi})^2 + c^2 (\partial_{\tau} \vec{\varphi})^2 + r \vec{\varphi}^2 \right) + \frac{u}{4!} (\vec{\varphi}^2)^2 \right]$$

The ground state for  $r > 0$  has no broken symmetry and a gapped S=1 quasiparticle excitation  
(oscillations of  $\vec{\varphi}$  about  $\vec{\varphi} = 0$ )

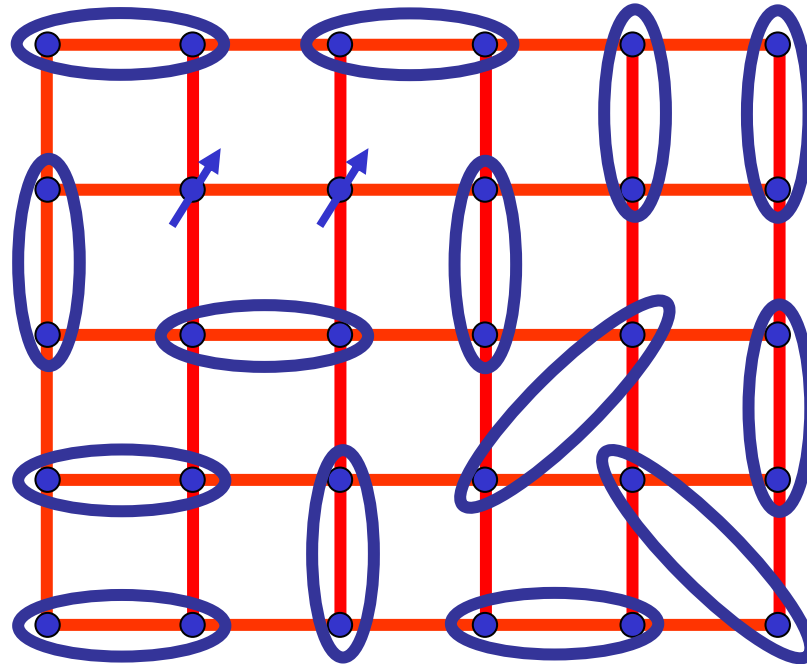
**Problem: there is no state with a gapped, stable**  
 **$S=1$  quasiparticle and no broken symmetries**

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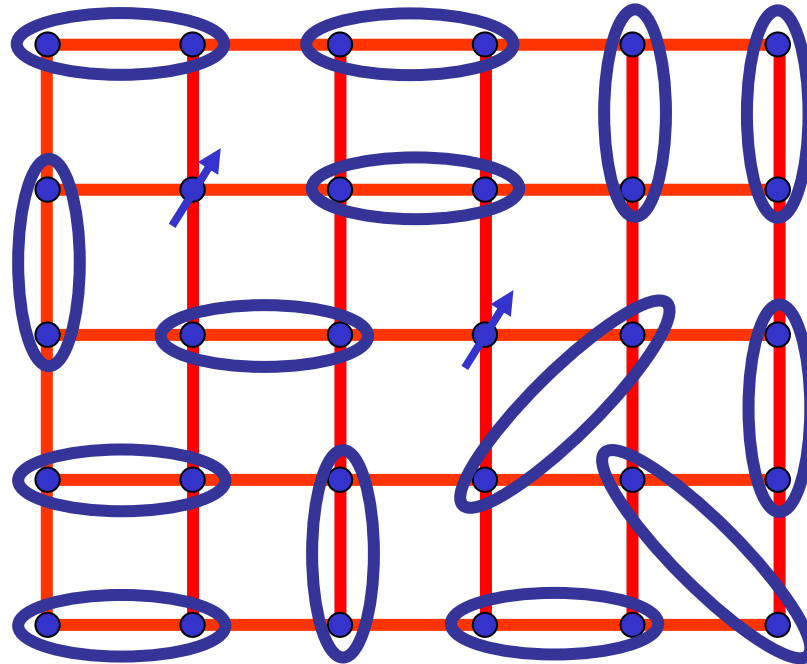
“Liquid” of valence bonds has  
fractionalized  $S=1/2$  excitations

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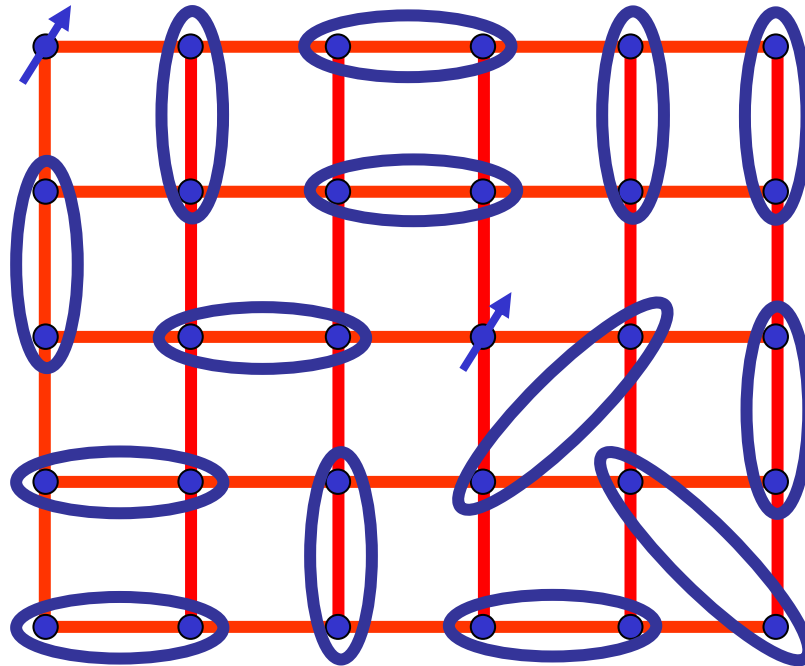
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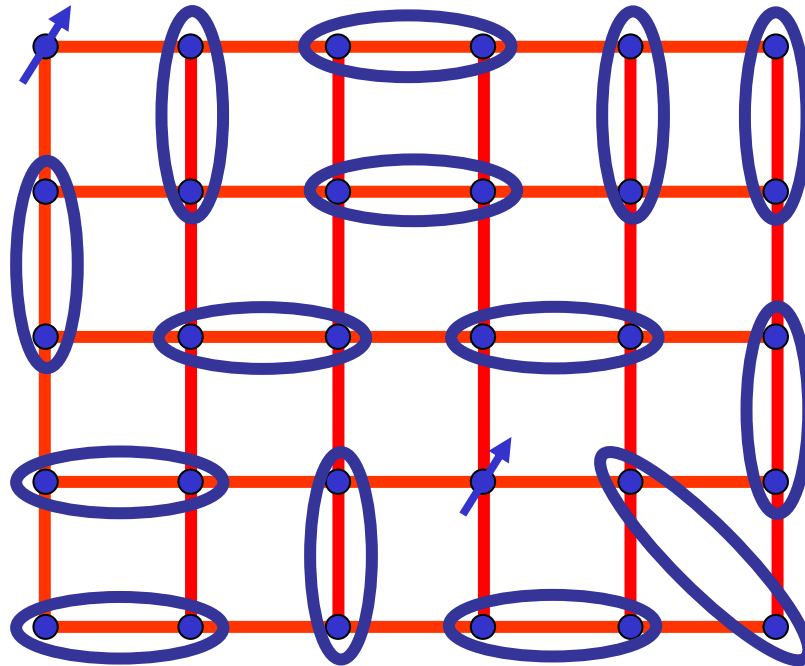


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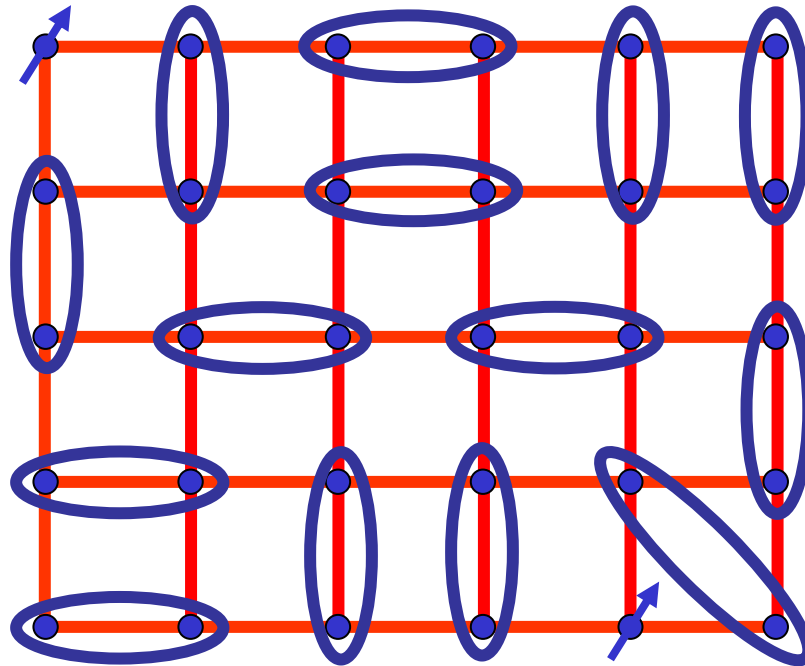
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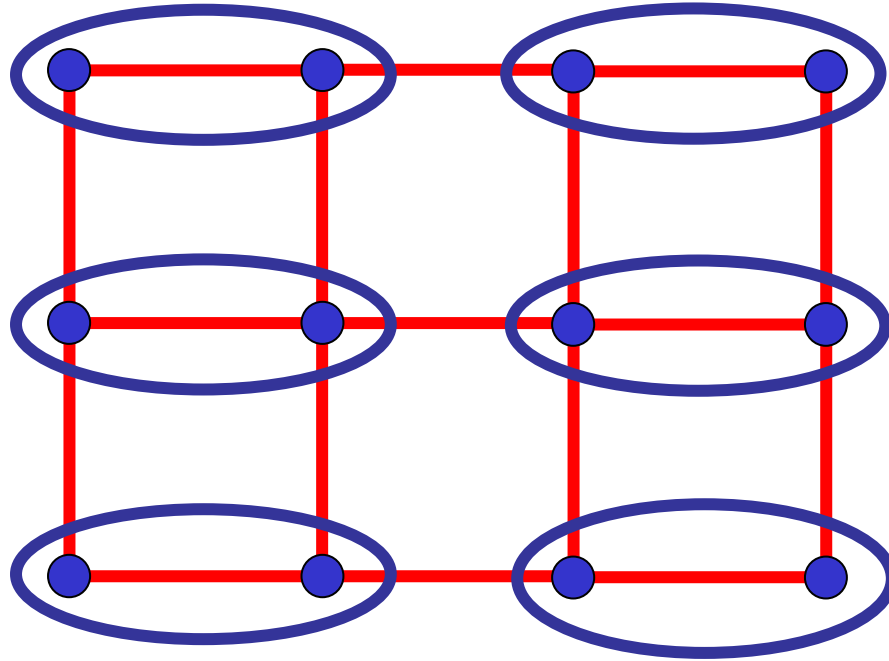
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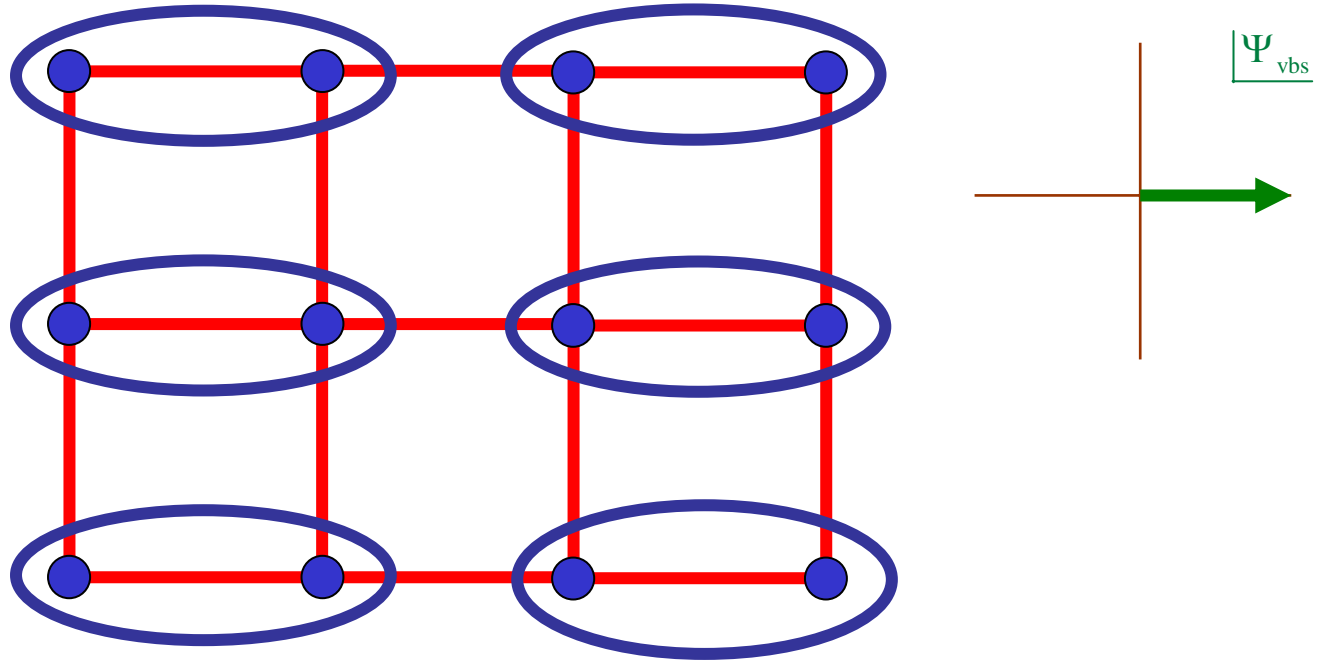


