

# Breakdown of the Landau-Ginzburg-Wilson paradigm at quantum phase transitions

*Science* **303**, 1490 (2004); cond-mat/0312617  
cond-mat/0401041

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# Outline

A. Magnetic quantum phase transitions in “dimerized”  
Mott insulators

*Landau-Ginzburg-Wilson (LGW) theory*

B. Mott insulators with spin  $S=1/2$  per unit cell

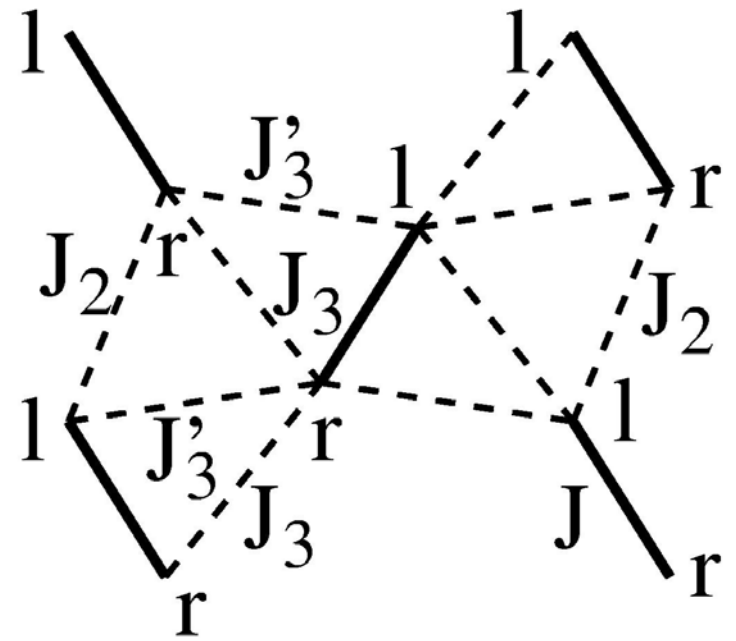
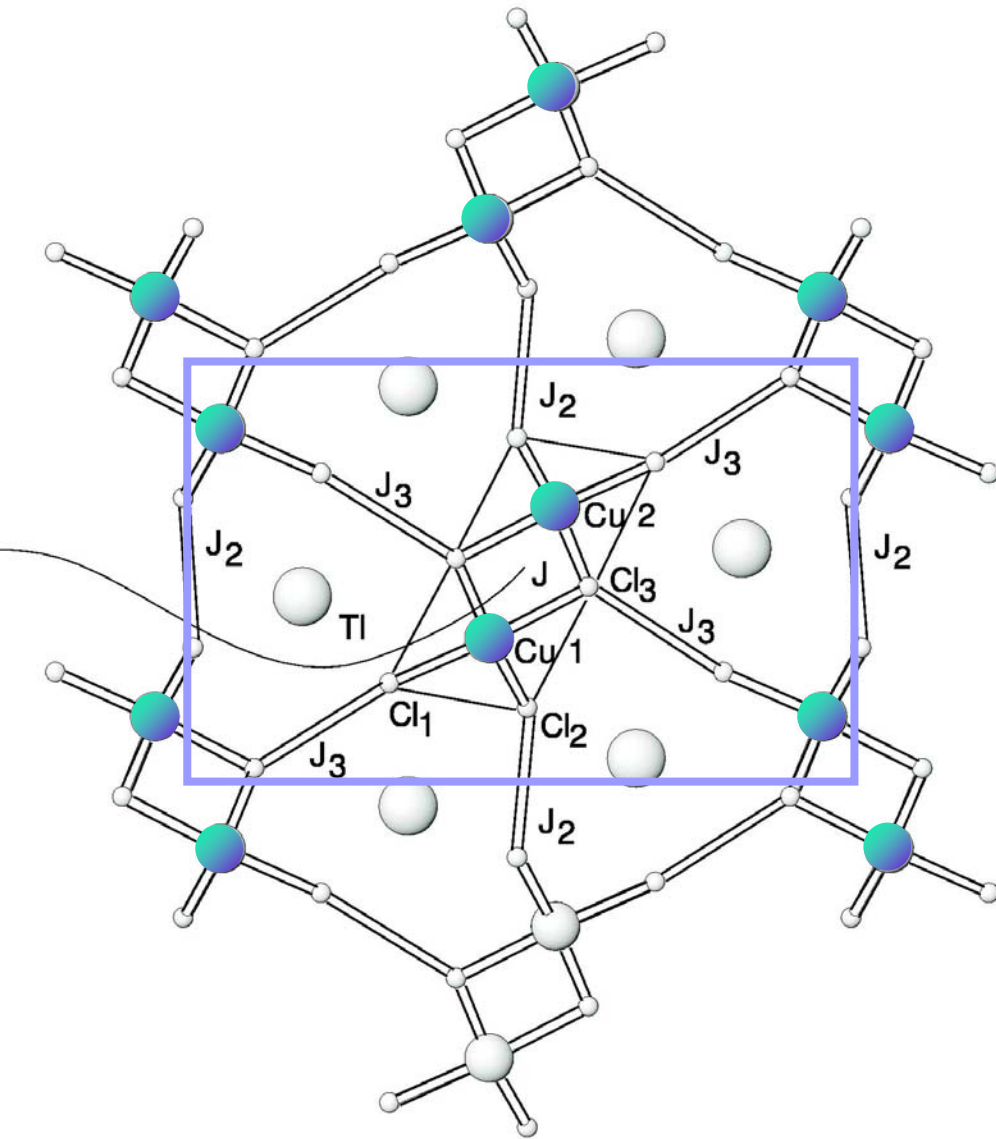
*Berry phases, bond order, and the  
breakdown of the LGW paradigm*

A. 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

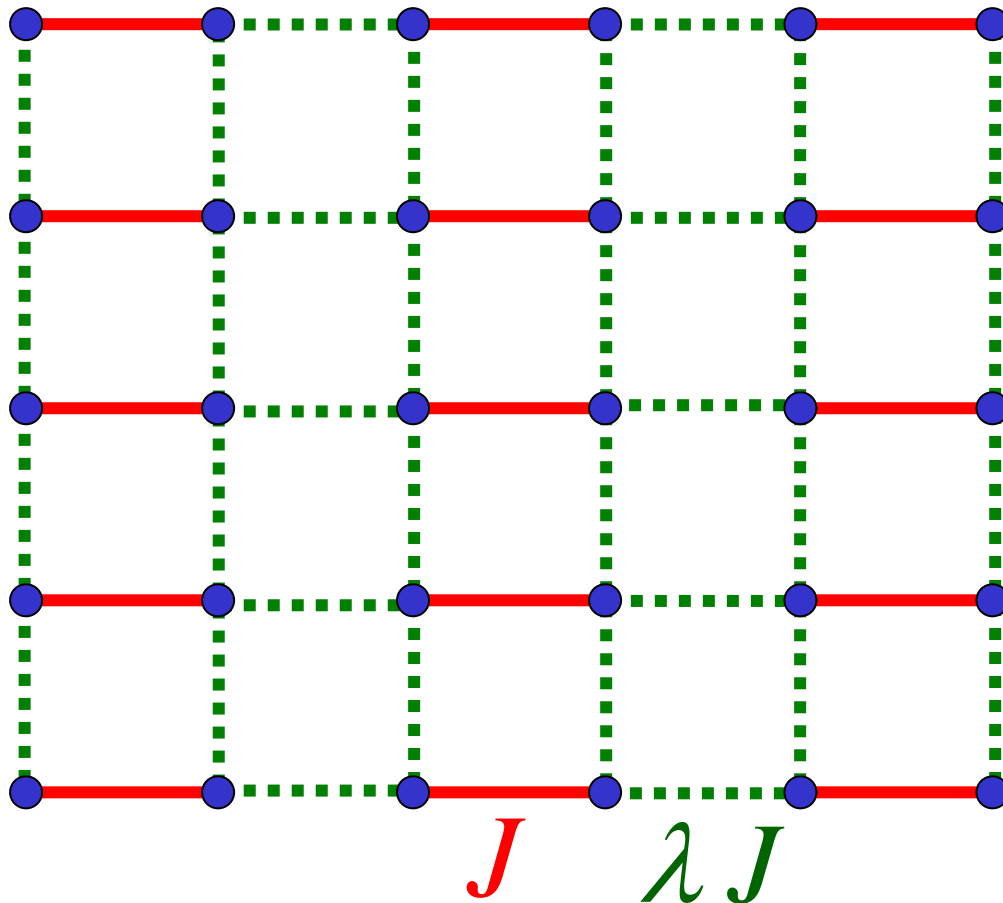
M. P. Gelfand, R. R. P. Singh, and D. A. Huse, *Phys. Rev. B* **40**, 10801-10809 (1989).

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).

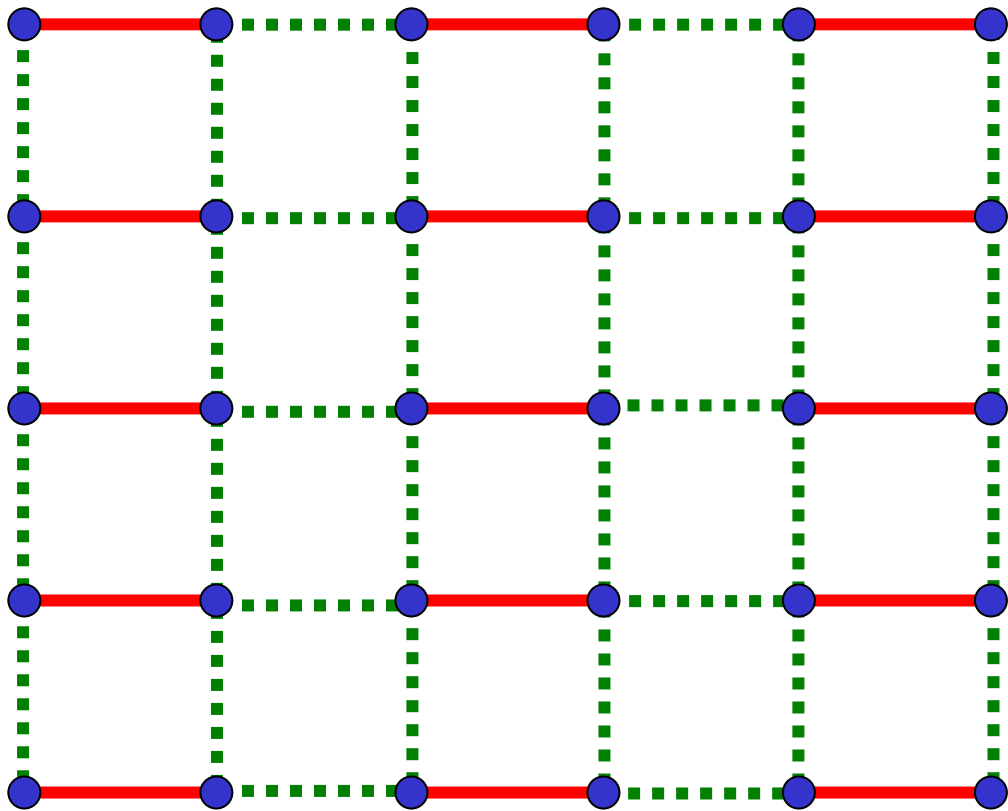
M. Matsumoto, C. Yasuda, S. Todo, and H. Takayama, *Phys. Rev. B* **65**, 014407 (2002).

$S=1/2$  spins on coupled dimers



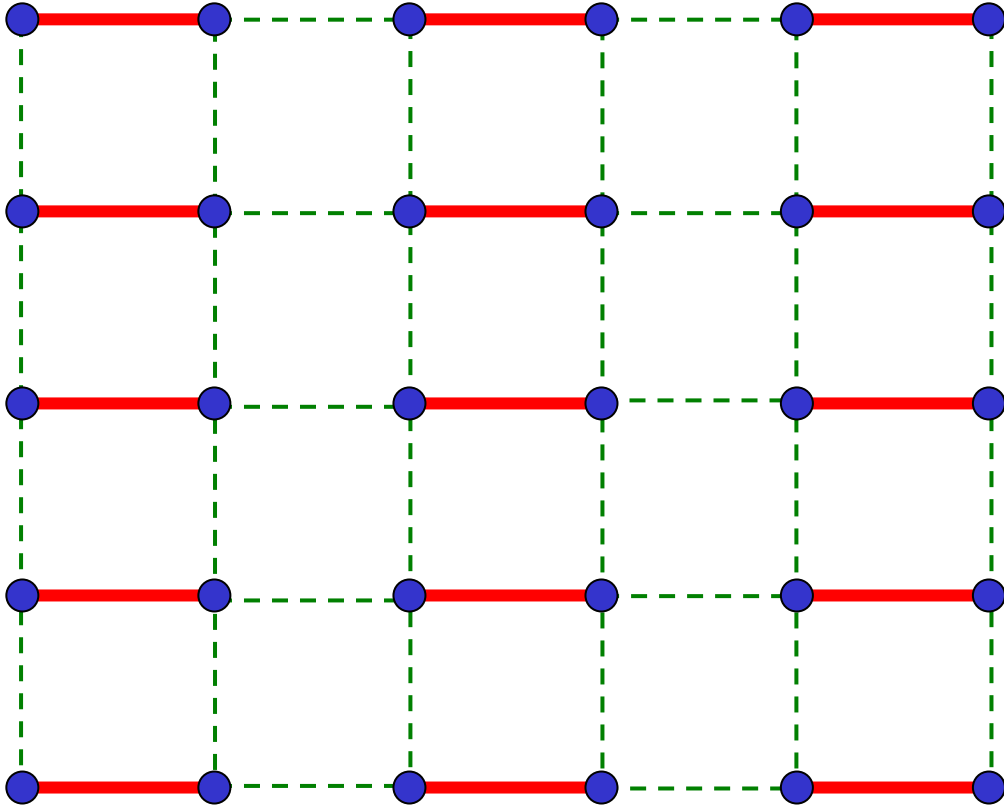
$$H = \sum_{\langle ij \rangle} J_{ij} \vec{S}_i \cdot \vec{S}_j$$

