

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

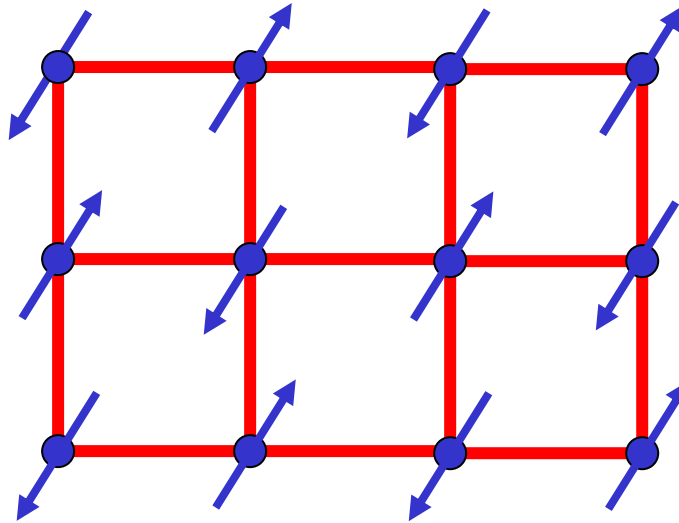
*Science* **303**, 1490 (2004); cond-mat/0312617  
cond-mat/0401041

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Ashvin Vishwanath (MIT)



Parent compound of the high temperature  
superconductors:  $\text{La}_2\text{CuO}_4$

### A Mott insulator



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

$\vec{S}_i \Rightarrow$  spin operator with  
angular momentum  $S=1/2$

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

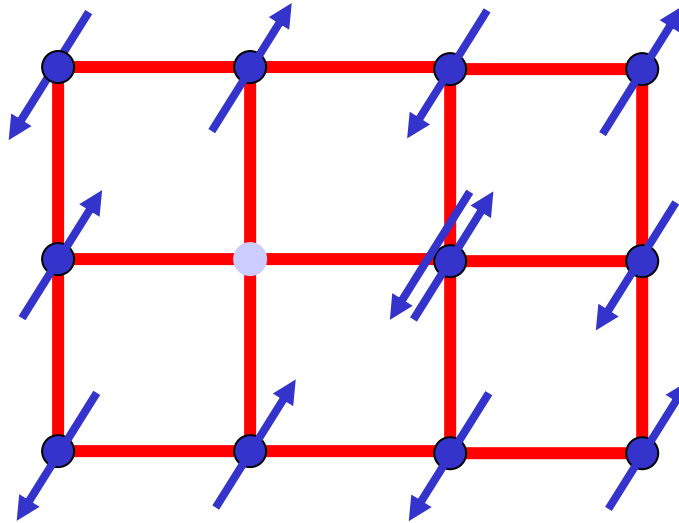
spin density wave order parameter:

$$\vec{\varphi} = \eta_i \frac{\vec{S}_i}{S} \quad ; \quad \eta_i = \pm 1 \text{ on two sublattices}$$

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

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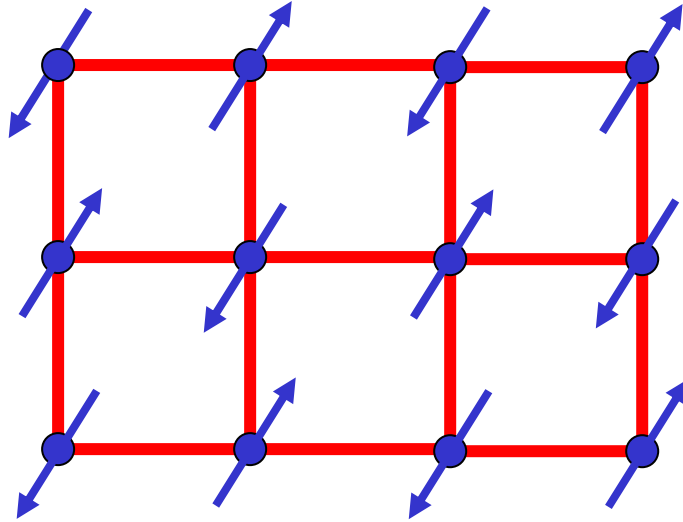
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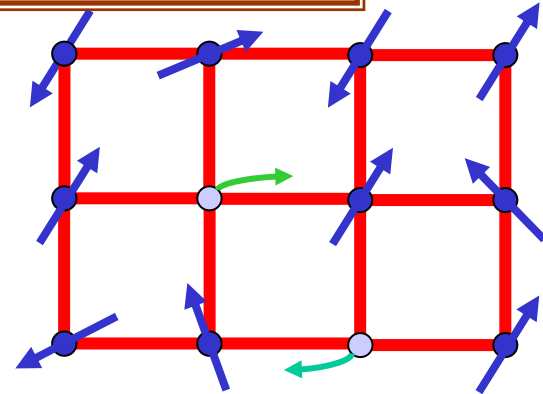
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# Superconductivity in a doped Mott insulator

Introduce mobile carriers of density  $\delta$   
by substitutional doping of out-of-plane  
ions *e.g.*  $\text{La}_{2-\delta}\text{Sr}_\delta\text{CuO}_4$



Doped state is a paramagnet with  $\langle \vec{\phi} \rangle = 0$

and also a high temperature superconductor with

the BCS pairing order parameter  $\langle \Psi_{\text{BCS}} \rangle \neq 0$ .

$\Rightarrow$  With increasing  $\delta$ , there must be one or more  
quantum phase transitions involving

(i) onset of a non-zero  $\langle \Psi_{\text{BCS}} \rangle$

(ii) restoration of spin rotation invariance by a transition

from  $\langle \vec{\phi} \rangle \neq 0$  to  $\langle \vec{\phi} \rangle = 0$

First study magnetic transition in Mott insulators.....

# 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*

C. Technical details

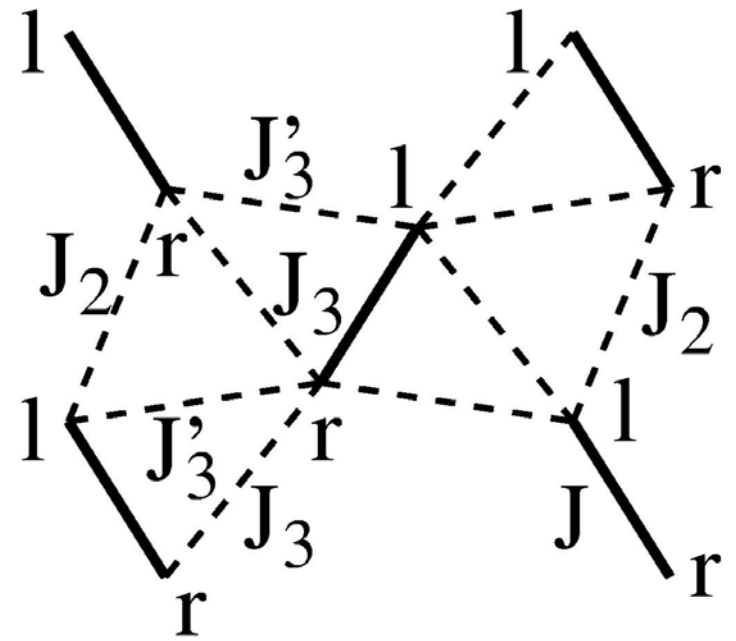
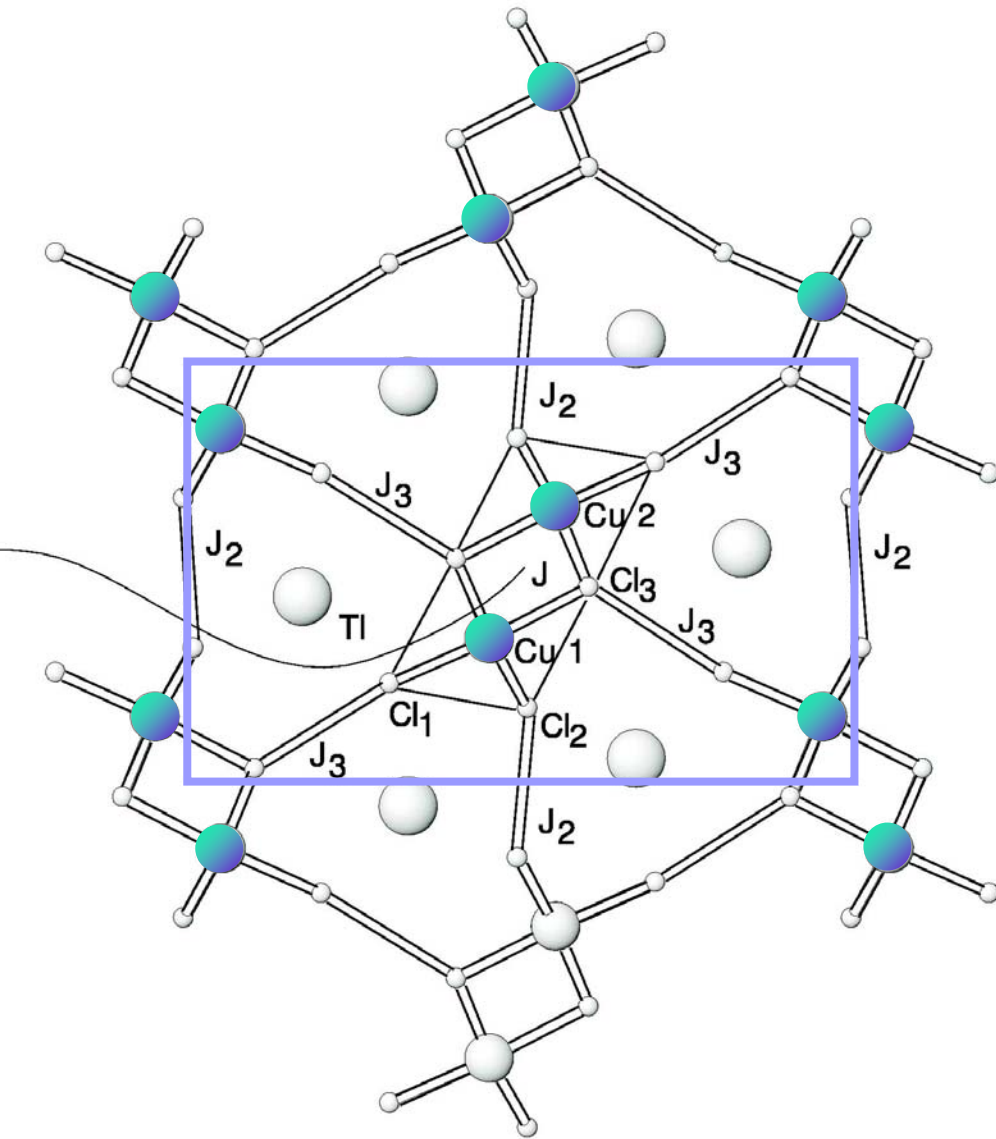
*Duality and dangerously irrelevant operators*

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

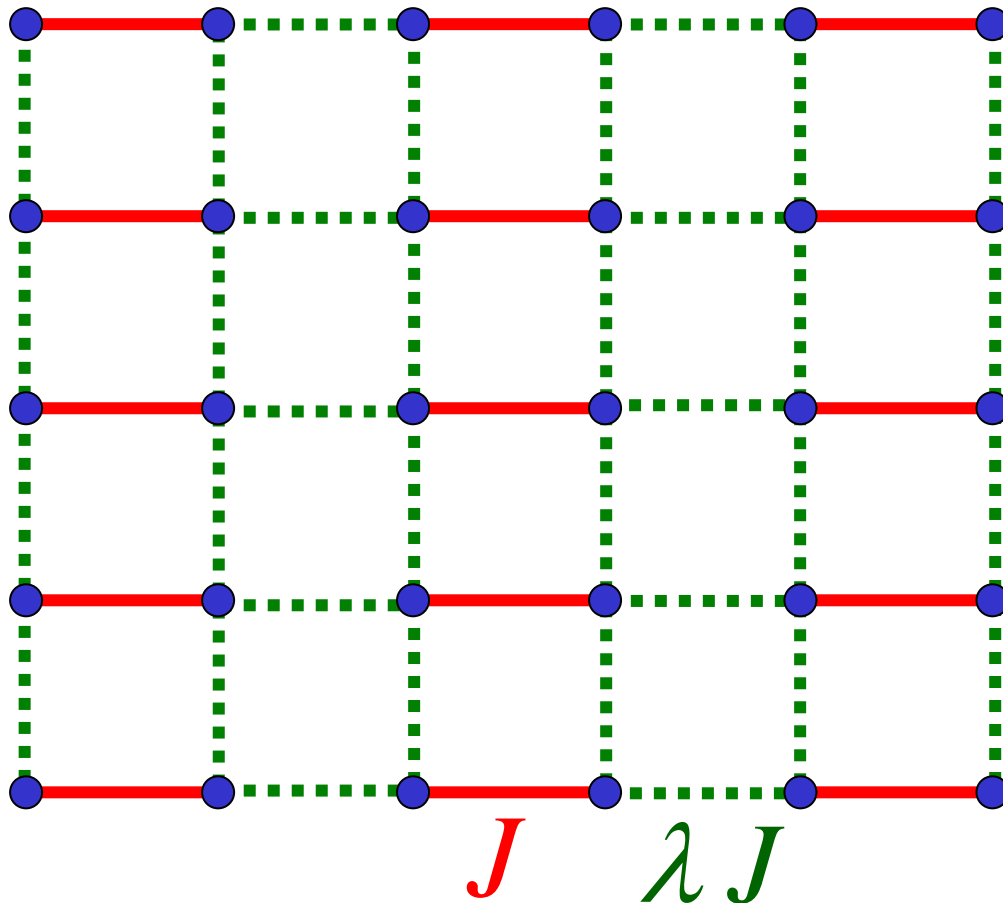
M. P. Gelfand, R. R. P. Singh, and D. A. Huse, *Phys. Rev. B* **40**, 10801-10809 (1989).

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).

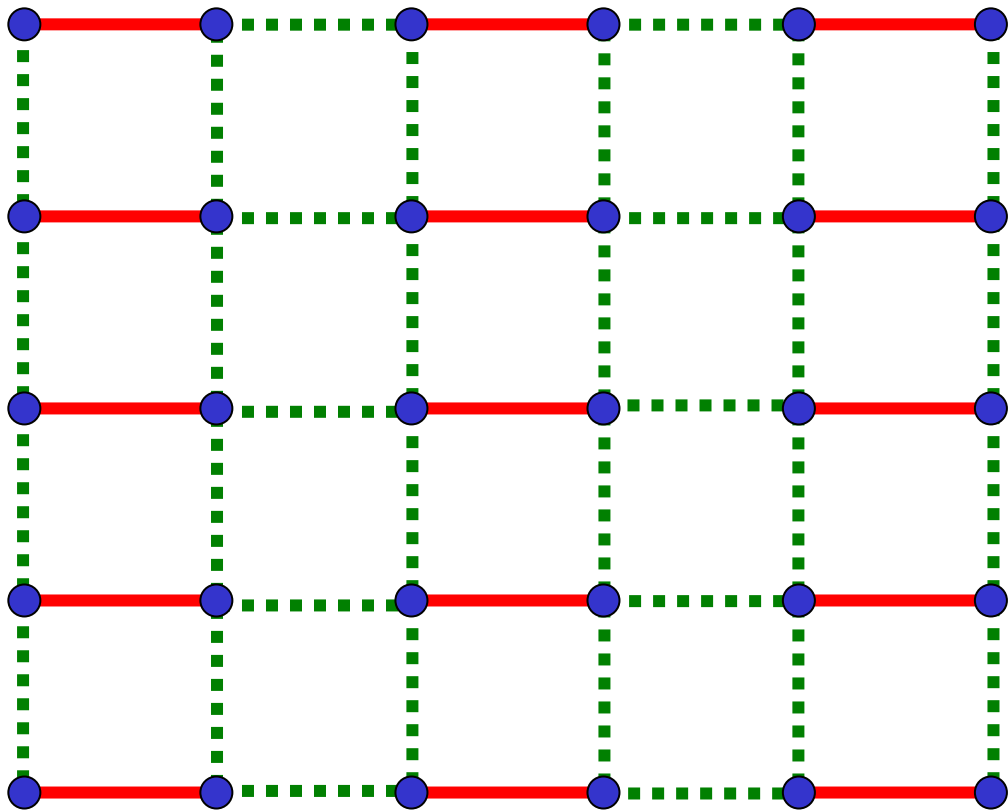
M. Matsumoto, C. Yasuda, S. Todo, and H. Takayama, *Phys. Rev. B* **65**, 014407 (2002).

$S=1/2$  spins on coupled dimers



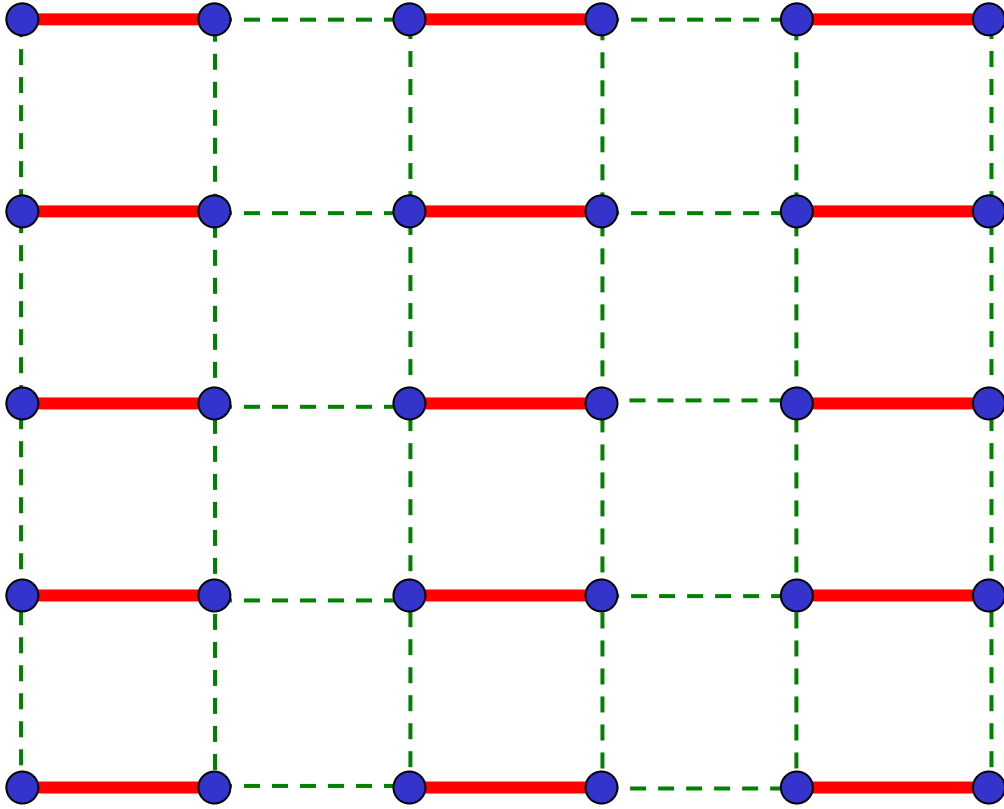
$$H = \sum_{\langle ij \rangle} J_{ij} \vec{S}_i \cdot \vec{S}_j$$

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



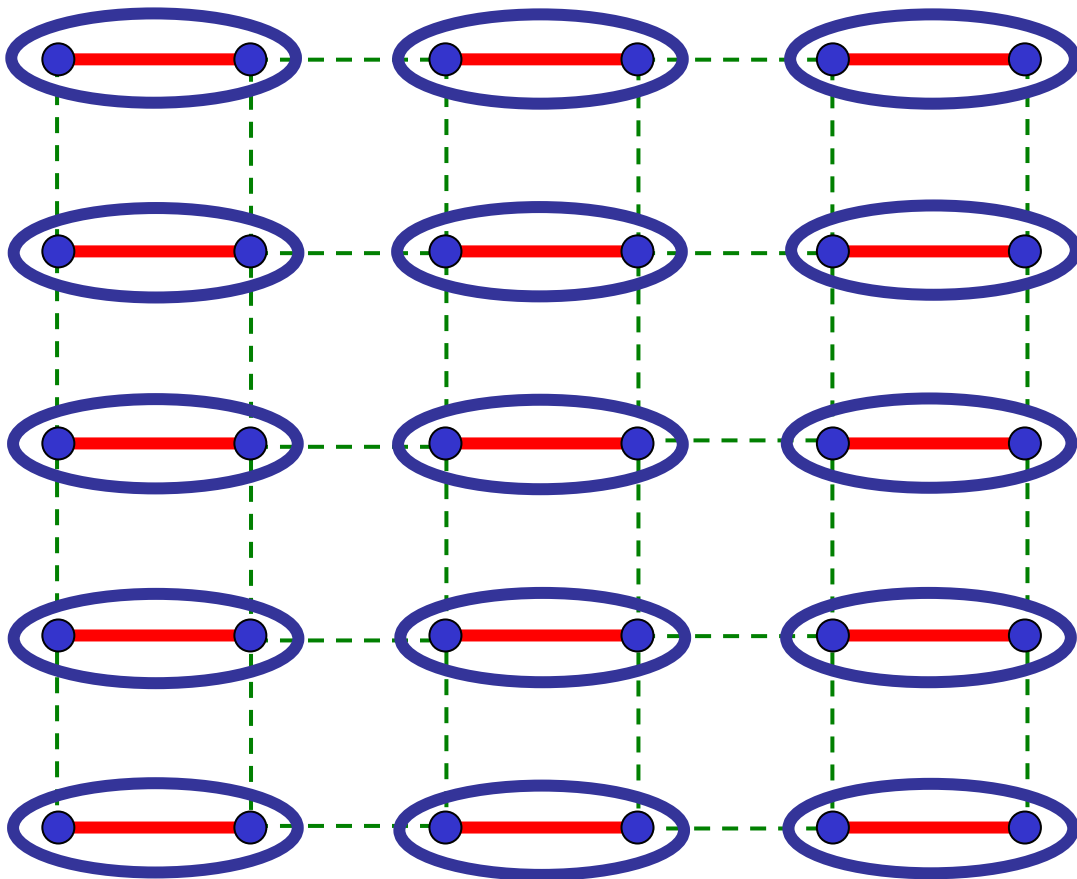
$\lambda$  close to 0

Weakly coupled dimers



$\lambda$  close to 0

Weakly coupled dimers



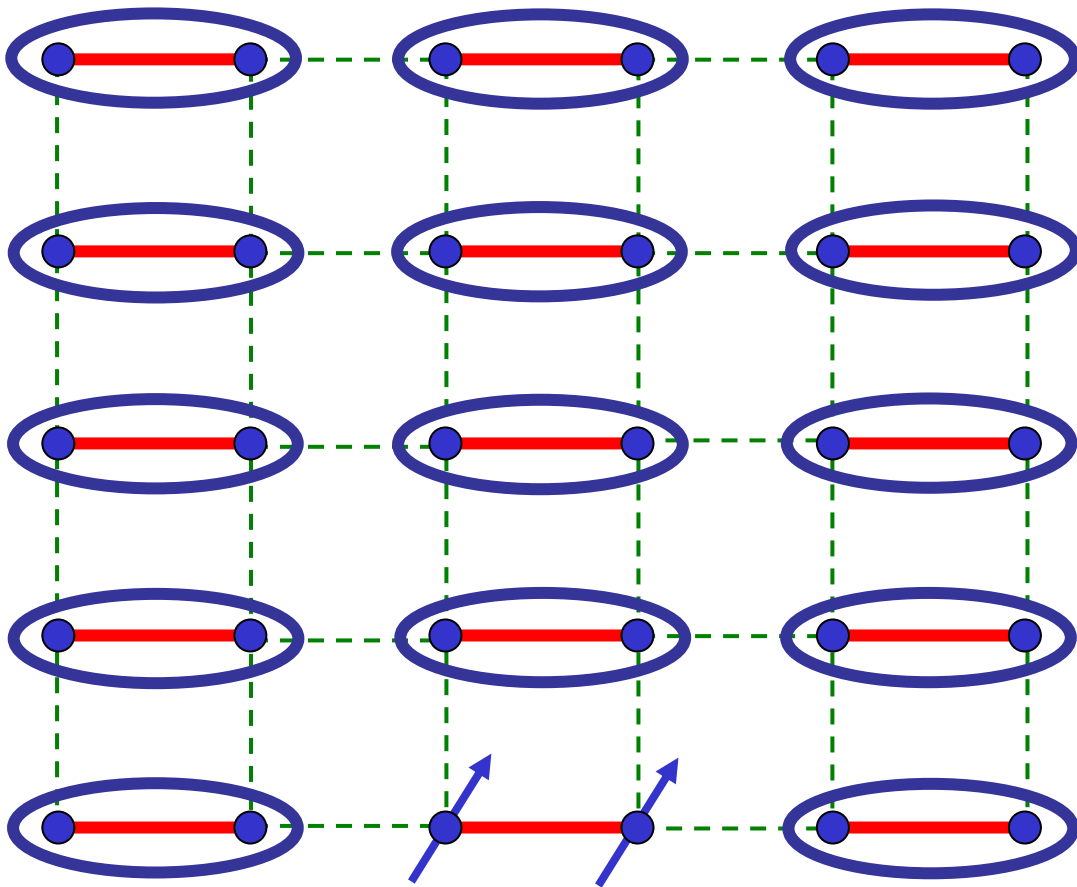
$$\text{dimer} = \frac{1}{\sqrt{2}} (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$$

