

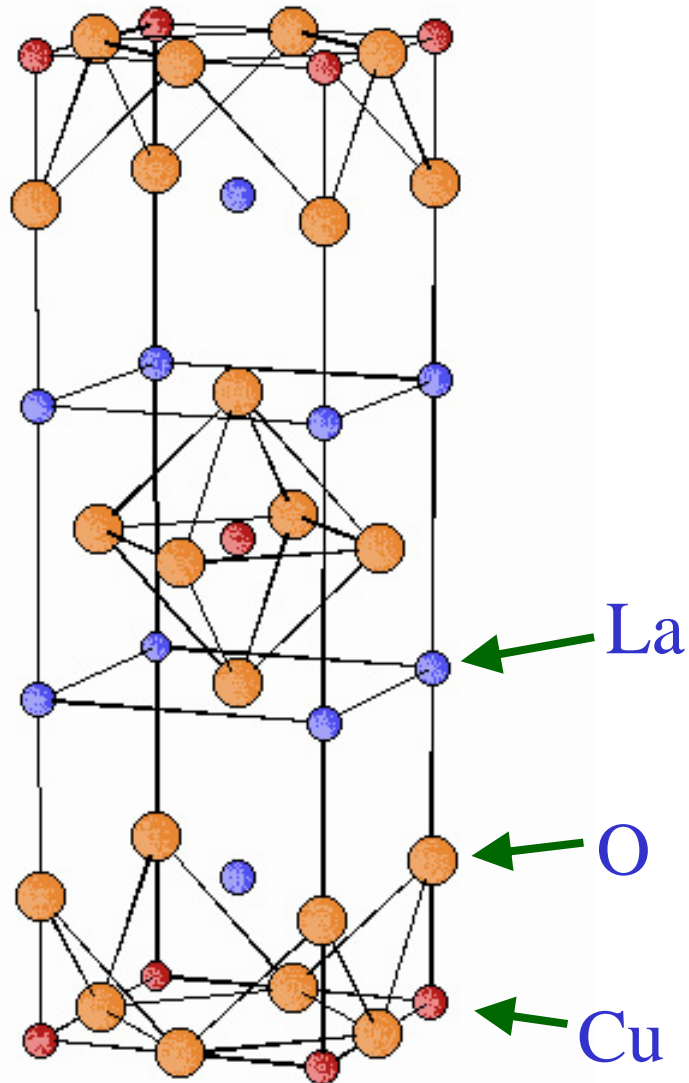
# Quantum phase transitions: from Mott insulators to the cuprate superconductors

Colloquium article in *Reviews of Modern Physics* **75**, 913 (2003)

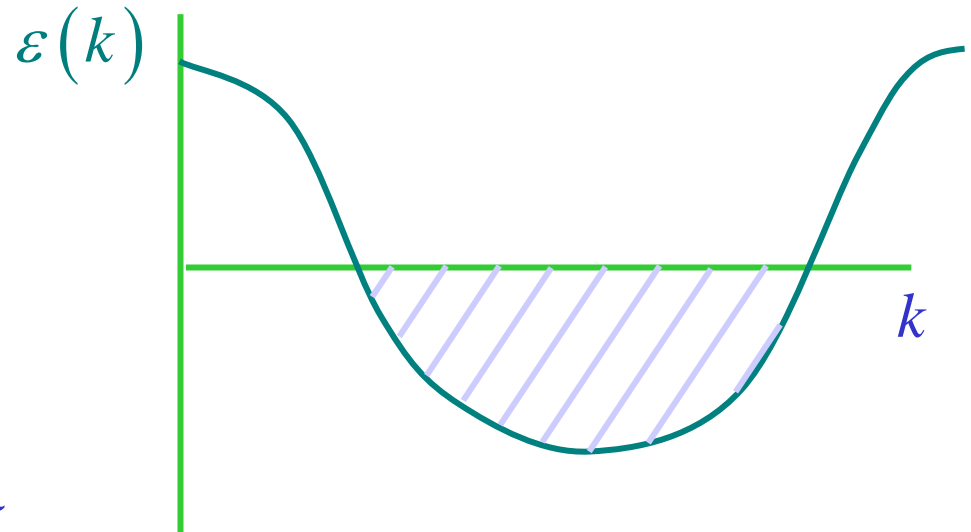
Leon Balents (UCSB)  
Eugene Demler (Harvard)  
Matthew Fisher (UCSB)  
Kwon Park (Maryland)  
Anatoli Polkovnikov (Harvard)  
T. Senthil (MIT)  
Ashvin Vishwanath (MIT)  
Matthias Vojtá (Karlsruhe)  
Ying Zhang (Maryland)



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



Band theory

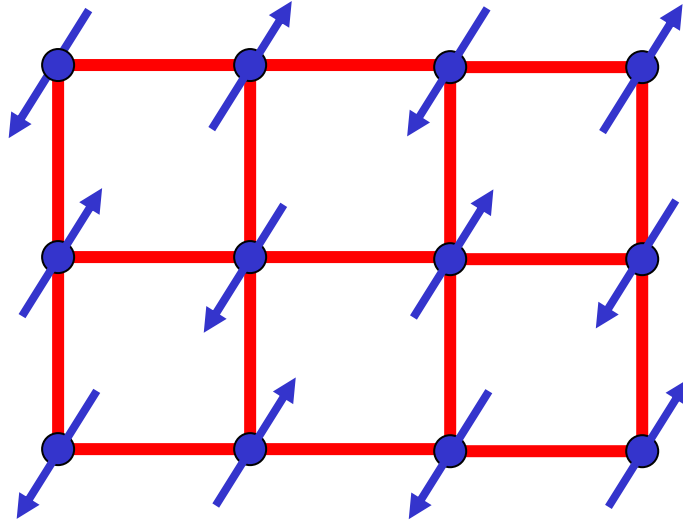


Half-filled band of Cu 3d orbitals –  
ground state is predicted by  
band theory to be a metal.