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



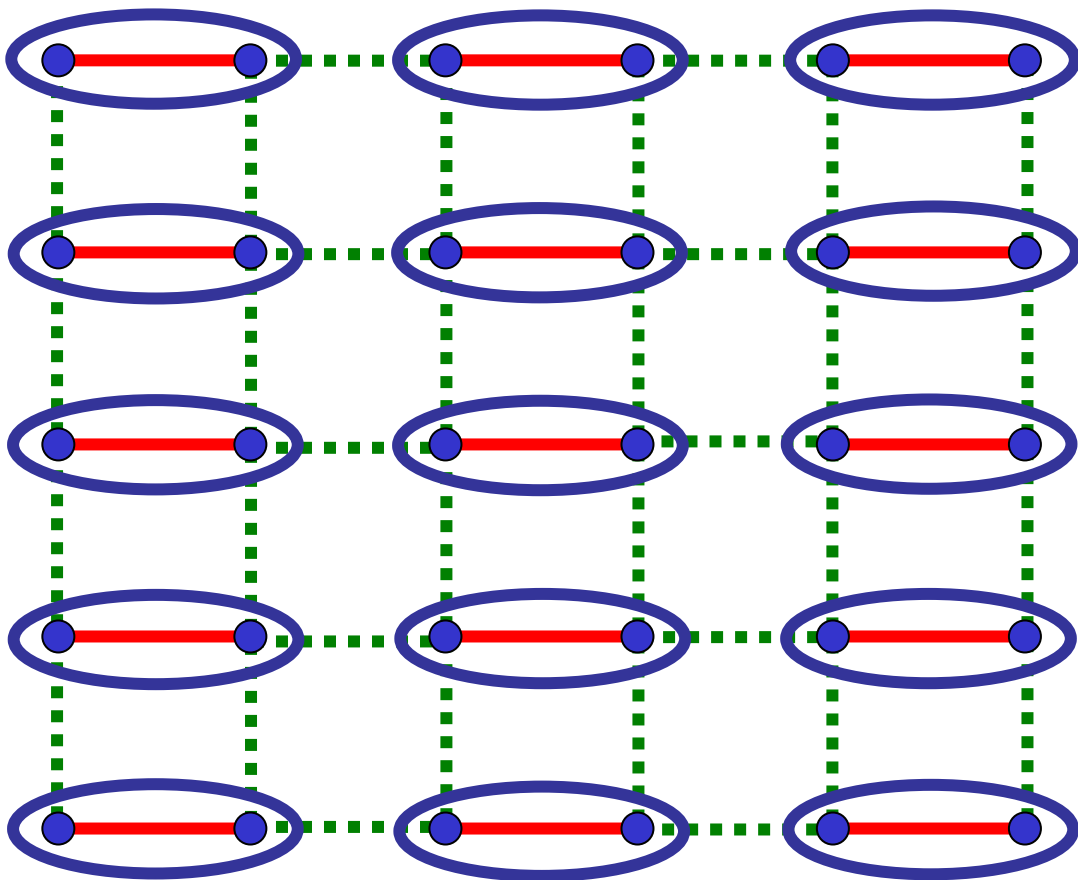
$\lambda$  close to 0

Weakly coupled dimers



$\lambda$  close to 0

Weakly coupled dimers



Paramagnetic ground state

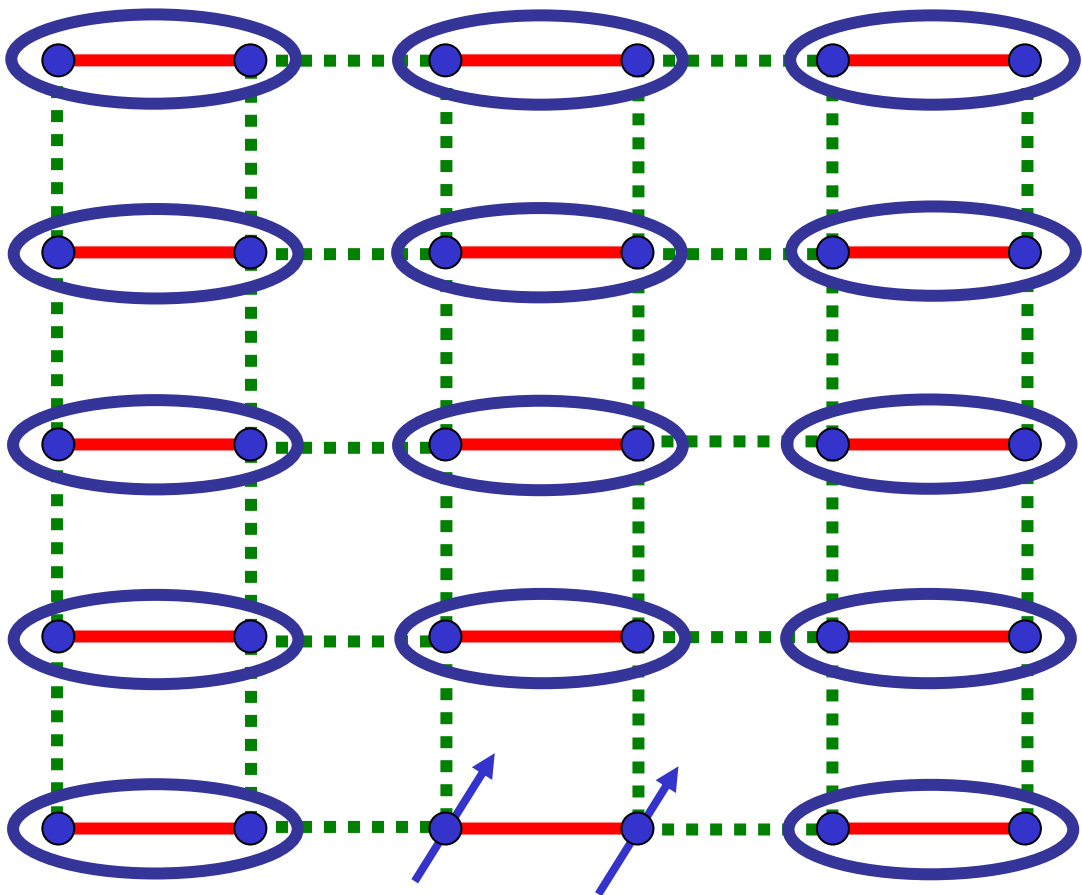
$$\text{dimer} = \frac{1}{\sqrt{2}} (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$$

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



$\lambda$  close to 0

Weakly coupled dimers

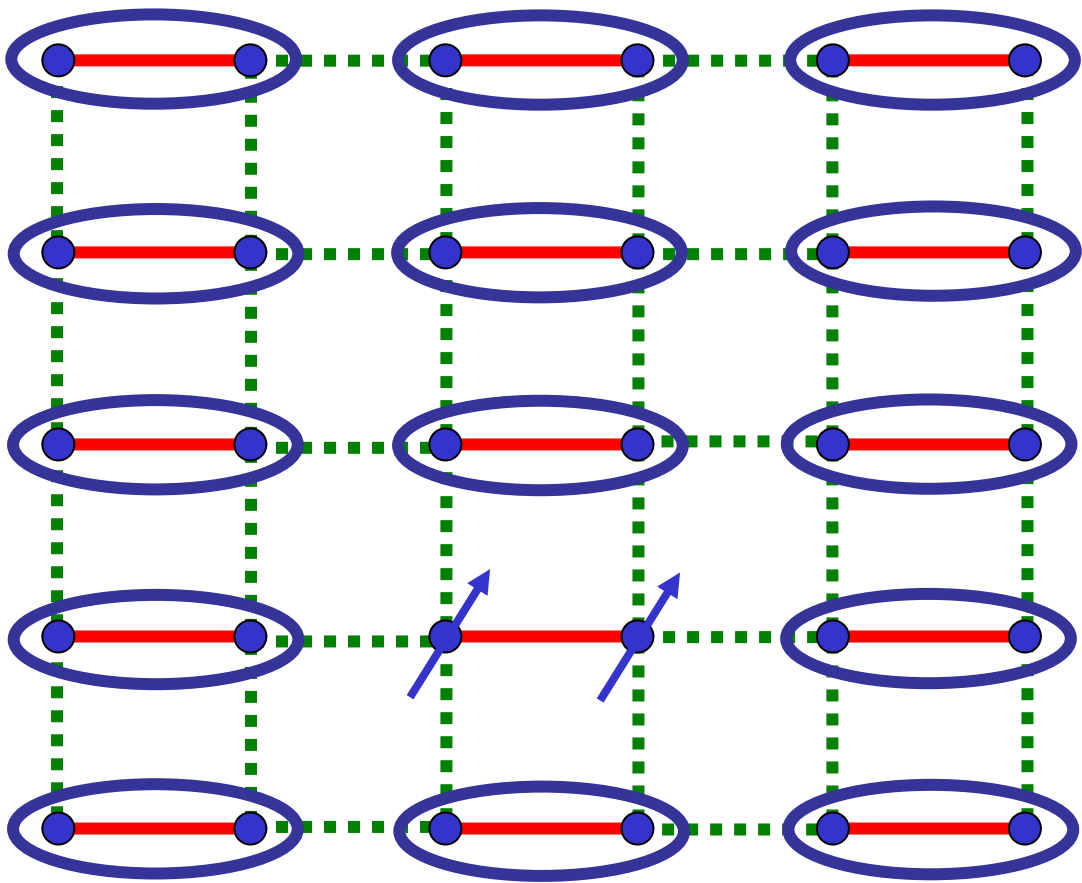


$$\text{dimer} = \frac{1}{\sqrt{2}} (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$$

Excitation:  $S=1$  *triplon*

$\lambda$  close to 0

Weakly coupled dimers

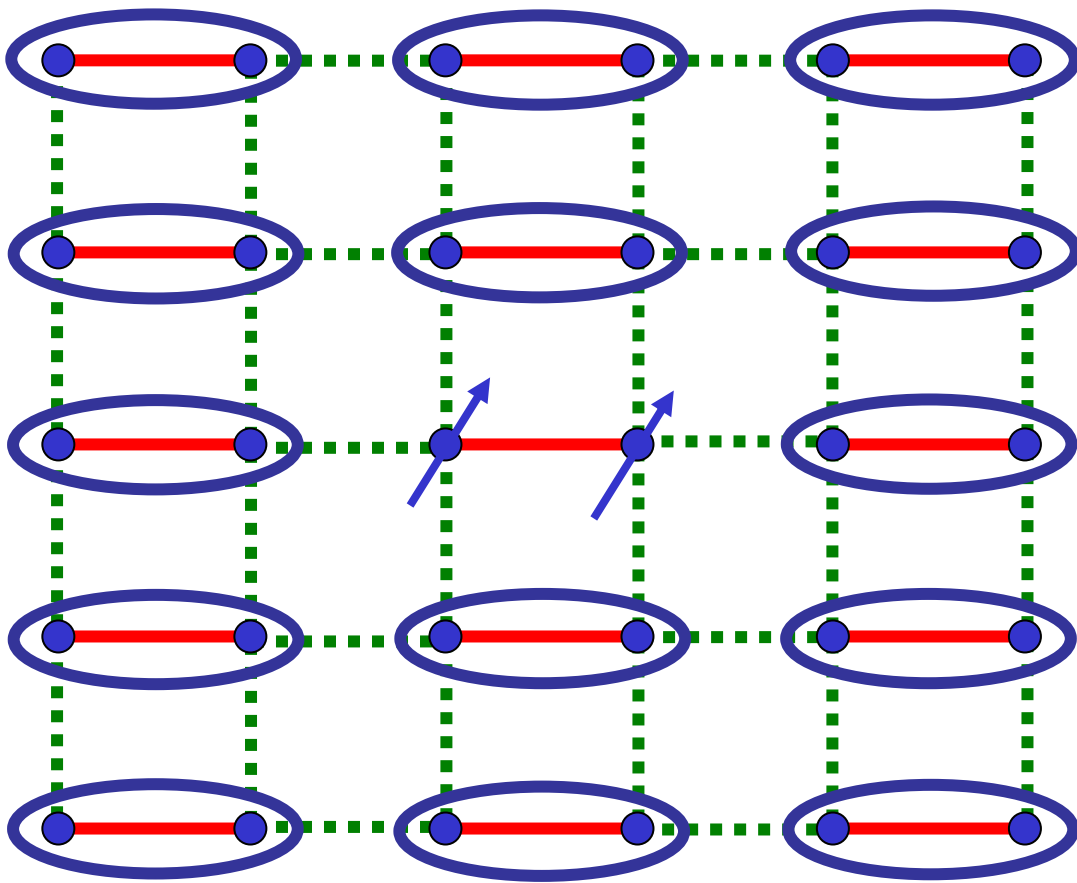


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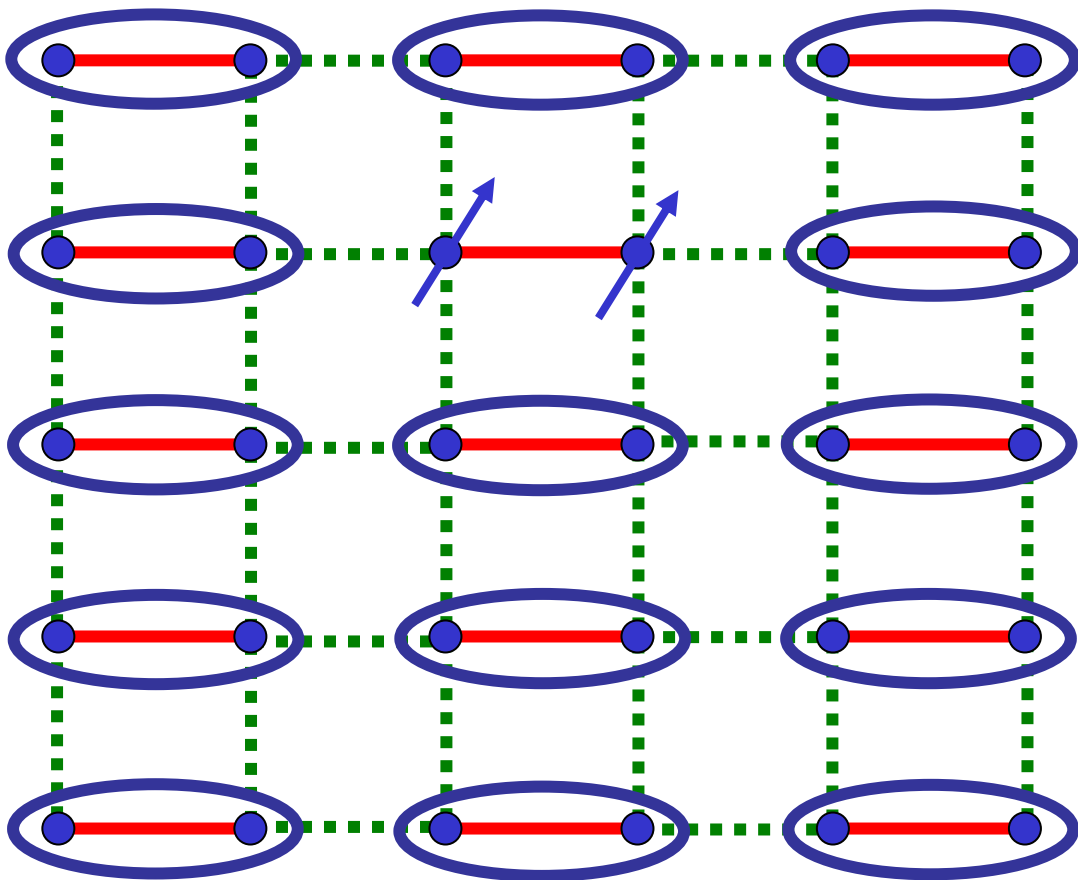