“Liquid” of valence bonds has fractionalized  $S=1/2$  excitations

Another possible state, with  $\langle \vec{\phi} \rangle = 0$ , is the valence bond solid (VBS)



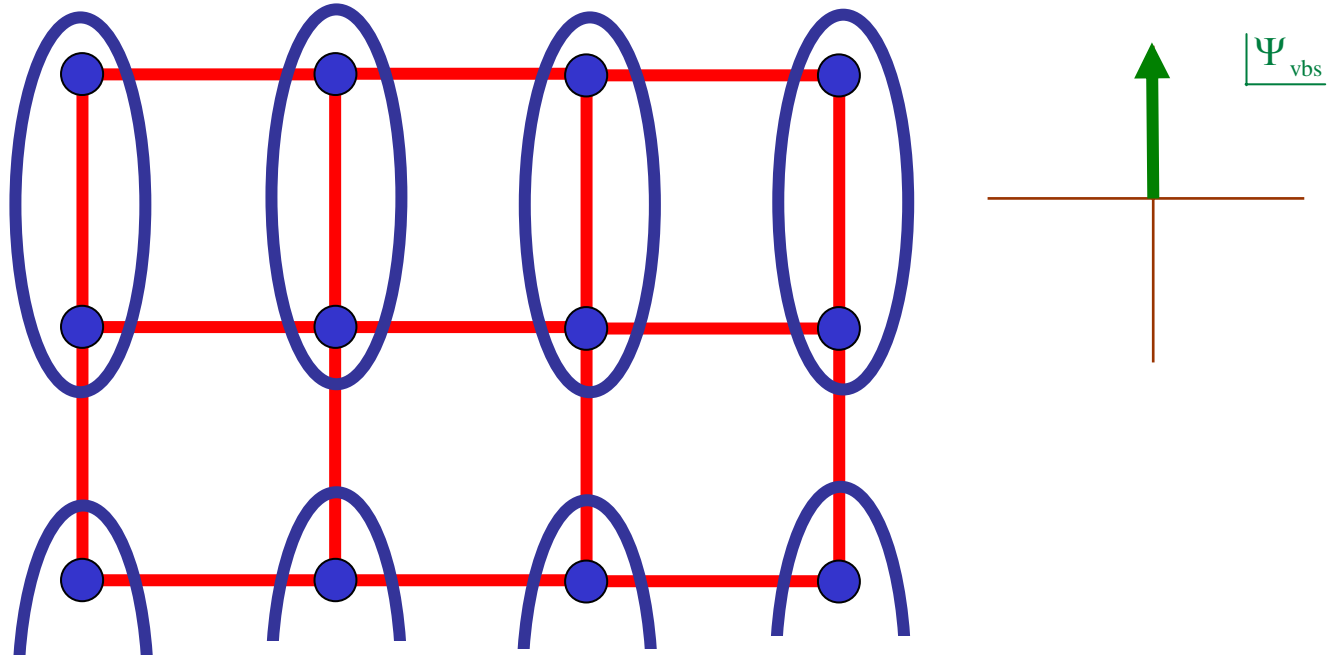
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Such a state breaks the symmetry of rotations by  $n\pi/2$  about lattice sites,  
and has  $\langle \Psi_{\text{vbs}} \rangle \neq 0$ , where  $\Psi_{\text{vbs}}$  is the *VBS order parameter*

$$\Psi_{\text{vbs}}(i) = \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j e^{i \arctan(\mathbf{r}_j - \mathbf{r}_i)}$$

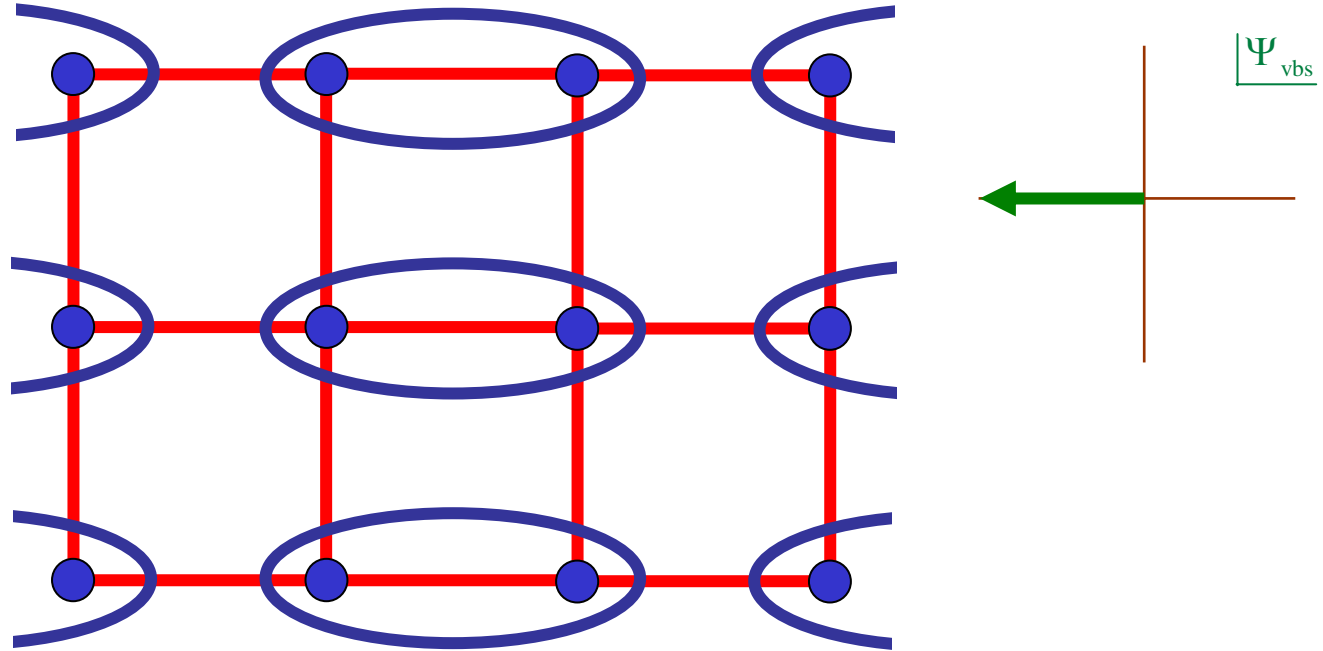
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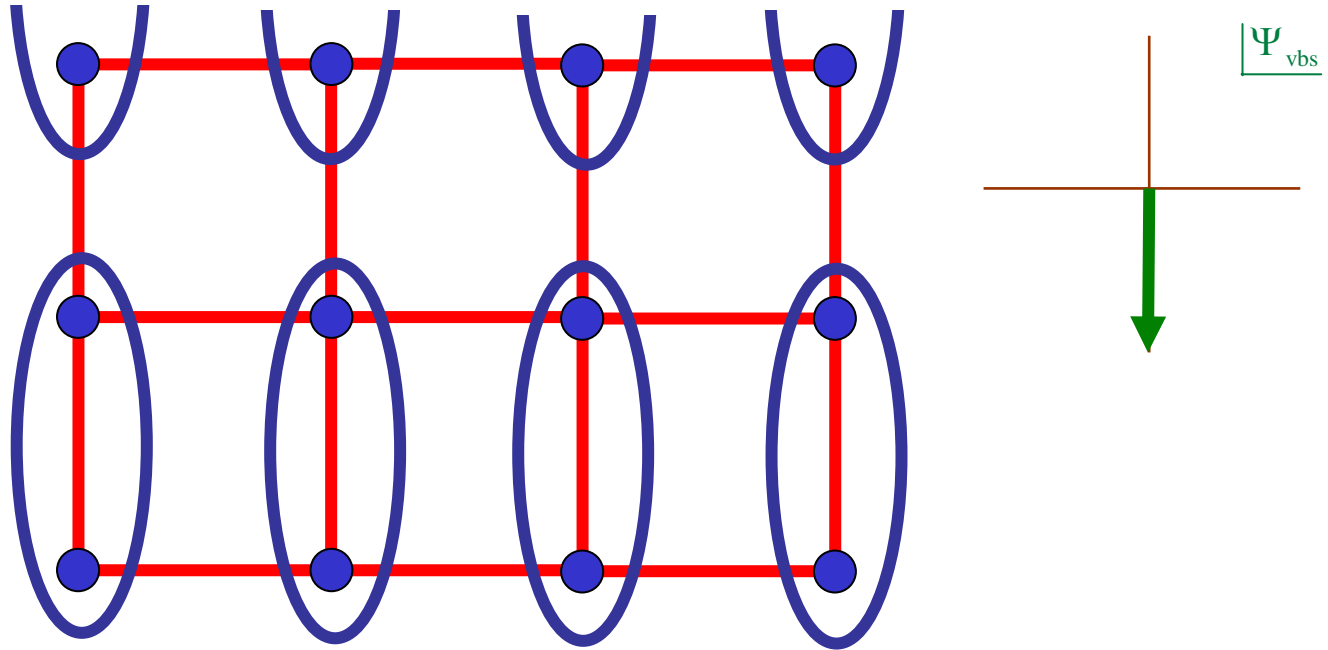
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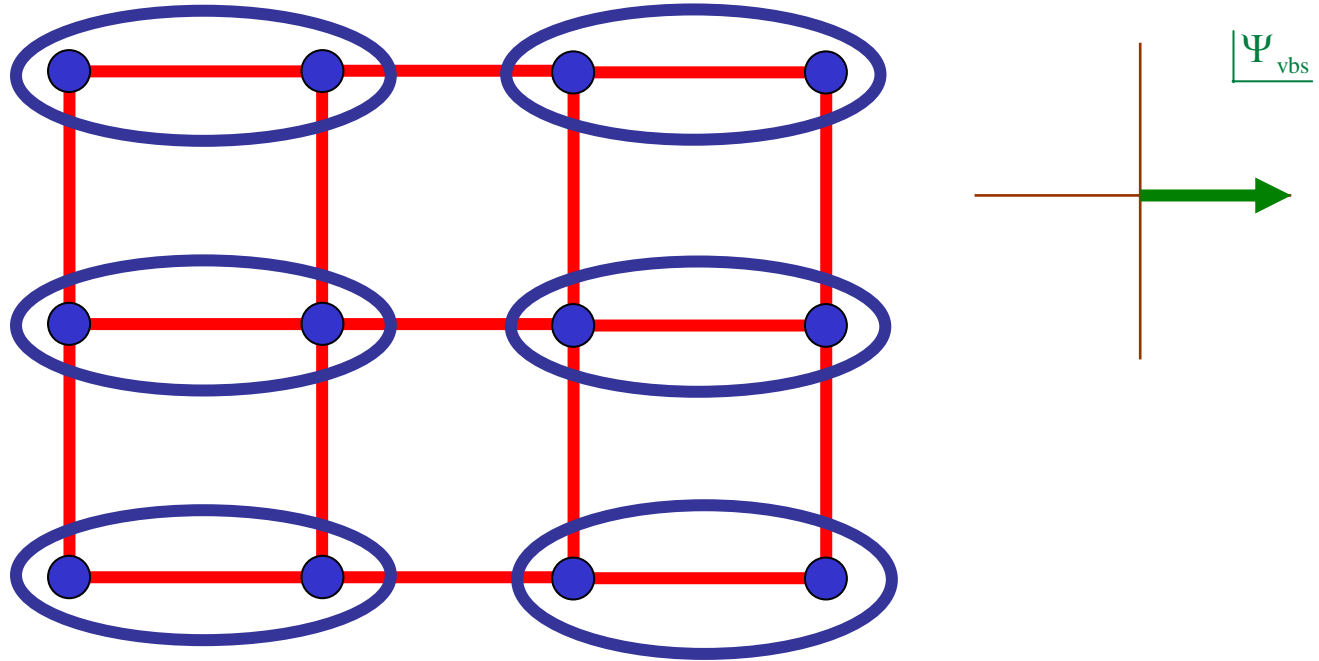