However,  $\text{La}_2\text{CuO}_4$  is a  
very good insulator

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### 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  $\mathbf{K} = (\pi, \pi)$

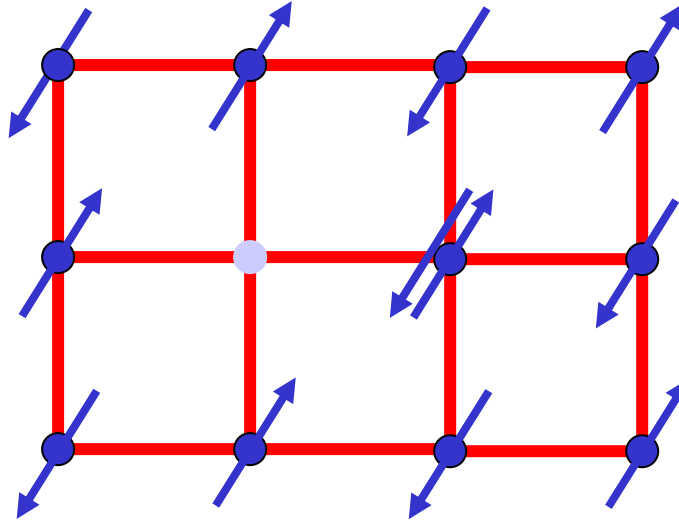
spin density wave order parameter:

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

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

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

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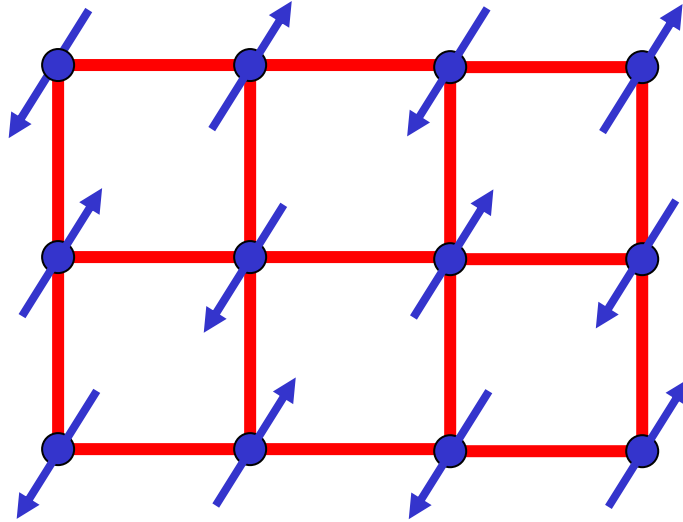
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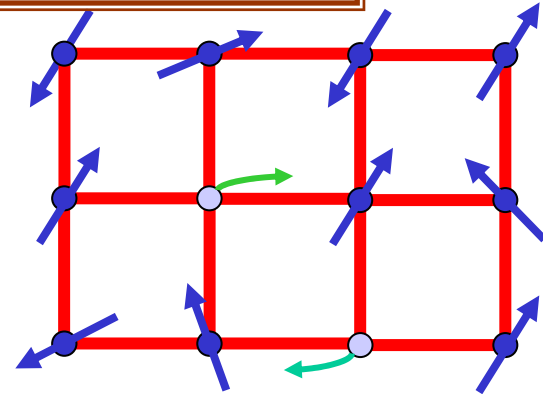
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$$\langle \vec{\varphi} \rangle \neq 0$$