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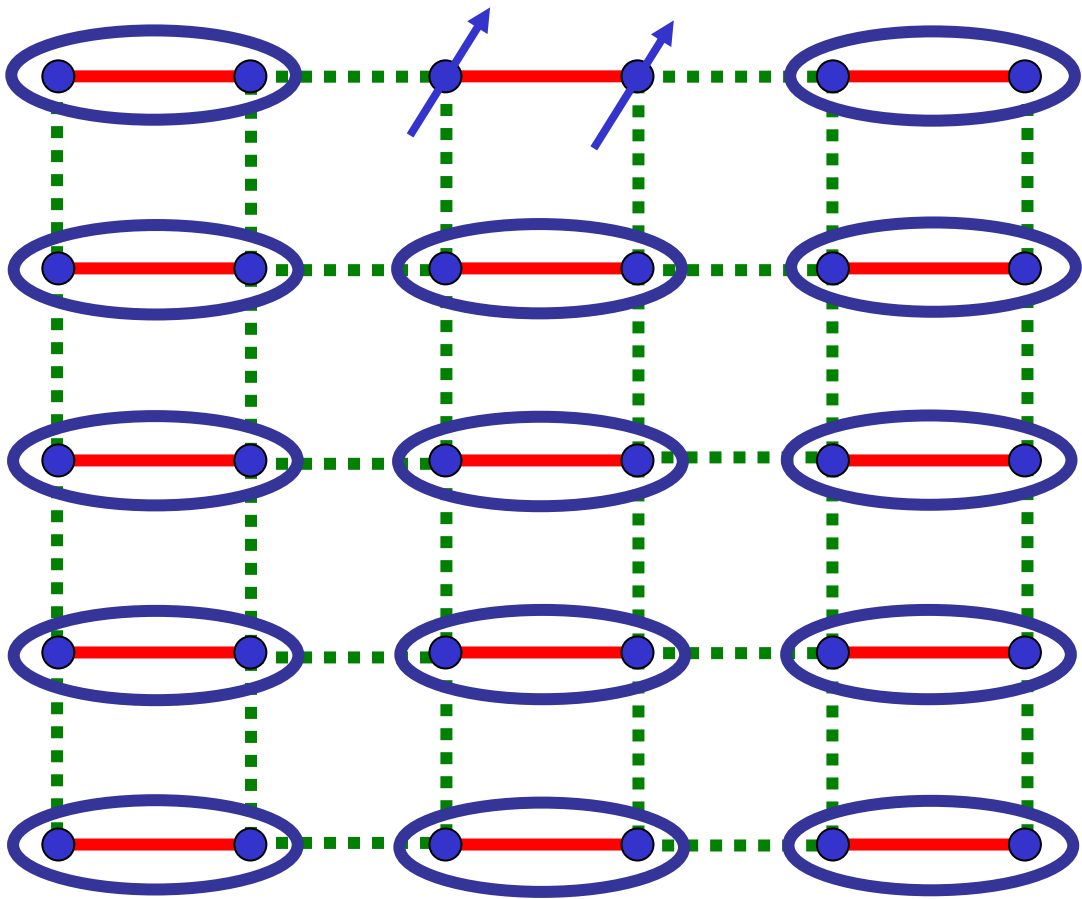


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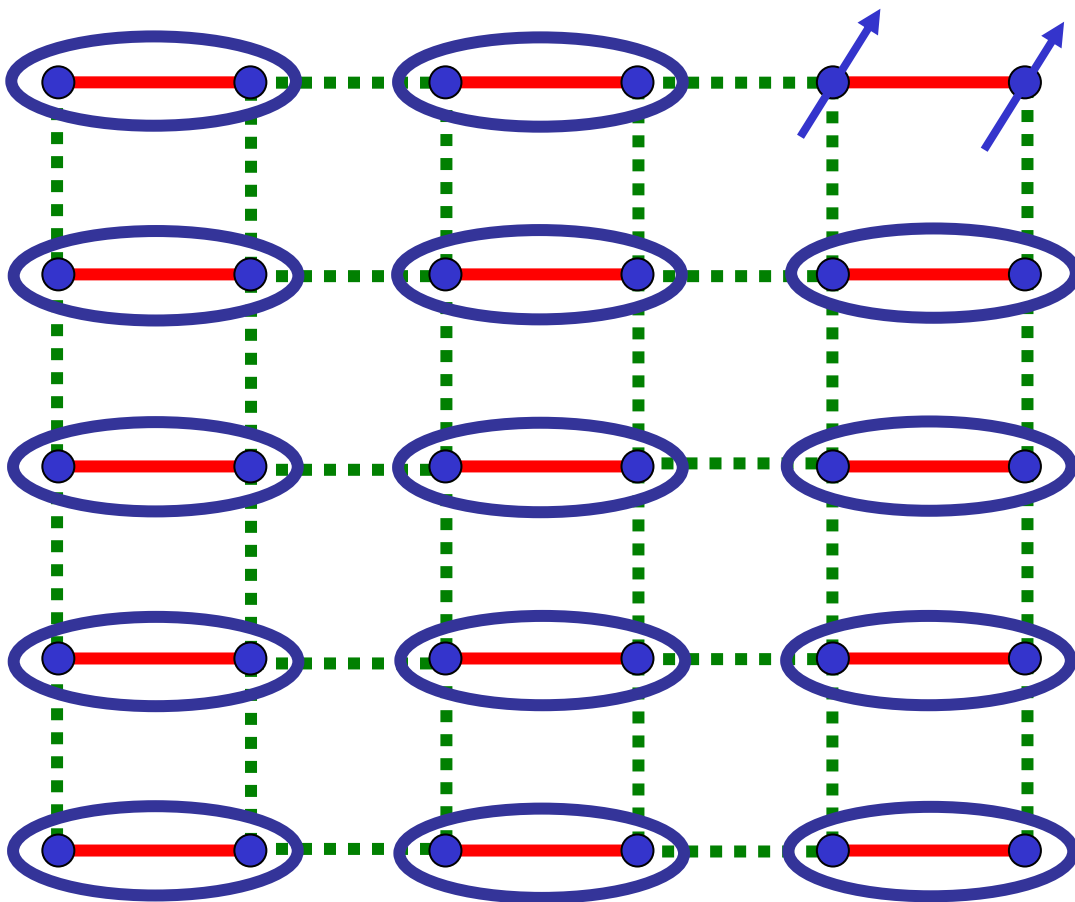


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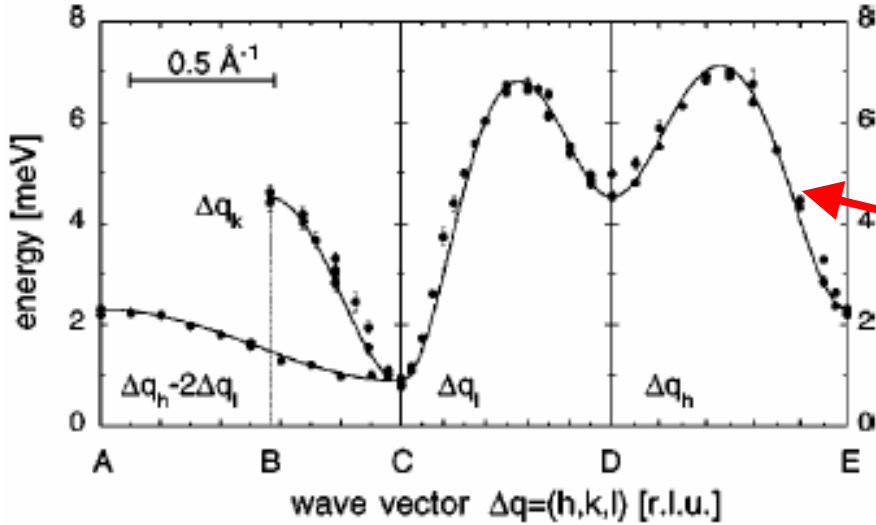
Excitation:  $S=1$  *triplon*  
(*exciton*, spin collective mode)

Energy dispersion away from  
antiferromagnetic wavevector

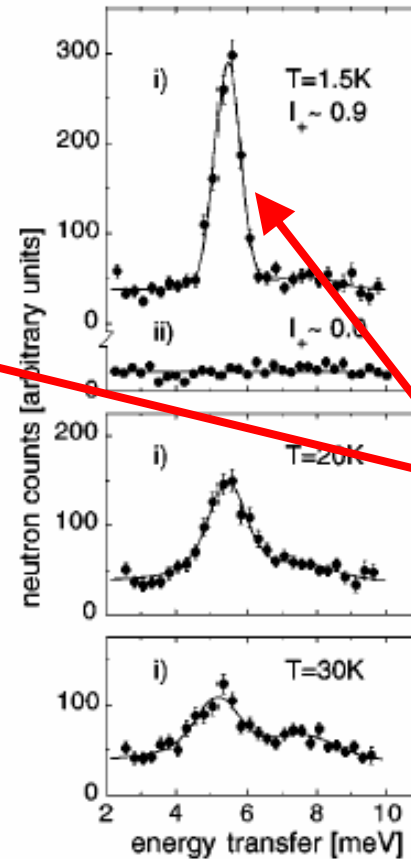
$$\varepsilon_p = \Delta + \frac{c_x^2 p_x^2 + c_y^2 p_y^2}{2\Delta}$$

$\Delta \rightarrow$  spin gap

# TiCuCl<sub>3</sub>



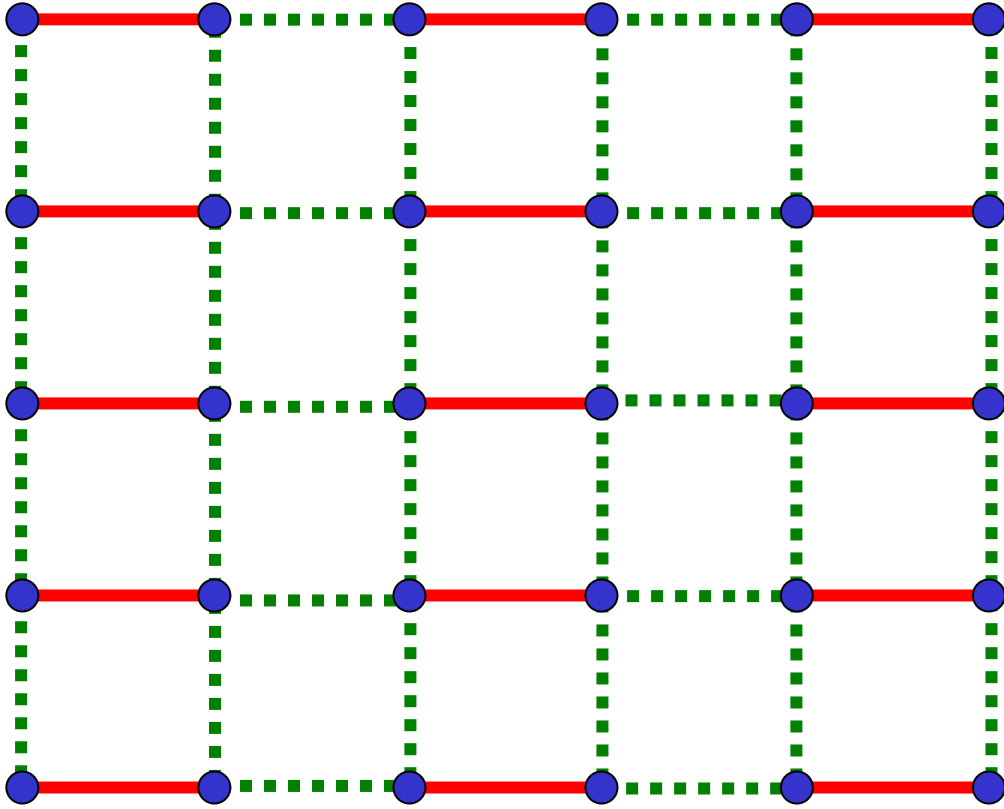
N. Cavadini, G. Heigold, W. Henggeler, A. Furrer,  
 H.-U. Güdel, K. Krämer and H. Mutka, *Phys. Rev.*  
 B 63 172414 (2001).