Paramagnetic ground state

$$\langle \vec{S}_i \rangle = 0, \quad \langle \vec{\phi} \rangle = 0$$

$\lambda$  close to 0

Weakly coupled dimers

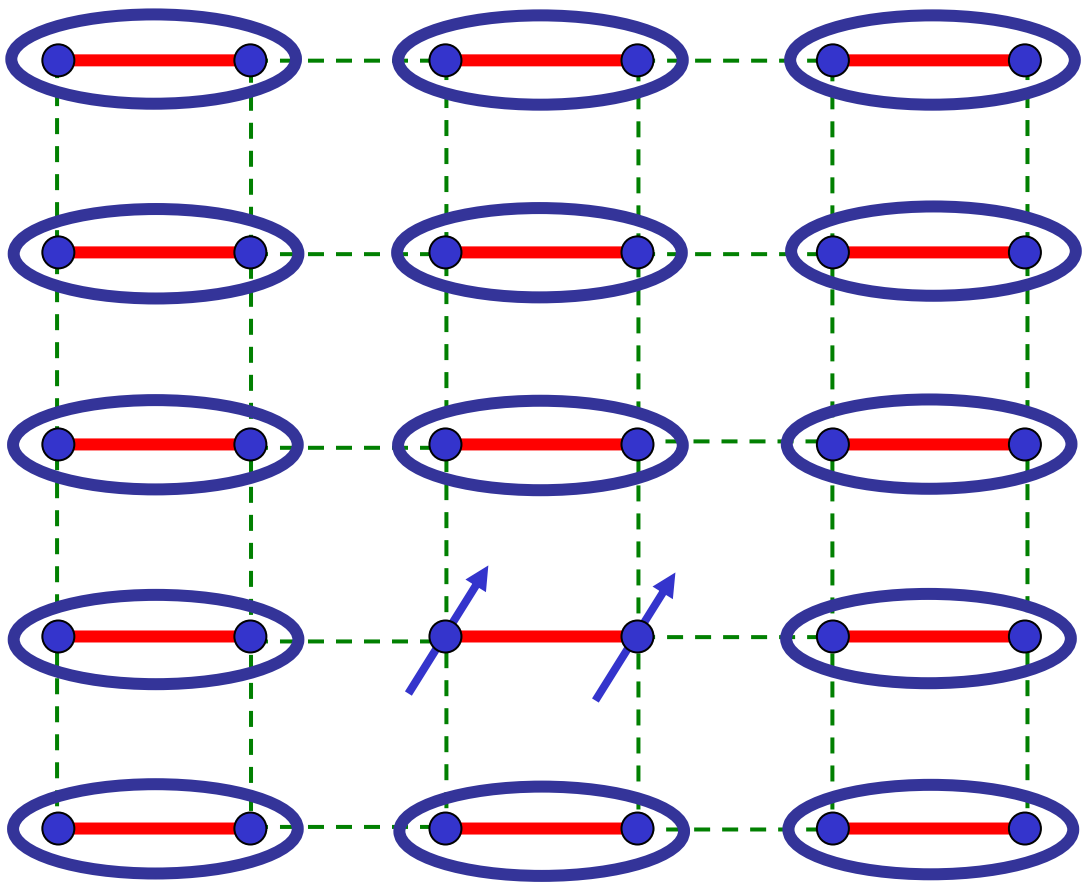


$$\text{dimer} = \frac{1}{\sqrt{2}} (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$$

Excitation:  $S=1$  *triplon*

$\lambda$  close to 0

Weakly coupled dimers

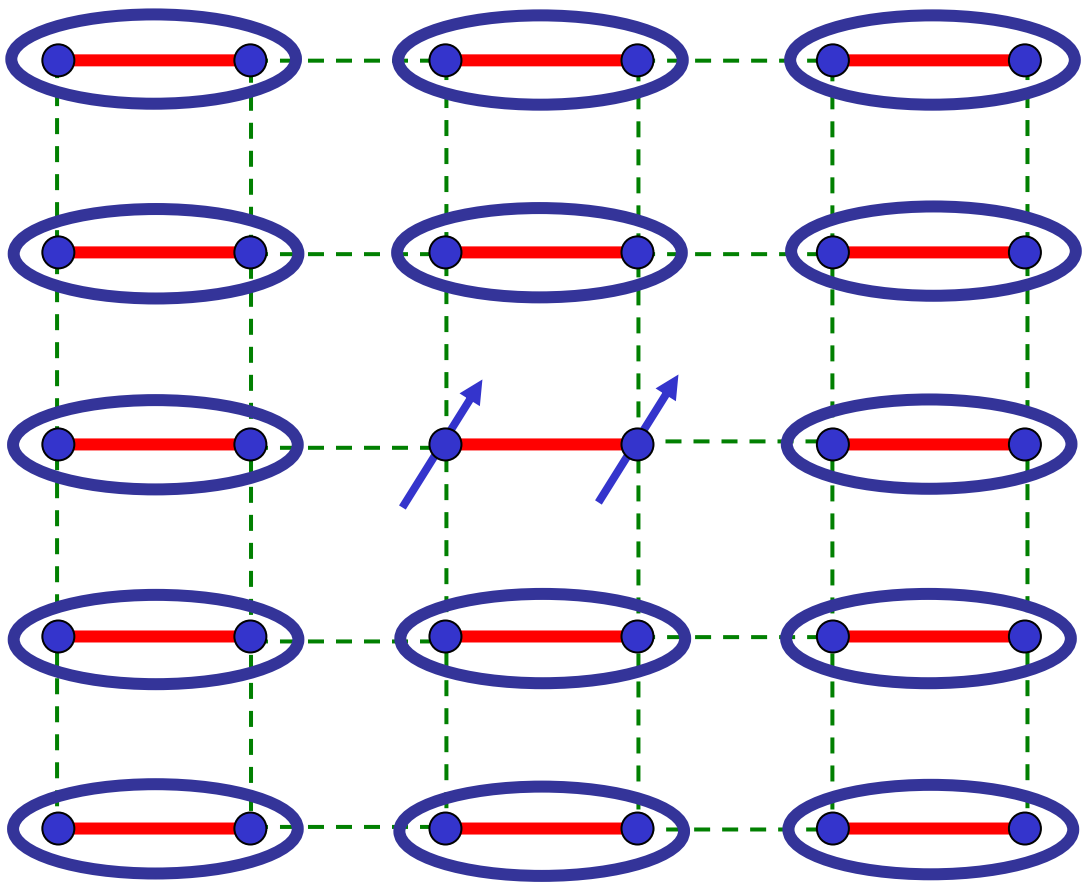


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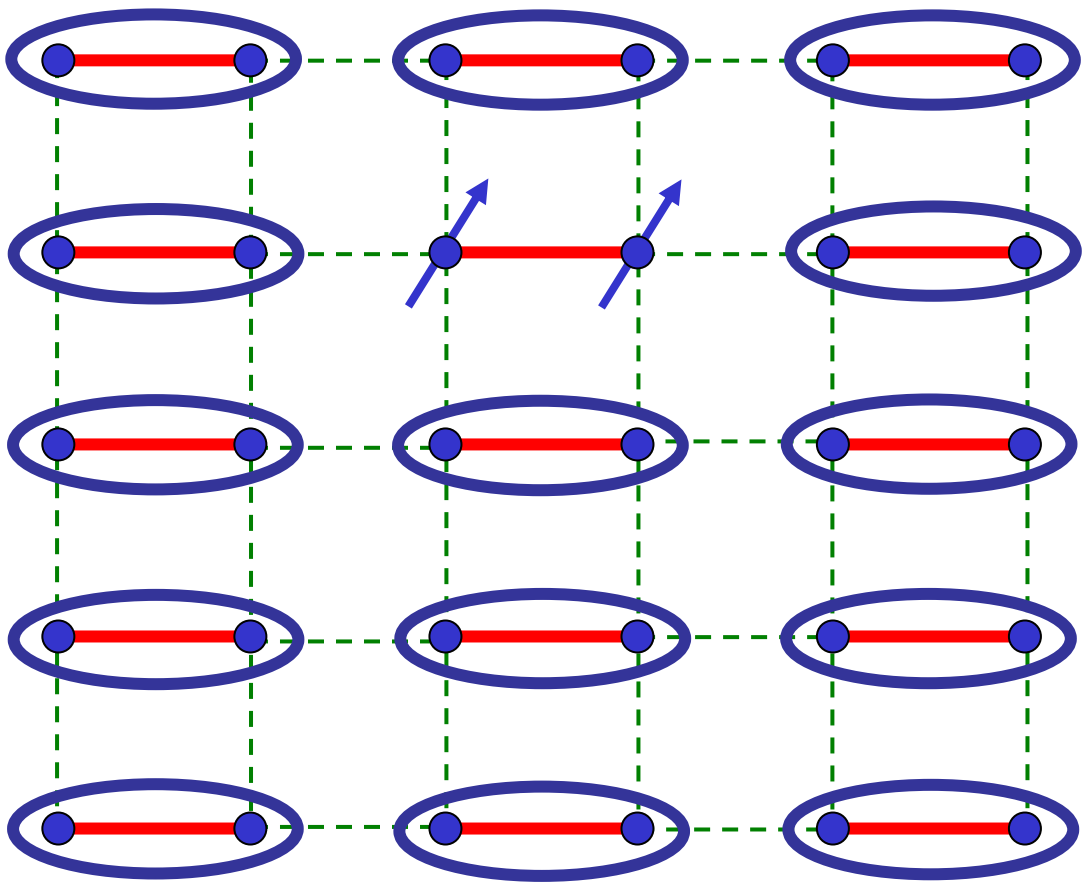


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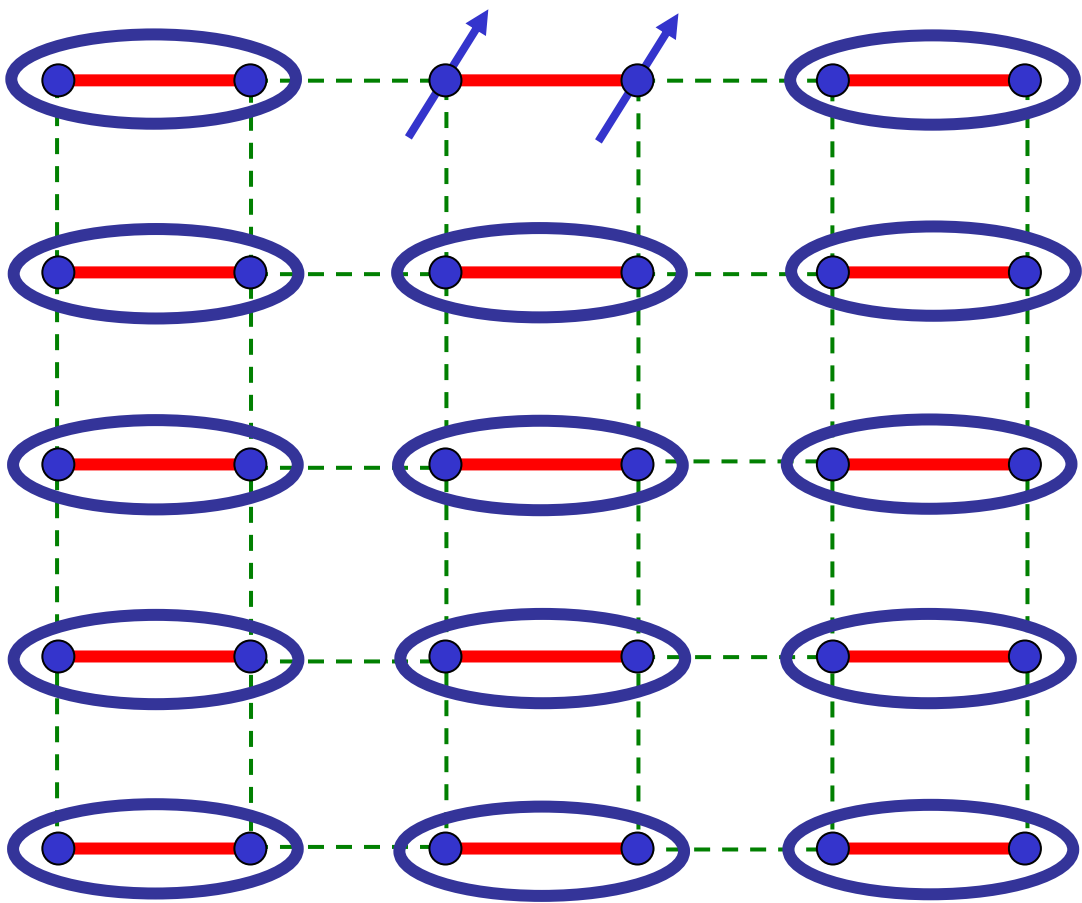
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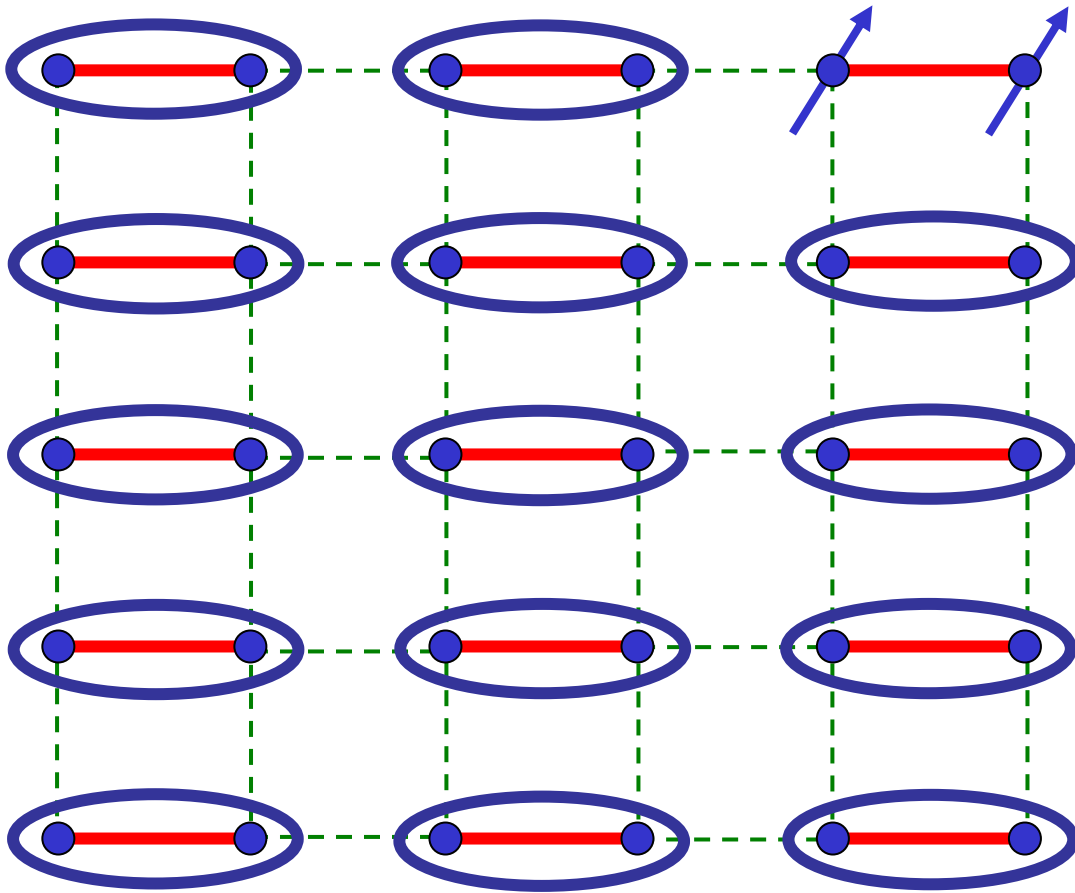


$$\text{Dimer} = \frac{1}{\sqrt{2}} (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$$

Excitation:  $S=1$  *triplon*

$\lambda$  close to 0

Weakly coupled dimers



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

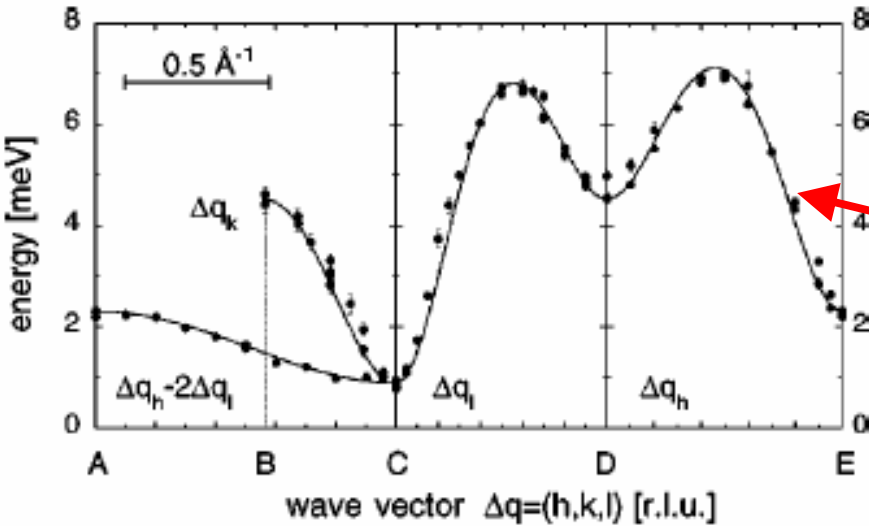
Excitation:  $S=1$  *triplon*  
(*exciton*, spin collective mode)

Energy dispersion away from  
antiferromagnetic wavevector

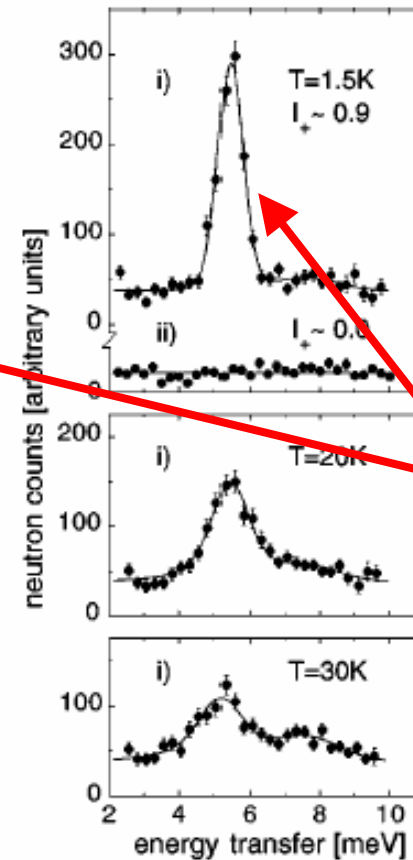
$$\varepsilon_p = \Delta + \frac{c_x^2 p_x^2 + c_y^2 p_y^2}{2\Delta}$$

$\Delta \rightarrow$  spin gap

# TlCuCl<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 TlCuCl<sub>3</sub> for  $i=(1.35,0,0)$ ,  $ii=(0,0,3.15)$  [r.l.u.]. The spectrum at  $T=1.5$  K