# 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. Cuprate Superconductors

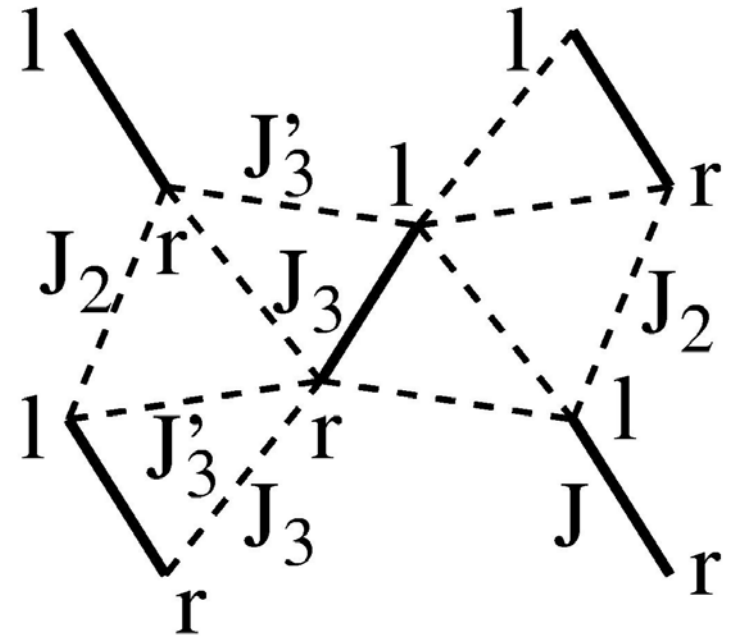
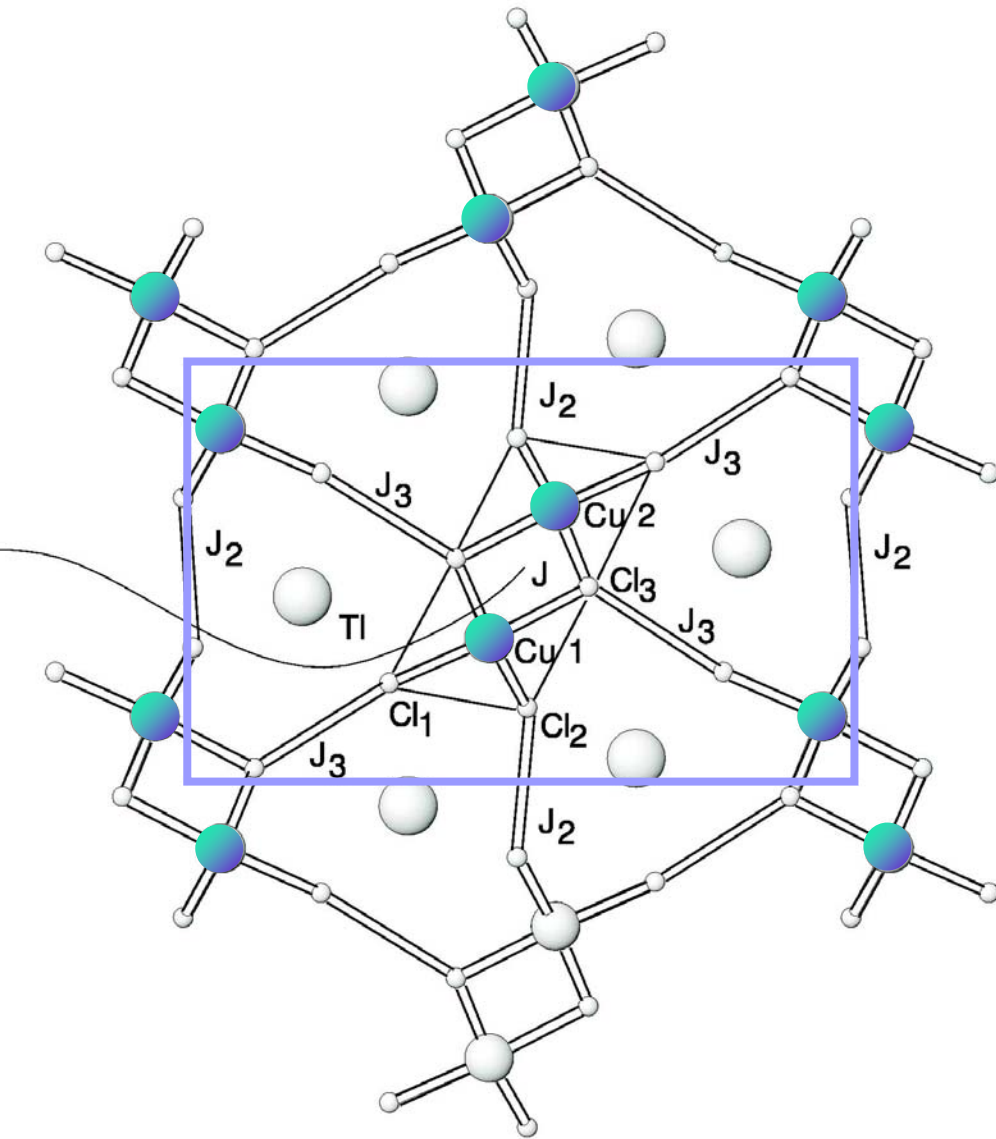
*Competing orders and recent experiments*

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

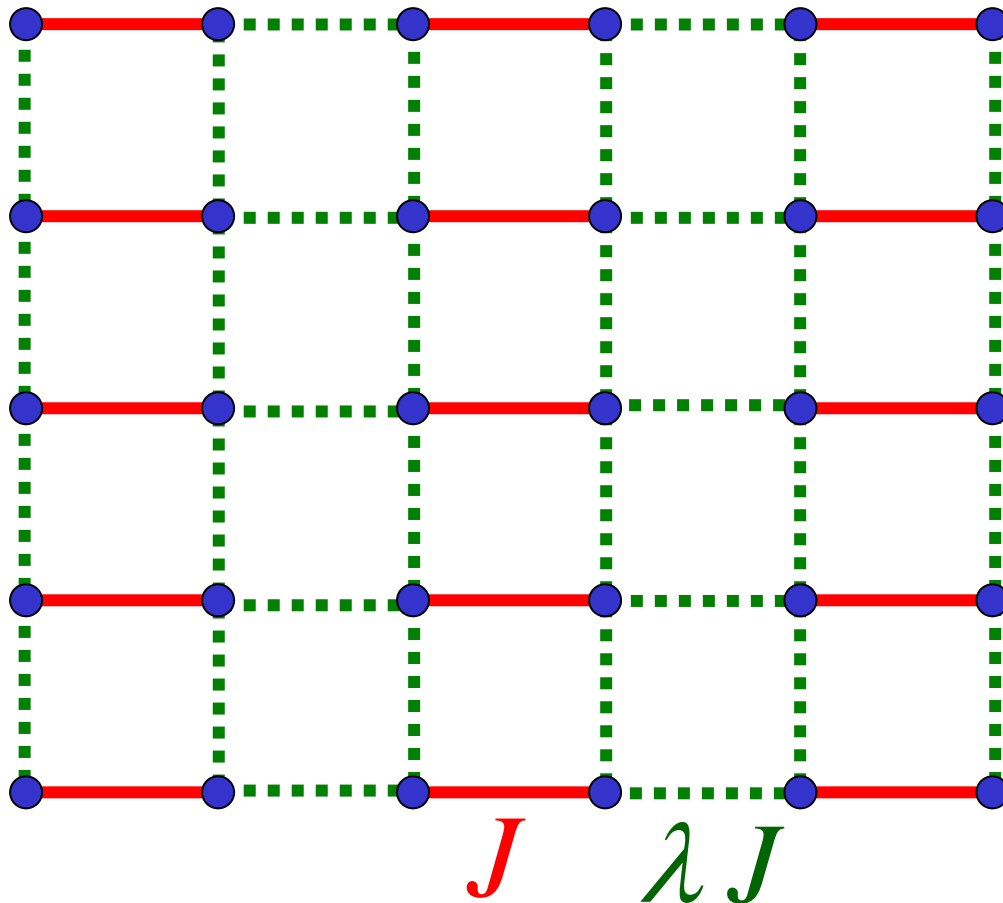
M. P. Gelfand, R. R. P. Singh, and D. A. Huse, *Phys. Rev. B* **40**, 10801-10809 (1989).