“triplon”

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

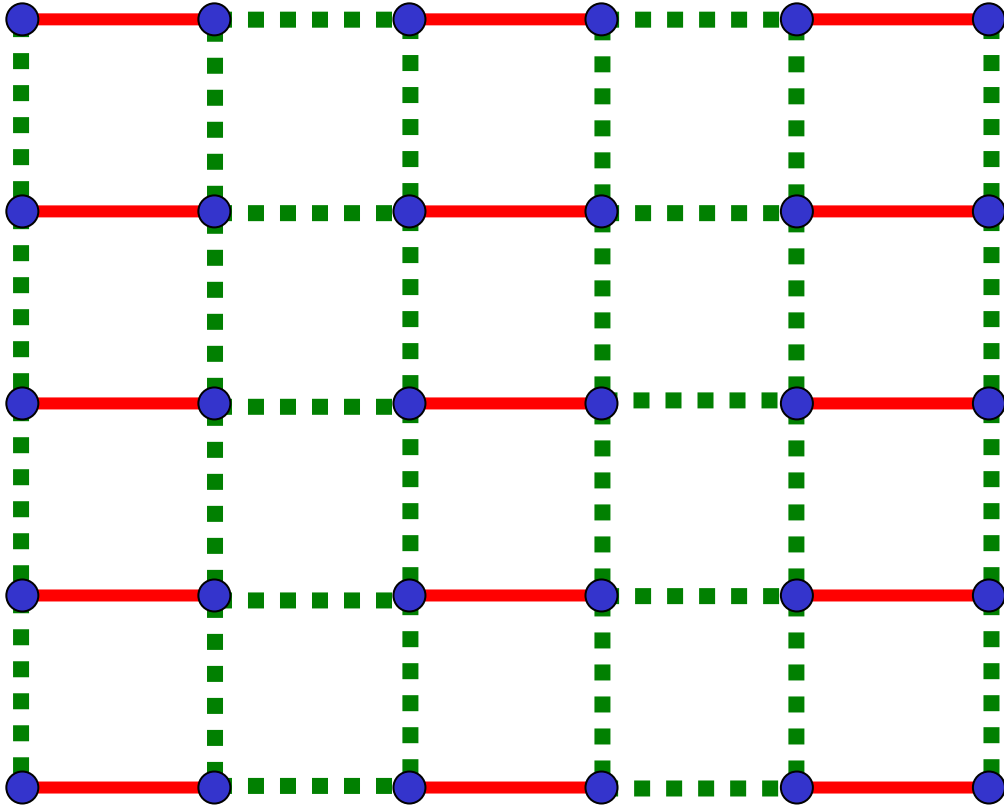
# Coupled Dimer Antiferromagnet





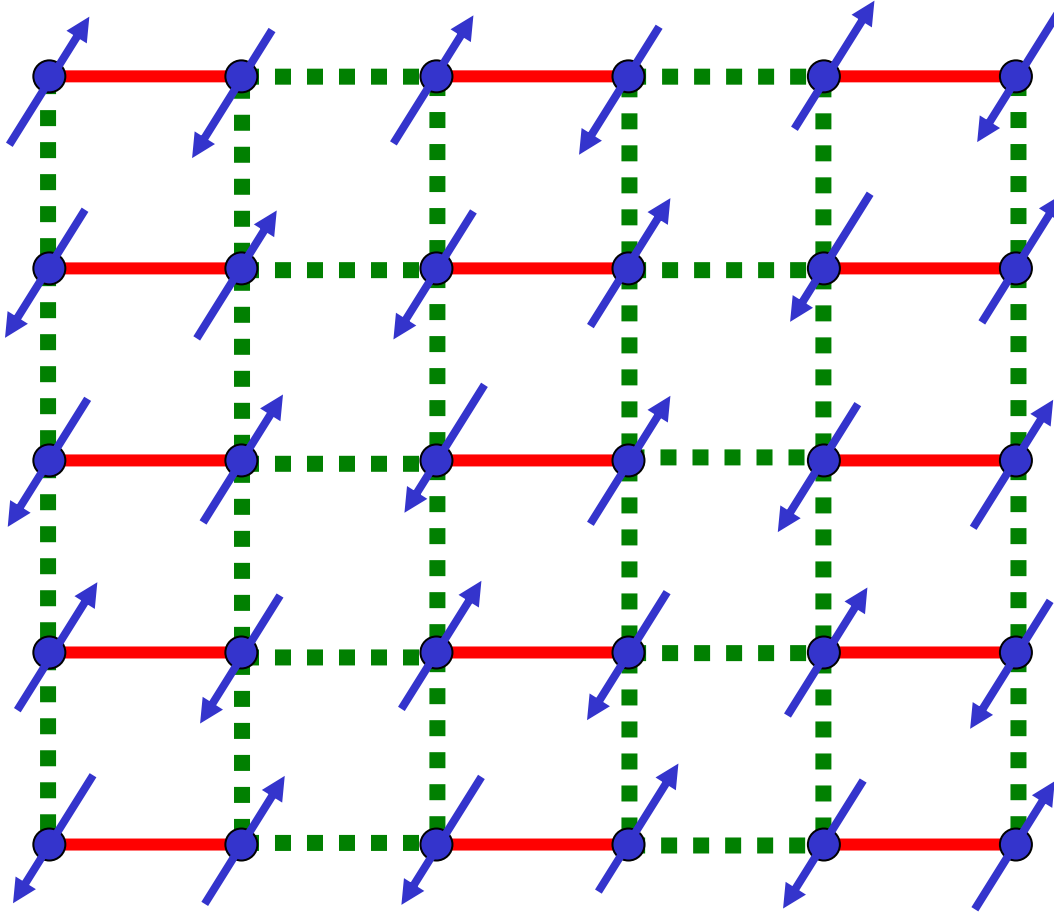
$\lambda$  close to 1

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>

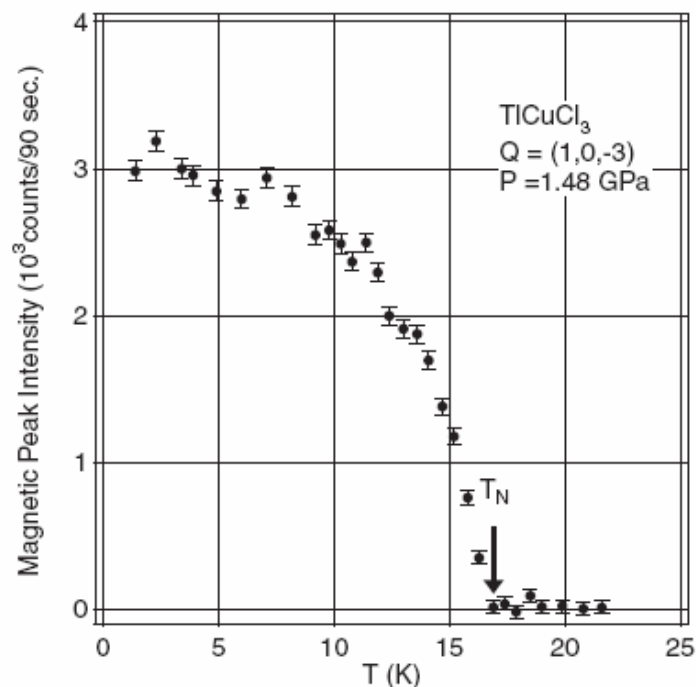
Akira OOSAWA\*, Masashi FUJISAWA<sup>1</sup>, Toyotaka OSAKABE, Kazuhisa KAKURAI and Hidekazu TANAKA<sup>2</sup>

*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)



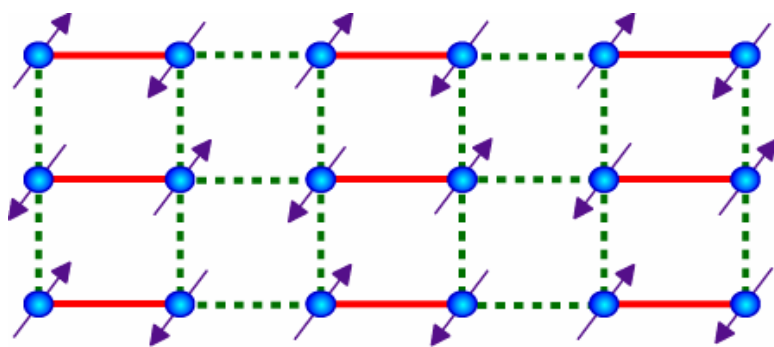
*J. Phys. Soc. Jpn* **72**, 1026 (2003)

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>.

$T=0$

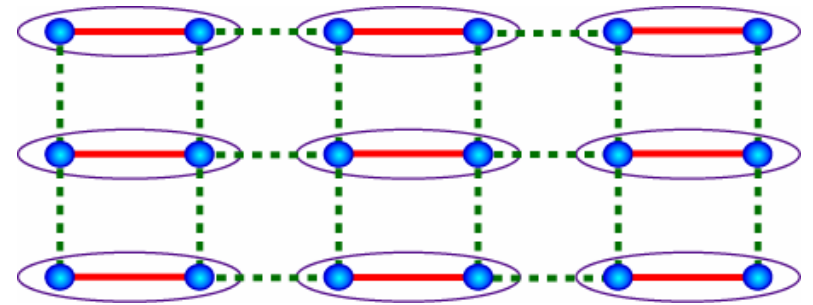
$$\lambda_c = 0.52337(3)$$

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

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



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)

## Key reason for validity of LGW theory

**Classical statistical mechanics:** There is a simple high temperature disordered state with  $\langle \vec{\phi} \rangle = 0$  and exponentially decaying correlations

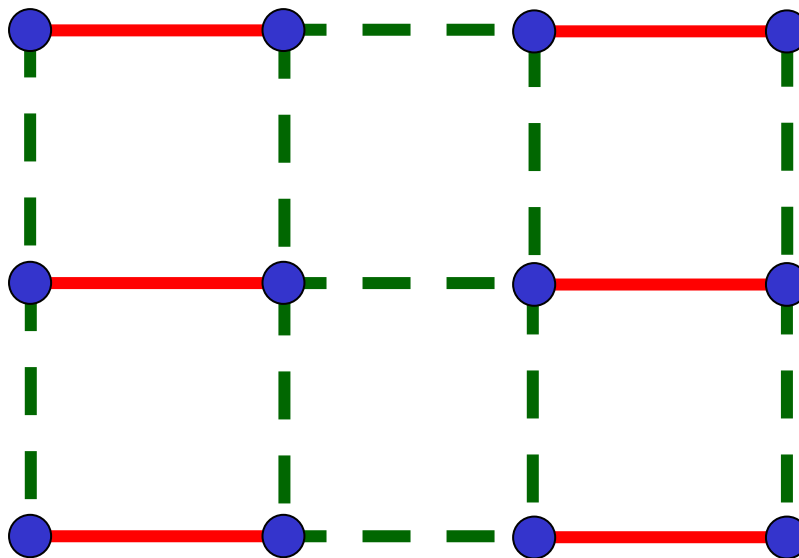
**Quantum mechanics:** There is a "*quantum disordered*" non-degenerate ground state with  $\langle \vec{\phi} \rangle = 0$  and an energy gap to all excitations

B. Mott insulators with  
spin  $S=1/2$  per unit cell:

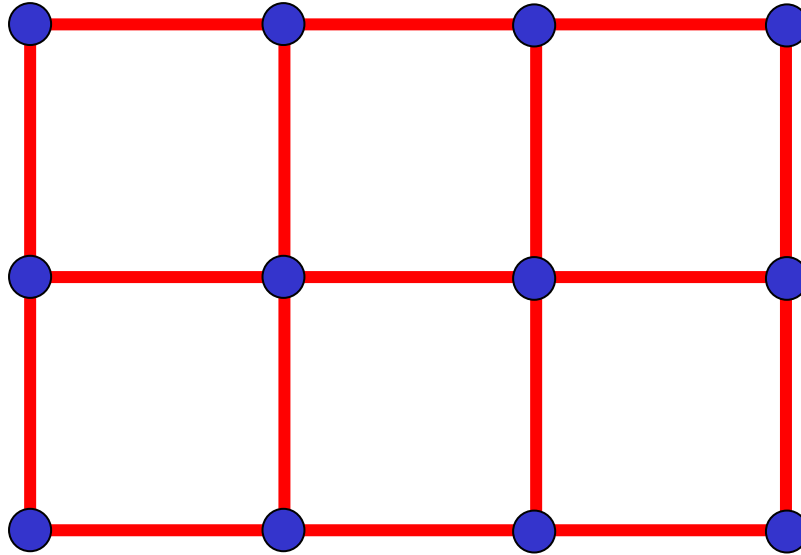
*Berry phases, bond order, and the  
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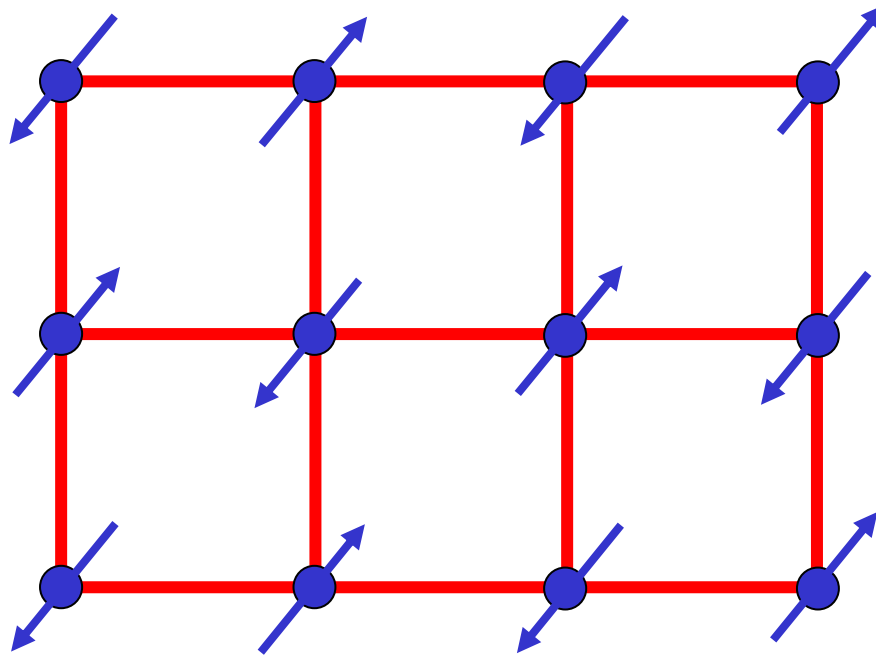
Mott insulator with two  $S=1/2$  spins per unit cell