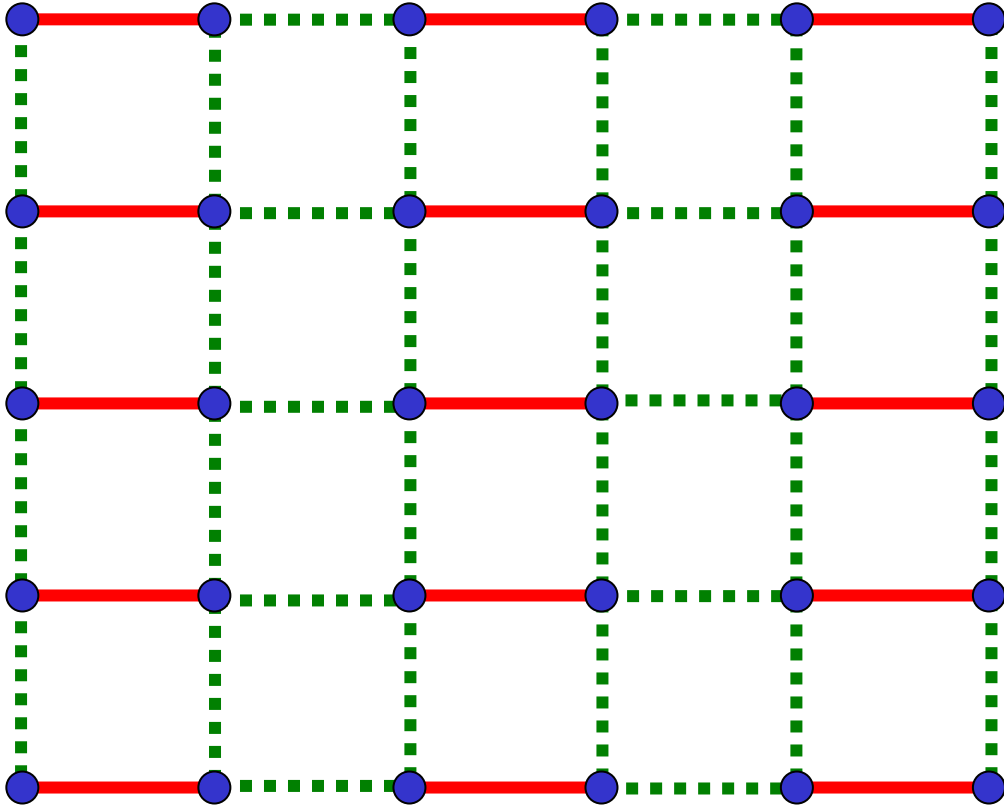
For quasi-one-dimensional systems, the triplon linewidth takes

the exact universal value  $= 1.20k_B T e^{-\Delta/k_B T}$  at low T

K. Damle and S. Sachdev, *Phys. Rev. B* **57**, 8307 (1998)

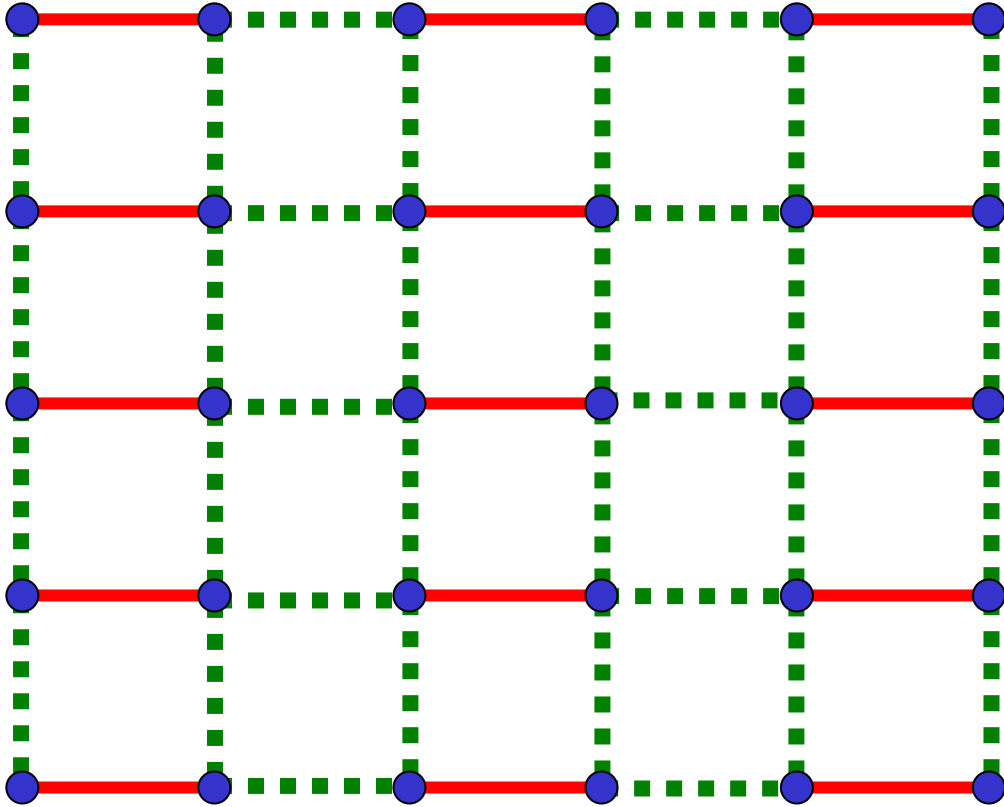
This result is in good agreement with observations in CsNiCl<sub>3</sub> (M. Kenzelmann, R. A. Cowley, W. J. L. Buyers, R. Coldea, M. Enderle, and D. F. McMorrow *Phys. Rev. B* **66**, 174412 (2002)) and Y<sub>2</sub>NiBaO<sub>5</sub> (G. Xu, C. Broholm, G. Aeppli, J. F. DiTusa, T. Ito, K. Oka, and H. Takagi, preprint).

# Coupled Dimer Antiferromagnet



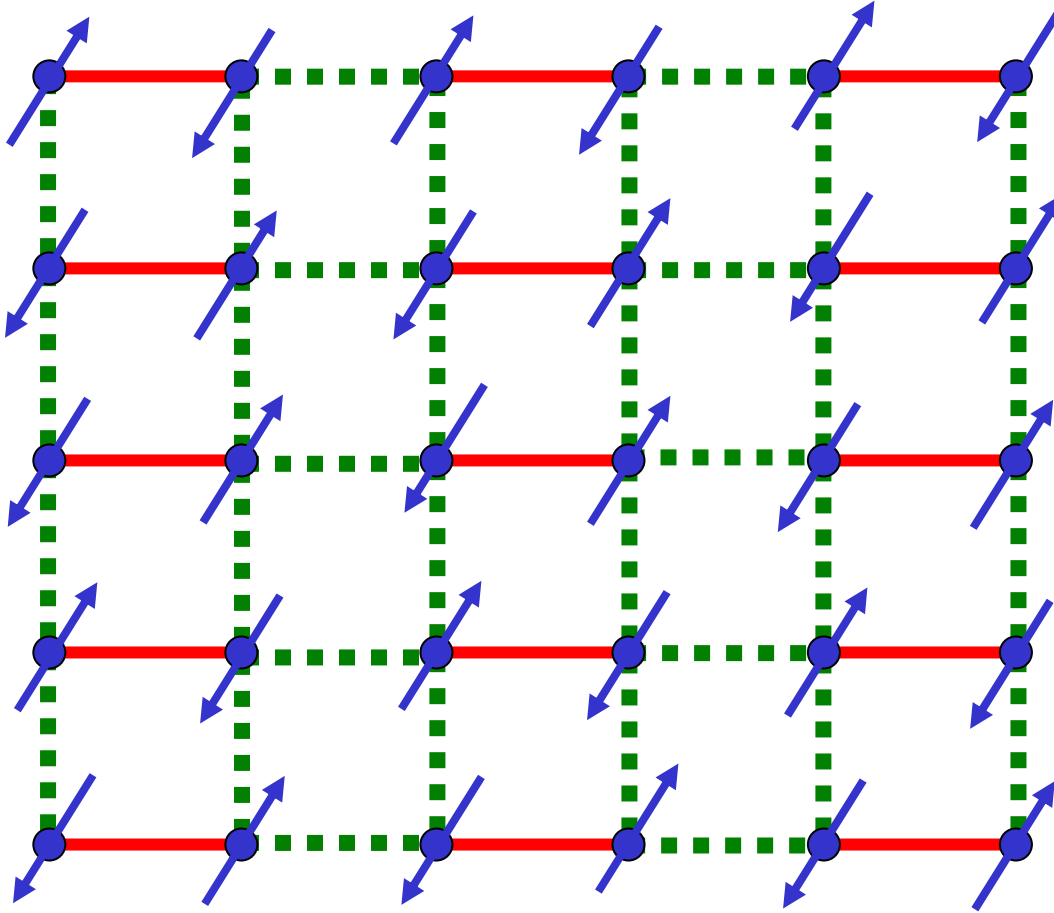
$\lambda$  close to 1

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>

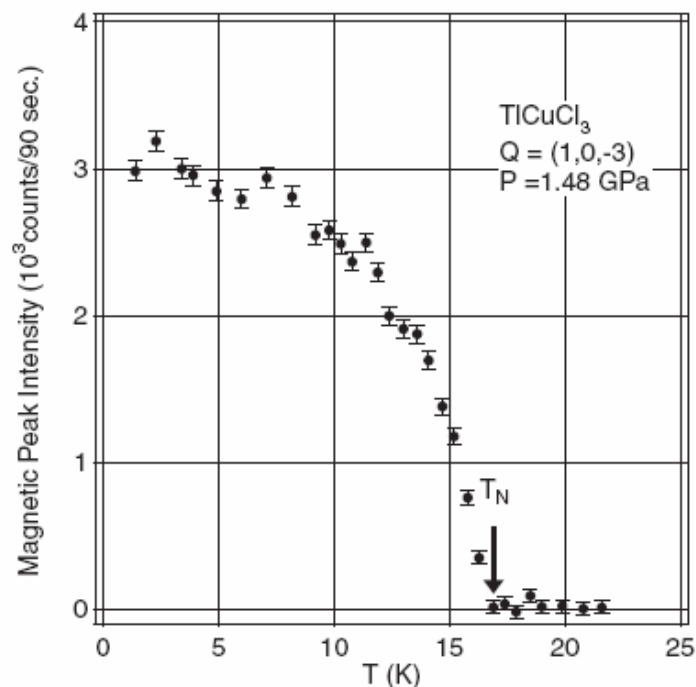
Akira OOSAWA\*, Masashi FUJISAWA<sup>1</sup>, Toyotaka OSAKABE, Kazuhisa KAKURAI and Hidekazu TANAKA<sup>2</sup>

*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)



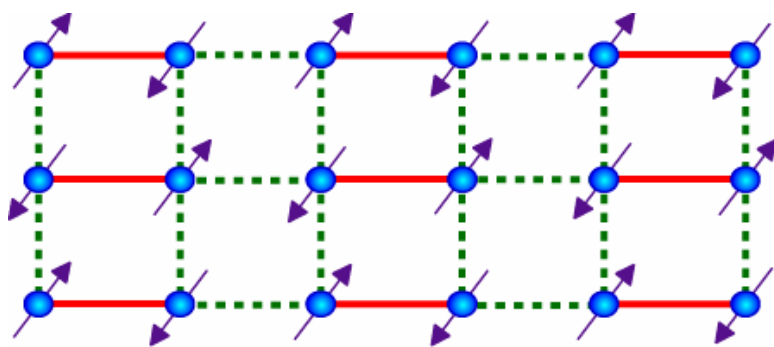
*J. Phys. Soc. Jpn* **72**, 1026 (2003)

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>.

$T=0$

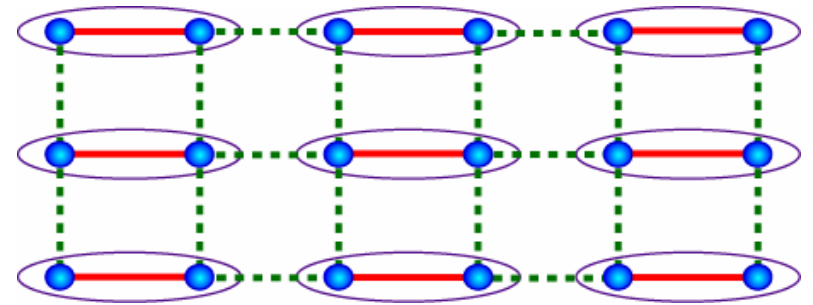
$$\lambda_c = 0.52337(3)$$

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

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



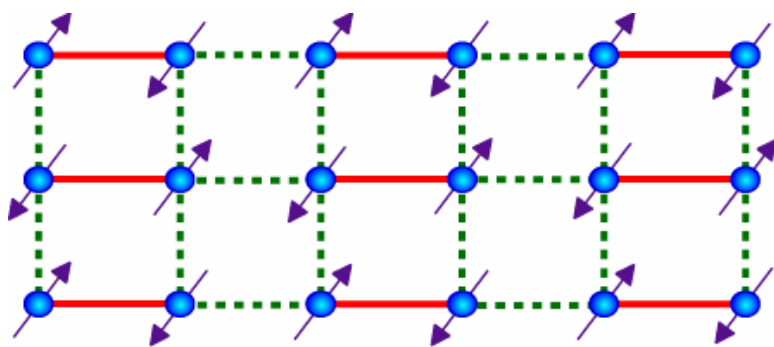
The method of bond operators (S. Sachdev and R.N. Bhatt, *Phys. Rev. B* **41**, 9323 (1990)) provides a quantitative description of spin excitations in  $\text{TlCuCl}_3$  across the quantum phase transition (M. Matsumoto, B. Normand, T.M. Rice, and M. Sigrist, *Phys. Rev. Lett.* **89**, 077203 (2002))



T=0

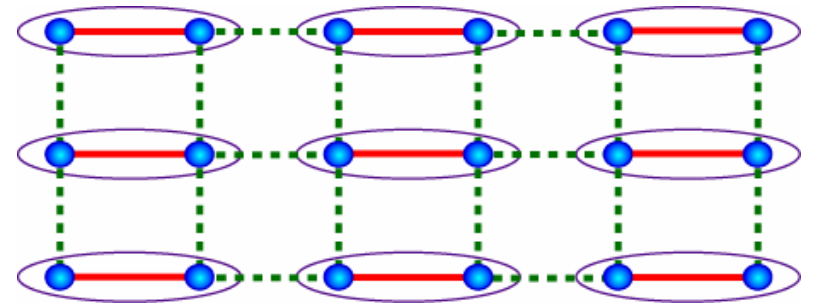
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Néel state

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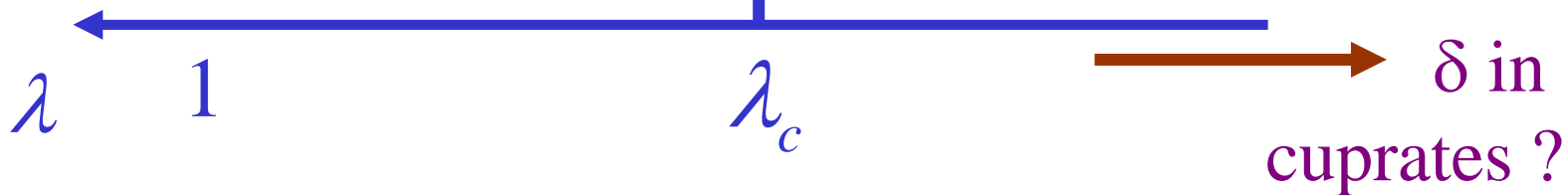


Quantum paramagnet

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

Magnetic order as in  $\text{La}_2\text{CuO}_4$

Electrons in charge-localized Cooper pairs



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# LGW theory for quantum criticality

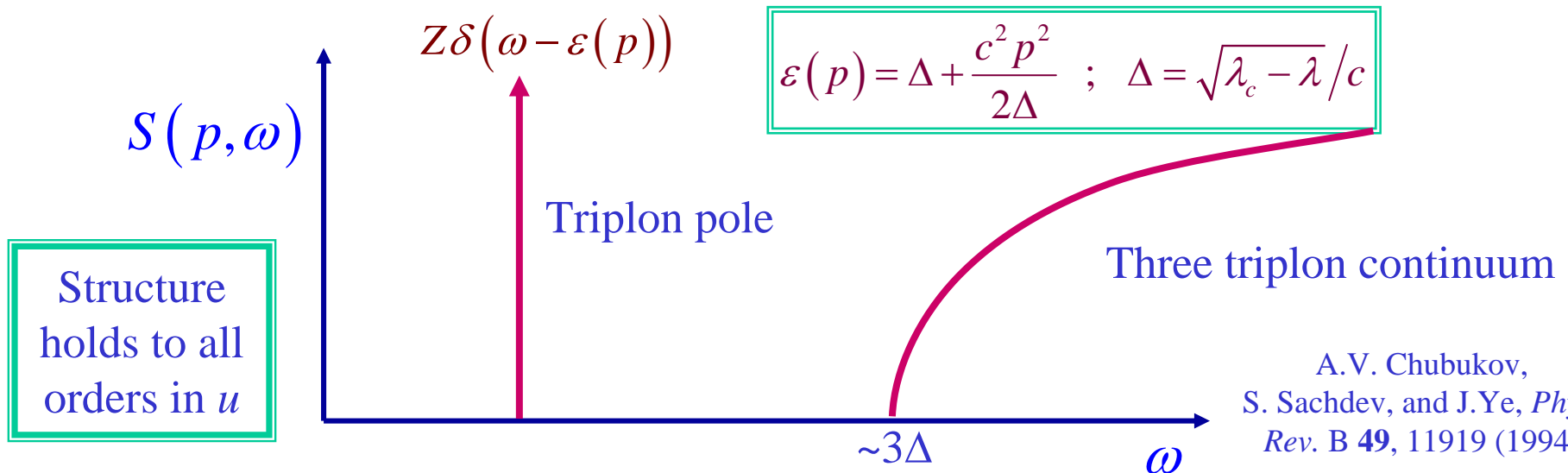
Landau-Ginzburg-Wilson theory: write down an effective action for the antiferromagnetic order parameter  $\vec{\varphi}$  by expanding in powers of  $\vec{\varphi}$  and its spatial and temporal derivatives, while preserving all symmetries of the microscopic Hamiltonian

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

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

For  $\lambda < \lambda_c$  oscillations of  $\vec{\varphi}$  about  $\vec{\varphi} = 0$  lead to the

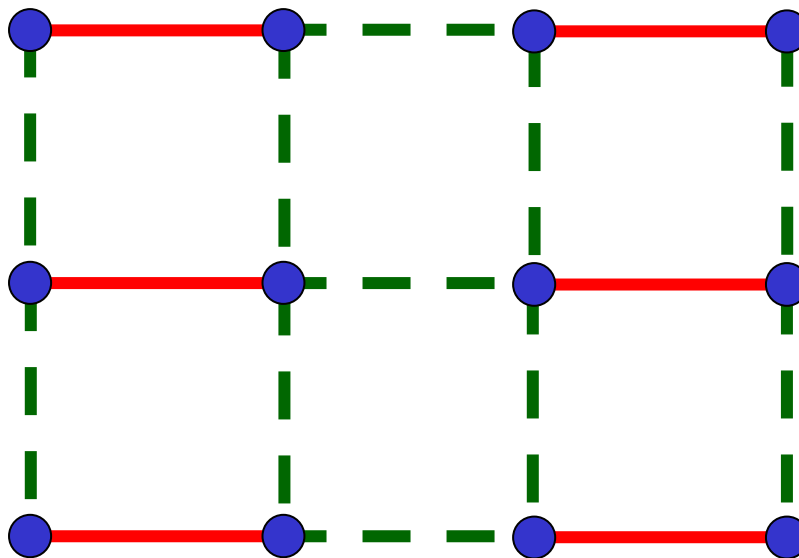
following structure in the dynamic structure factor  $S(p, \omega)$



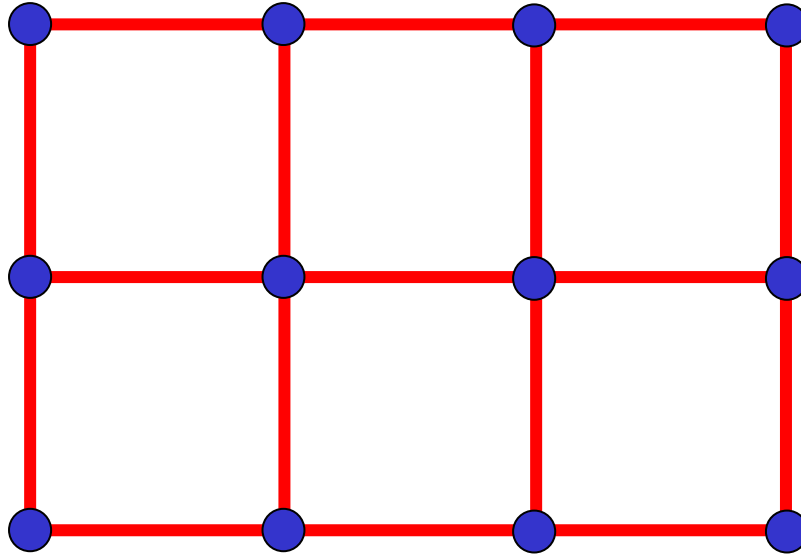
B. Mott insulators with  
spin  $S=1/2$  per unit cell:

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

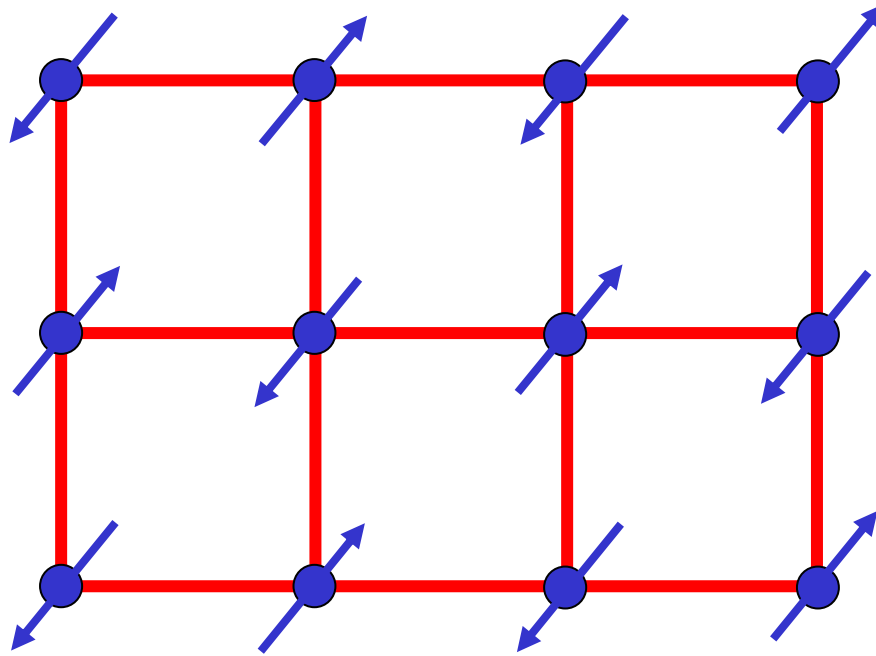
Mott insulator with two  $S=1/2$  spins per unit cell



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

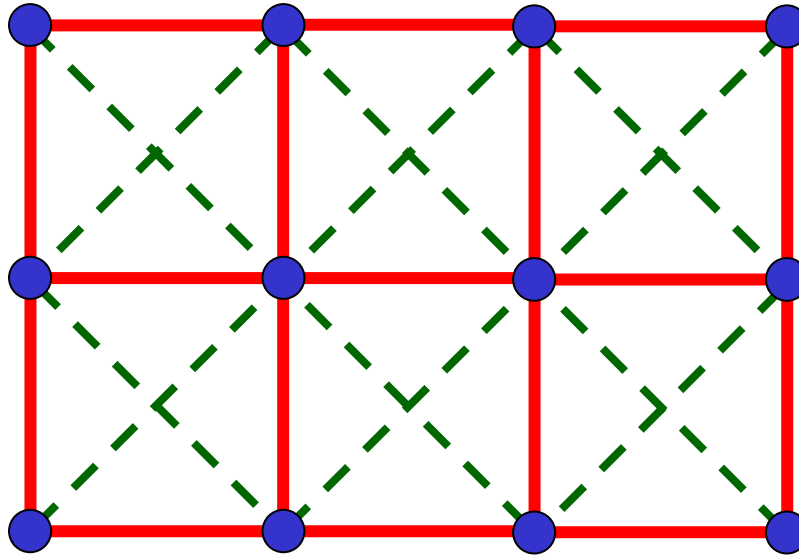


Mott insulator with one  $S=1/2$  spin per unit cell



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

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



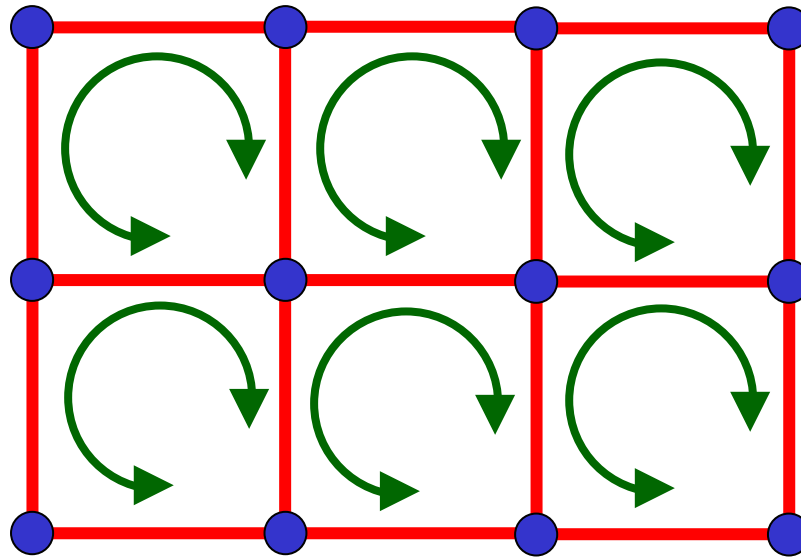
Destroy Neel order by perturbations which preserve full square lattice symmetry *e.g.* second-neighbor or ring exchange.