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).

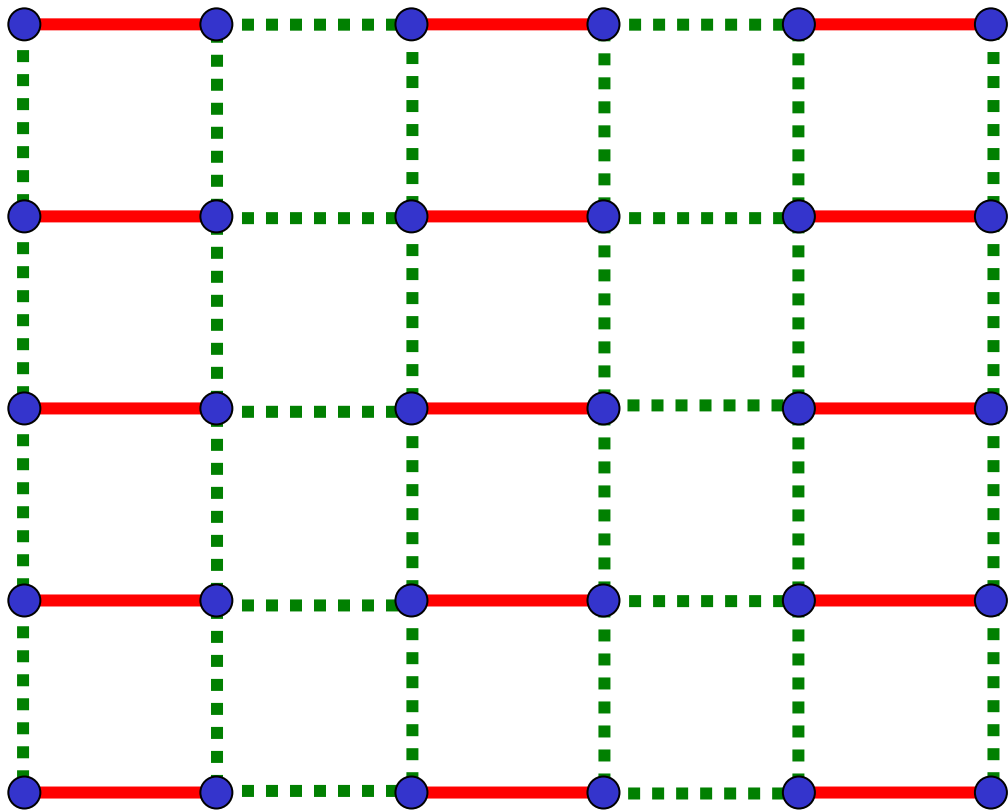
M. Matsumoto, C. Yasuda, S. Todo, and H. Takayama, *Phys. Rev. B* **65**, 014407 (2002).

$S=1/2$  spins on coupled dimers



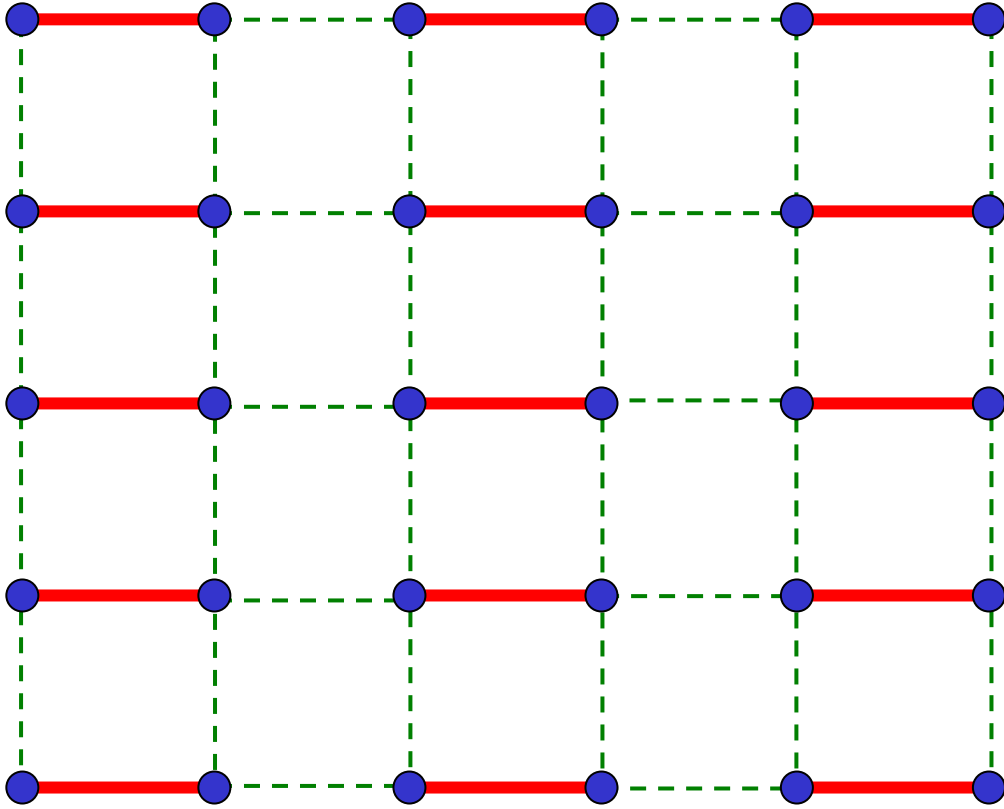
$$H = \sum_{\langle ij \rangle} J_{ij} \vec{S}_i \cdot \vec{S}_j$$