Mott insulator with one  $S=1/2$  spin per unit cell

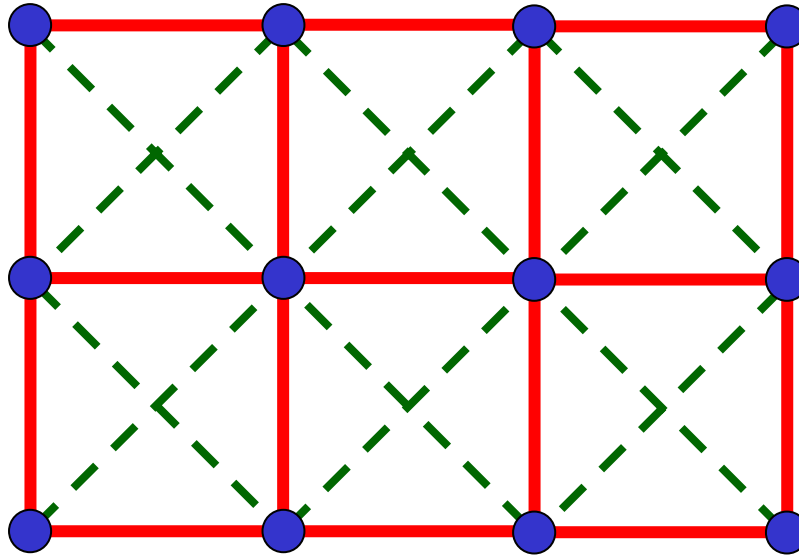


Mott insulator with one  $S=1/2$  spin per unit cell



Ground state has Neel order with  $\vec{\phi} \neq 0$

## Mott insulator with one $S=1/2$ spin per unit cell



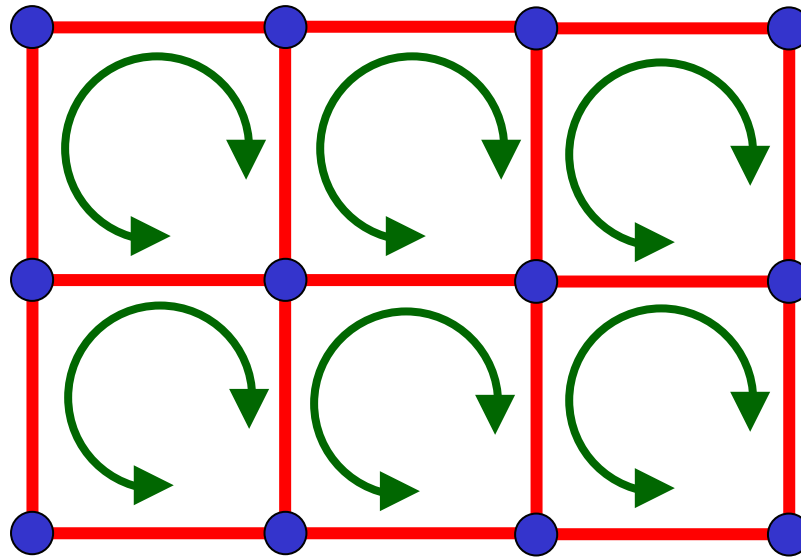
Destroy Neel order by perturbations which preserve full square lattice symmetry *e.g.* second-neighbor or ring exchange.

The strength of this perturbation is measured by a coupling  $g$ .

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

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

## Mott insulator with one $S=1/2$ spin per unit cell



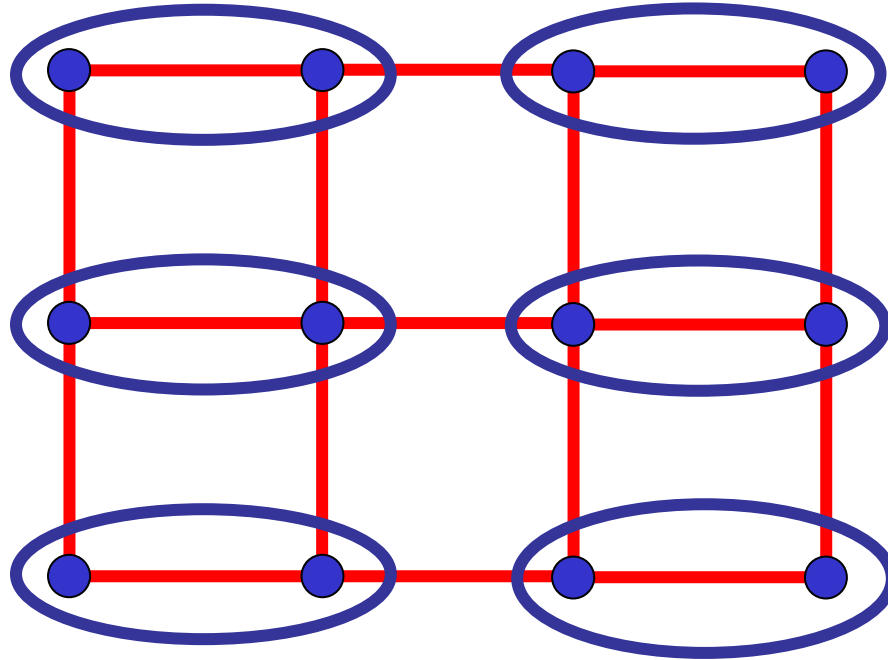
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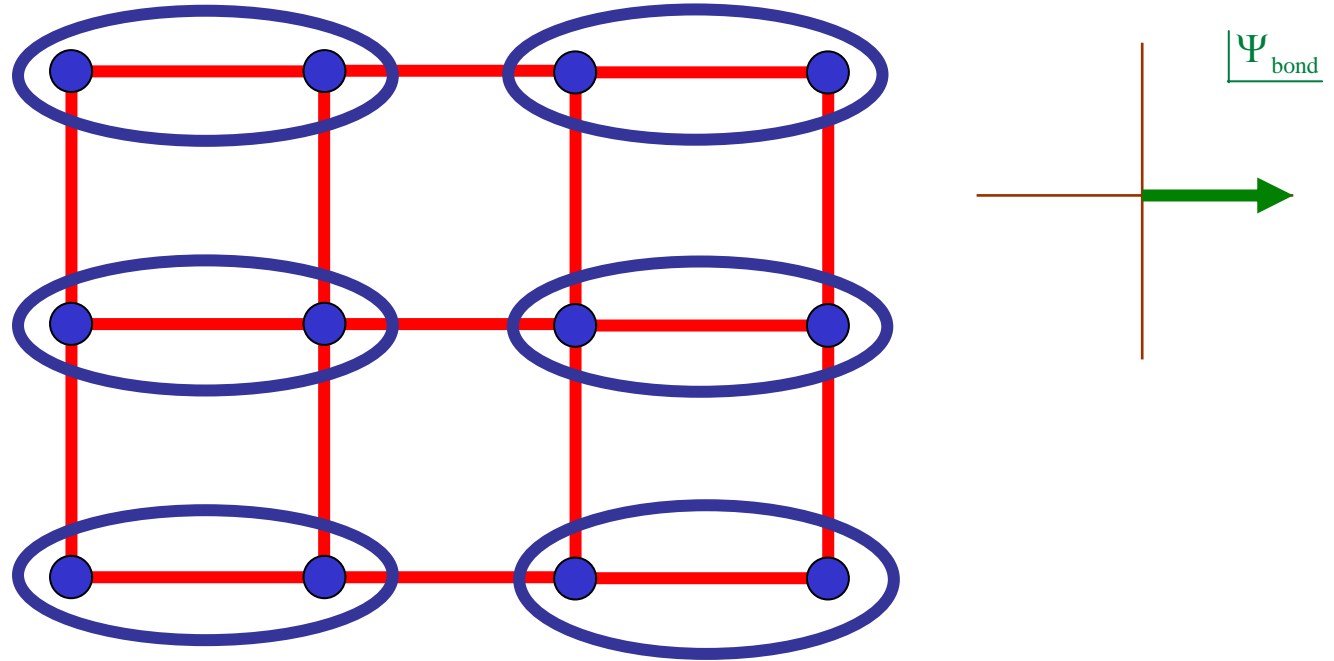
Large  $g \Rightarrow$  paramagnetic ground state with  $\langle \vec{\phi} \rangle = 0$

Mott insulator with one  $S=1/2$  spin per unit cell



Possible large  $g$  paramagnetic ground state with  $\langle \vec{\phi} \rangle = 0$

## Mott insulator with one $S=1/2$ spin per unit cell

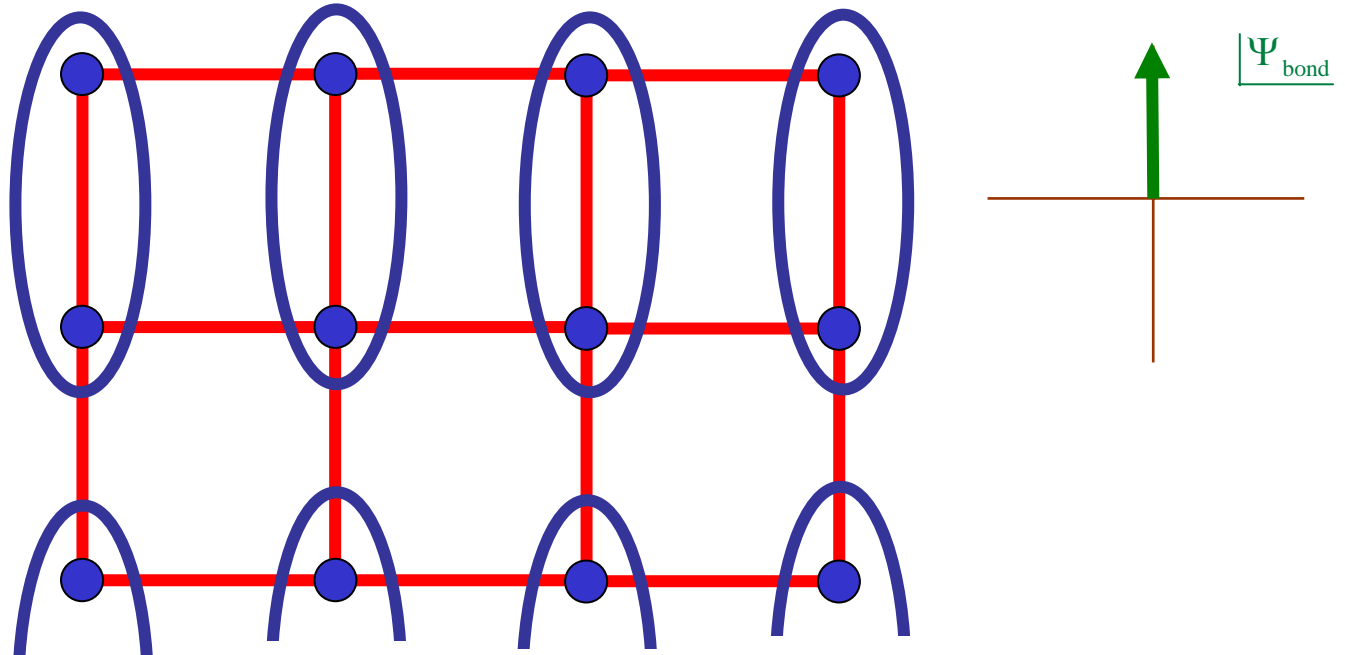


Possible large  $g$  paramagnetic ground state with  $\langle \vec{\phi} \rangle = 0$

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

$$\Psi_{\text{bond}}(i) = \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j e^{i \arctan(r_j - r_i)}$$

## Mott insulator with one $S=1/2$ spin per unit cell



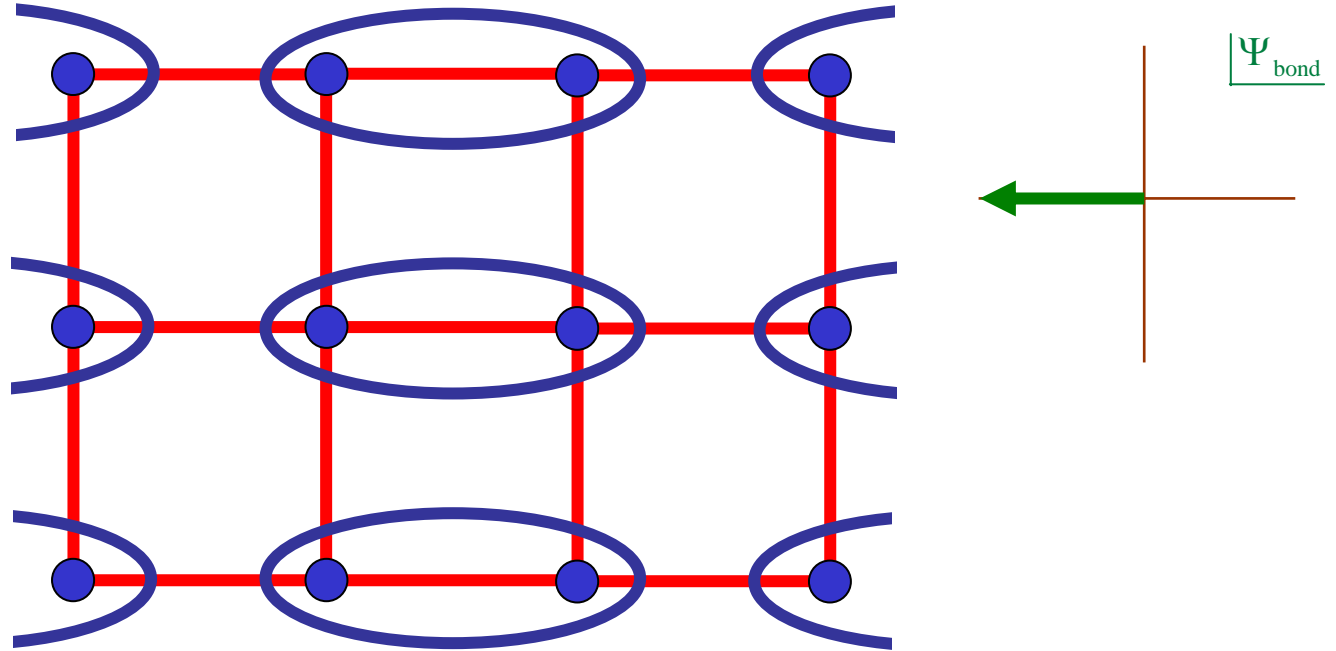
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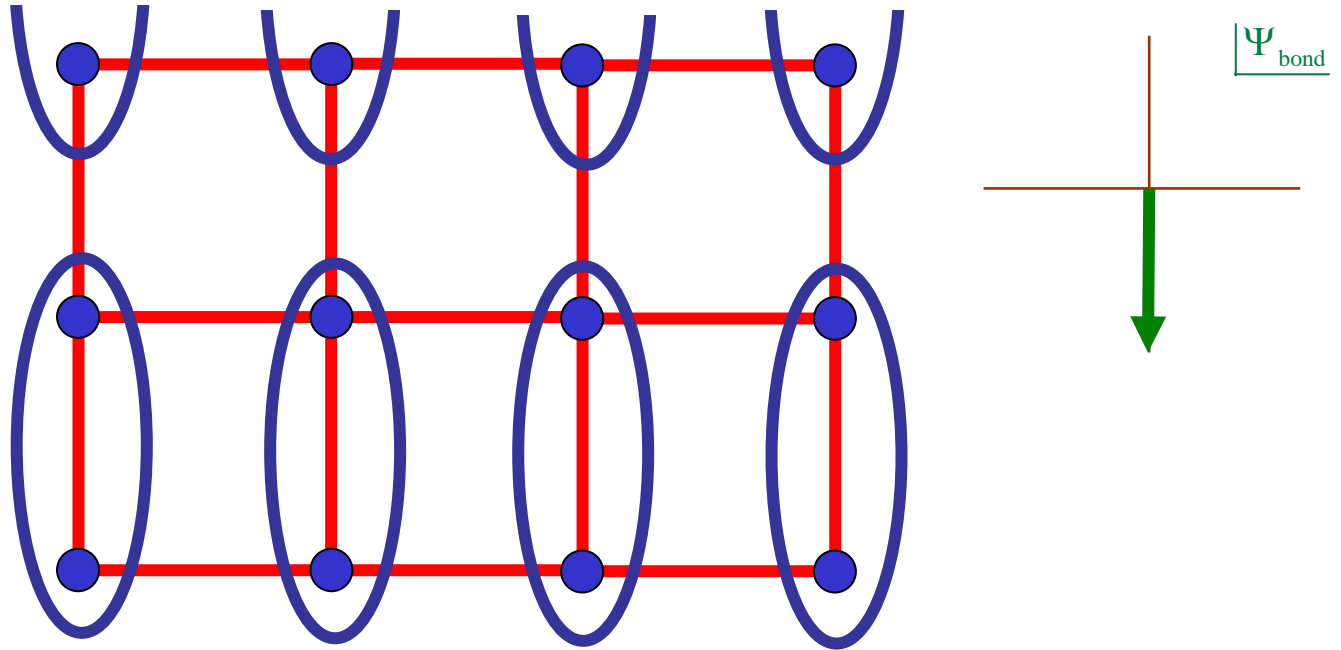