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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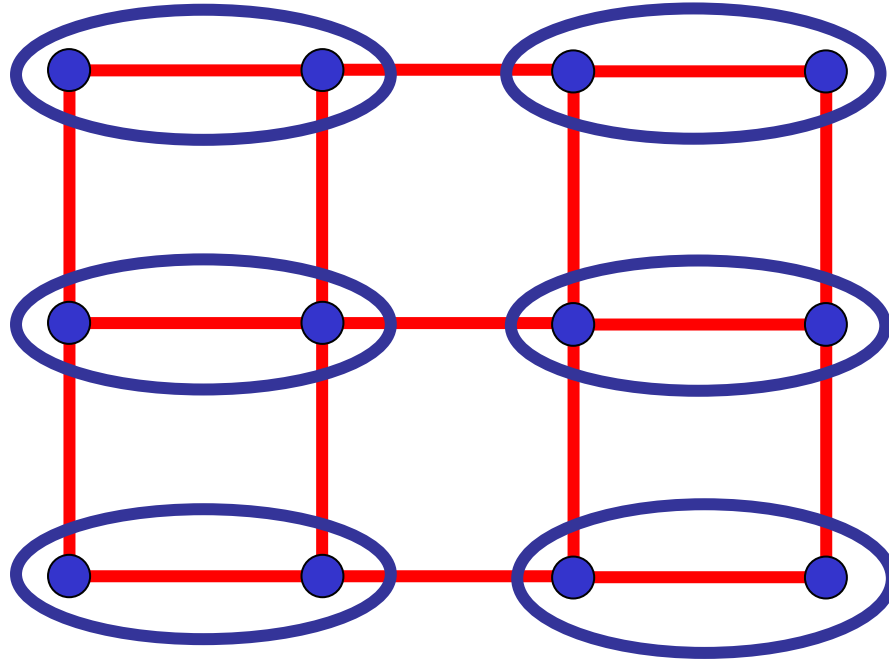
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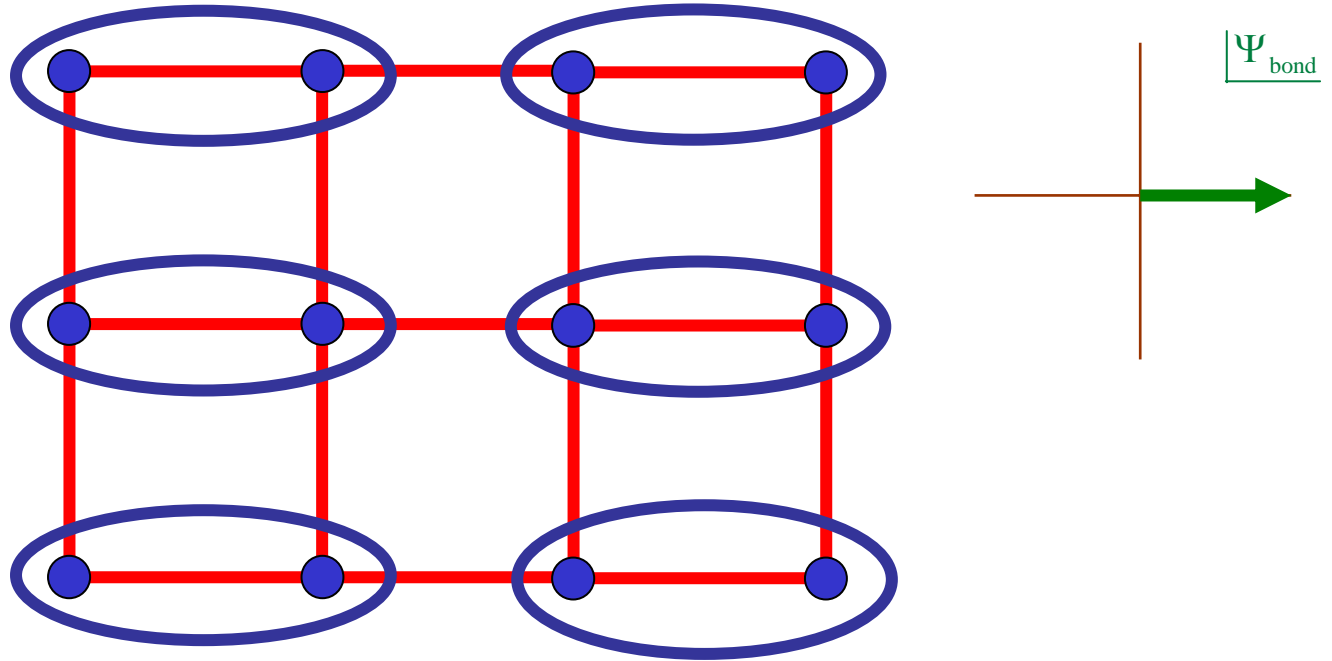


Mott insulator with one  $S=1/2$  spin per unit cell



Possible large  $g$  paramagnetic ground state (**Class A**) with  $\langle \vec{\phi} \rangle = 0$

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

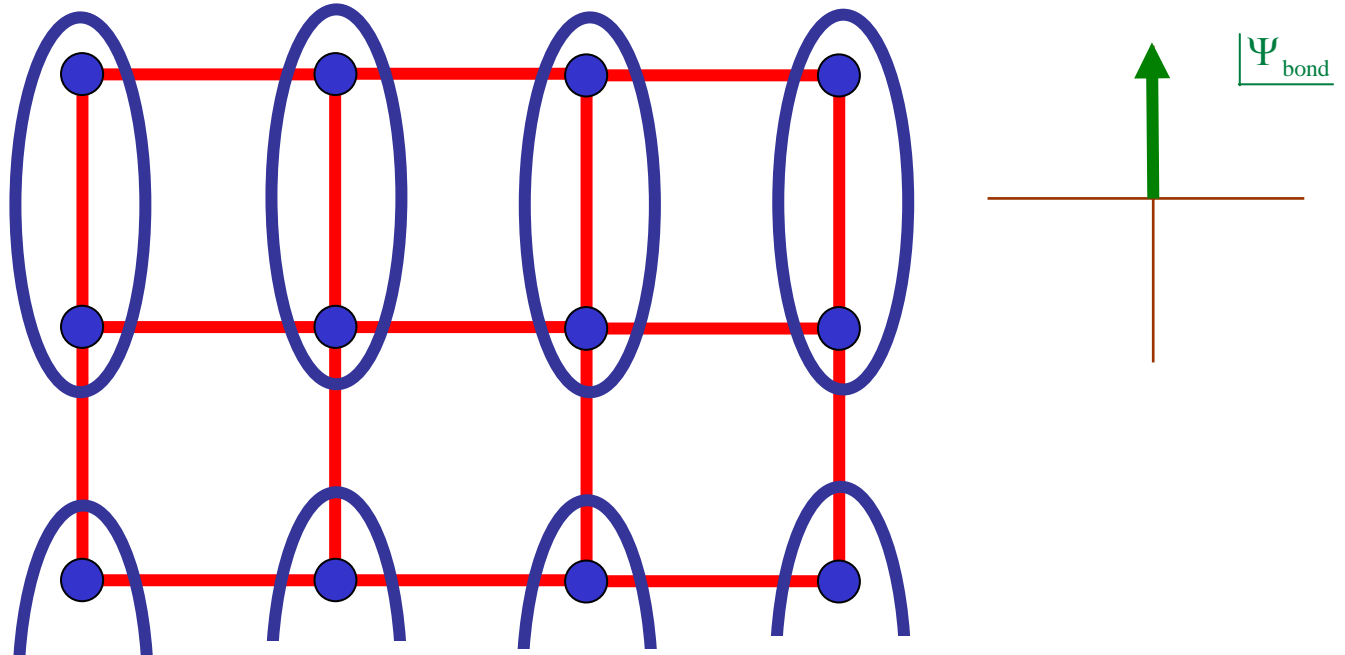


Possible large  $g$  paramagnetic ground state (**Class A**) with  $\langle \vec{\phi} \rangle = 0$

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

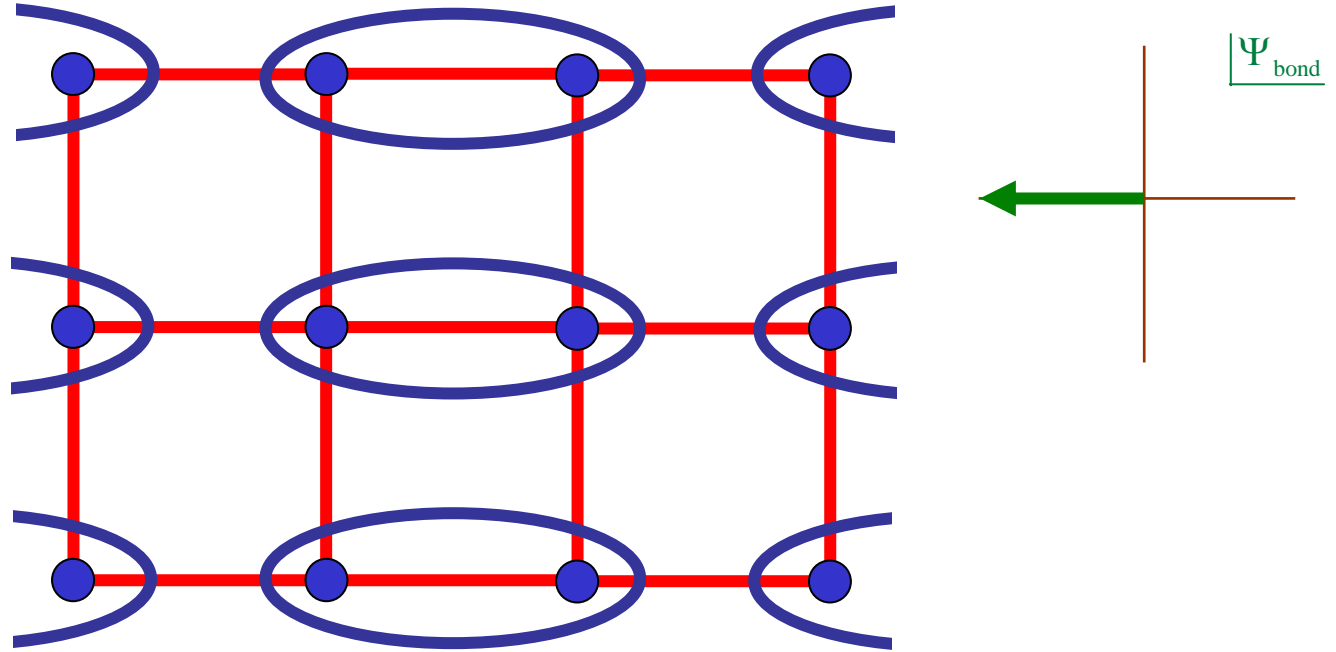


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## Mott insulator with one $S=1/2$ spin per unit cell

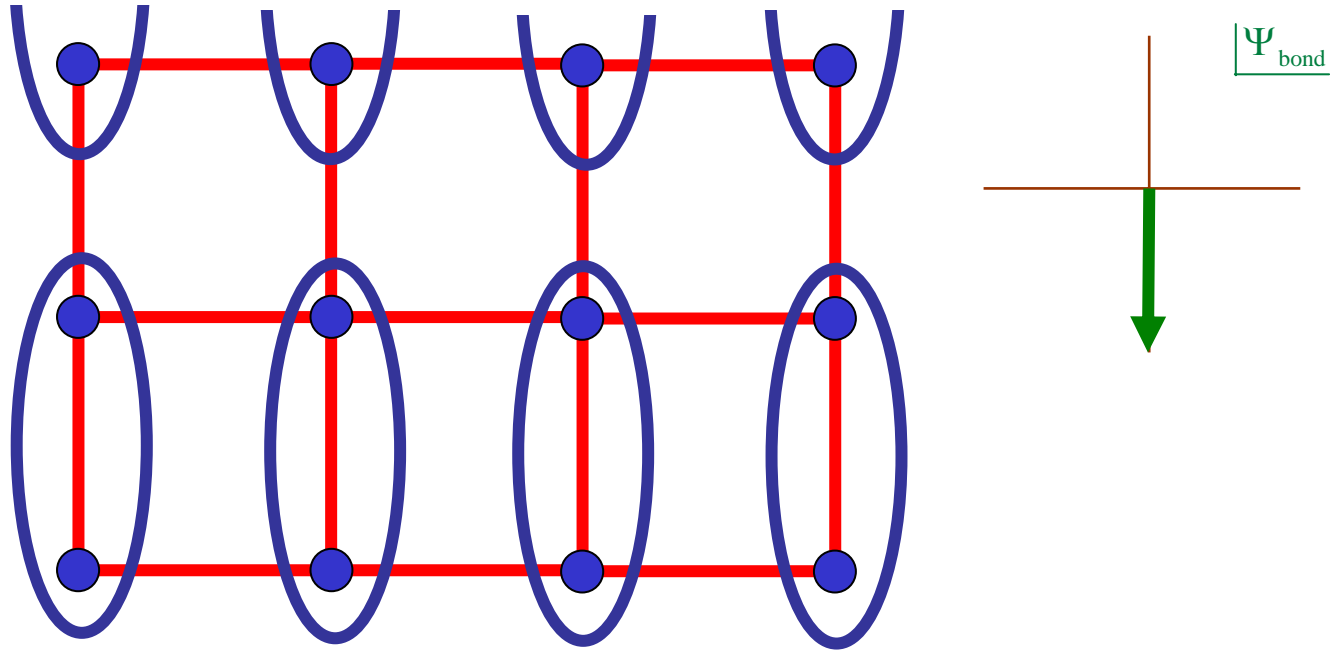


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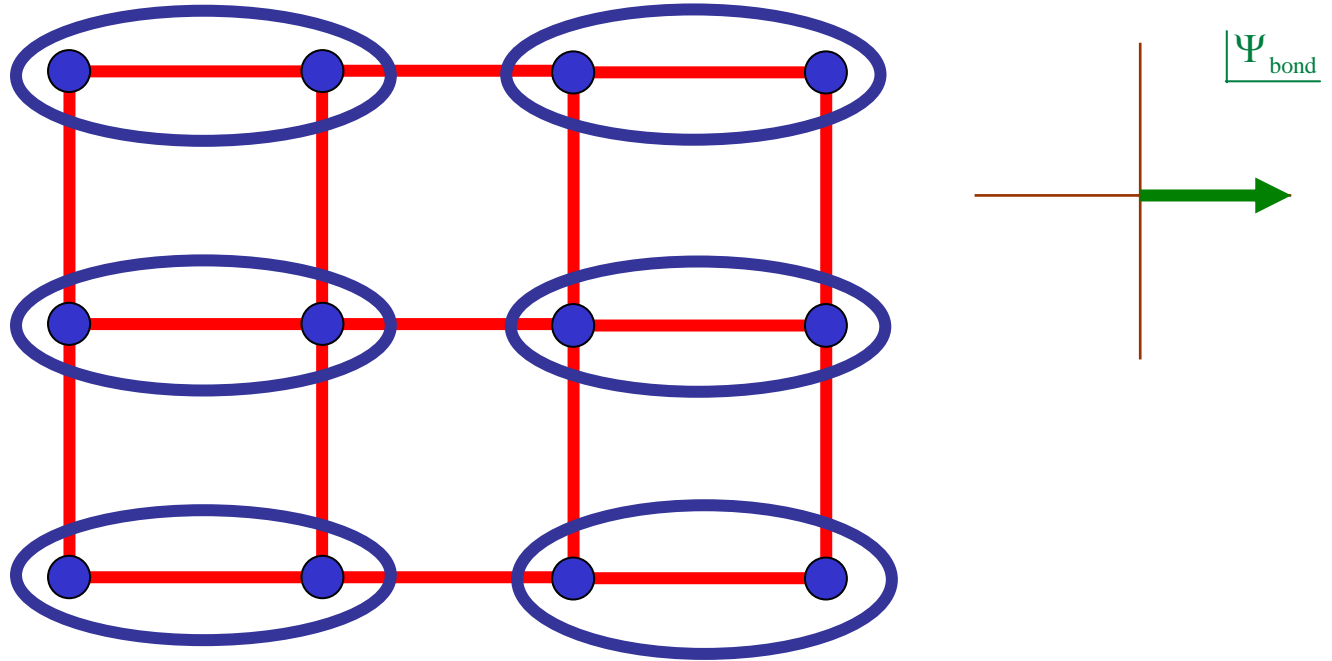


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## Mott insulator with one $S=1/2$ spin per unit cell

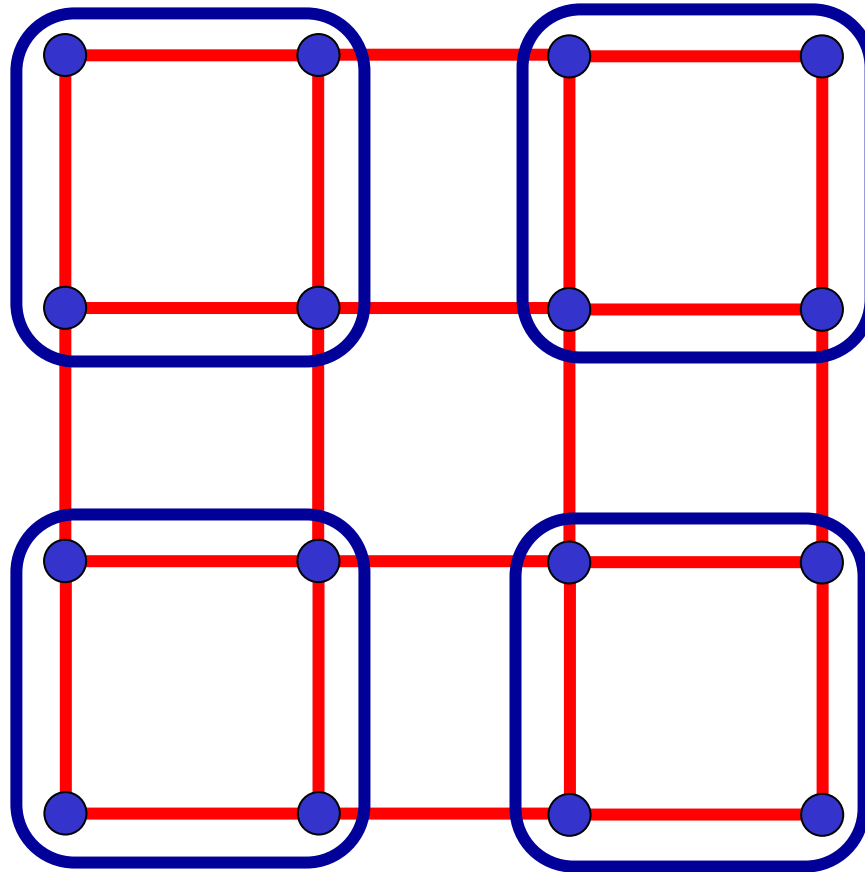


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$$\Psi_{\text{bond}}(i) = \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j e^{i \arctan(\mathbf{r}_j - \mathbf{r}_i)}$$