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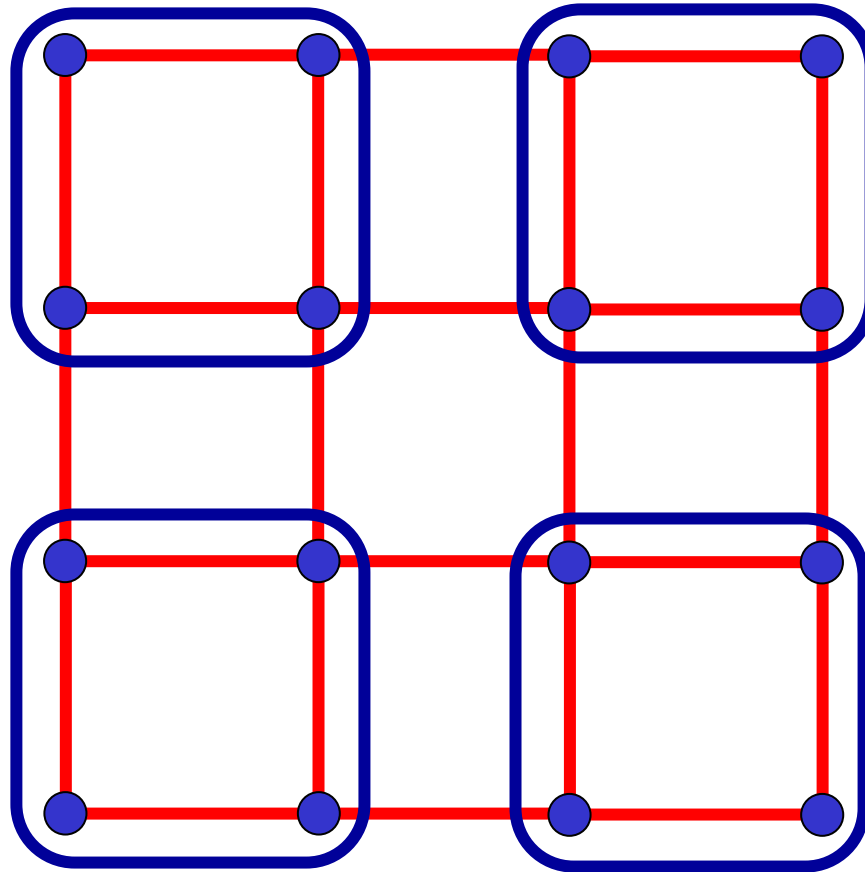
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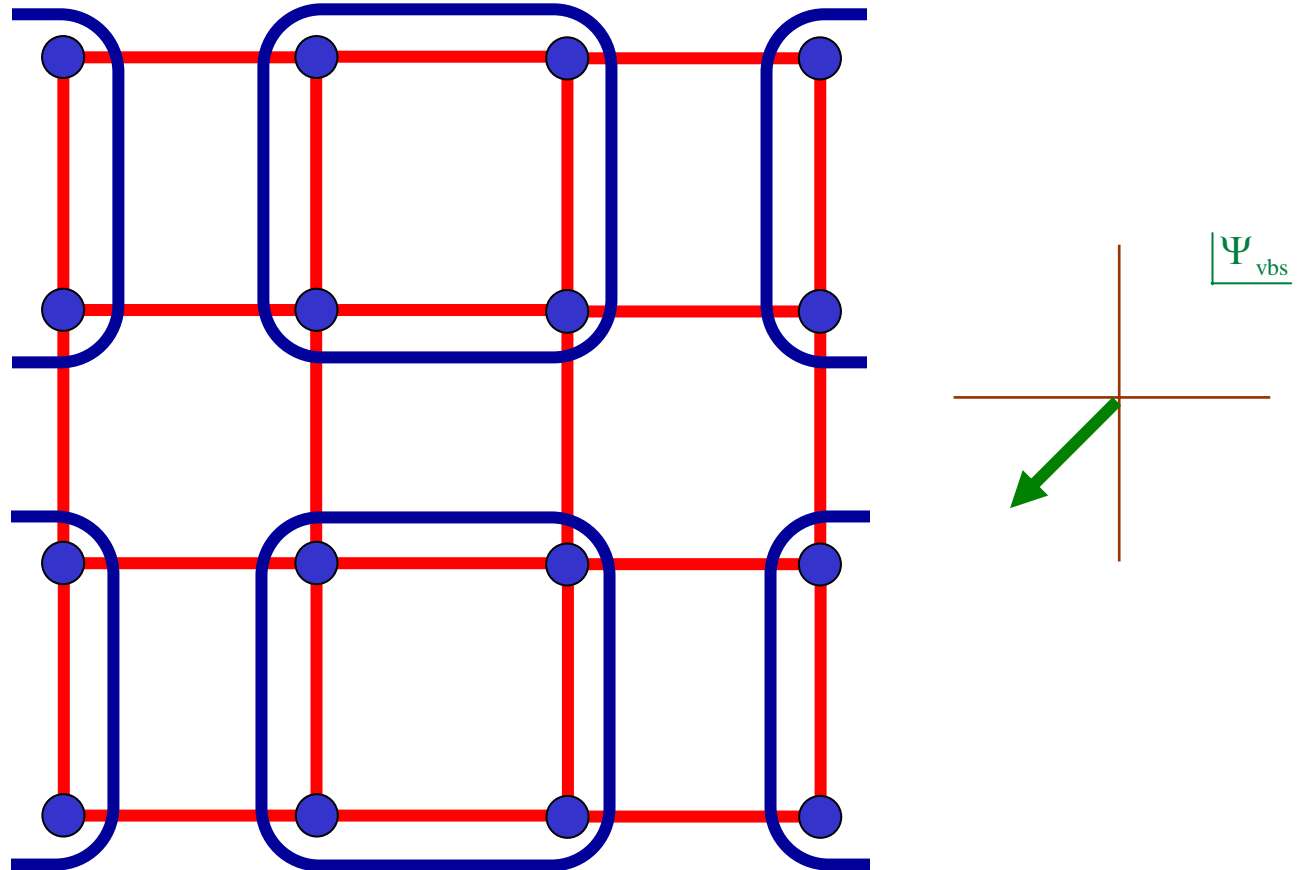
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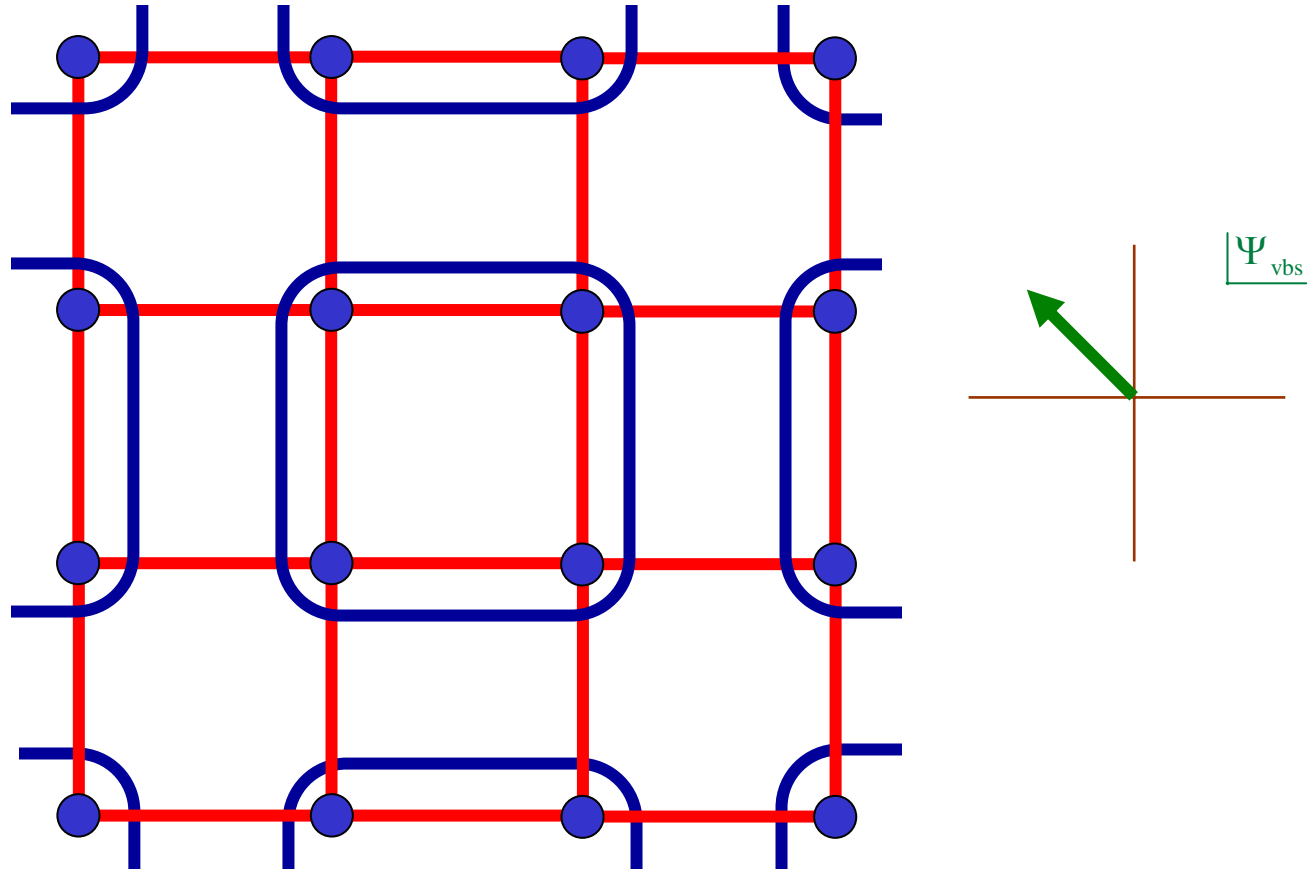
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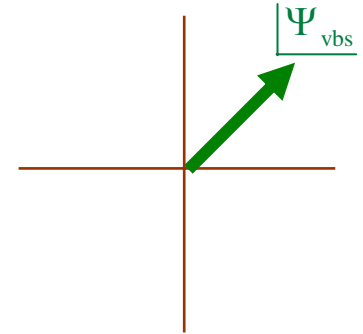
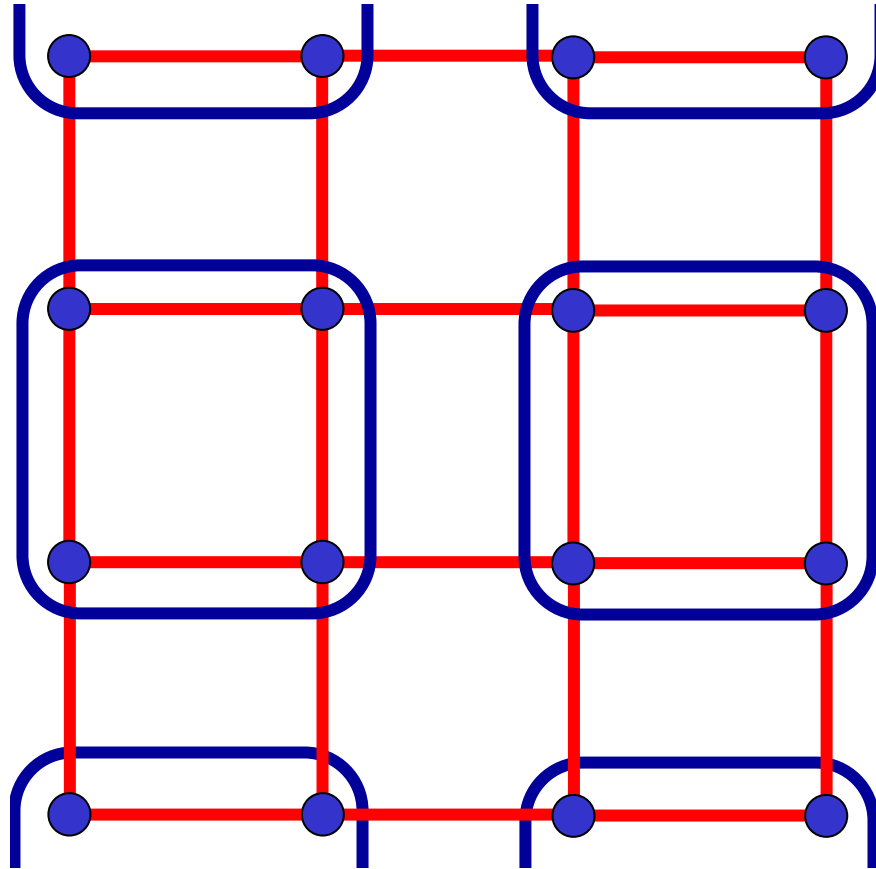
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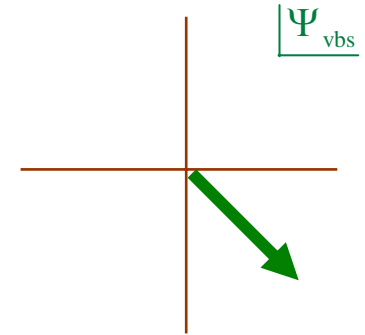
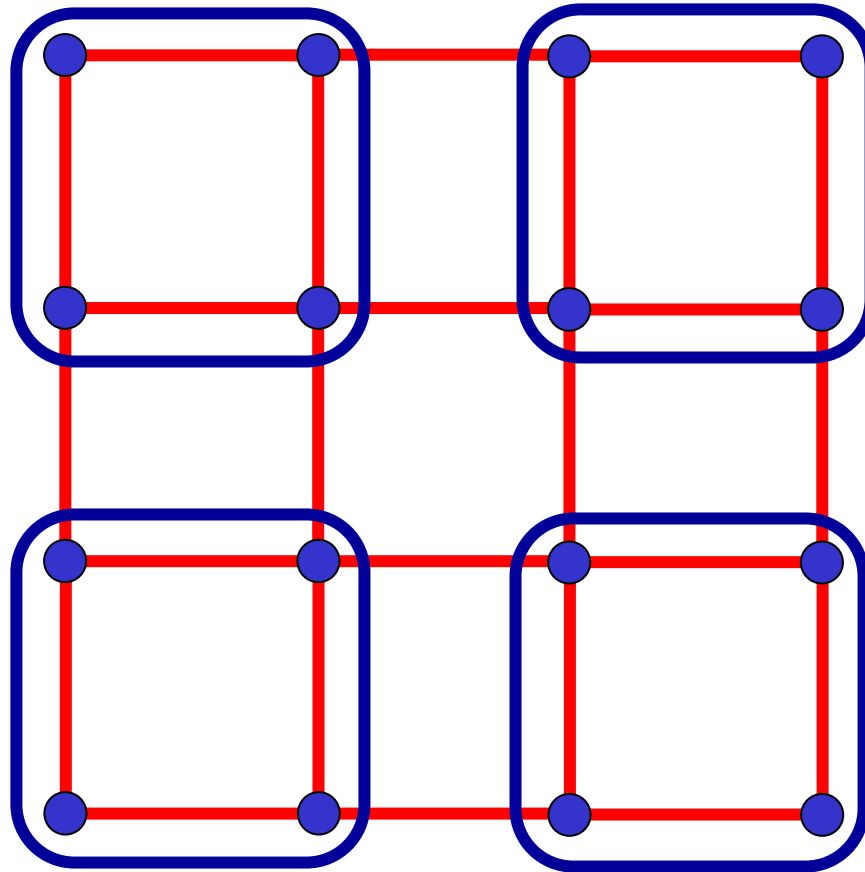
Another possible state, with  $\langle \vec{\phi} \rangle = 0$ , is the valence bond solid (VBS)