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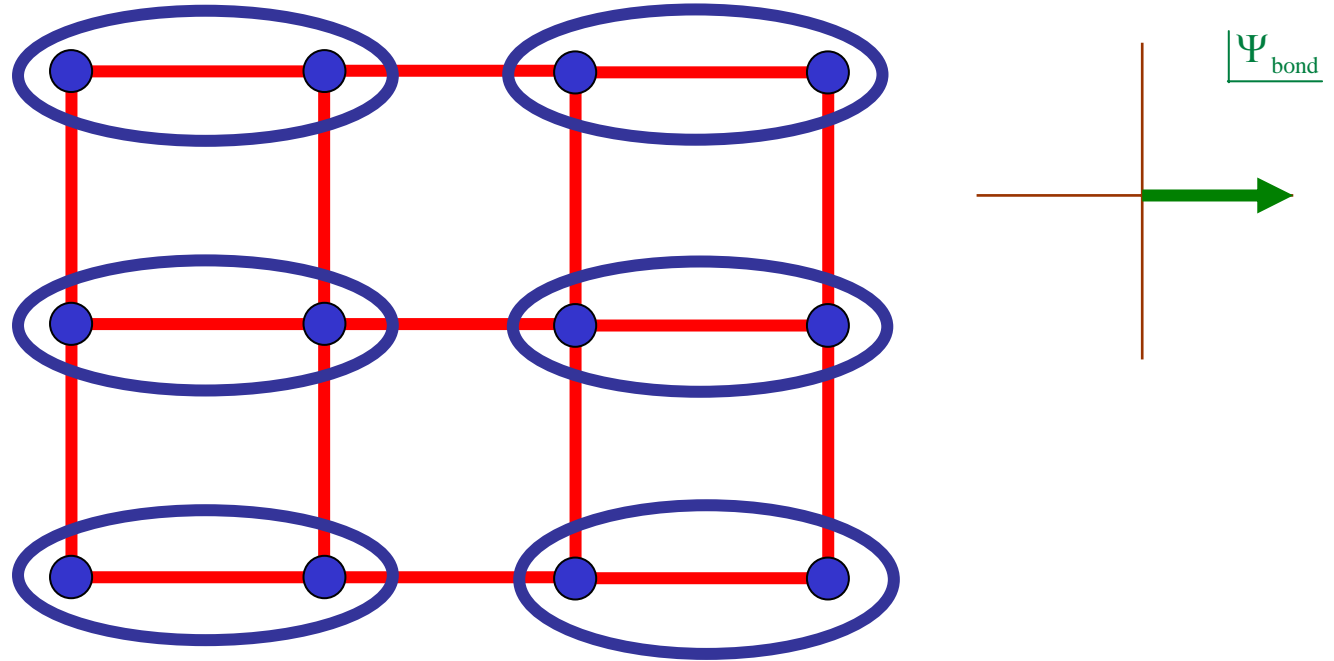


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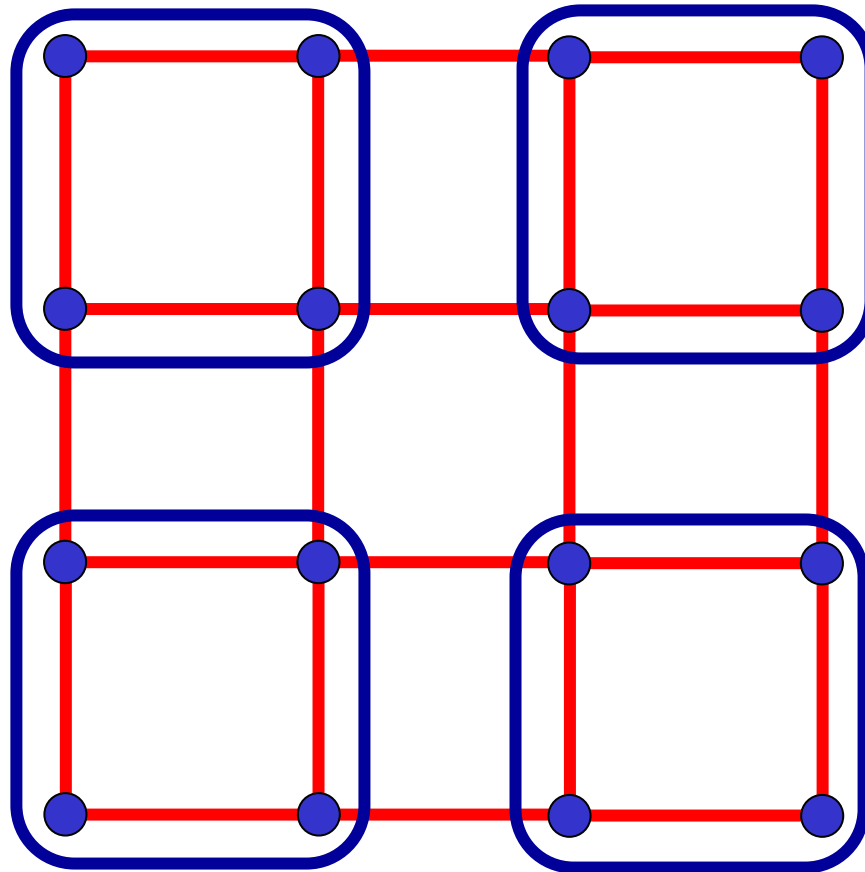


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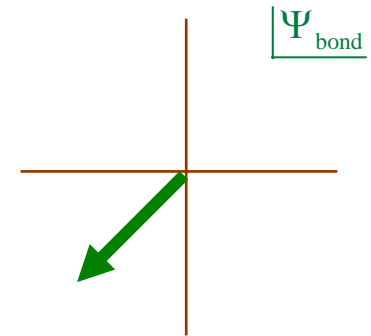
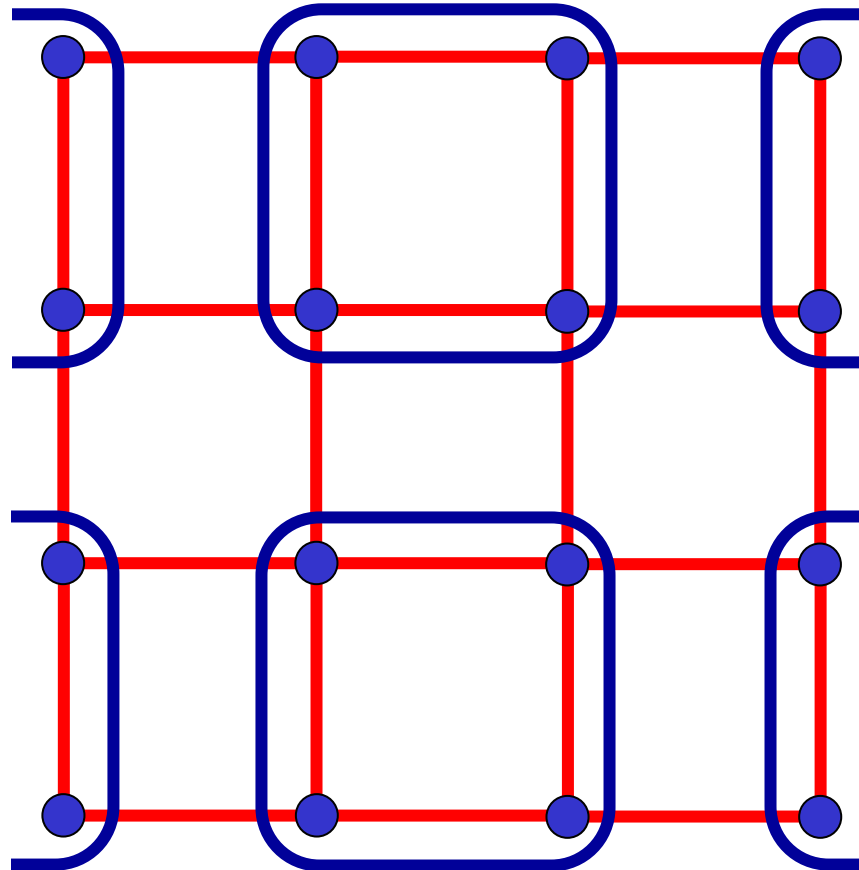


Possible large  $g$  paramagnetic ground state with  $\langle \vec{\phi} \rangle = 0$

Another state breaking the symmetry of rotations by  $n\pi/2$  about lattice sites, which also has  $\langle \Psi_{\text{bond}} \rangle \neq 0$ , where  $\Psi_{\text{bond}}$  is the *bond order parameter*

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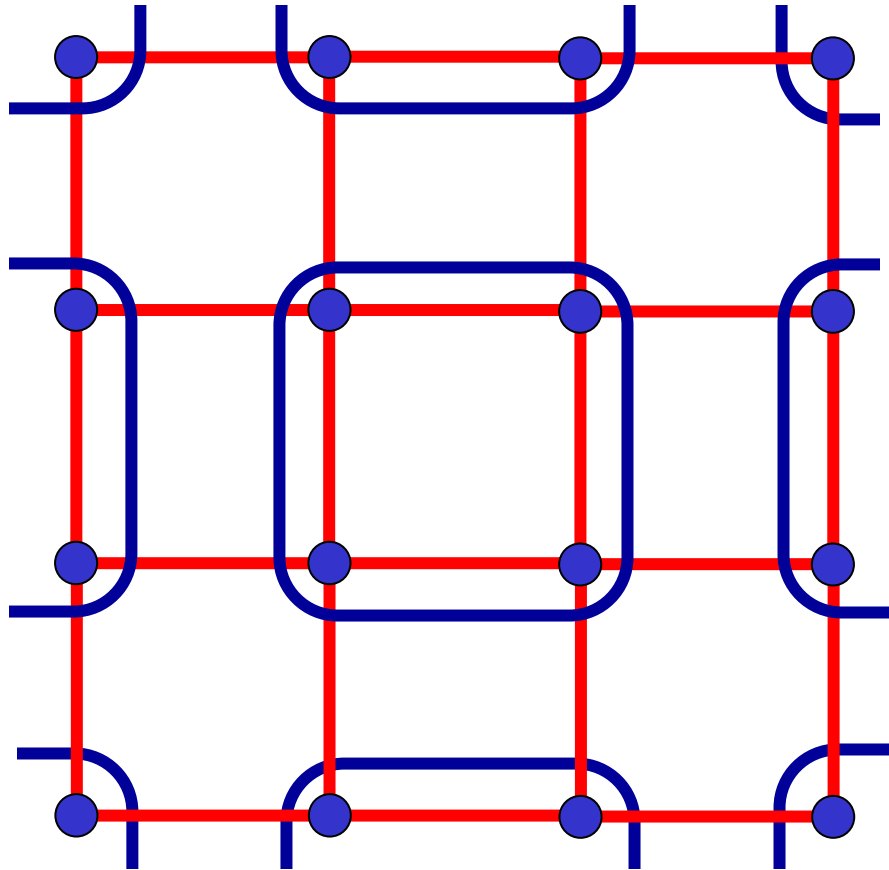