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

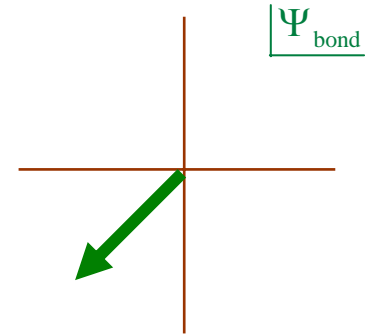
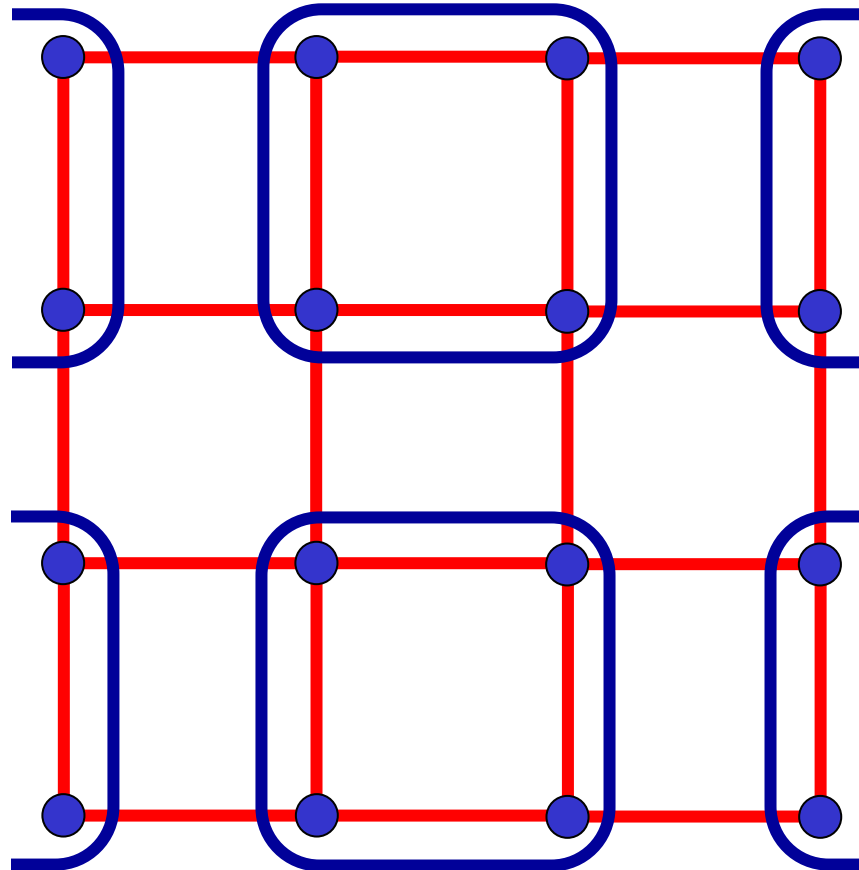


Possible large  $g$  paramagnetic ground state (**Class A**) with  $\langle \vec{\phi} \rangle = 0$

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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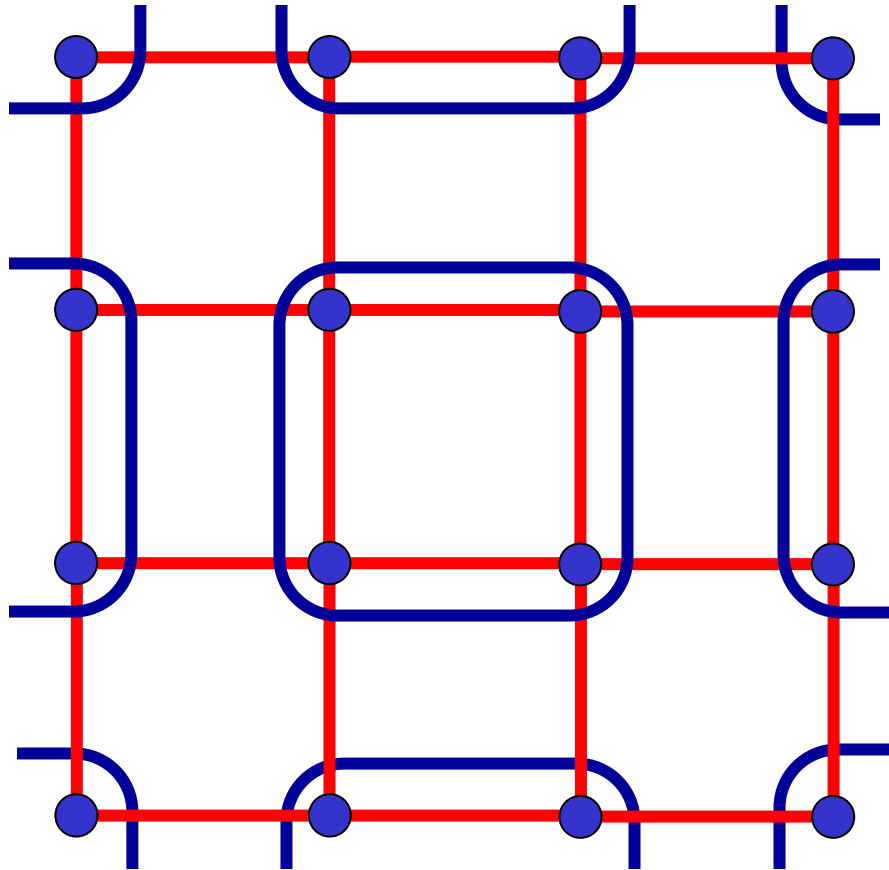
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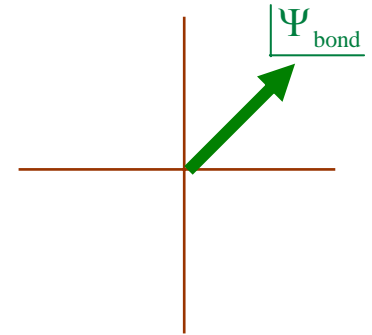
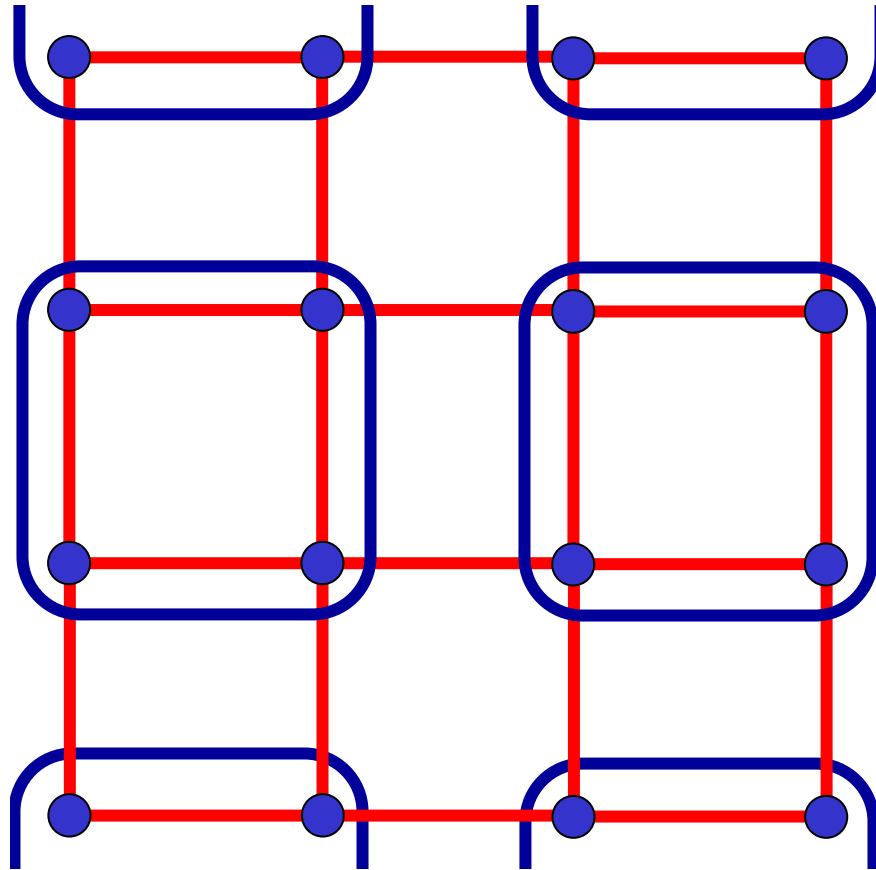


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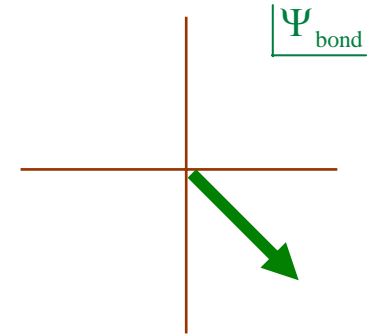
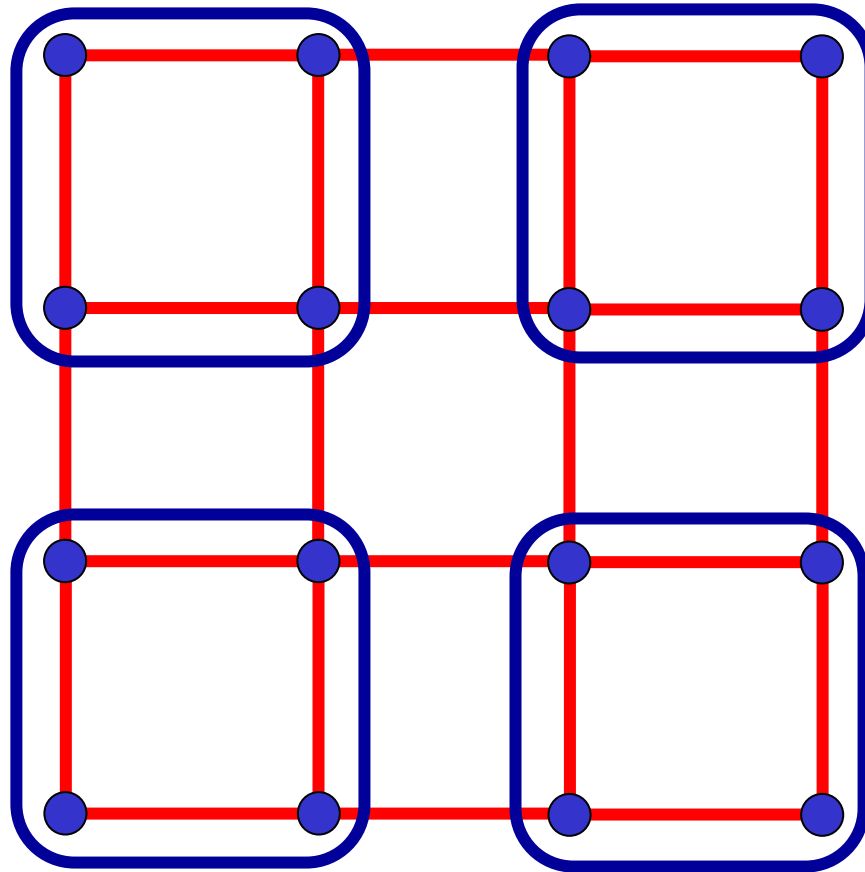


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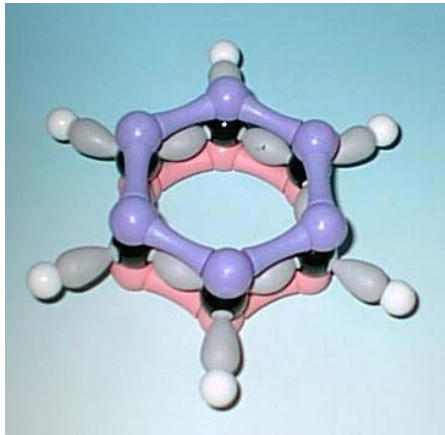
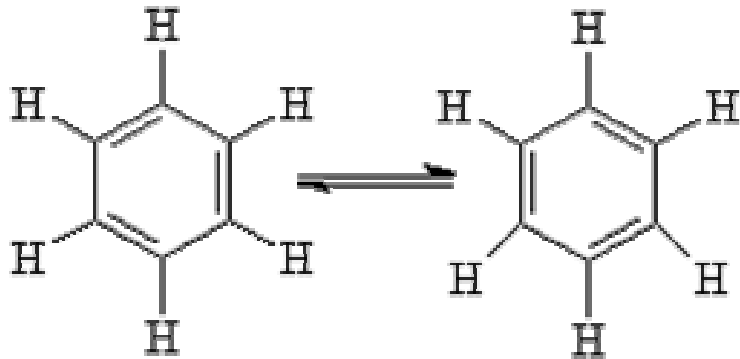


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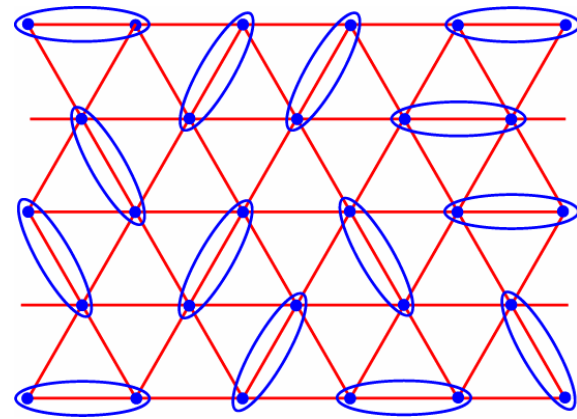
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# Resonating valence bonds



Resonance in benzene leads to a symmetric configuration of valence bonds  
(F. Kekulé, L. Pauling)



Different valence bond pairings resonate with each other, leading to a resonating valence bond *liquid*, (Class B paramagnet) with  $\langle \Psi_{\text{bond}} \rangle = 0$

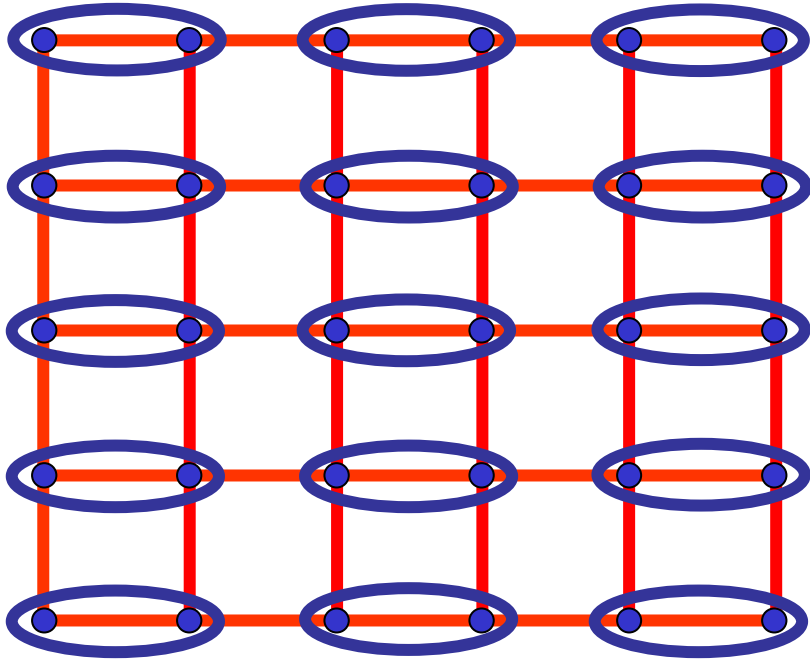
P. Fazekas and P.W. Anderson, *Phil Mag* **30**, 23 (1974); P.W. Anderson 1987

Such states are associated with non-collinear spin correlations,  $Z_2$  gauge theory, and topological order.

N. Read and S. Sachdev, *Phys. Rev. Lett.* **66**, 1773 (1991); X. G. Wen, *Phys. Rev. B* **44**, 2664 (1991).

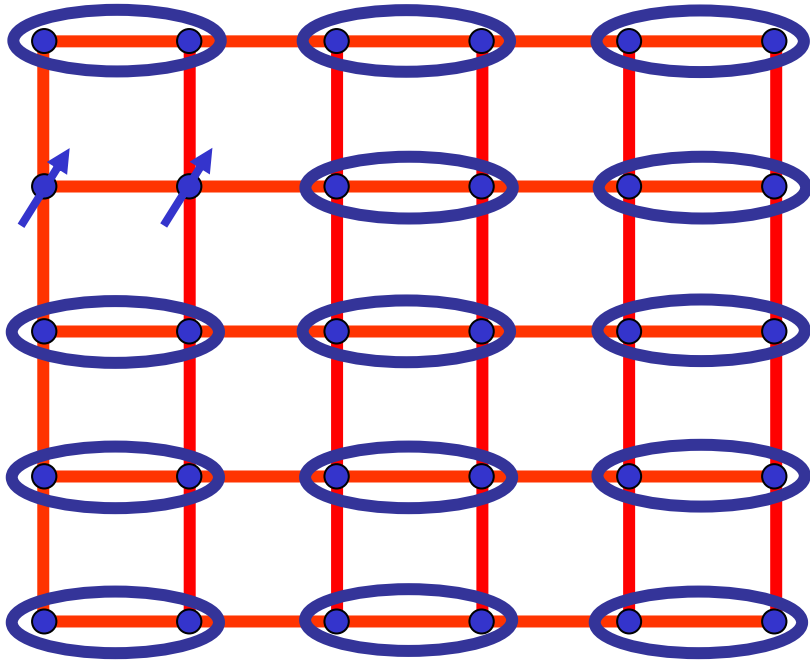
# Excitations of the paramagnet with non-zero spin

$\langle \Psi_{\text{bond}} \rangle \neq 0$ ; Class A



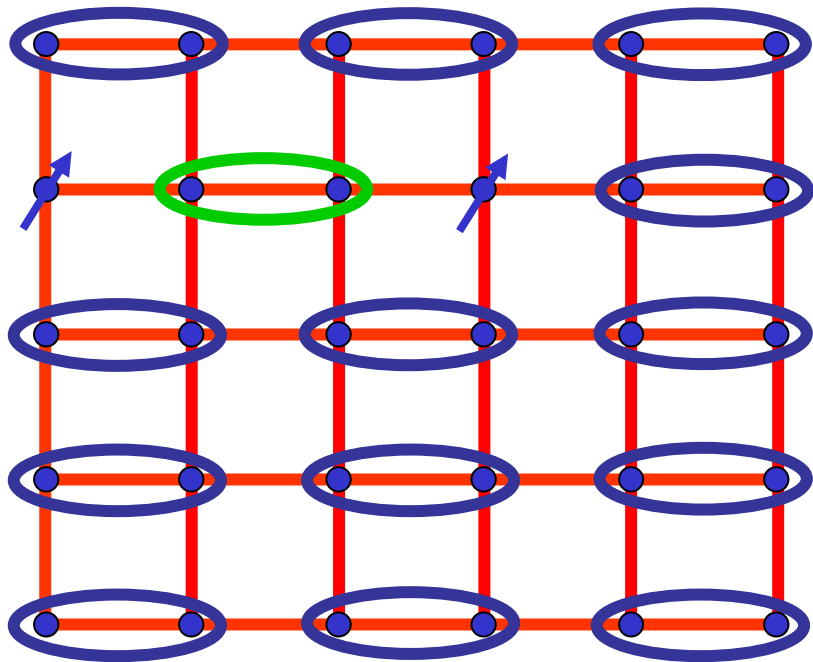
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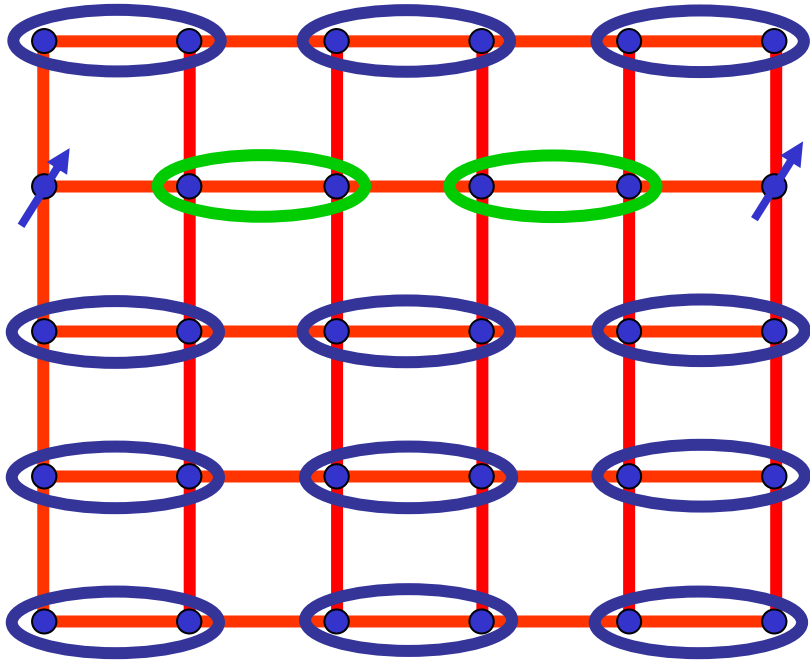
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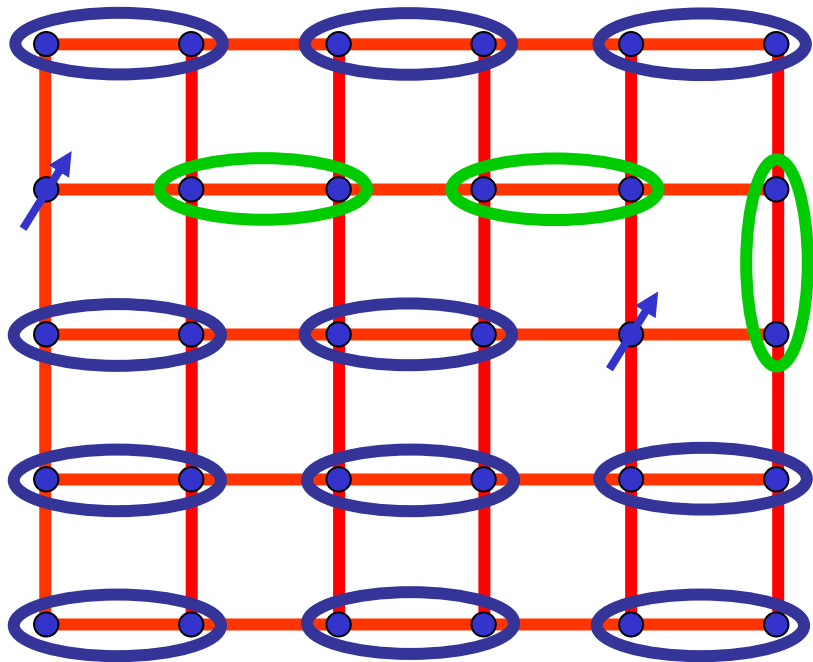
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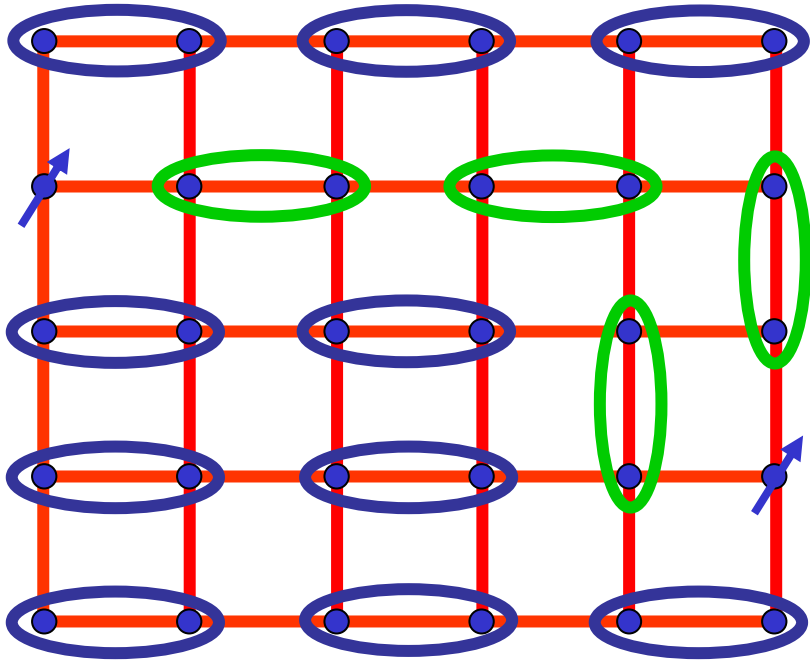
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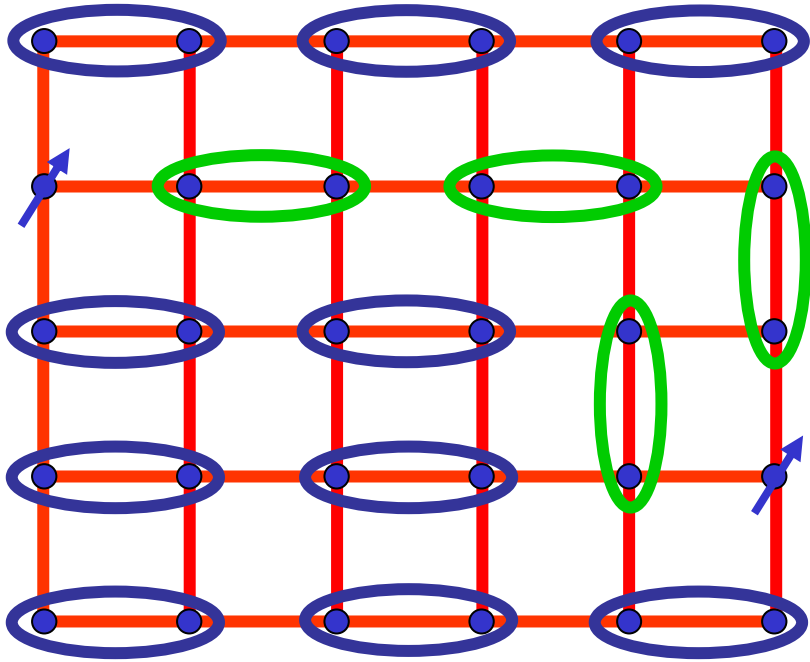