Such a state breaks the symmetry of rotations by  $n\pi/2$  about lattice sites, and has  $\langle \Psi_{\text{vbs}} \rangle \neq 0$ , where  $\Psi_{\text{vbs}}$  is the *VBS order parameter*

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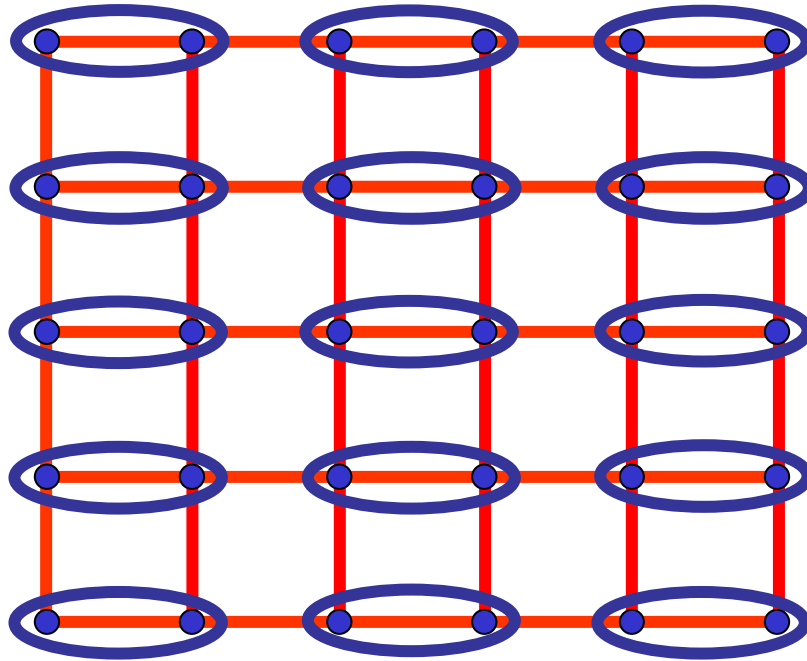


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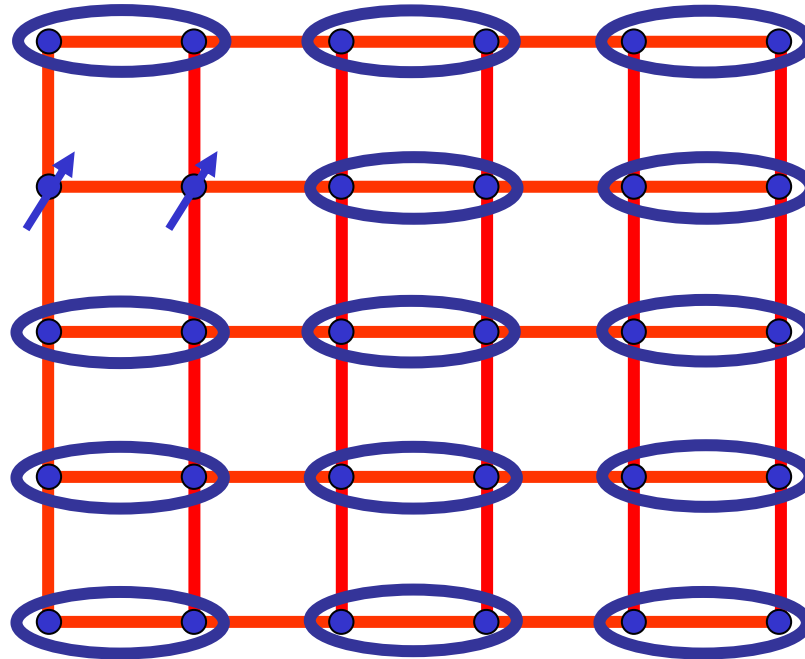
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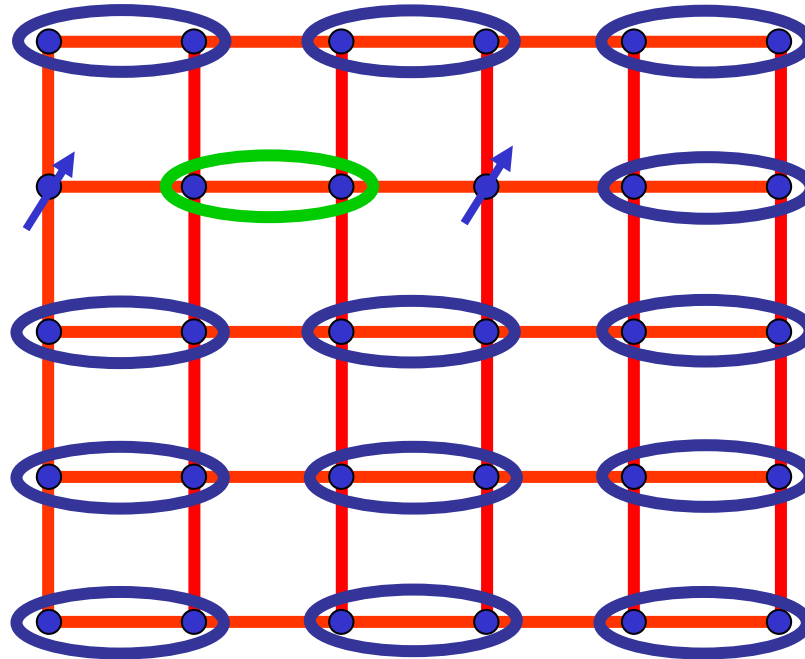
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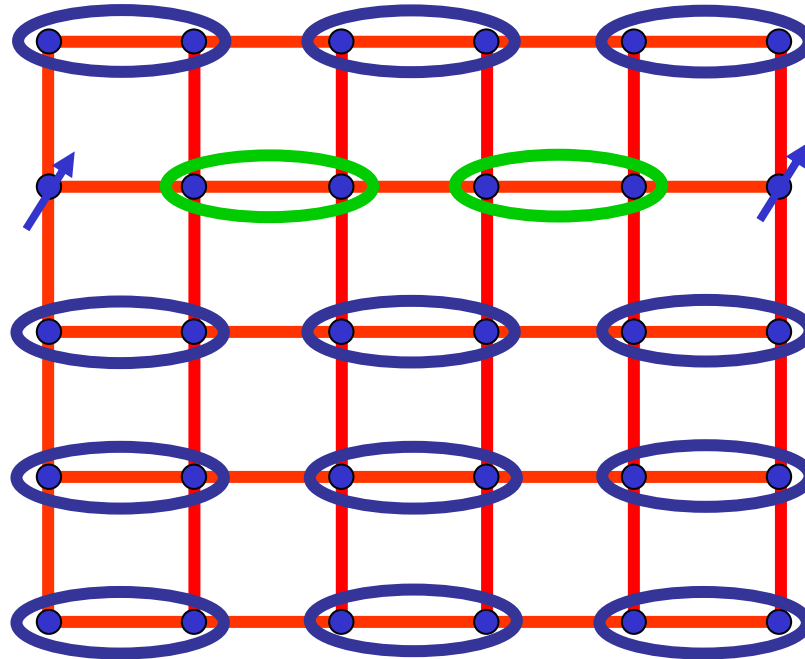
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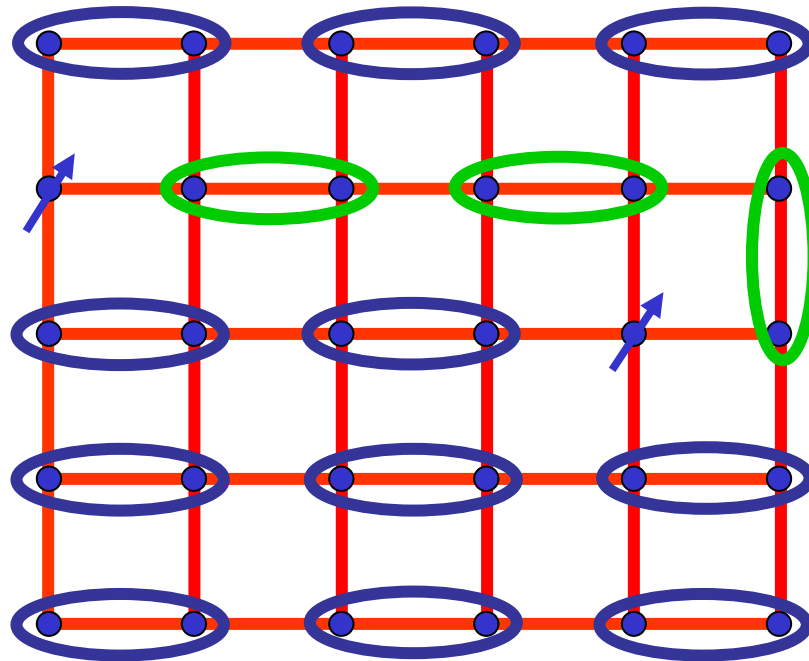
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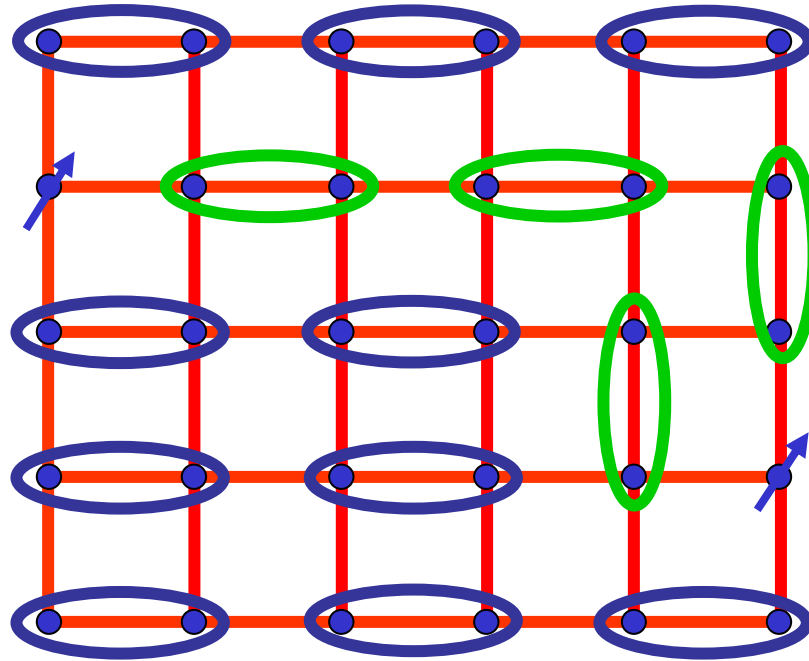
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# LGW theory of multiple order parameters

$$F = F_{\text{vbs}} [\Psi_{\text{vbs}}] + F_{\varphi} [\vec{\varphi}] + F_{\text{int}}$$