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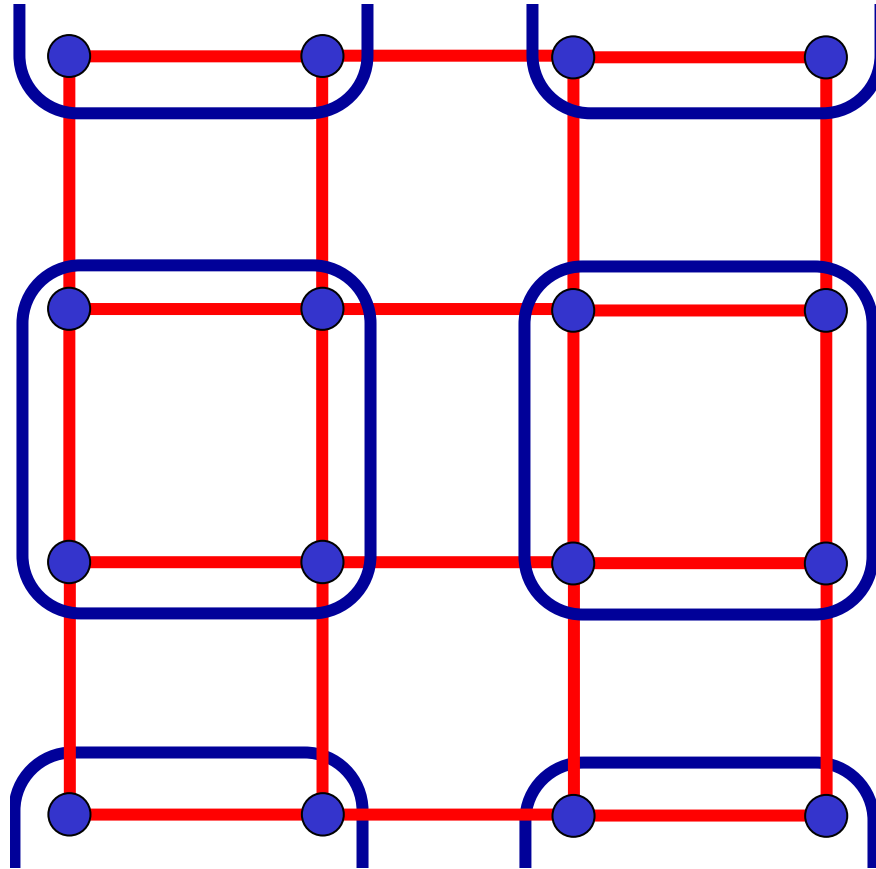


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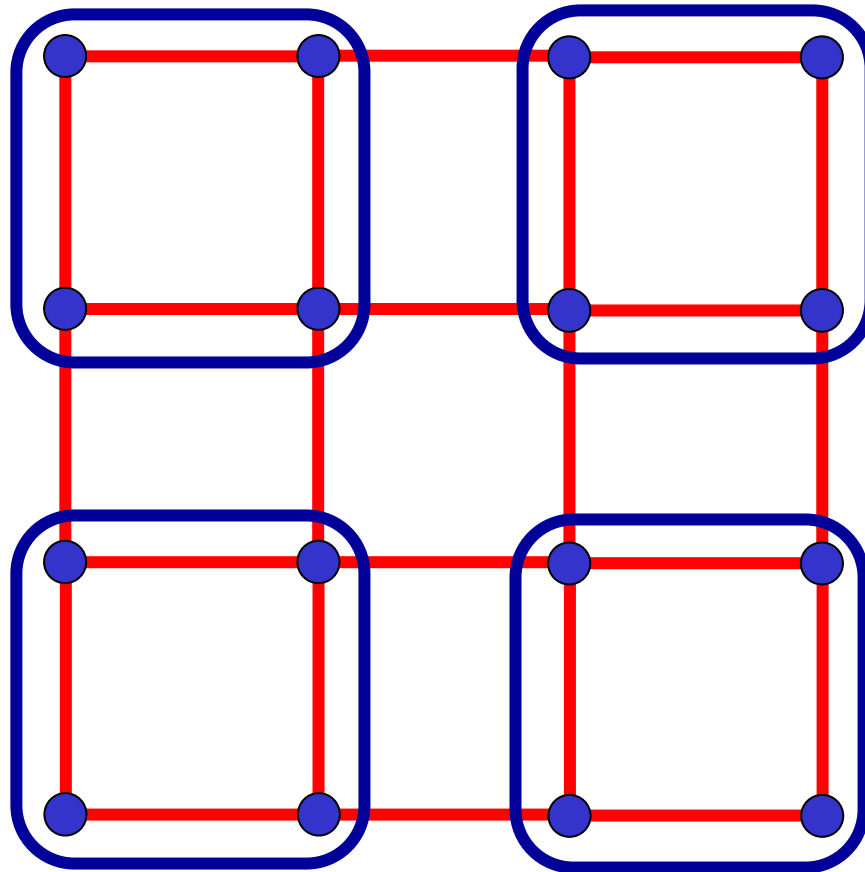


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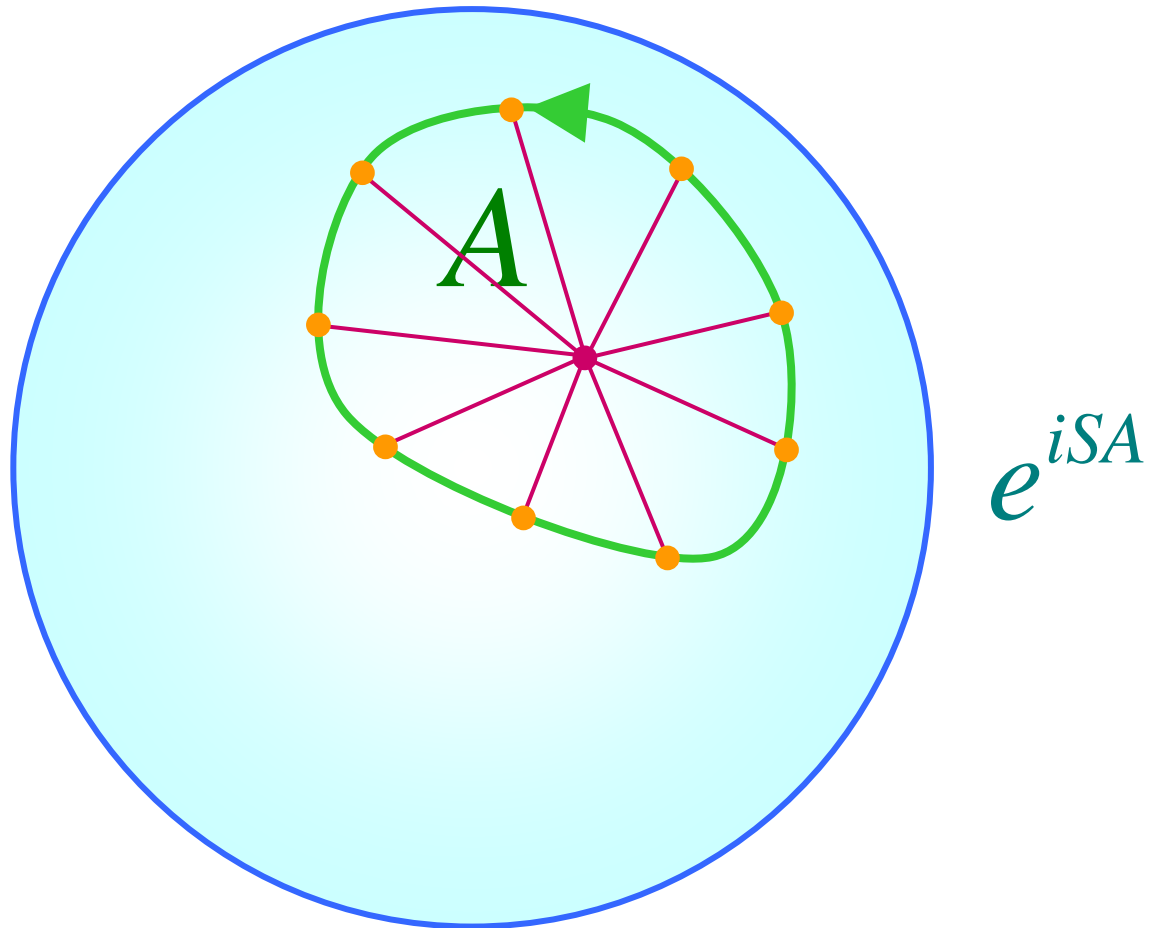
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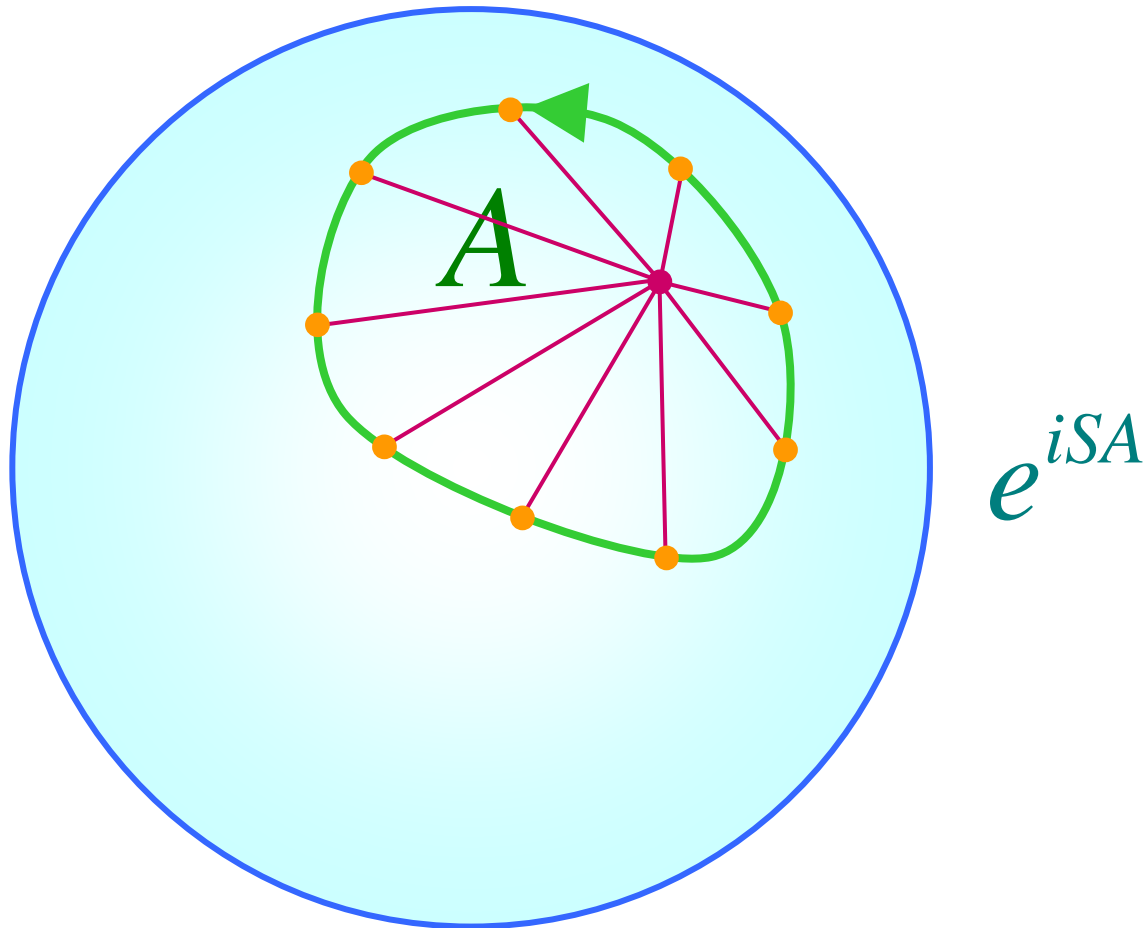
# Quantum theory for destruction of Neel order

## Ingredient missing from LGW theory: Spin Berry Phases

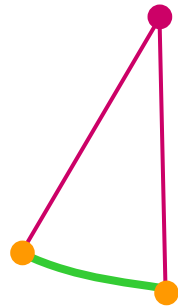


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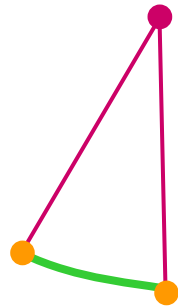


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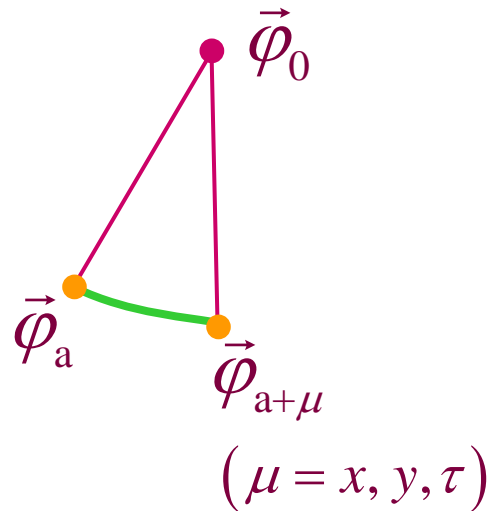
Discretize imaginary time: path integral is over fields on the sites of a cubic lattice of points  $a$



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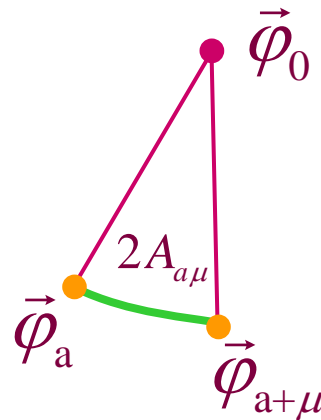
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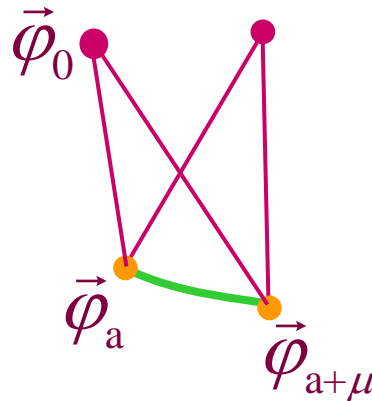
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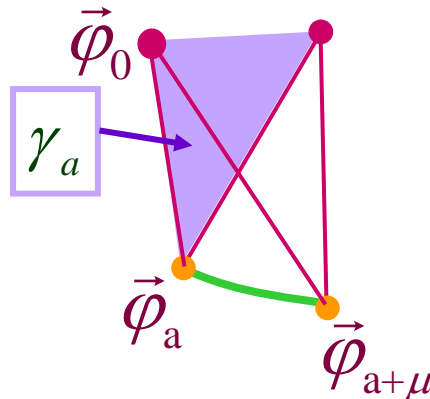
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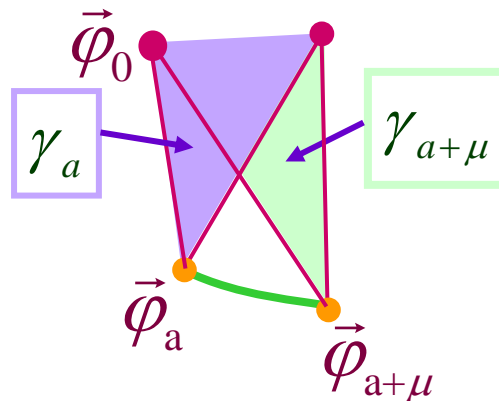
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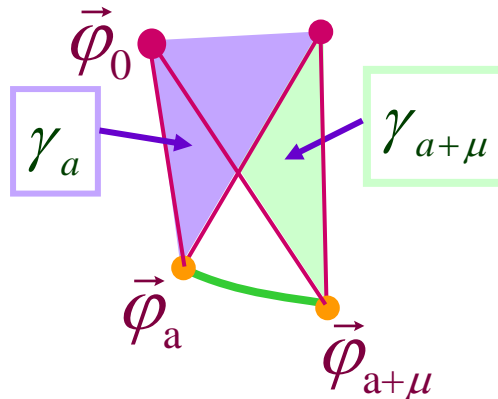
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Change in choice of  $\vec{\varphi}_0$  is like a “gauge transformation”