$S=1/2$  *spinons*,  $z_\alpha$ , are  
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*triplon*,  $\vec{\varphi}$

$$\vec{\varphi} \sim z_\alpha^* \vec{\sigma}_{\alpha\beta} z_\beta$$

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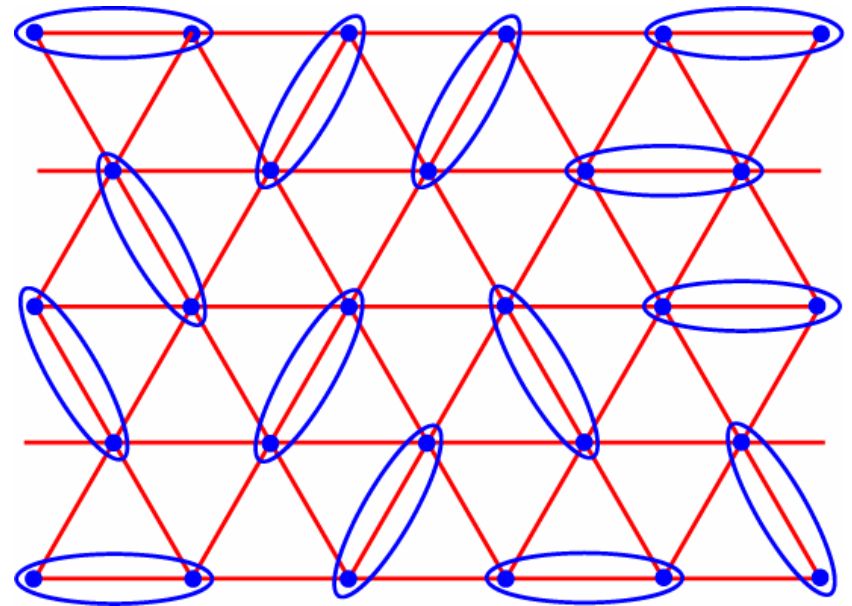
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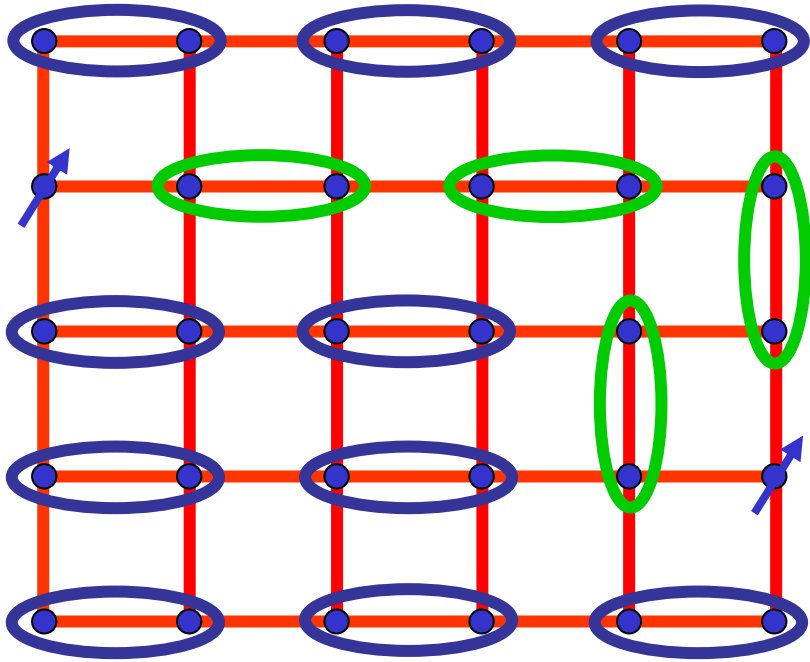
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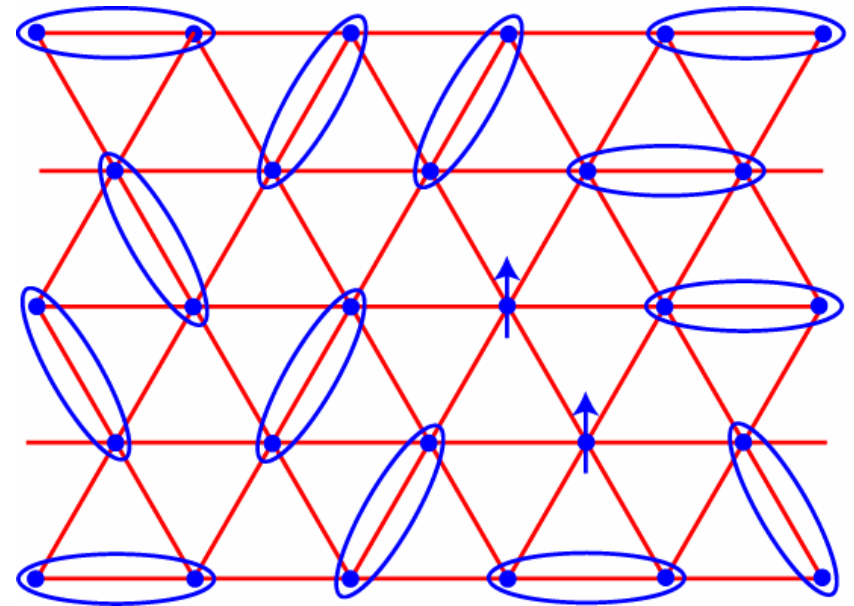
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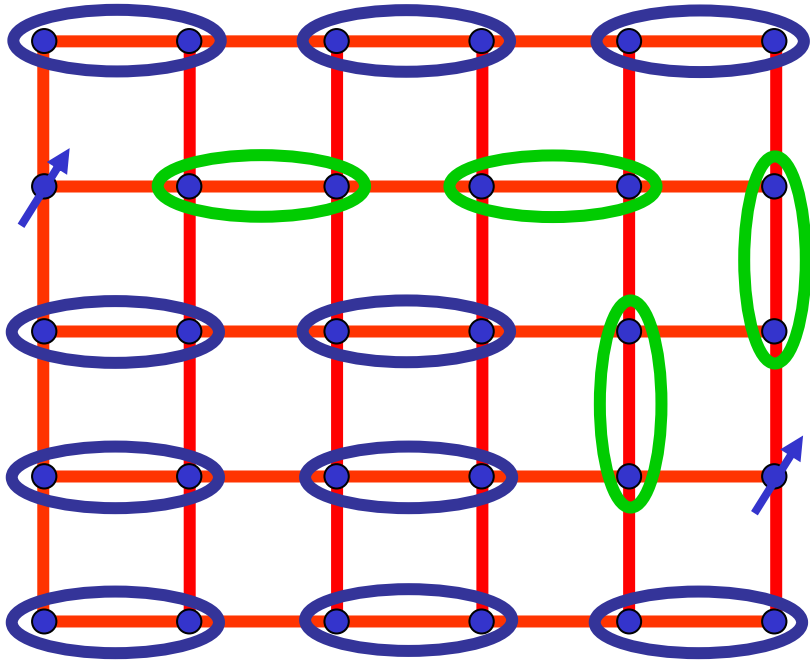
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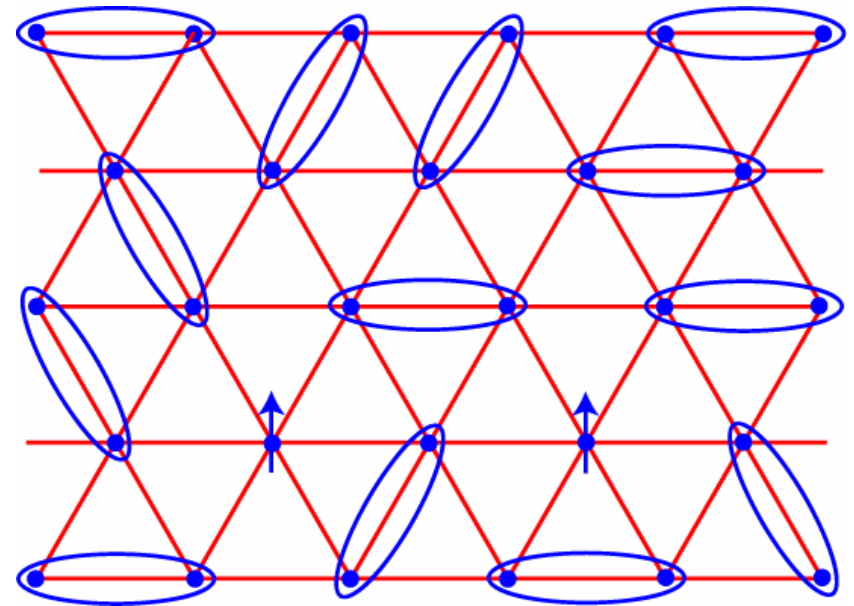
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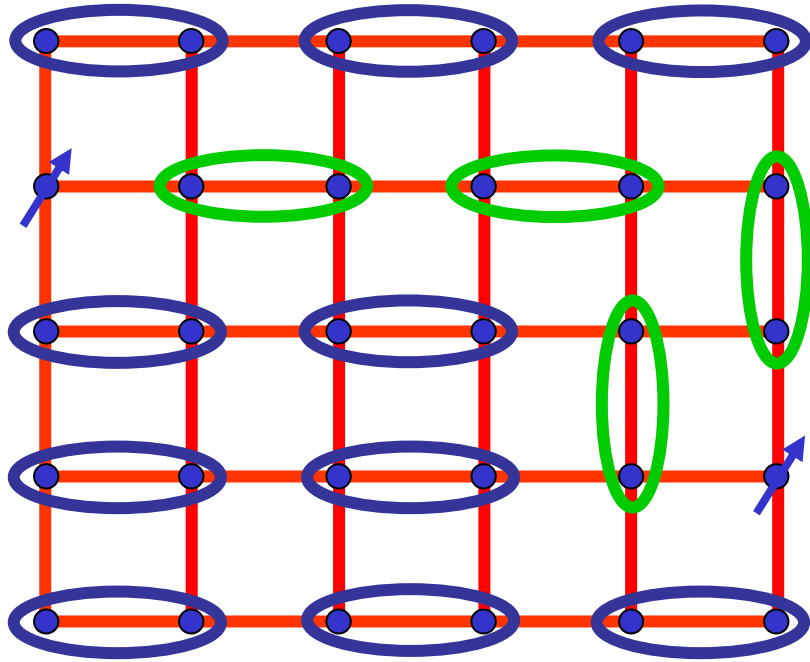
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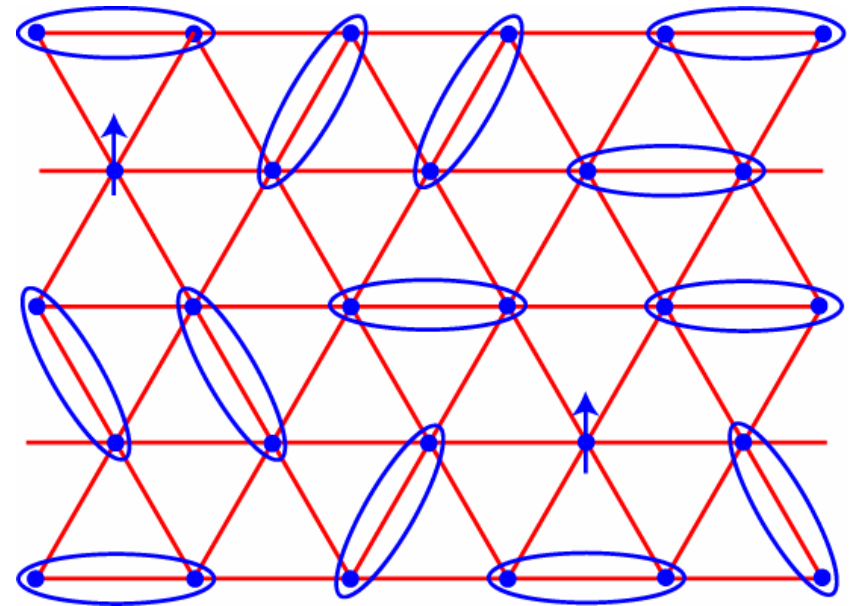
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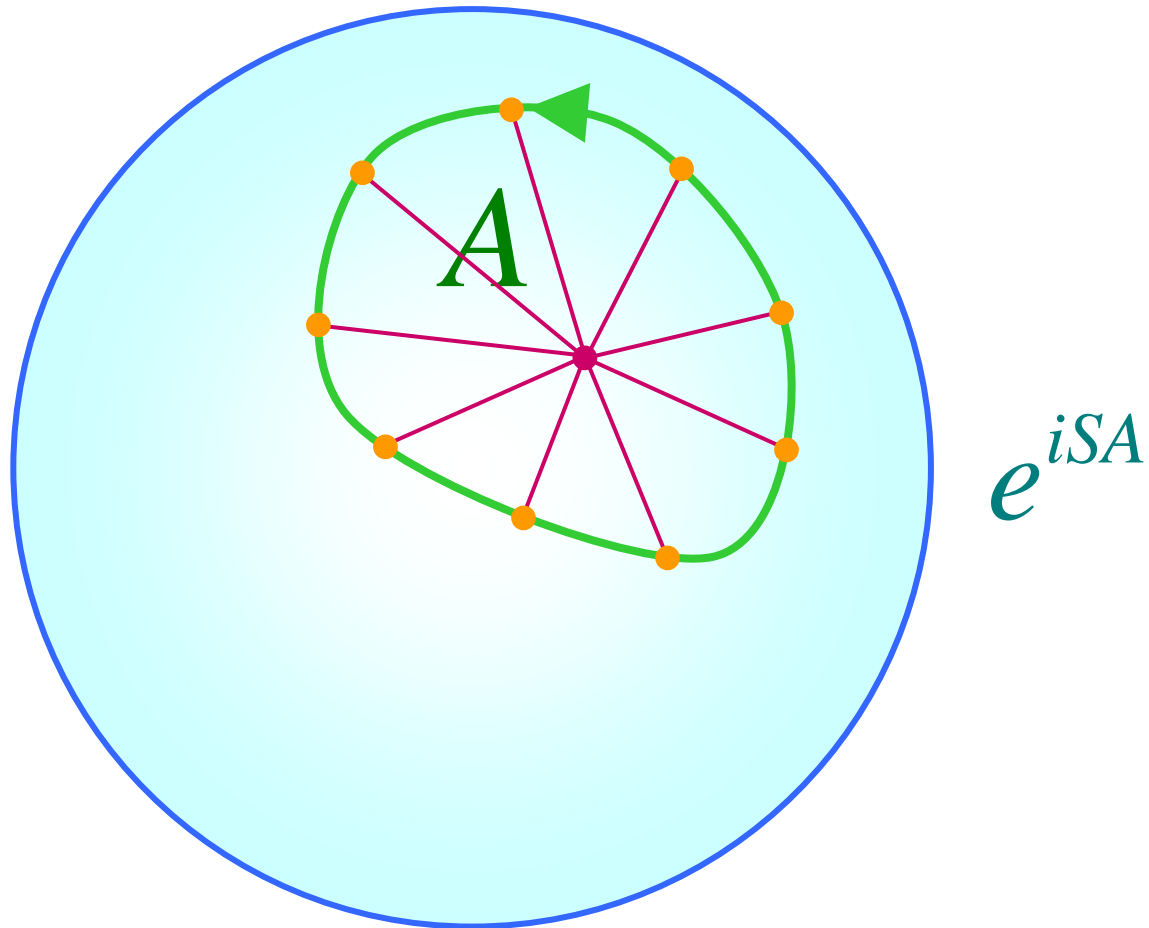
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$S=1/2$  spinons can  
 propagate  
 independently across  
 the lattice

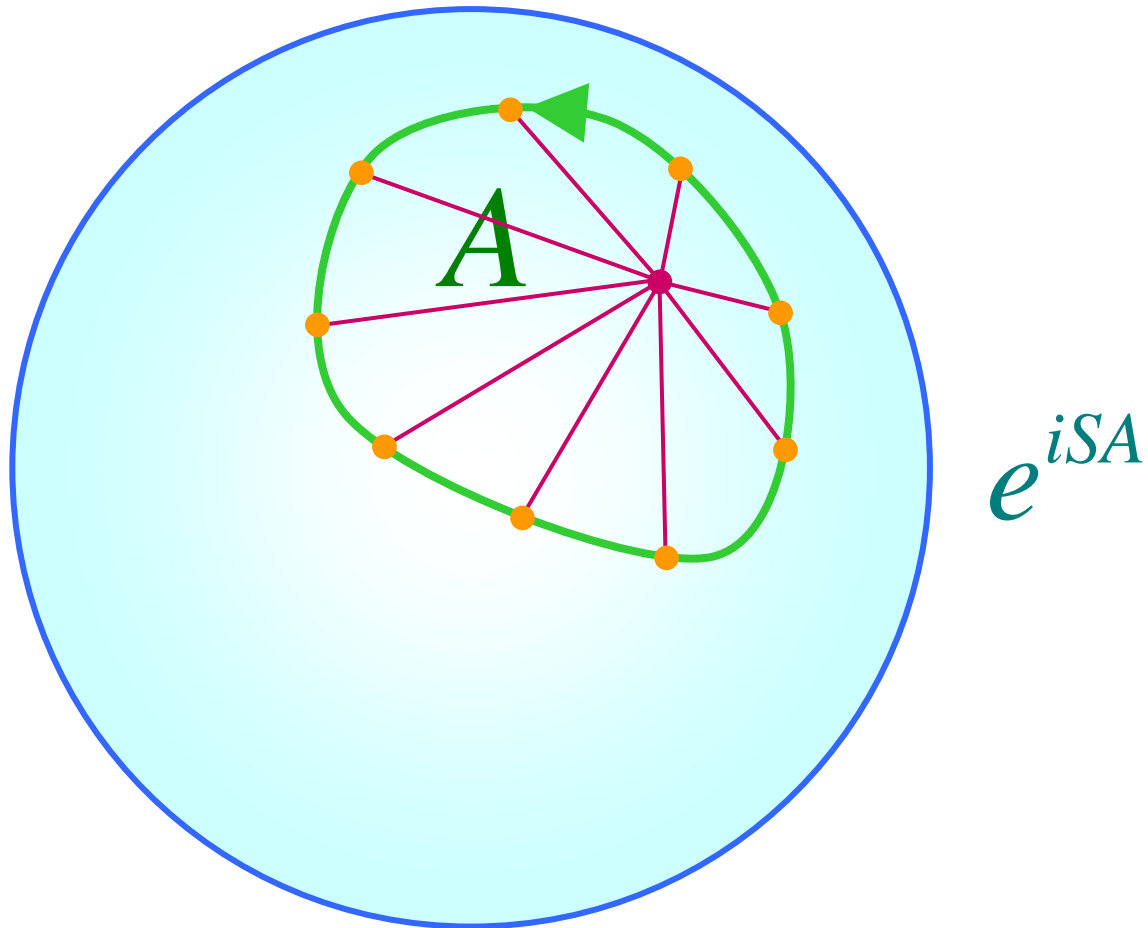
# Quantum theory for destruction of Neel order

## Ingredient missing from LGW theory: Spin Berry Phases



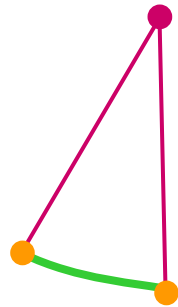
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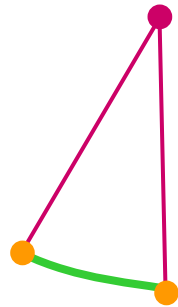