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



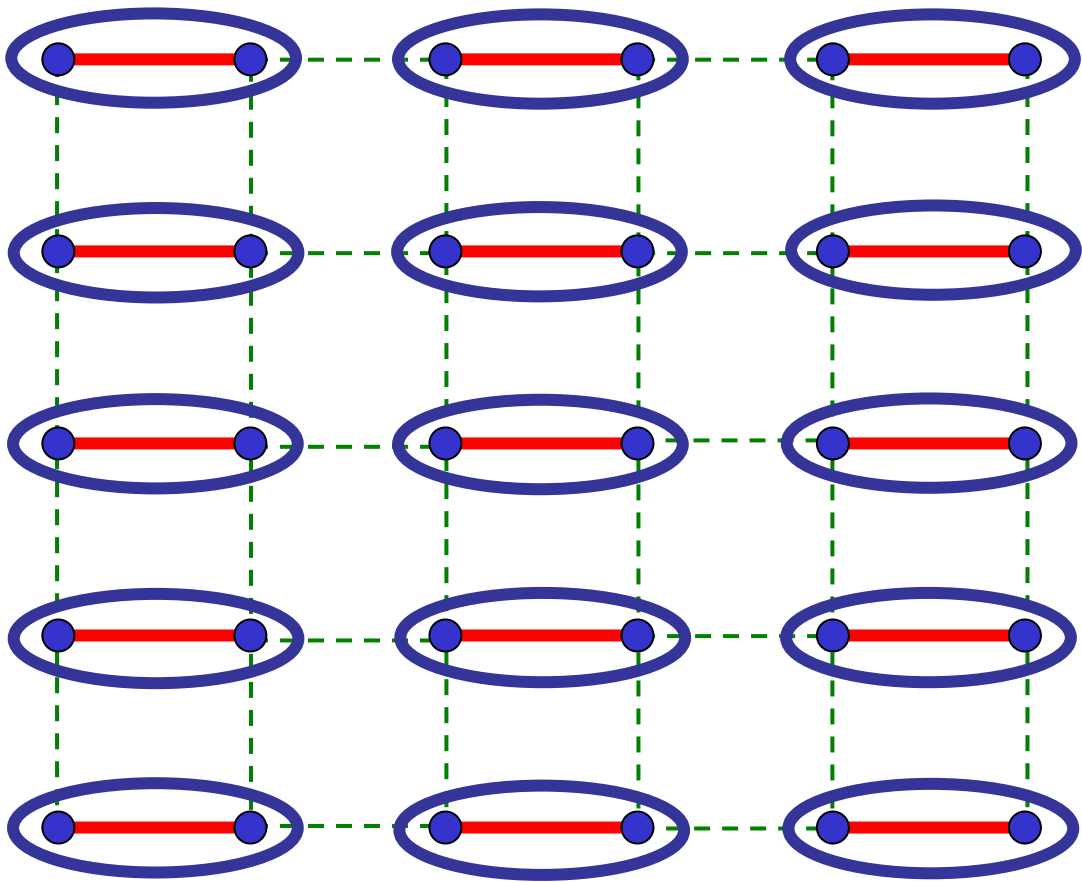
$\lambda$  close to 0

Weakly coupled dimers



$\lambda$  close to 0

Weakly coupled dimers



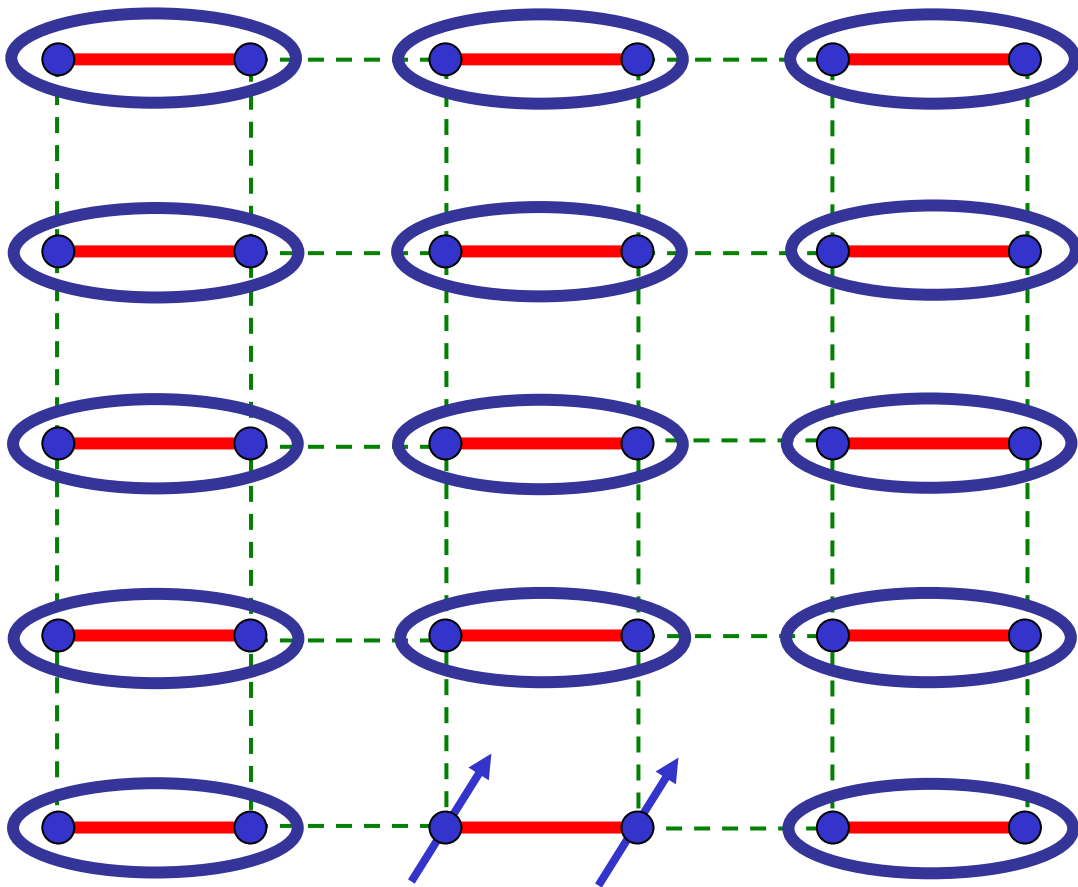
$$\text{dimer} = \frac{1}{\sqrt{2}} (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$$