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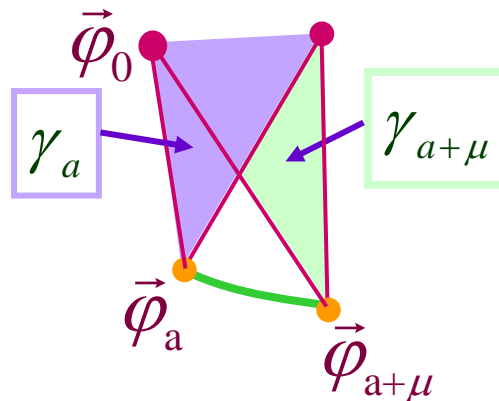
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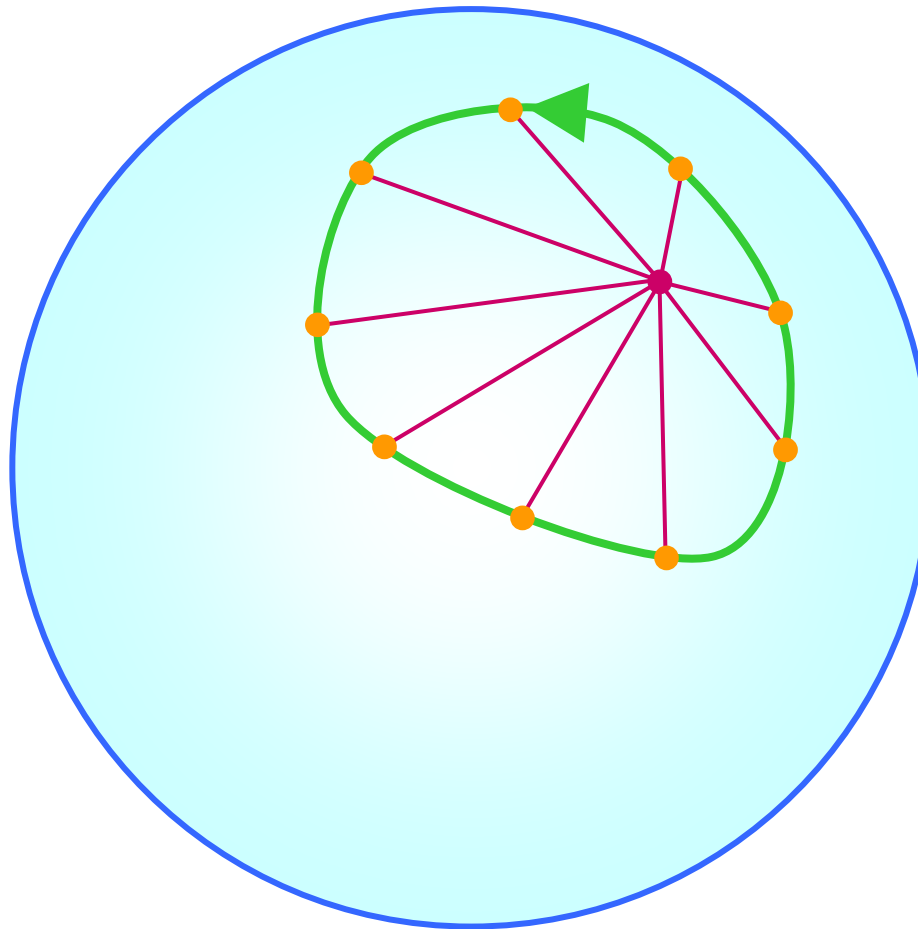
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The area of the triangle is uncertain modulo  $4\pi$ , and the action has to be invariant under  $A_{a\mu} \rightarrow A_{a\mu} + 2\pi$

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

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

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

Simplest large  $g$  effective action for the  $A_{a\mu}$

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

with  $e^2 \sim g^2$

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

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

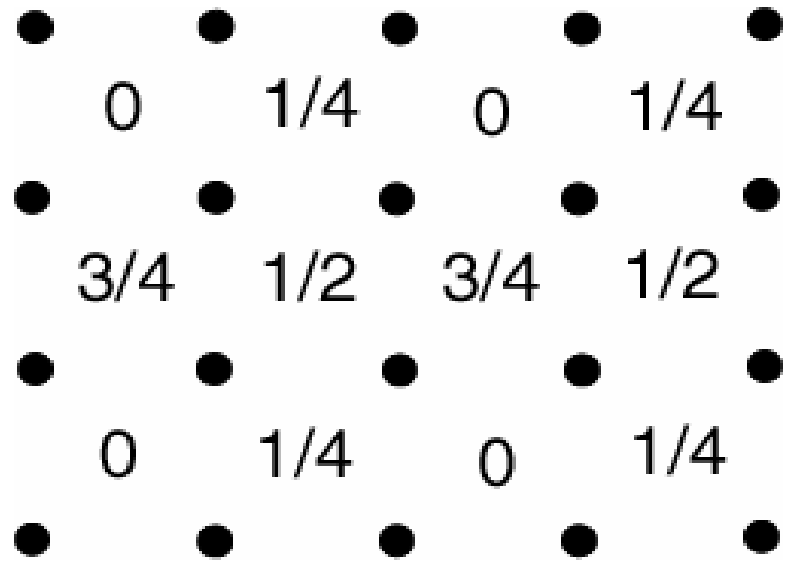
S. Sachdev and R. Jalabert, *Mod. Phys. Lett. B* **4**, 1043 (1990).

S. Sachdev and K. Park, *Annals of Physics*, **298**, 58 (2002)

Exact duality transform on periodic Gaussian (“Villain”) action for compact QED yields a representation in terms of a Coulomb gas of monopoles

$$Z_{\text{dual}} = \sum_{\{m_{\bar{j}}\}} \exp \left( -\frac{\pi}{2e^2} \sum_{\bar{j}, \bar{j}'} \frac{m_{\bar{j}} m_{\bar{j}'}}{|r_{\bar{j}} - r_{\bar{j}'}|} + 2\pi i \sum_{\bar{j}} m_{\bar{j}} \mathcal{X}_{\bar{j}} \right)$$

with the  $m_{\bar{j}}$  integer monopole charges. Each monopole carries a Berry phase (F.D.M. Haldane, *Phys. Rev. Lett.* **61**, 1029 (1988)) determined by the fixed  $\mathcal{X}_{\bar{j}} = 0, 1/4, 1/2, 3/4$  on the four dual sublattices.



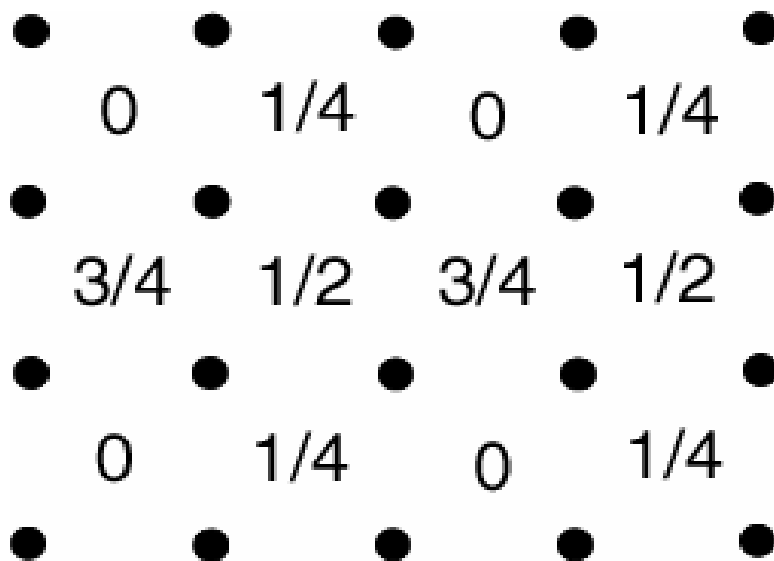


Alternative representation is in terms of a “height” model

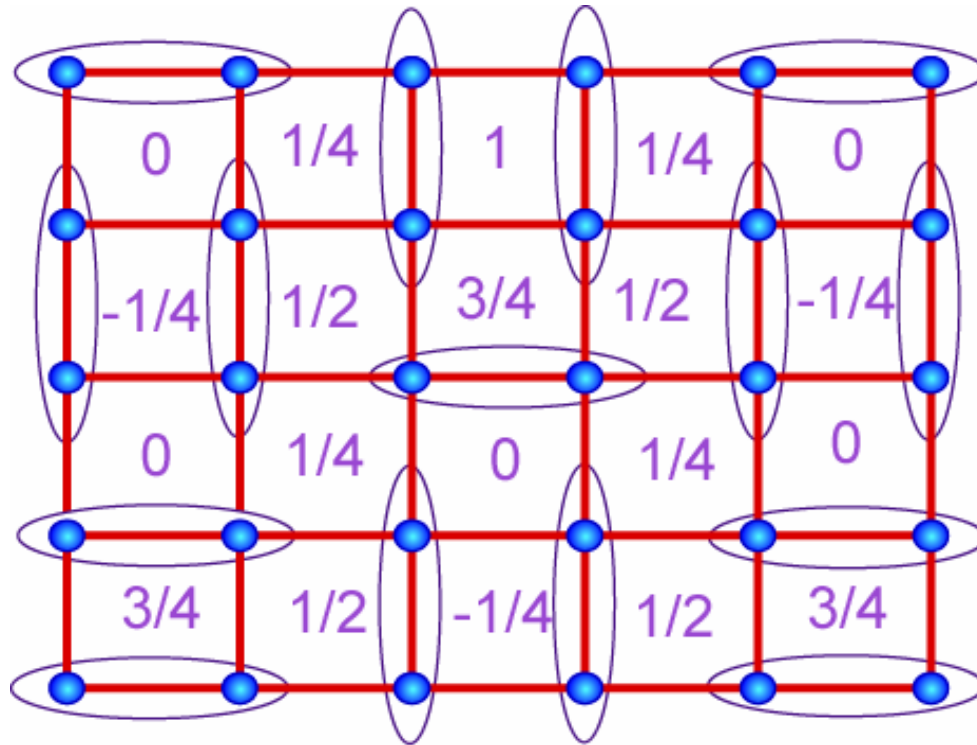
$$Z_{\text{dual}} = \sum_{\{h_{\bar{j}}\}} \exp \left( -\frac{e^2}{2} \sum_{\bar{j}} (\Delta_{\mu} h_{\bar{j}} - \Delta_{\mu} \mathcal{X}_{\bar{j}})^2 \right)$$

with the  $h_{\bar{j}}$  integer heights.

The Berry phases now lead to height ‘offsets’  $\mathcal{X}_{\bar{j}} = 0, 1/4, 1/2, 3/4$  on the four dual sublattices.



For large  $e^2$ , low energy height configurations are in exact one-to-one correspondence with nearest-neighbor valence bond pairings of the sites square lattice



There is no roughening transition for three dimensional interfaces, which are smooth for all couplings

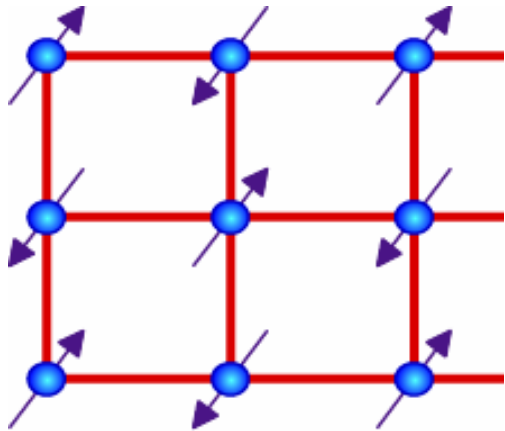
D.S. Fisher and J.D. Weeks, *Phys. Rev. Lett.* **50**, 1077 (1983).

⇒ There is a definite average height of the interface

⇒ **Ground state has bond order.**

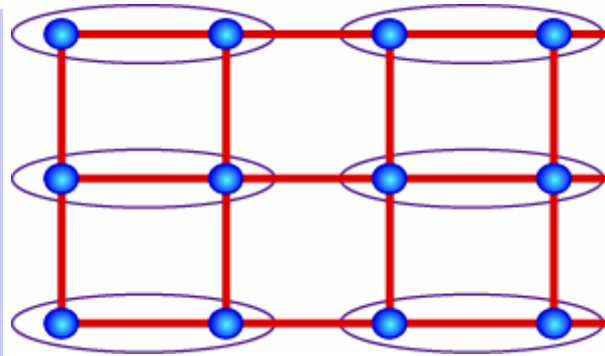
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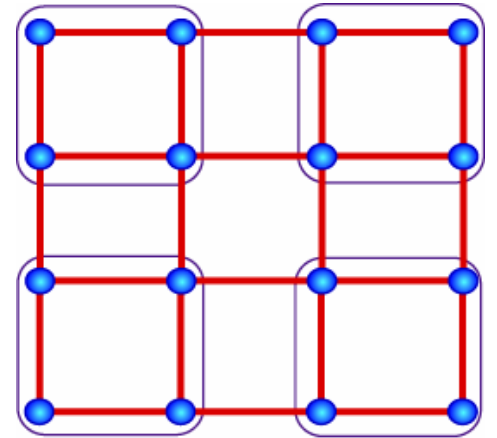


Neel order

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



or



Bond order

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

Not present in

LGW theory

of  $\vec{\varphi}$  order

0

$g$