# Quantum theory for destruction of Neel order



## Quantum theory for destruction of Neel order

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

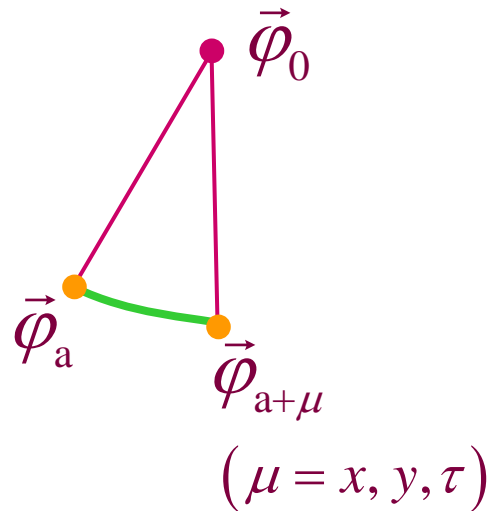


## Quantum theory for destruction of Neel order

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

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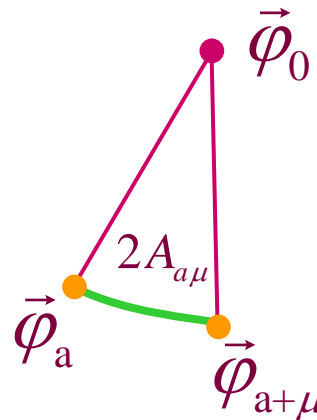
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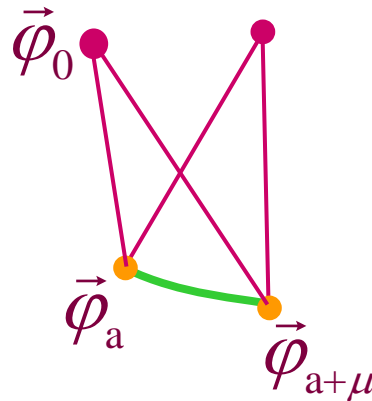
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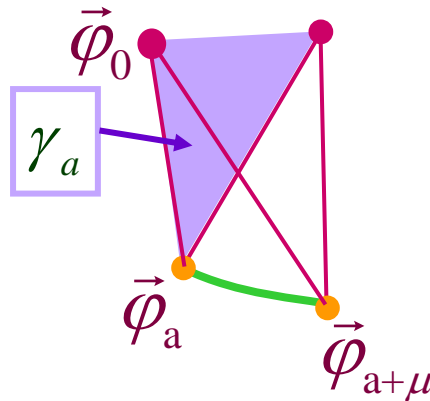
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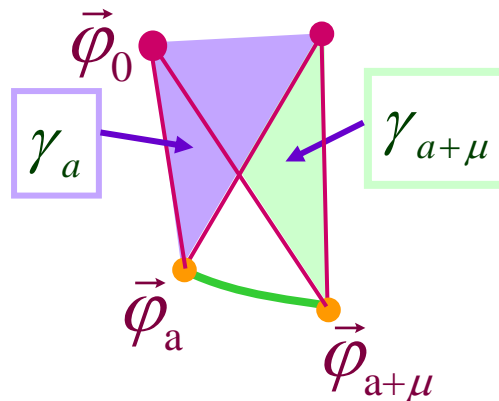
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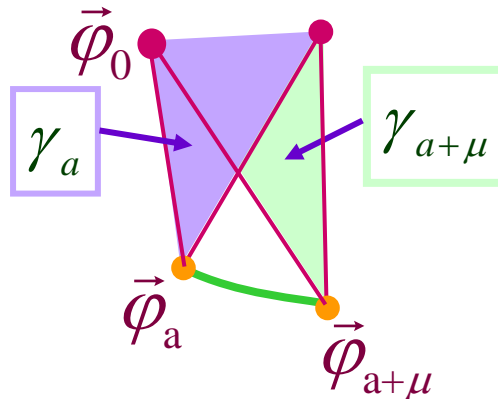
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$$2A_{a\mu} \rightarrow 2A_{a\mu} - \gamma_{a+\mu} + \gamma_a$$

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





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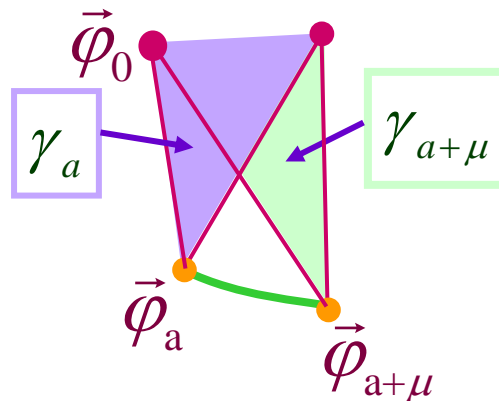
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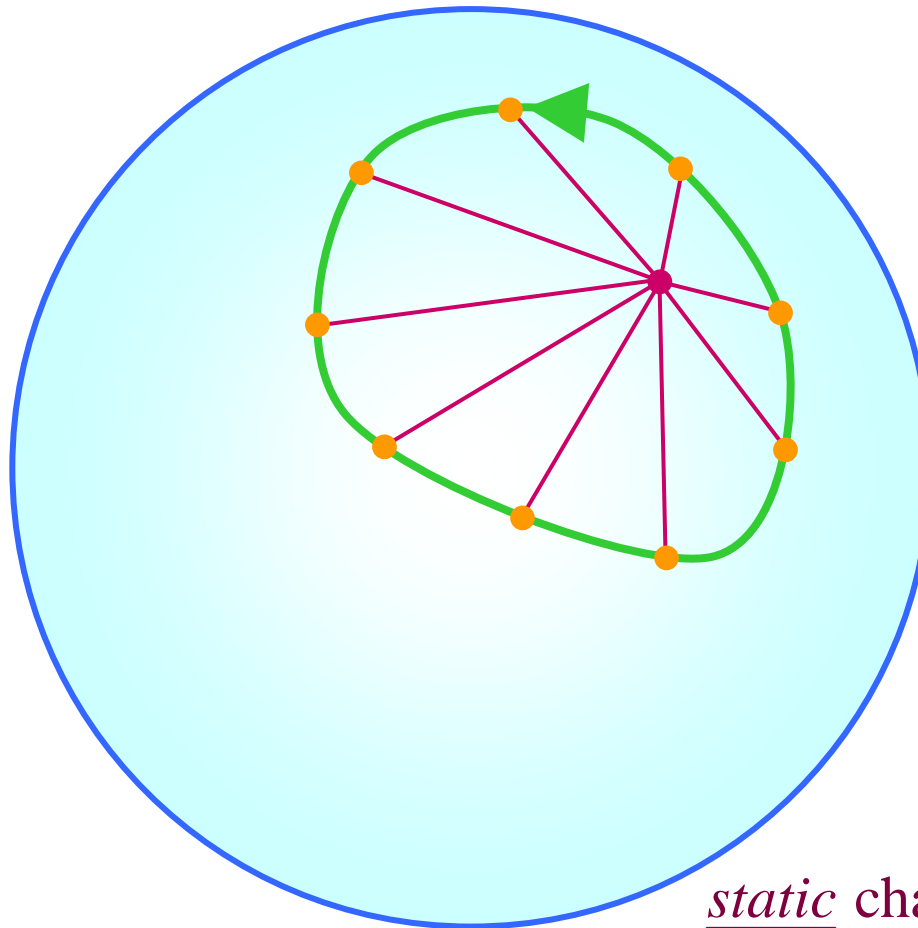
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The area of the triangle is uncertain modulo  $4\pi$ , and the action has to be invariant under  $A_{a\mu} \rightarrow A_{a\mu} + 2\pi$

# 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.

$$= \exp\left(i\sum_{a,\mu} J_{a\mu} A_{a\mu}\right)$$

with "current"  $J_{a\mu}$  of static charges  $\pm 1$  on sublattices

## Quantum theory for destruction of Neel order

Partition function on cubic lattice

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

Modulus of weights in partition function: 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  $\langle \vec{\varphi} \rangle = 0$

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).

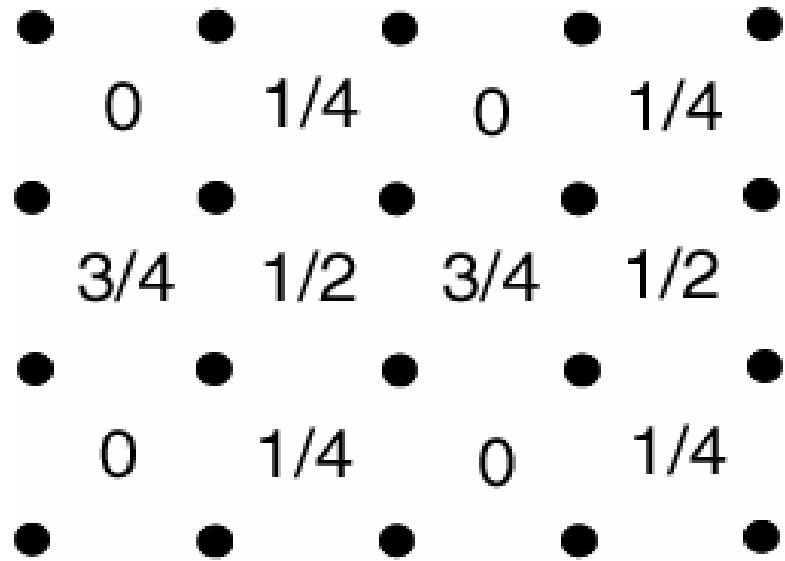
S. Sachdev and R. Jalabert, *Mod. Phys. Lett. B* **4**, 1043 (1990).

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.

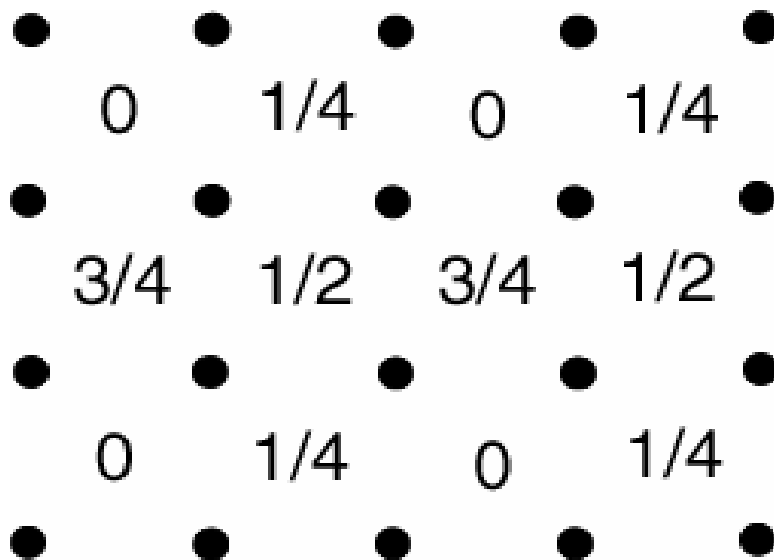


Alternative representation is in terms of a “height” model

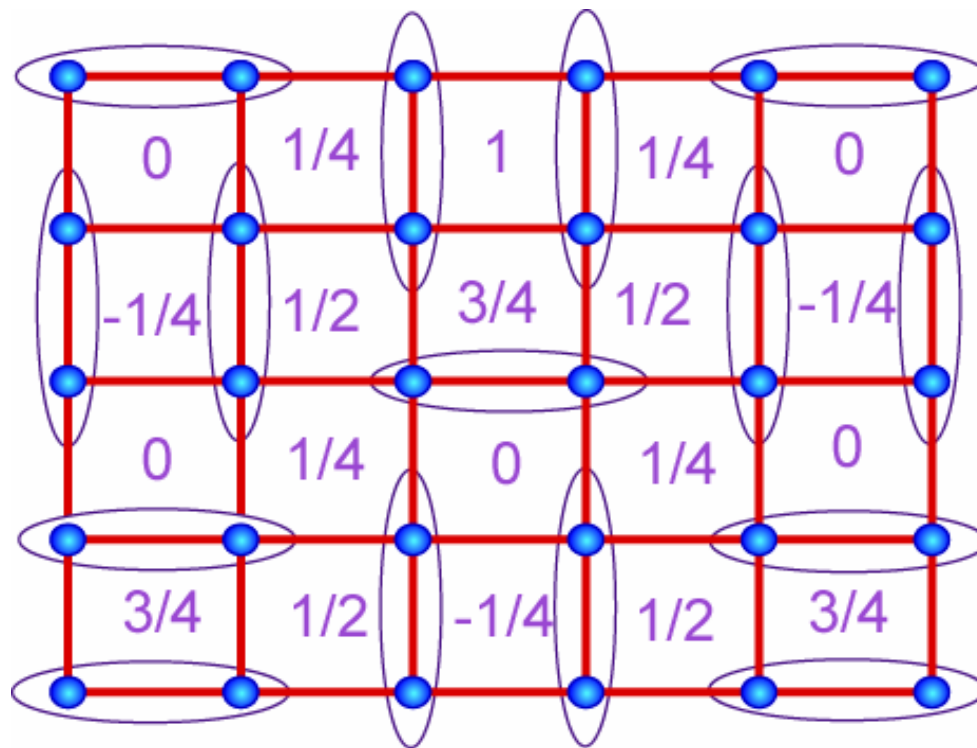
$$Z_{\text{dual}} = \sum_{\{h_{\bar{j}}\}} \exp \left( -\frac{e^2}{2} \sum_{\bar{j}} (\Delta_{\mu} h_{\bar{j}} - \Delta_{\mu} \mathcal{X}_{\bar{j}})^2 \right)$$

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.



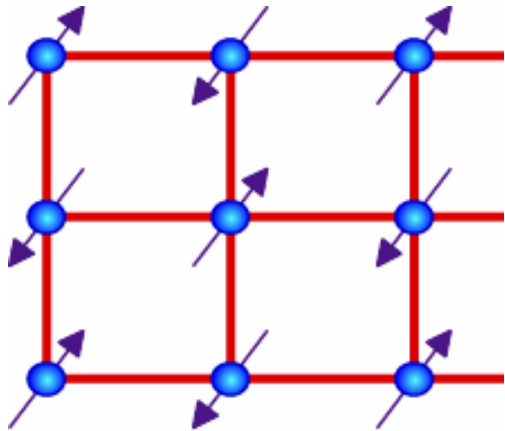
For large  $e^2$ , low energy height configurations are in exact one-to-one correspondence with nearest-neighbor valence bond pairings of the sites square lattice



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

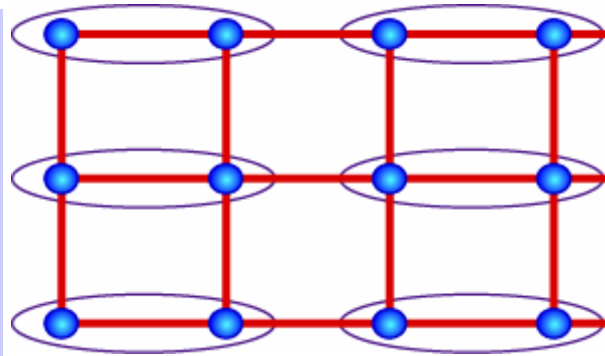
- ⇒ There is a definite average height of the interface
- ⇒ Ground state has bond order.

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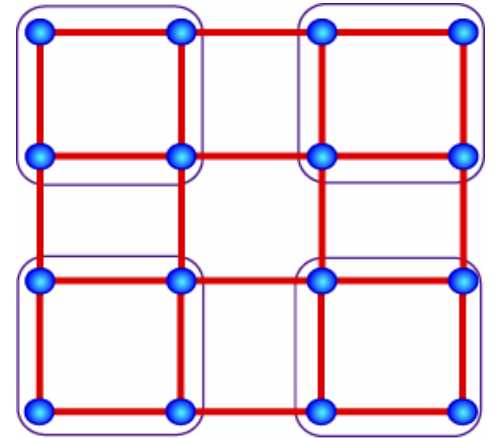


Neel order

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



or



Bond order

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

Not present in

LGW theory

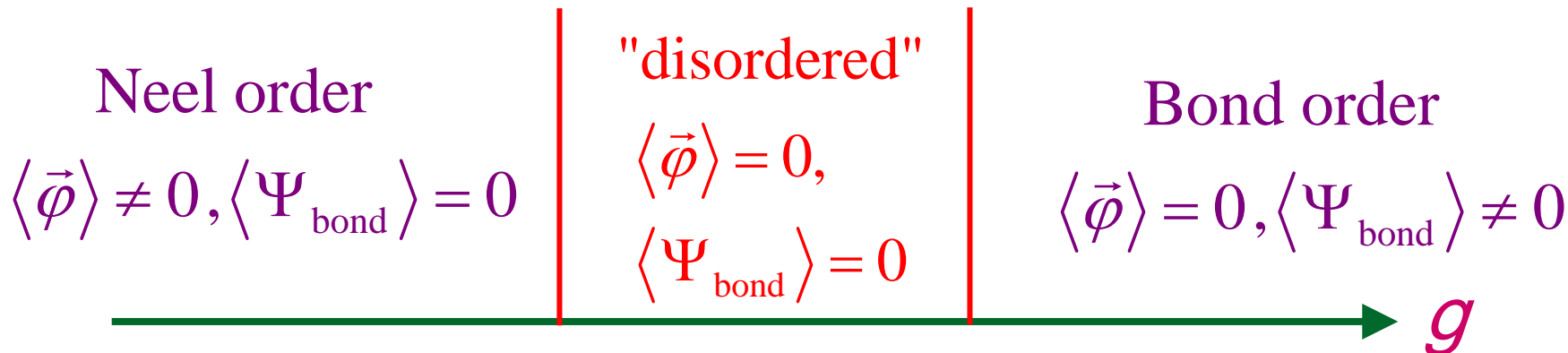
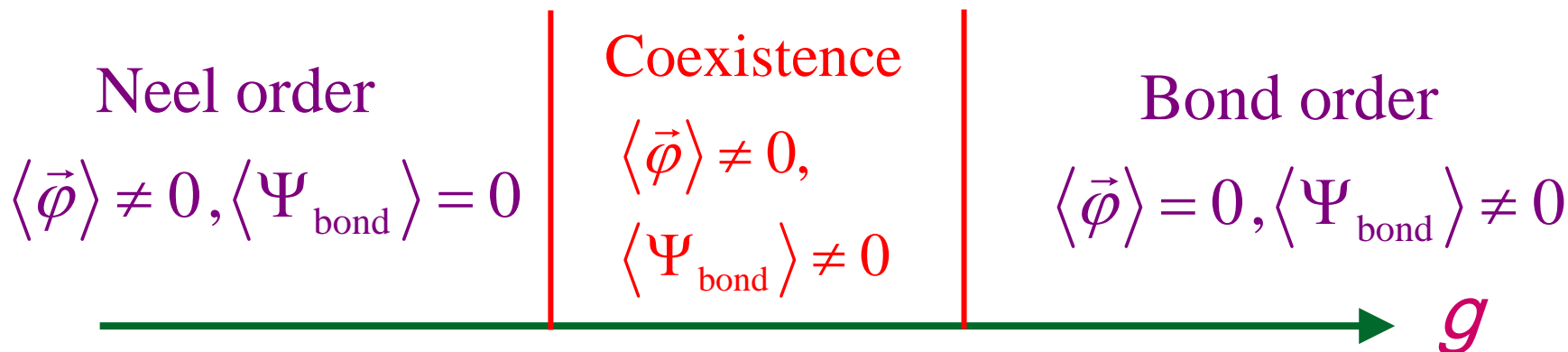
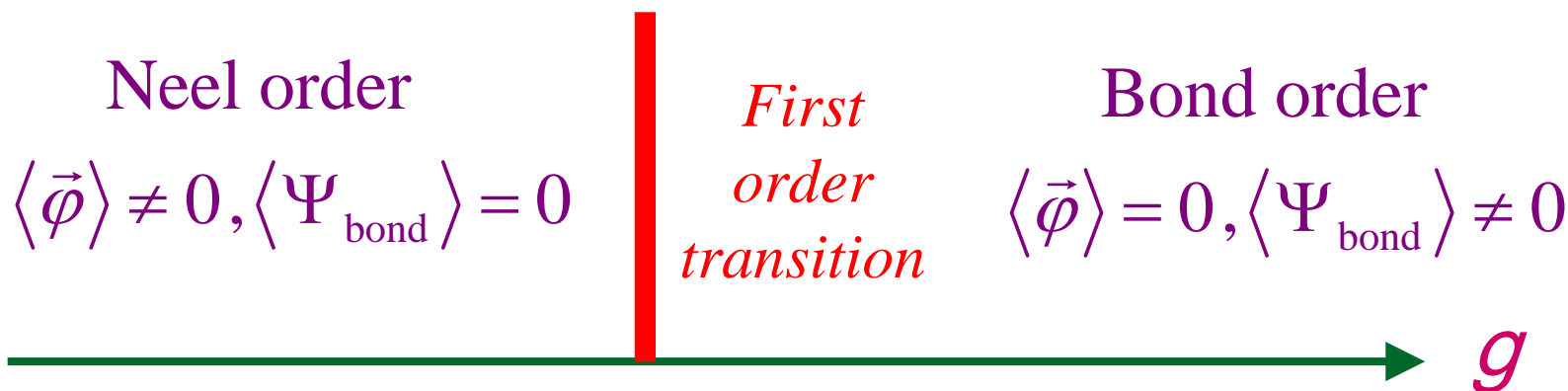
of  $\vec{\varphi}$  order

0

$g$



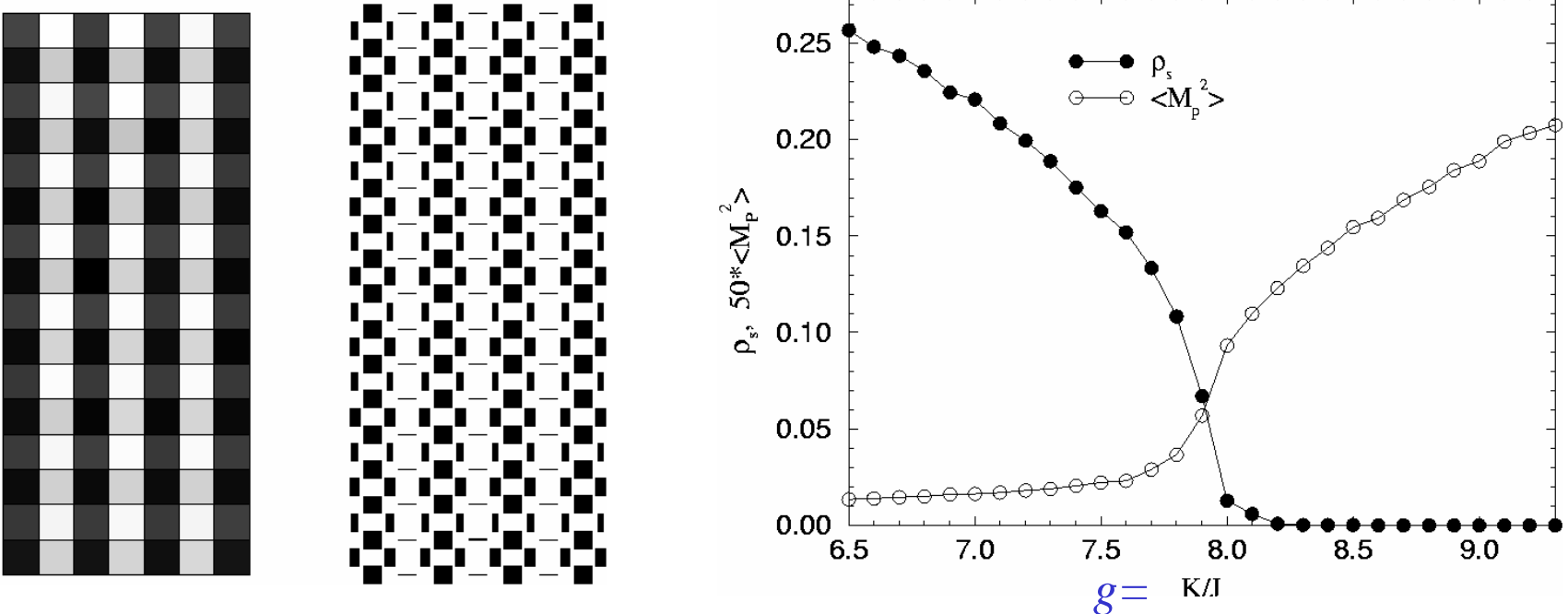
# Naïve approach: add bond order parameter to LGW theory “by hand”