Paramagnetic ground state

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

$\lambda$  close to 0

Weakly coupled dimers

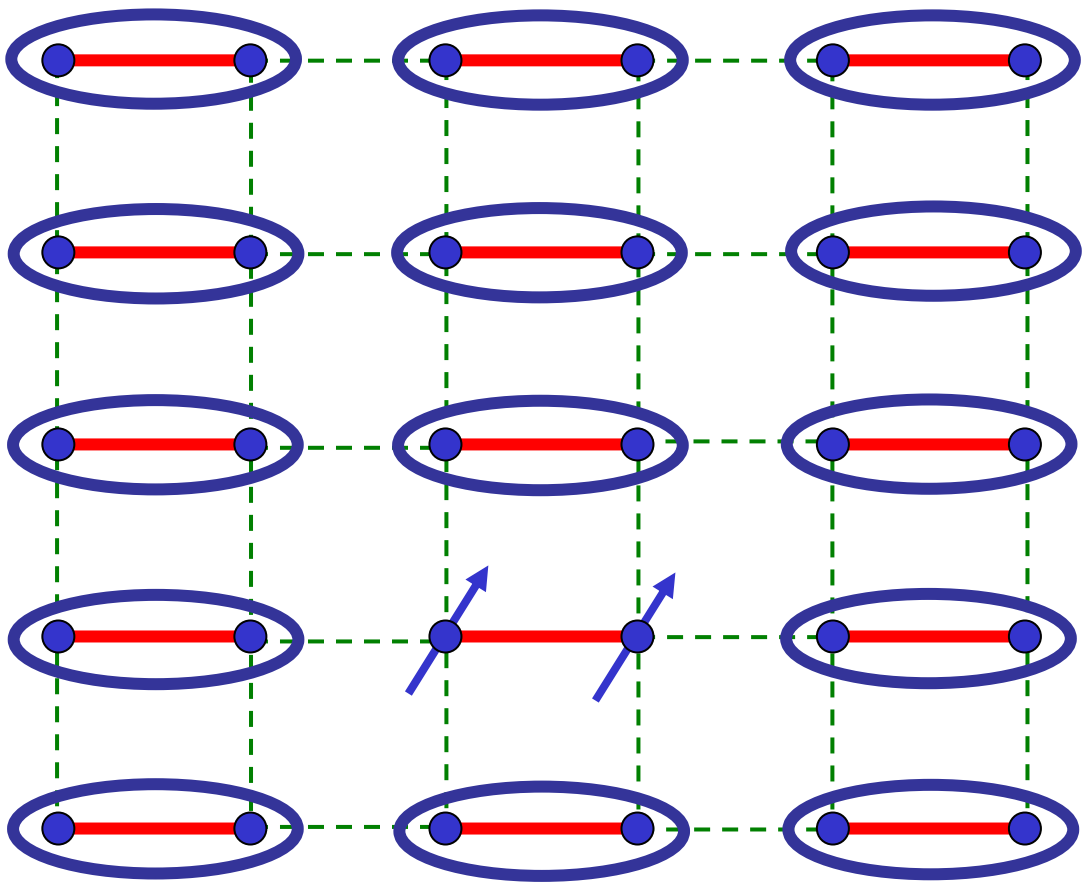


$$\text{dimer} = \frac{1}{\sqrt{2}} (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$$