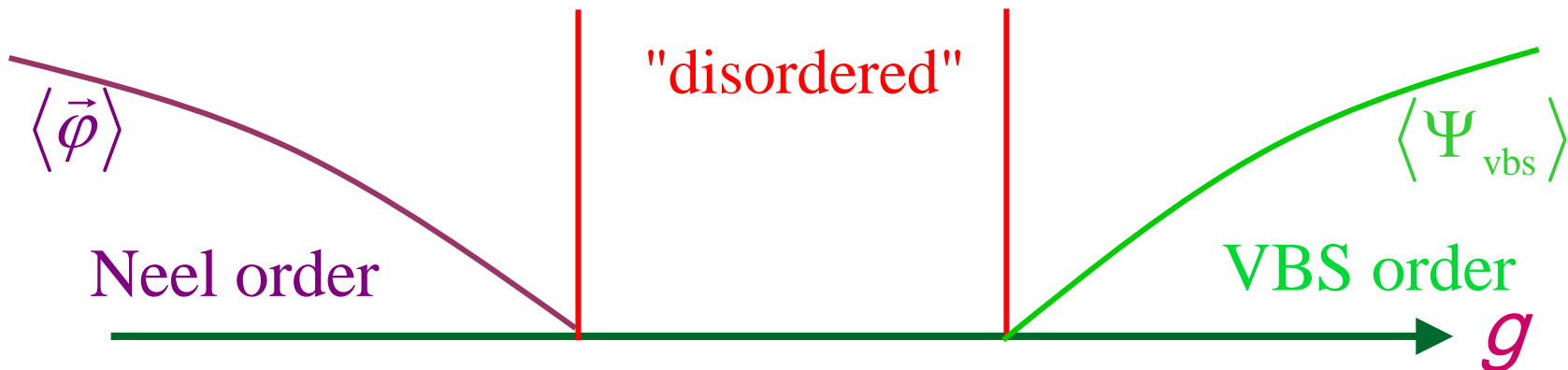
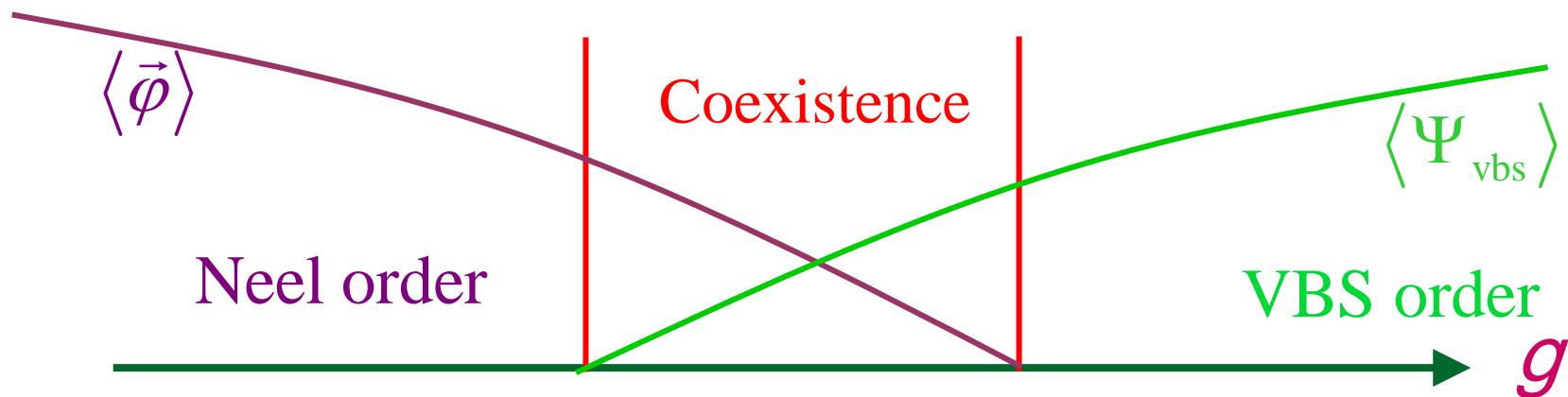
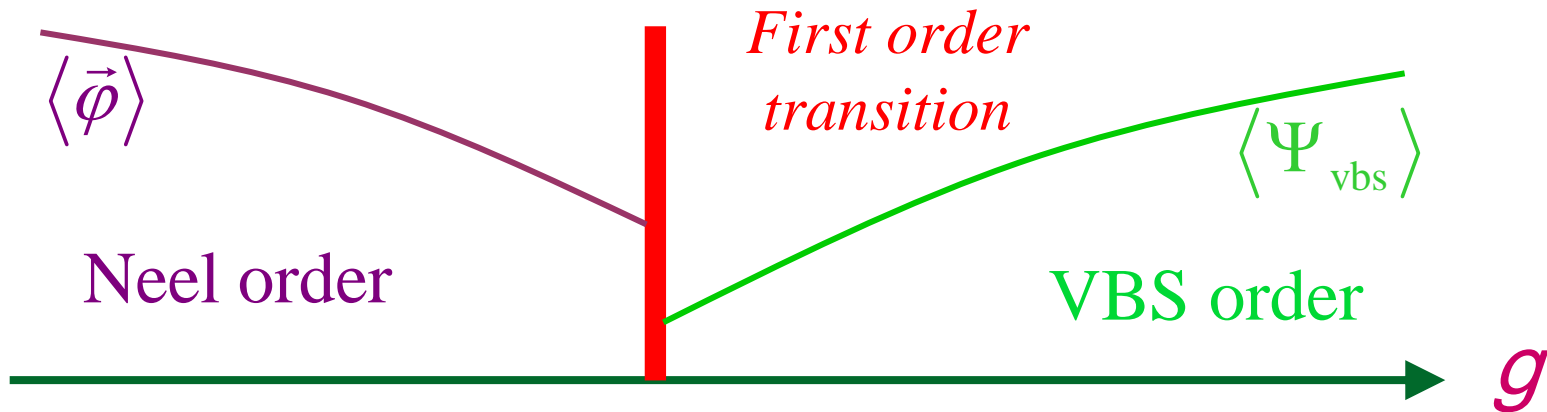
$$F_{\text{vbs}} [\Psi_{\text{vbs}}] = r_1 |\Psi_{\text{vbs}}|^2 + u_1 |\Psi_{\text{vbs}}|^4 + \dots$$

$$F_{\varphi} [\vec{\varphi}] = r_2 |\vec{\varphi}|^2 + u_2 |\vec{\varphi}|^4 + \dots$$

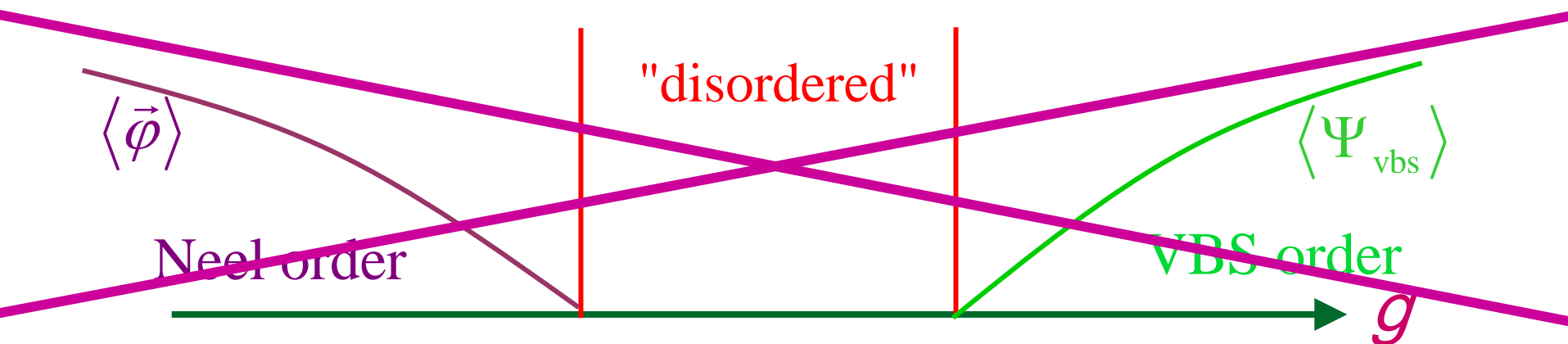
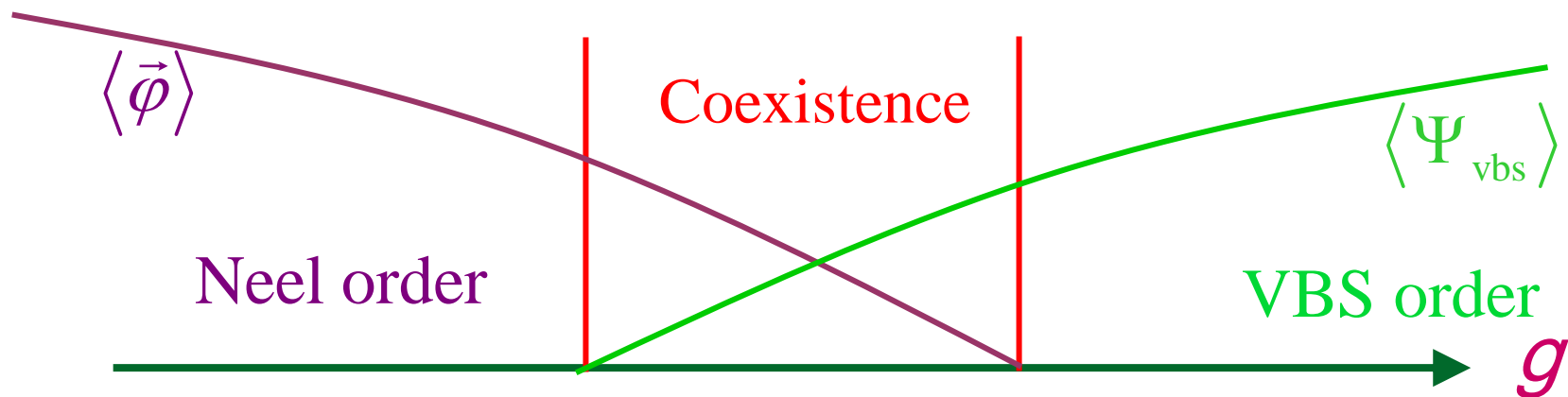
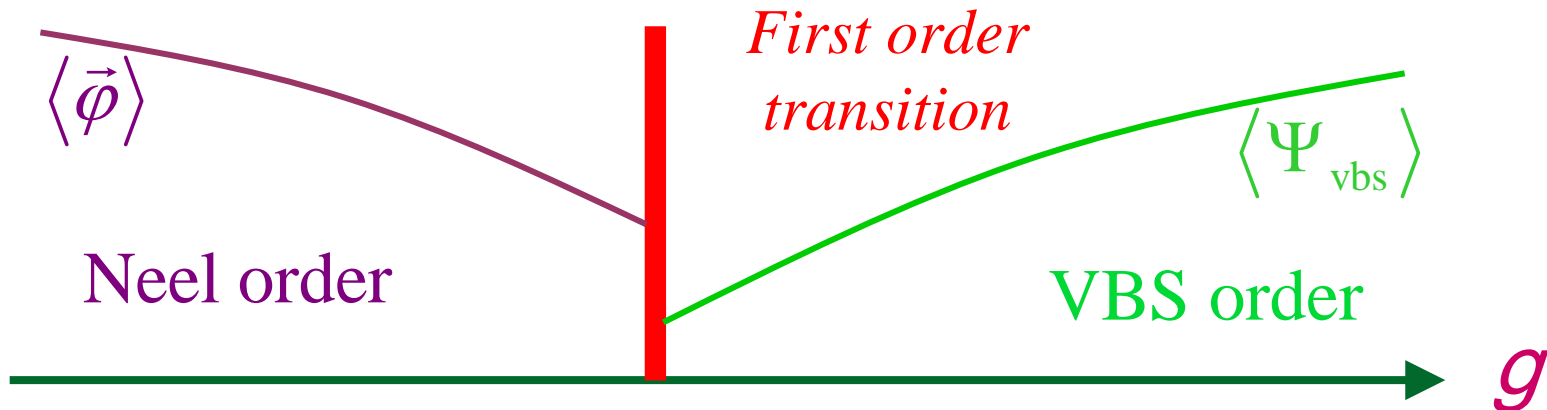
$$F_{\text{int}} = v |\Psi_{\text{vbs}}|^2 |\vec{\varphi}|^2 + \dots$$

Distinct symmetries of order parameters permit couplings only between their energy densities

# LGW theory of multiple order parameters



# LGW theory of multiple order parameters



# Outline

- I. Magnetic quantum phase transitions in “dimerized”  
Mott insulators:  
*Landau-Ginzburg-Wilson (LGW) theory*
  
- II. Magnetic quantum phase transitions of Mott insulators  
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  - A. *Breakdown of LGW theory*
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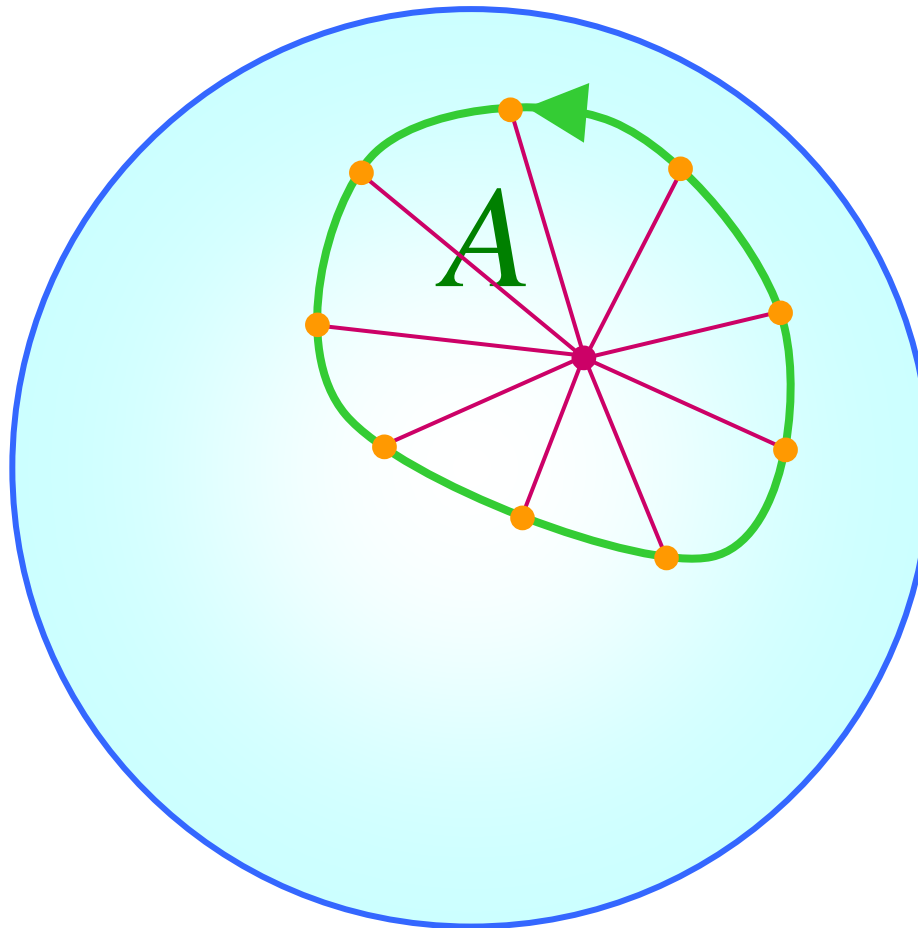