# Bond order in a frustrated $S=1/2$ XY magnet

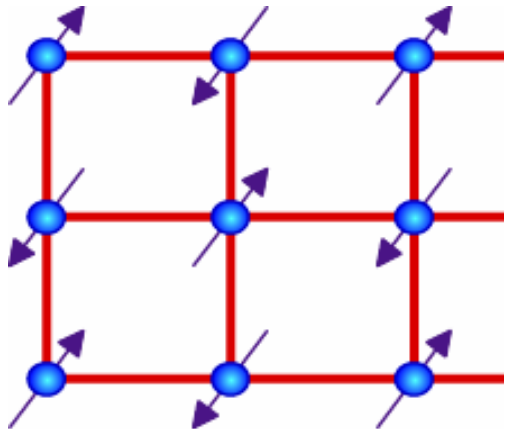
A. W. Sandvik, S. Daul, R. R. P. Singh, and D. J. Scalapino, *Phys. Rev. Lett.* **89**, 247201 (2002)

First *large scale* ( $> 8000$  spins) numerical study of the destruction of Neel order in a  $S=1/2$  antiferromagnet with full square lattice symmetry



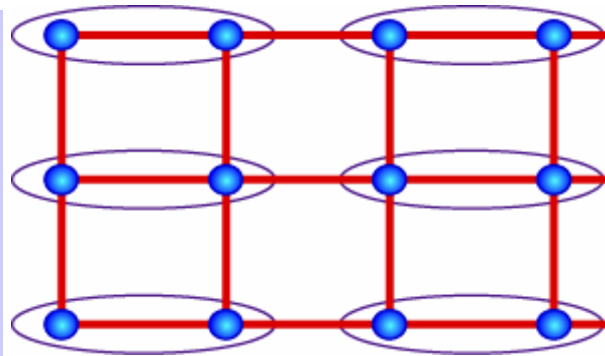
$$H = 2J \sum_{\langle ij \rangle} (S_i^x S_j^x + S_i^y S_j^y) - K \sum_{\langle ijkl \rangle \square} (S_i^+ S_j^- S_k^+ S_l^- + S_i^- S_j^+ S_k^- S_l^+)$$

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

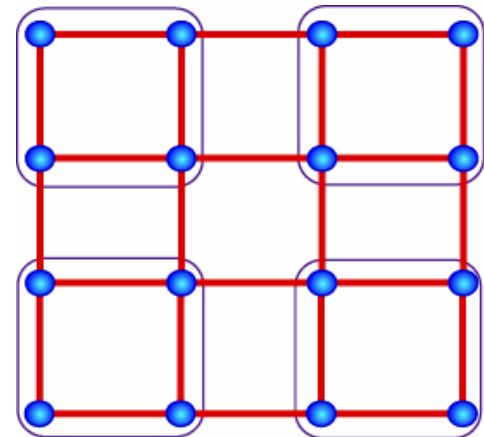


Neel order

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



or



Bond order

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

Not present in

LGW theory

of  $\vec{\varphi}$  order

0

$g$

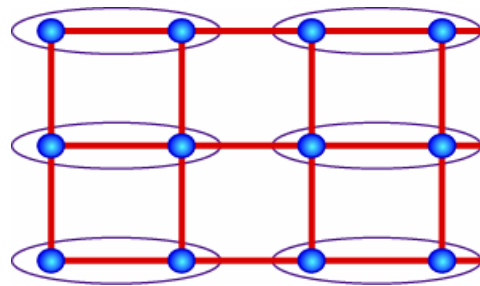
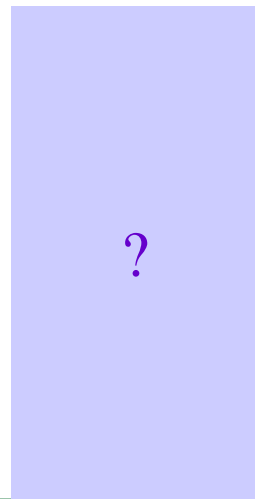
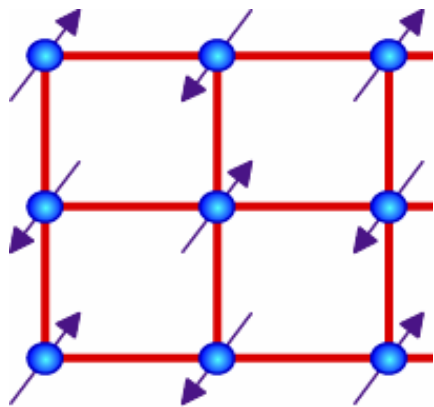
## Alternative formulation to describe transition:

Express theory in terms of a complex spinor  $z_{a\alpha}$ ,  $\alpha = \uparrow, \downarrow$ , with

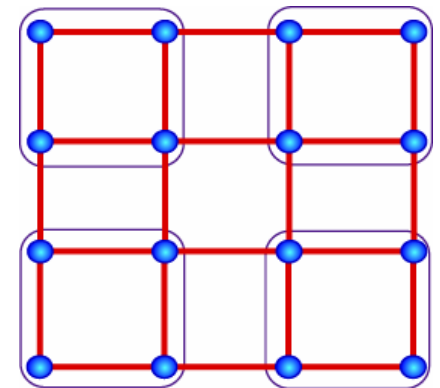
$$\mathbf{n}_a = z_{a\alpha}^* \boldsymbol{\sigma}_{\alpha\beta} z_{a\beta}$$

$$Z = \prod_a \int dz_{a\alpha} dA_{a\mu} \delta(|z_{a\alpha}|^2 - 1)$$

$$\exp \left( \frac{1}{g} \sum_{a,\mu} z_{a\alpha}^* e^{iA_{a\mu}} z_{a+\mu,\alpha} + \text{c.c.} + i \sum_a \eta_a A_{a\tau} \right)$$



or



0

$g$

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

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

# Theory of a second-order quantum phase transition between Neel and bond-ordered 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.

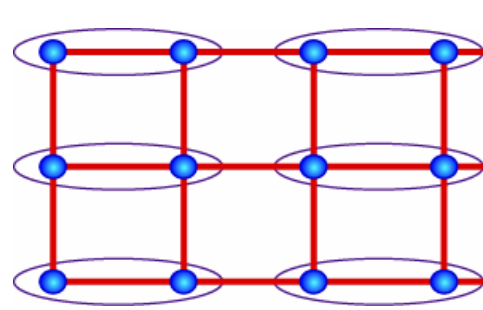
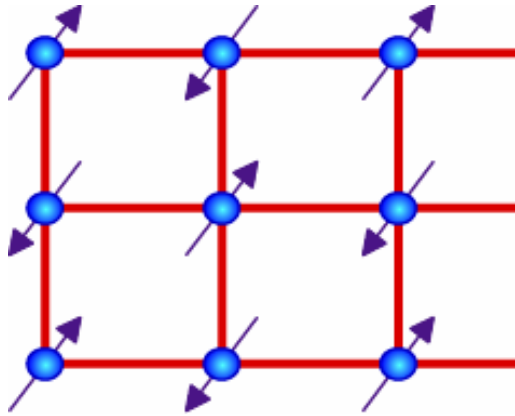
*Second-order critical point described by emergent fractionalized degrees of freedom ( $A_\mu$  and  $z_\alpha$ ); Order parameters ( $\vec{\varphi}$  and  $\Psi_{\text{bond}}$ ) are “composites” and of secondary importance*

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);

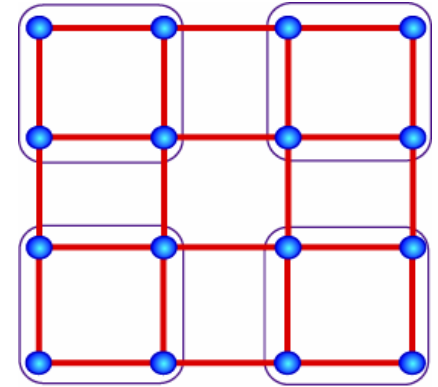
O. Motrunich and A. Vishwanath, cond-mat/0311222.

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



or



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

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

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

$S = 1$  triplon excitations

Neel order

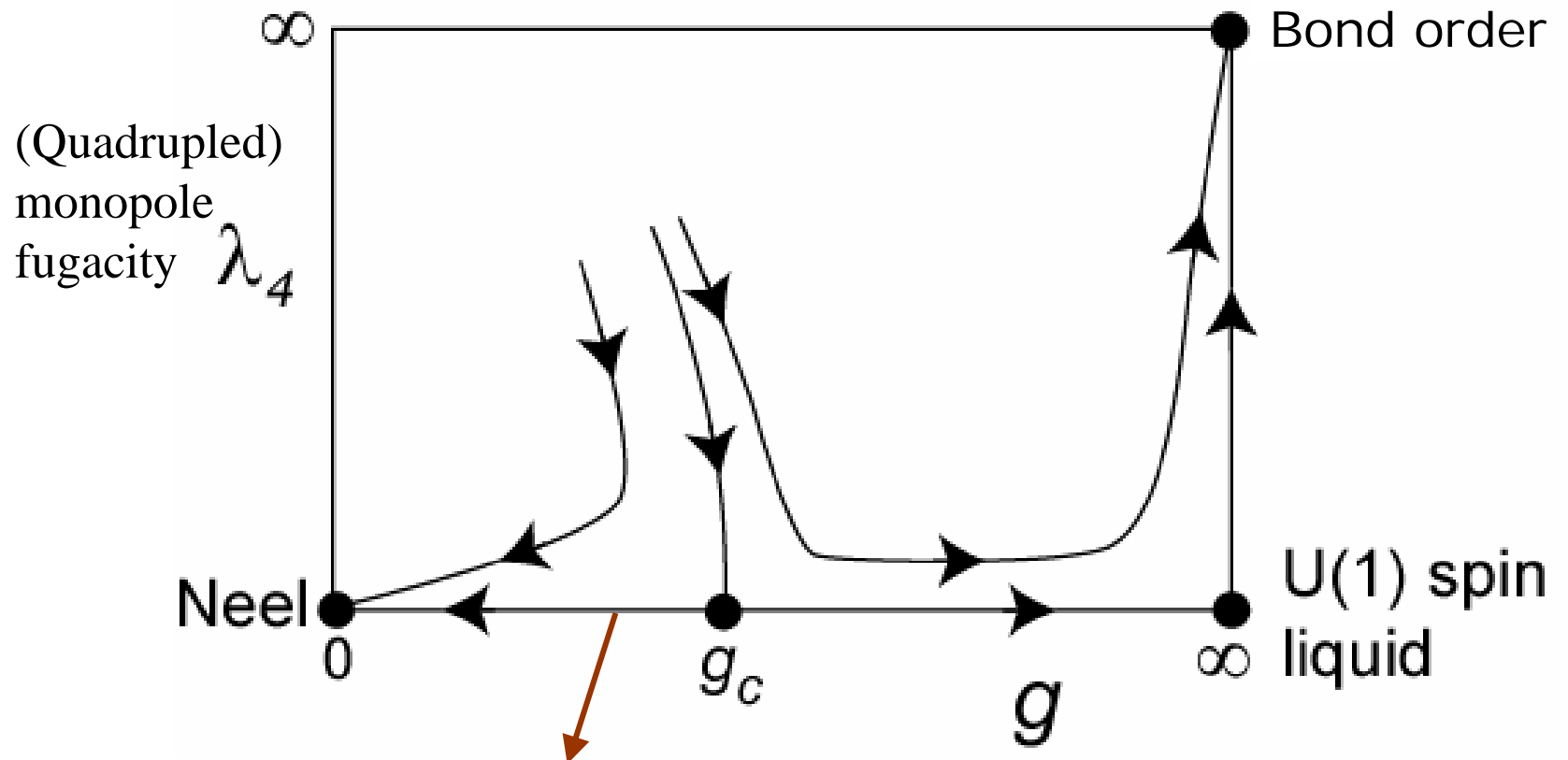
$$\langle \vec{\phi} \rangle \sim \langle z_\alpha^* \vec{\sigma}_{\alpha\beta} z_\beta \rangle \neq 0$$



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*



The line  $\lambda_4 = 0$  is described by

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

where  $A_\mu$  is non-compact

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

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

*Order parameters/broken symmetry*

+

*Emergent gauge excitations, fractionalization.*



## C. Technical details

*Duality and dangerously irrelevant operators*

## Nature of quantum critical point

$$Z = \prod_a \int dz_{a\alpha} dA_{a\mu} \delta(|z_{a\alpha}|^2 - 1) \exp \left( \frac{1}{g} \sum_{a,\mu} z_{a\alpha}^* e^{iA_{a\mu}} z_{a+\mu,\alpha} + \text{c.c.} + i \sum_a \eta_a A_{a\tau} + \frac{1}{e^2} \sum_{\square} \cos(\Delta_\mu A_{a\nu} - \Delta_\nu A_{a\mu}) \right)$$

Use a sequence of simpler models which can be analyzed by duality mappings

- A. Non-compact QED with scalar matter
- B. Compact QED with scalar matter
- C.  $N=1$ : Compact QED with scalar matter and Berry phases
- D.  $N \rightarrow \infty$  theory
- E. Easy plane case for  $N=2$

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## A. $N=1$ , non-compact $U(1)$ , no Berry phases

Use  $z_a = e^{i\theta_a}$  and then

$$Z = \prod_a \int d\theta_a dA_{a\mu} \exp \left( -\frac{1}{2e^2} \sum_{\square} (\Delta_{\mu} A_{a\nu} - \Delta_{\nu} A_{a\mu})^2 + \frac{1}{g} \sum_{a,\mu} \cos(\Delta_{\mu} \theta_a - A_{a\mu}) \right)$$

Standard duality maps, similar to those discussed earlier, show that this theory is equivalent to an **inverted XY model**, described by the field theory

$$Z_{\text{dual}} = \int \mathcal{D}\psi \exp \left( - \int d^2x d\tau \left( |\partial_{\mu} \psi|^2 + r|\psi|^2 + \frac{u}{2} |\psi|^4 \right) \right)$$

Here  $\psi$  is a *dual* field which orders in the paramagnetic phase *i.e.*  $\langle \psi \rangle \neq 0$  where  $\langle e^{i\theta} \rangle = 0$ , and vice versa. The field  $\psi$  is a creation operator for *vortices* in the original theory of a “Ginzburg-Landau superconductor” coupled to “electromagnetism”.

C. Dasgupta and B.I. Halperin, *Phys. Rev. Lett.* **47**, 1556 (1981).

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## B. $N=1$ , compact $U(1)$ , no Berry phases

Use  $z_a = e^{i\theta_a}$  and then

$$Z = \prod_a \int d\theta_a dA_{a\mu} \exp \left( \frac{1}{e^2} \sum_{\square} \cos (\Delta_{\mu} A_{a\nu} - \Delta_{\nu} A_{a\mu}) + \frac{1}{g} \sum_{a,\mu} \cos (\Delta_{\mu} \theta_a - A_{a\mu}) \right)$$

The Dasgupta-Halperin mapping now yields the dual theory

$$Z_{\text{dual}} = \int \mathcal{D}\psi \exp \left( - \int d^2x d\tau \left( |\partial_{\mu} \psi|^2 + r|\psi|^2 + \frac{u}{2} |\psi|^4 - y_m (\psi + \psi^*) \right) \right)$$

Here  $y_m$  is a *monopole fugacity*, and the last term in  $Z_{\text{dual}}$  accounts for the fact that vortex lines can end in monopoles.

This dual theory is an **inverted XY model in a “magnetic” field** and it has no phase transition. In the direct theory, the monopoles are a relevant perturbation, and they destroy the “superconducting” phase.



## Nature of quantum critical point

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## C. $N=1$ , compact $U(1)$ , Berry phases

Upon including Berry phases, the previous theory becomes

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

The Dasgupta-Halperin duality can also be extended to this theory, and we obtain

$$Z_{\text{dual}} = \int \mathcal{D}\psi \exp \left( - \int d^2x d\tau \left( |\partial_{\mu} \psi|^2 + r|\psi|^2 + \frac{u}{2} |\psi|^4 - \tilde{y}_m (\psi^4 + \psi^{*4}) \right) \right)$$

## C. $N=1$ , compact $U(1)$ , Berry phases

$$Z_{\text{dual}} = \int \mathcal{D}\psi \exp \left( - \int d^2x d\tau \left( |\partial_\mu \psi|^2 + r|\psi|^2 + \frac{u}{2}|\psi|^4 - \tilde{y}_m(\psi^4 + \psi^{*4}) \right) \right)$$

This is an **inverted XY model with a four-fold anisotropy**, *i.e.* a  $Z_4$  clock model. The four-fold anisotropy is irrelevant at the critical point (J.M. Carmona, A. Pelissetto, E. Vicari, Phys. Rev. B **61**, 15136 (2000)), and hence there is a XY transition to a four-fold degenerate state with  $\langle \psi \rangle \neq 0$ . In the direct theory, this is the *bond-ordered* paramagnet.

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

## C. $N=1$ , compact $U(1)$ , Berry phases

$$Z_{\text{dual}} = \int \mathcal{D}\psi \exp \left( - \int d^2x d\tau \left( |\partial_\mu \psi|^2 + r|\psi|^2 + \frac{u}{2}|\psi|^4 - \tilde{y}_m(\psi^4 + \psi^{*4}) \right) \right)$$

Reinterpretation by T. Senthil: In the direct theory, the irrelevance of  $\tilde{y}_m$  implies that the Berry phases have cancelled out the monopole contributions. So monopoles are ‘dangerously irrelevant’ at the critical point, and the critical theory is *the same Dasgupta-Halperin inverted XY model describing the non-compact theory without monopoles or Berry phases!*

## Nature of quantum critical point

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**Identical critical theories !**



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**Identical critical theories !**



## D. $N \rightarrow \infty$ , compact U(1), Berry phases

Near the critical point of the  $N = \infty$  non-compact theory, integrate out  $z_\alpha$  quanta (with gap  $\Delta$ ) in the presence of a Dirac monopole with  $A_\mu = A_\mu^D$  with magnetic charge  $q$ . The functional determinant yields the action of such a monopole, and the scaling dimension of the monopole insertion

$$\mathcal{S}_{\text{monopole}} = N \text{Tr} \ln \left[ \frac{-(\partial_\mu - iA_\mu^D)^2 + \Delta^2 + V(r)}{-\partial_\mu^2 + \Delta^2} \right] - \frac{N}{g} \int d^3r V(r)$$

$$\text{where } \frac{\delta \mathcal{S}_{\text{monopole}}}{\delta V(r)} = 0 \text{ and } V(r \rightarrow \infty) = 0.$$

Evaluation of functional determinant for  $q = 4$  shows

$$\mathcal{S}_{\text{monopole}} = 0.815787N \ln \left( \frac{\Lambda}{\Delta} \right)$$

This computation shows that the scaling dimension of  $q = 4$  monopoles is  $3 - 0.815787N$

Monopoles are irrelevant both with and without Berry phases for large  $N$ .



## E. Easy plane case for $N=2$

Explicit duality mappings show that the physical situation is as for  $N = 1$ :

- monopoles are relevant without Berry phases,
- monopoles are irrelevant at the critical point in the presence of Berry phases, and
- monopoles drive the appearance of bond order in the paramagnetic phase.

$$Z_{\text{dual}} = \int \mathcal{D}\psi_1 \mathcal{D}\psi_2 \mathcal{D}a_\mu \exp \left( - \int d^2x d\tau \left( |(\partial_\mu - ia_\mu)\psi_1|^2 + |(\partial_\mu - ia_\mu)\psi_2|^2 \right. \right. \\ \left. \left. + r (|\psi_1|^2 + |\psi_2|^2) + \frac{u}{2} (|\psi_1|^4 + |\psi_2|^4) - \tilde{y}_m ((\psi_1^* \psi_2)^4 + (\psi_1 \psi_2^*)^4) \right) \right)$$

C. Lannert, M.P.A. Fisher, and T. Senthil, *Phys. Rev. B* **63**, 134510 (2001).

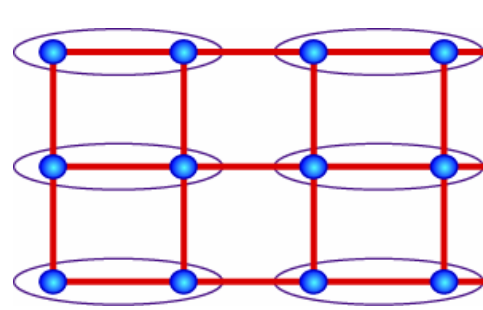
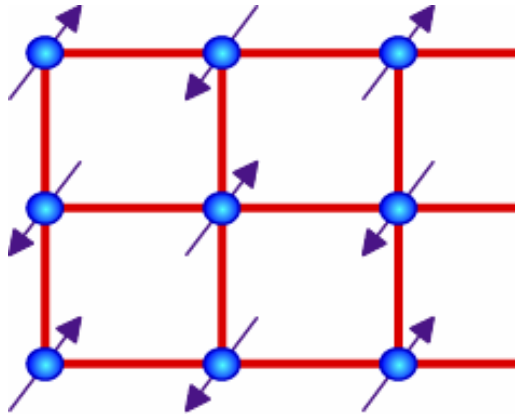
S. Sachdev and K. Park, *Annals of Physics*, **298**, 58 (2002).

O. Motrunich and A. Vishwanath, cond-mat/0311222

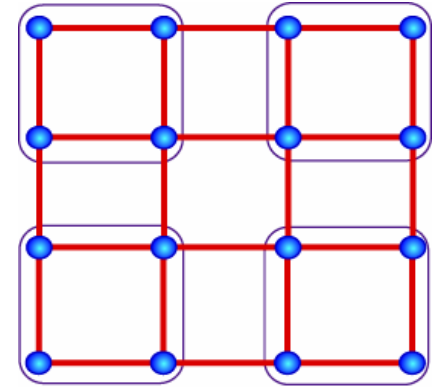
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# Phase diagram of S=1/2 square lattice antiferromagnet



or



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

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

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

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Second-order critical point described by

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