Excitation:  $S=1$  *triplon*

$\lambda$  close to 0

Weakly coupled dimers

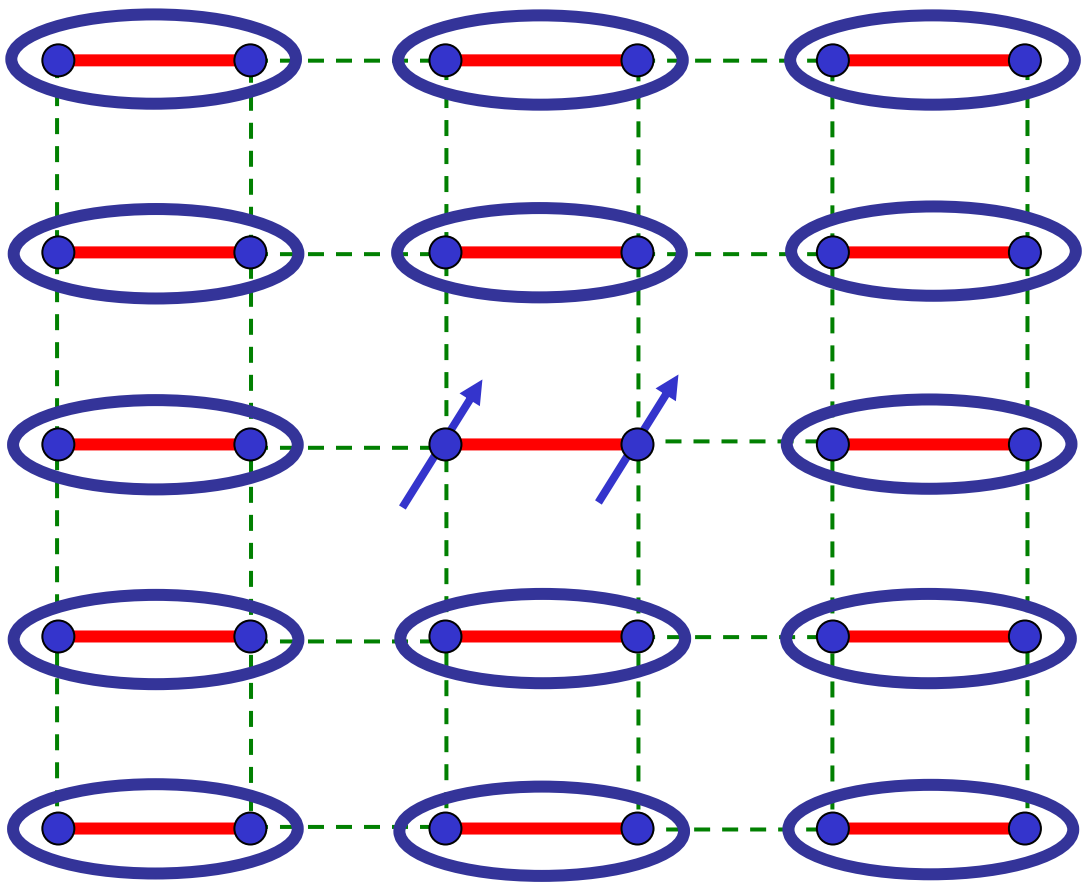


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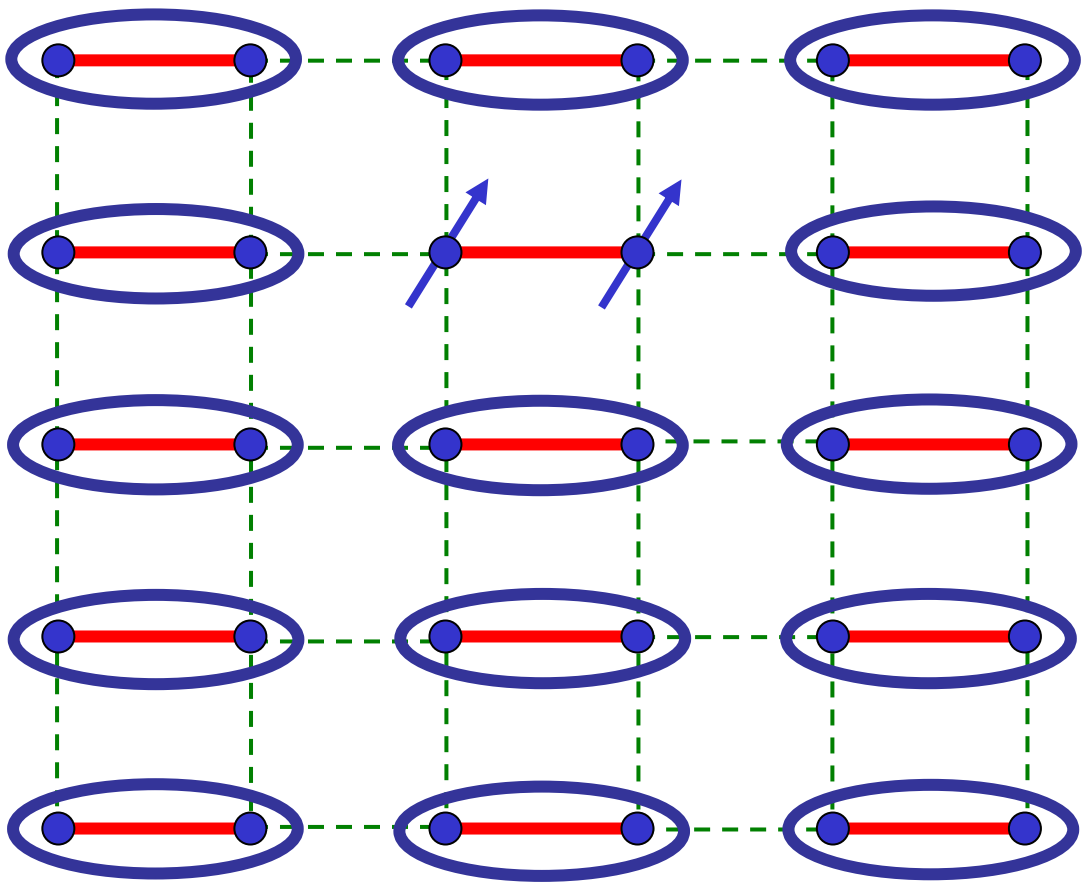