## II. Magnetic quantum phase transitions of Mott insulators on the square lattice:

### *B. Berry phases*

# Quantum theory for destruction of Neel order

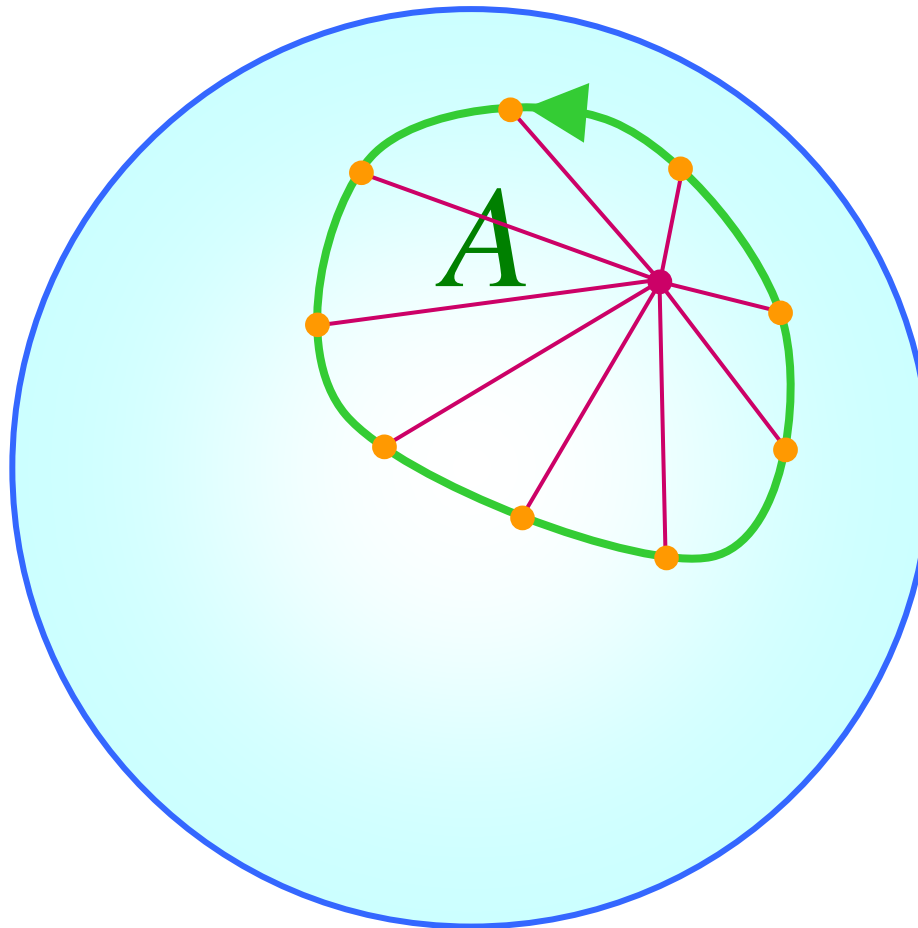
## Ingredient missing from LGW theory: Spin Berry Phases



$$e^{iSA}$$

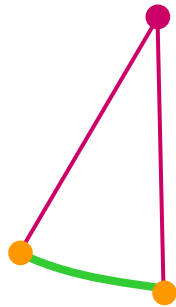
# Quantum theory for destruction of Neel order

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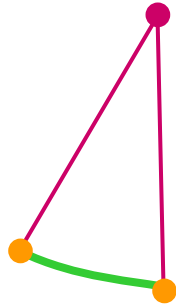
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# Quantum theory for destruction of Neel order



## Quantum theory for destruction of Neel order

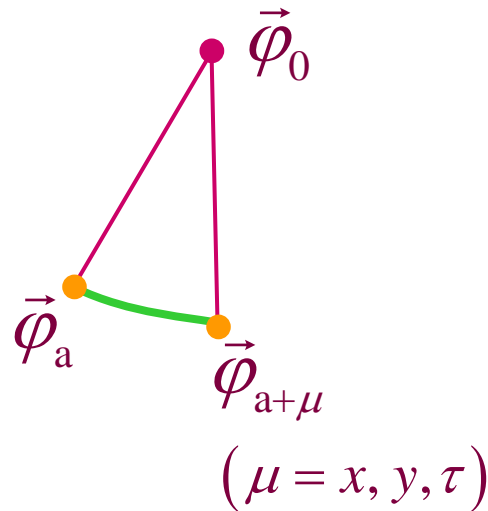
Discretize imaginary time: path integral is over fields on the sites of a cubic lattice of points  $a$



## Quantum theory for destruction of Neel order

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Recall  $\vec{\varphi}_a = 2\eta_a \vec{S}_a \rightarrow \vec{\varphi}_a = (0,0,1)$  in classical Neel state;  
 $\eta_a \rightarrow \pm 1$  on two square sublattices ;



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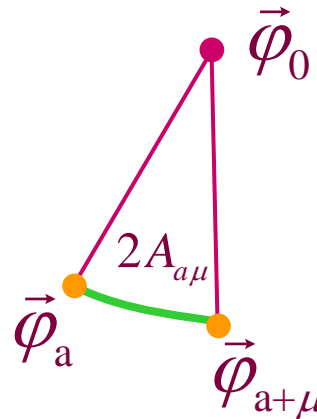
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$A_{a\mu} \rightarrow$  half oriented area of spherical triangle

formed by  $\vec{\varphi}_a$ ,  $\vec{\varphi}_{a+\mu}$ , and an arbitrary reference point  $\vec{\varphi}_0$



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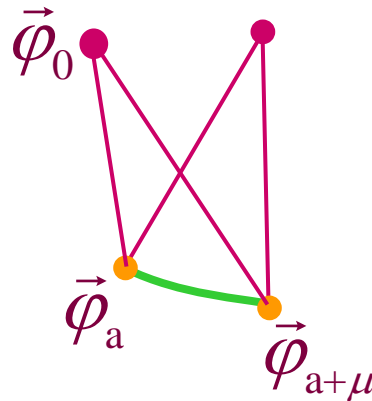
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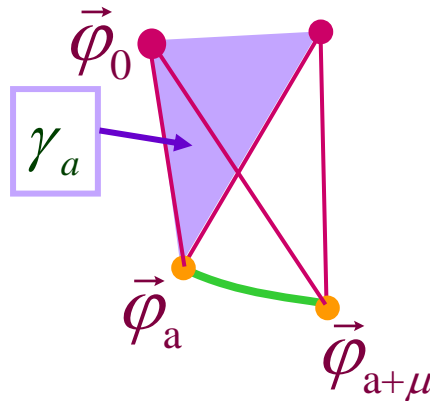
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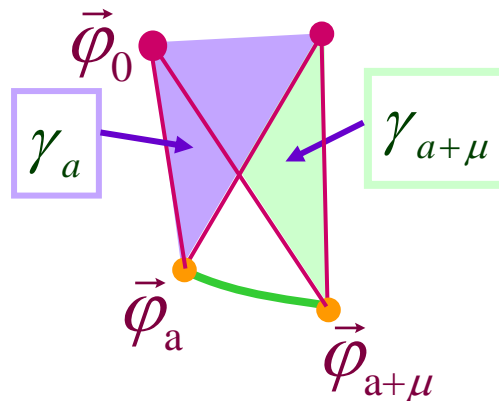
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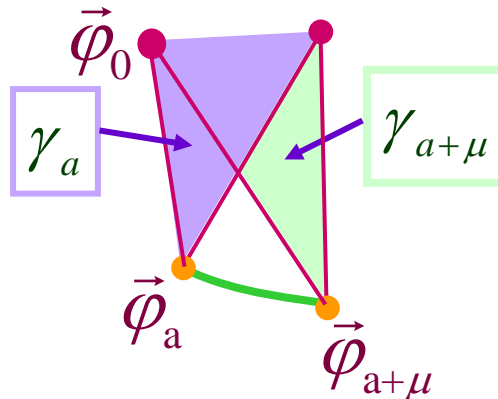
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$$2A_{a\mu} \rightarrow 2A_{a\mu} - \gamma_{a+\mu} + \gamma_a$$

Change in choice of  $\vec{\varphi}_0$  is like a “gauge transformation”



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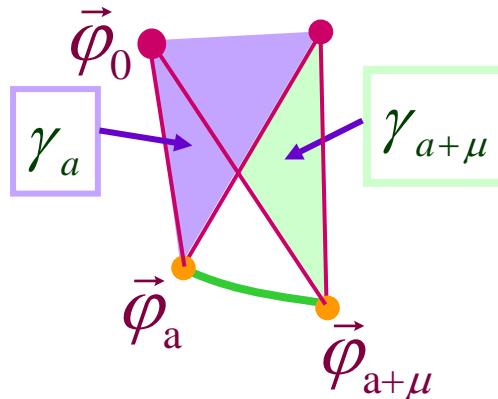
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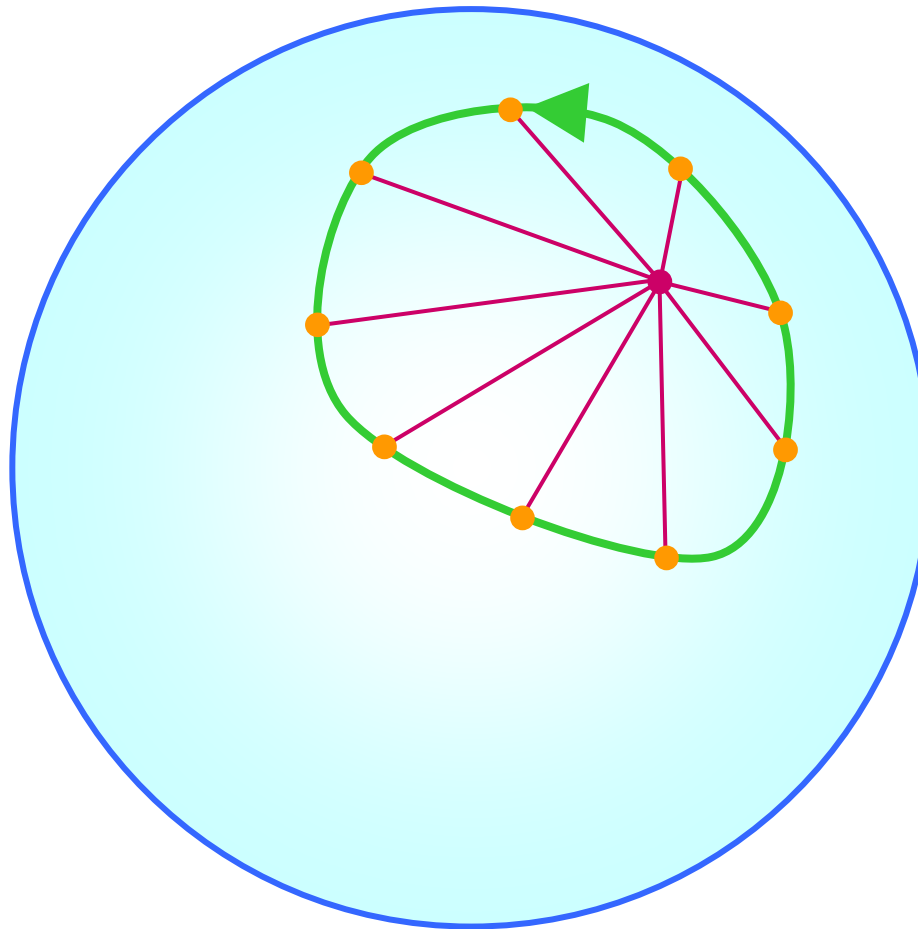
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The area of the triangle is uncertain modulo  $4\pi$ , and the action has to be invariant under  $A_{a\mu} \rightarrow A_{a\mu} + 2\pi$

# Quantum theory for destruction of Neel order

## Ingredient missing from LGW theory: Spin Berry Phases



$$\exp\left(i \sum_a \eta_a A_{a\tau}\right)$$

Sum of Berry phases of  
all spins on the square  
lattice.

## Quantum theory for destruction of Neel order

Partition function on cubic lattice

$$Z = \prod_a \int d\vec{\varphi}_a \delta(\vec{\varphi}_a^2 - 1) \exp\left(\frac{1}{g} \sum_{a,\mu} \vec{\varphi}_a \cdot \vec{\varphi}_{a+\mu}\right)$$

LGW theory: weights in partition function are those of a classical ferromagnet at a “temperature”  $g$

Small  $g \Rightarrow$  ground state has Neel order with  $\langle \vec{\varphi} \rangle \neq 0$

Large  $g \Rightarrow$  paramagnetic ground state with  $\langle \vec{\varphi} \rangle = 0$

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Berry phases lead to large cancellations between different time histories  $\rightarrow$  need an effective action for  $A_{a\mu}$  at large  $g$

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## II. Magnetic quantum phase transitions of Mott insulators on the square lattice:

### *C. Spinor formulation and deconfined criticality*

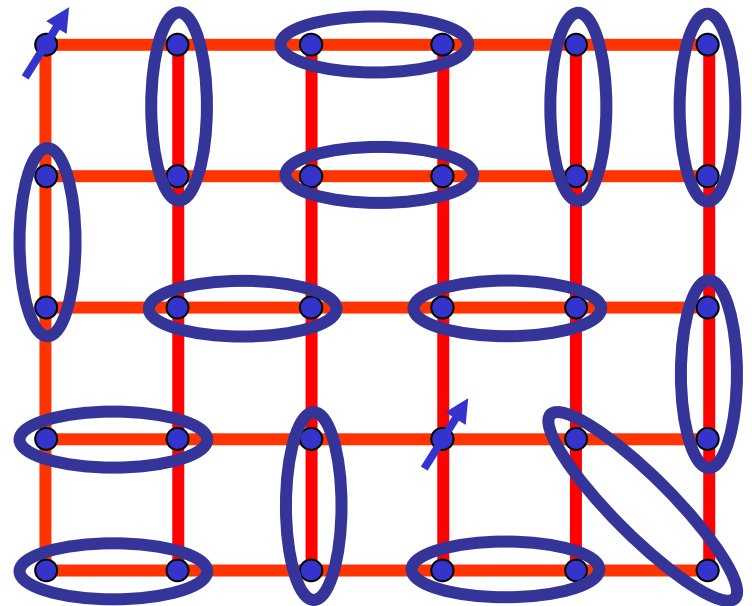
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Rewrite partition function in terms of spinors  $z_{a\alpha}$ ,  
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Remarkable identity from spherical trigonometry

$$\text{Arg} \left[ z_{a\alpha}^* z_{a+\mu,\alpha} \right] = A_{a\mu}$$

## Quantum theory for destruction of Neel order

Partition function on cubic lattice

$$Z = \prod_a \int d\vec{\varphi}_a \delta(\vec{\varphi}_a^2 - 1) \exp\left(\frac{1}{g} \sum_{a,\mu} \vec{\varphi}_a \cdot \vec{\varphi}_{a+\mu} + i \sum_a \eta_a A_{a\tau}\right)$$

Partition function expressed as a gauge theory of spinor degrees of freedom

$$Z \approx \prod_a \int dz_{a\alpha} dA_{a\mu} \delta(|z_{a\alpha}|^2 - 1) \times \exp\left(\frac{1}{g} \sum_{a,\mu} z_{a\alpha}^* e^{iA_{a\mu}} z_{a+\mu,\alpha} + i \sum_a \eta_a A_{a\tau}\right)$$

Large  $g$  effective action for the  $A_{a\mu}$  after integrating  $z_{\alpha\mu}$

$$Z = \prod_{a,\mu} \int dA_{a\mu} \exp \left( \frac{1}{2e^2} \sum_{\square} \cos \left( \Delta_{\mu} A_{a\nu} - \Delta_{\nu} A_{a\mu} \right) - i \sum_a \eta_a A_{a\tau} \right)$$

with  $e^2 \sim g^2$

This is compact QED in 3 spacetime dimensions with static charges  $\pm 1$  on two sublattices.

This theory can be reliably analyzed by a duality mapping.

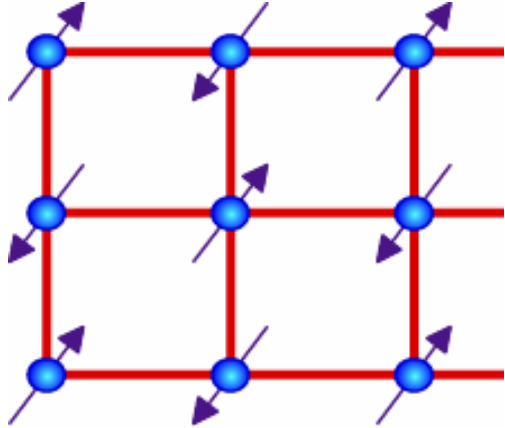
The gauge theory is in a **confining** phase, and there is VBS order in the ground state. (Proliferation of monopoles in the presence of Berry phases).

N. Read and S. Sachdev, *Phys. Rev. Lett.* **62**, 1694 (1989).

S. Sachdev and R. Jalabert, *Mod. Phys. Lett. B* **4**, 1043 (1990).

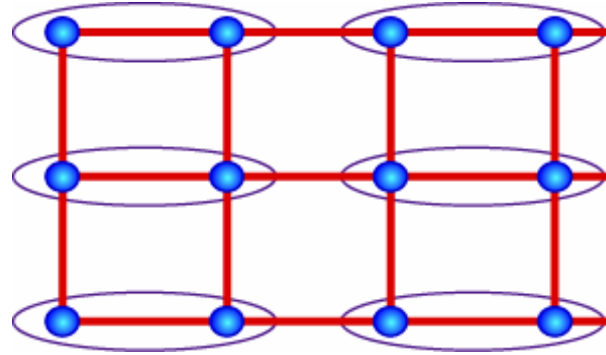
K. Park and S. Sachdev, *Phys. Rev. B* **65**, 220405 (2002).

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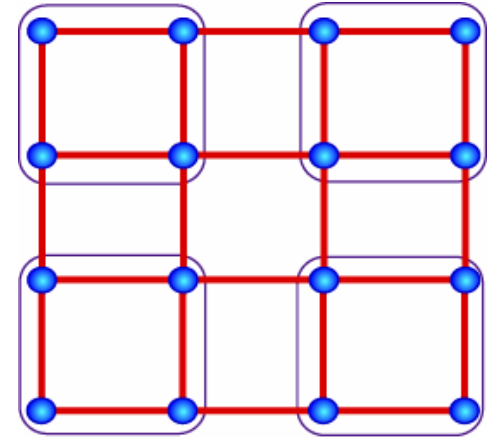


Neel order

$$\langle \vec{\phi} \rangle \neq 0$$



or



VBS order

$$\langle \Psi_{\text{vbs}} \rangle \neq 0$$

Not present in

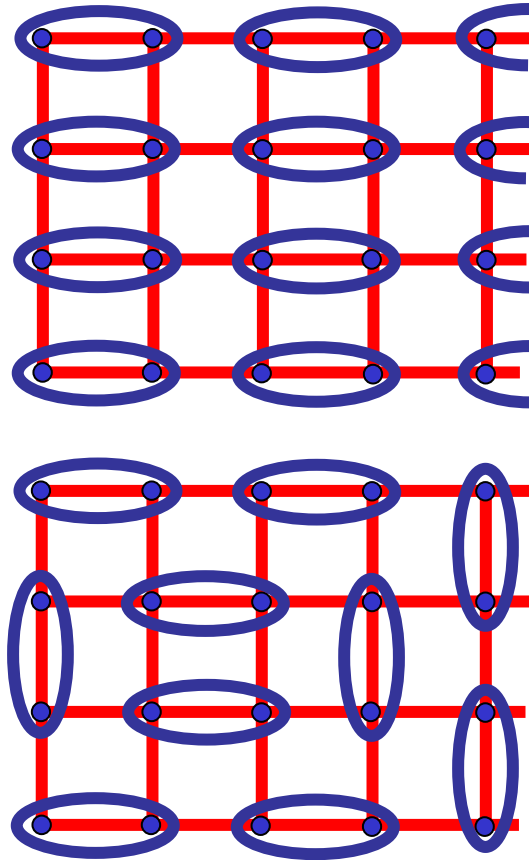
LGW theory

of  $\vec{\phi}$  order

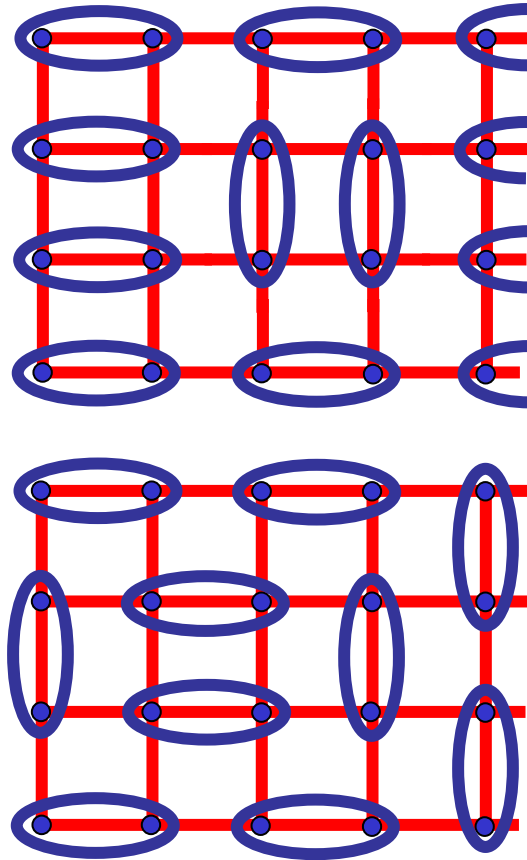
0

$g$

# Ordering by quantum fluctuations

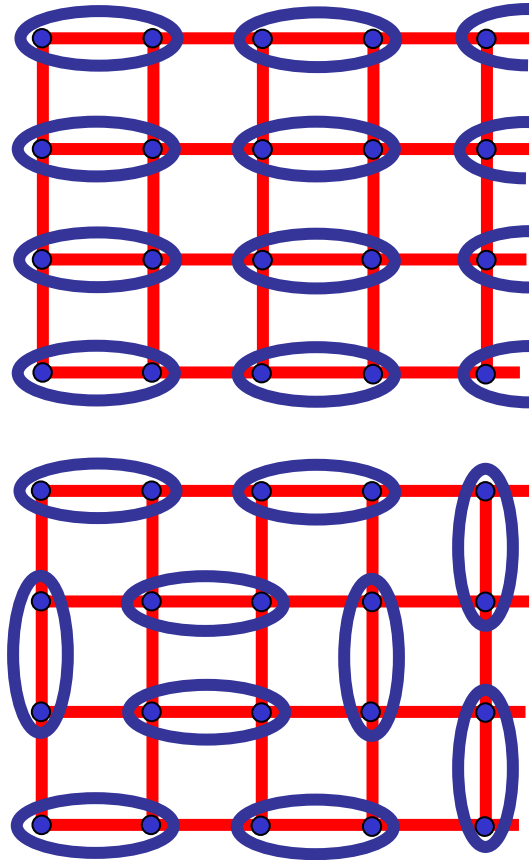


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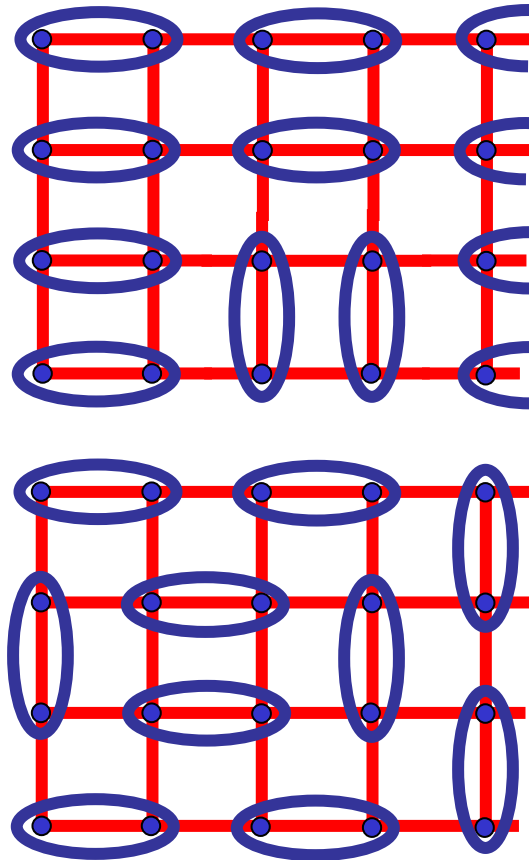




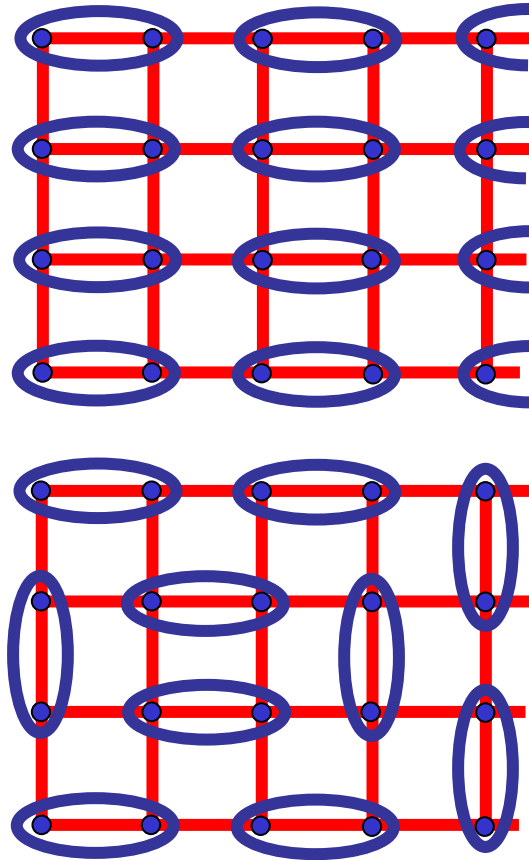
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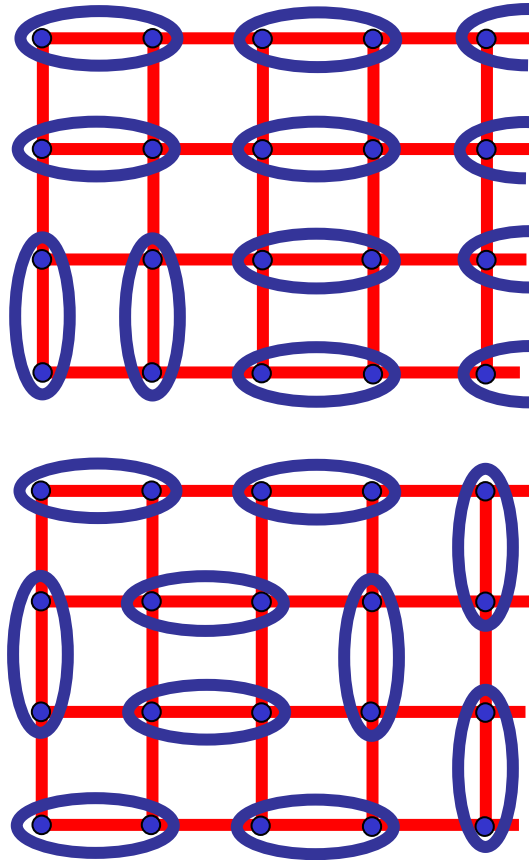
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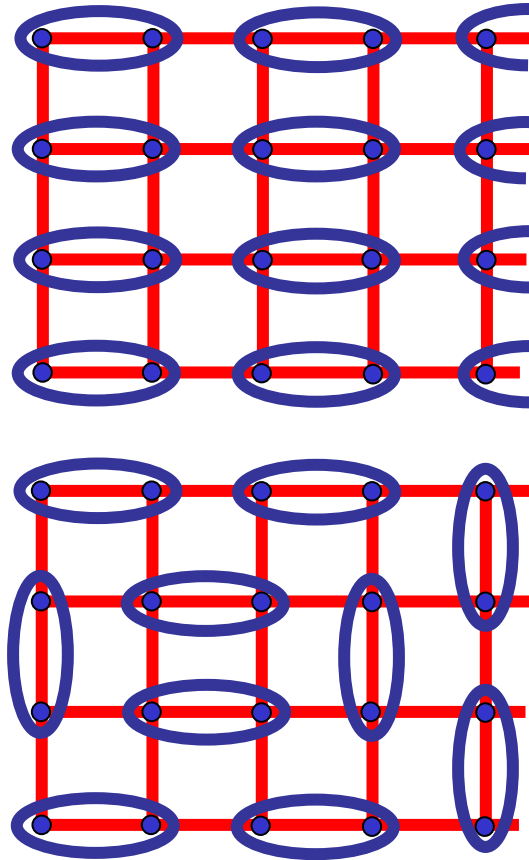
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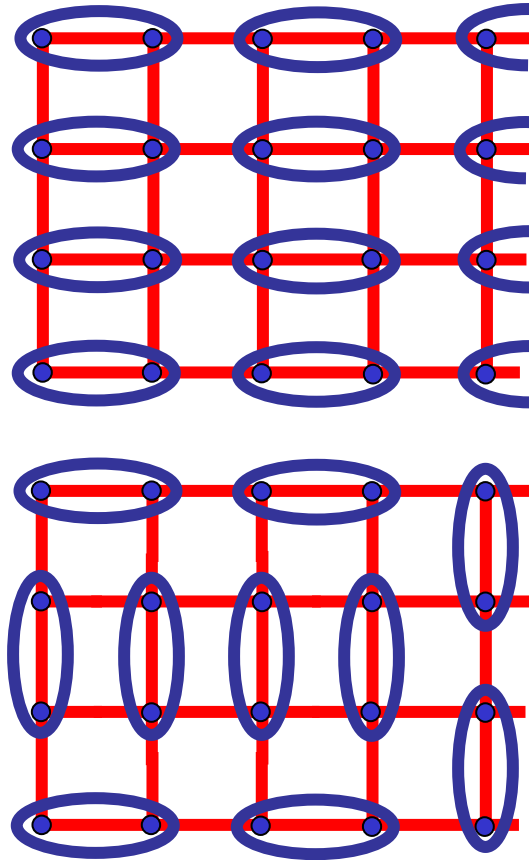
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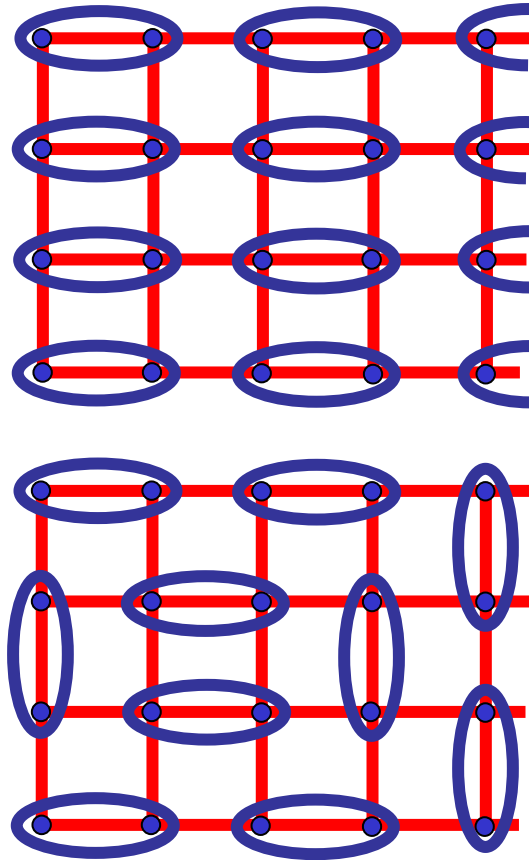
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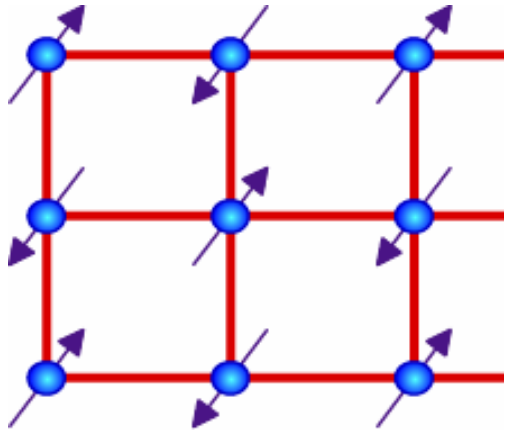
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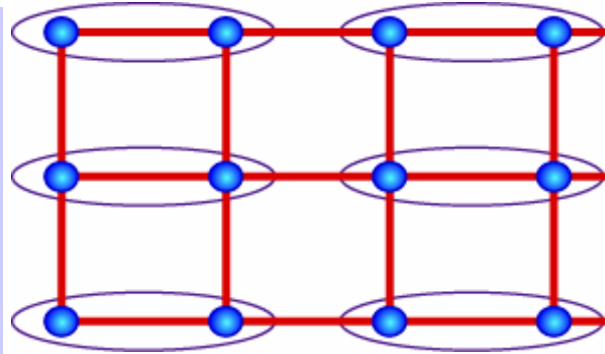


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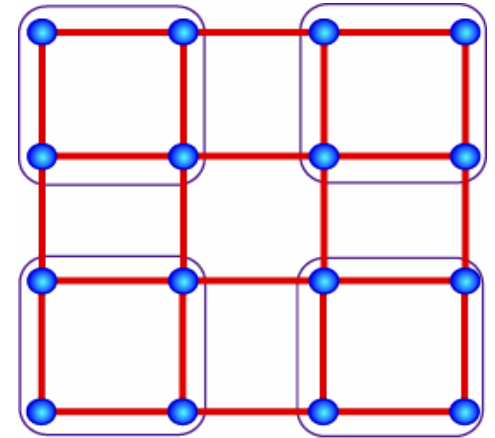


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Not present in

LGW theory

of  $\vec{\phi}$  order

0

$g$



## Theory of a second-order quantum phase transition between Neel and VBS phases

At the quantum critical point:

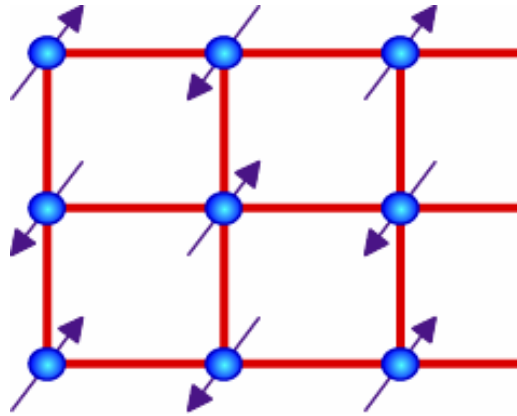
- $A_\mu \rightarrow A_\mu + 2\pi$  periodicity can be ignored  
(Monopoles interfere destructively and are dangerously irrelevant).
- $S=1/2$  spinons  $z_\alpha$ , with  $\vec{\varphi} \sim z_\alpha^* \vec{\sigma}_{\alpha\beta} z_\beta$ , are globally propagating degrees of freedom.

*Second-order critical point described by emergent fractionalized degrees of freedom ( $A_\mu$  and  $z_\alpha$ ); Order parameters ( $\vec{\varphi}$  and  $\Psi_{\text{vbs}}$ ) are “composites” and of secondary importance*

S. Sachdev and R. Jalabert, *Mod. Phys. Lett. B* **4**, 1043 (1990); G. Murthy and S. Sachdev, *Nuclear Physics B* **344**, 557 (1990); C. Lannert, M.P.A. Fisher, and T. Senthil, *Phys. Rev. B* **63**, 134510 (2001); S. Sachdev and K. Park, *Annals of Physics*, **298**, 58 (2002); O. Motrunich and A. Vishwanath, *Phys. Rev. B* **70**, 075104 (2004)

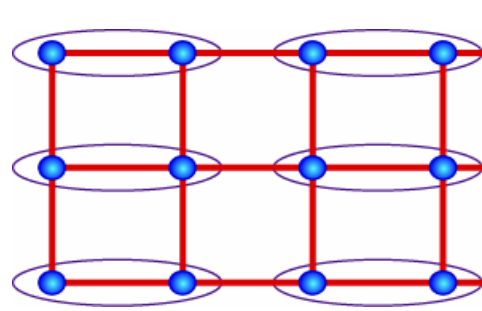
T. Senthil, A. Vishwanath, L. Balents, S. Sachdev and M.P.A. Fisher, *Science* **303**, 1490 (2004).

# Phase diagram of $S=1/2$ square lattice antiferromagnet

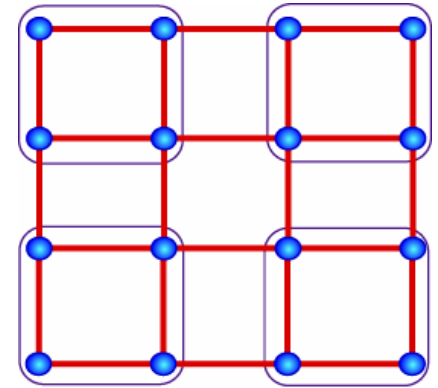


Neel order

$$\langle \vec{\phi} \rangle \sim \langle z_\alpha^* \vec{\sigma}_{\alpha\beta} z_\beta \rangle \neq 0$$



or



$$\text{VBS order } \langle \Psi_{\text{vbs}} \rangle \neq 0$$

(associated with condensation of monopoles in  $A_\mu$ ),

$S = 1/2$  spinons  $z_\alpha$  confined,

$S = 1$  triplon excitations



Second-order critical point described by

$$\mathcal{S}_{\text{critical}} = \int d^2x d\tau \left[ |(\partial_\mu - iA_\mu)z_\alpha|^2 + r |z_\alpha|^2 + \frac{u}{2} (|z_\alpha|^2)^2 + \frac{1}{4e^2} (\partial_\mu A_\nu - \partial_\nu A_\mu)^2 \right]$$

at its critical point  $r = r_c$ , where  $A_\mu$  is *non-compact*

## Conclusions

- New quantum phases induced by Berry phases: VBS order in the antiferromagnet
- Critical resonating-valence-bond states describes the quantum phase transition from the Neel to the VBS
- Emergent gauge fields are essential for a full description of the low energy physics.