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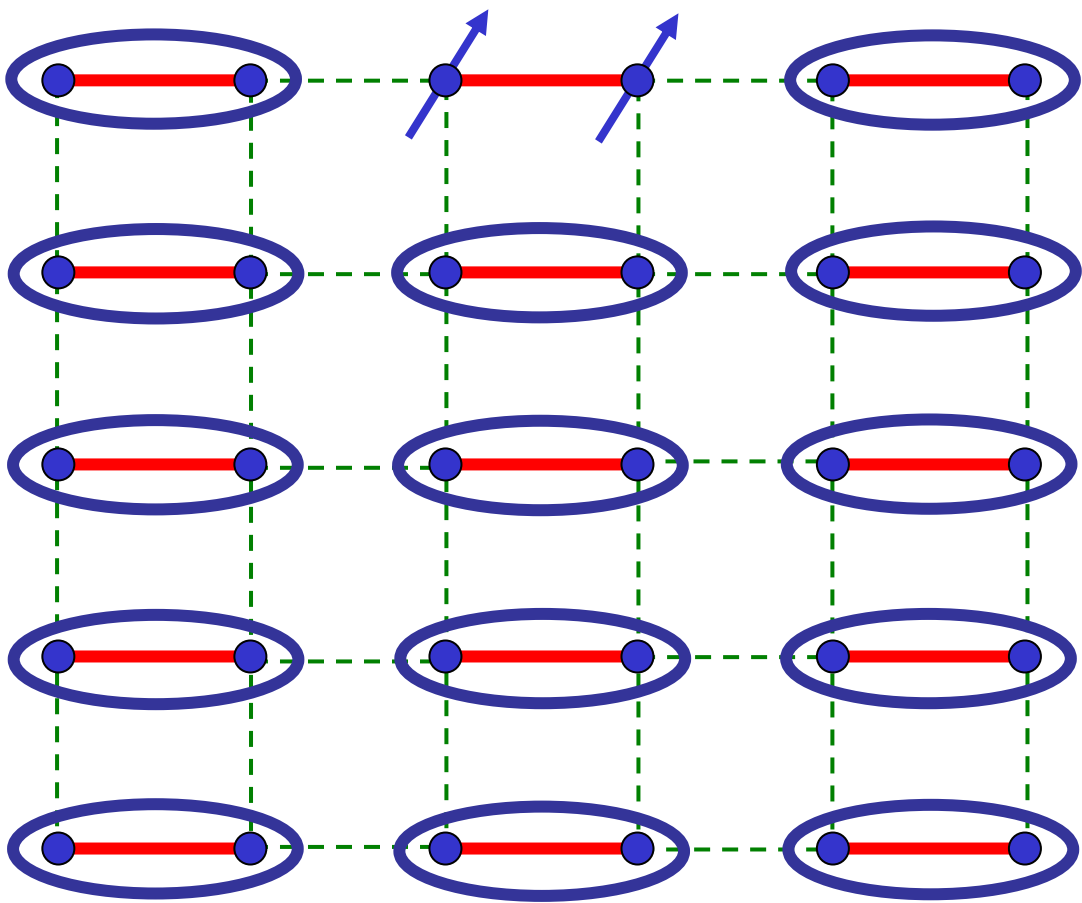


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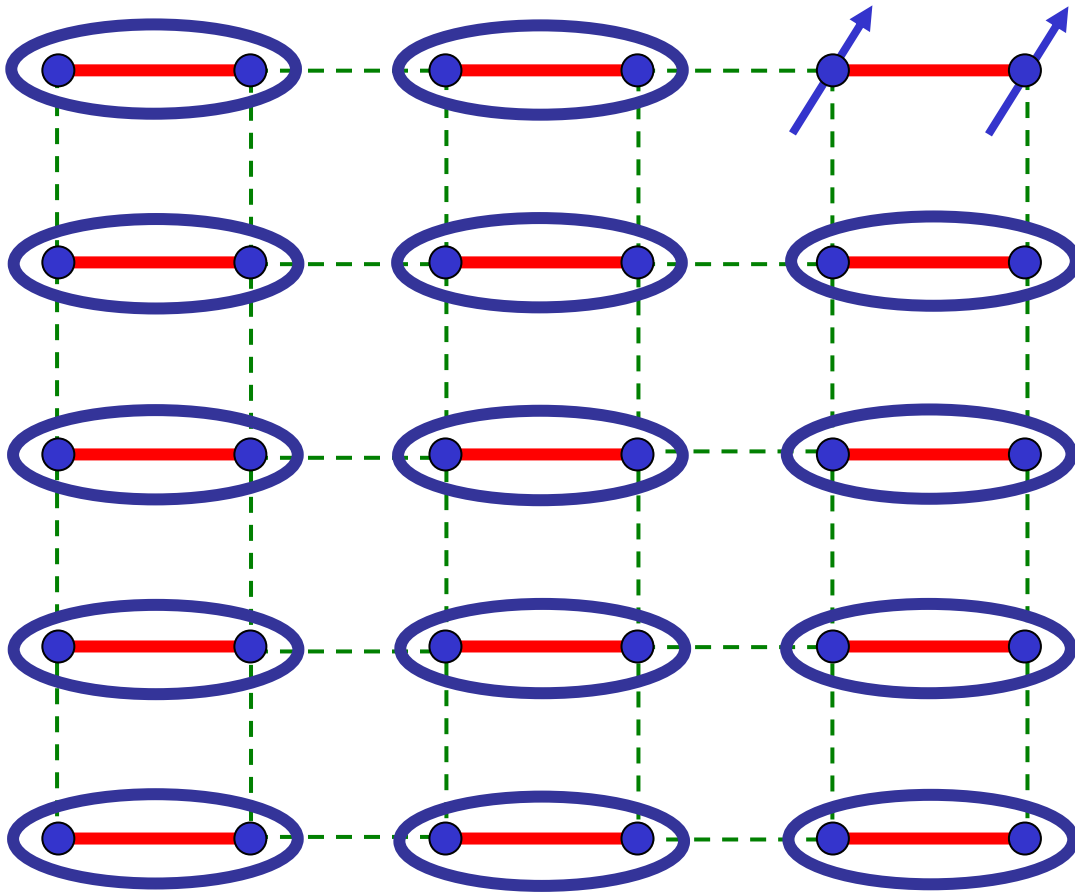


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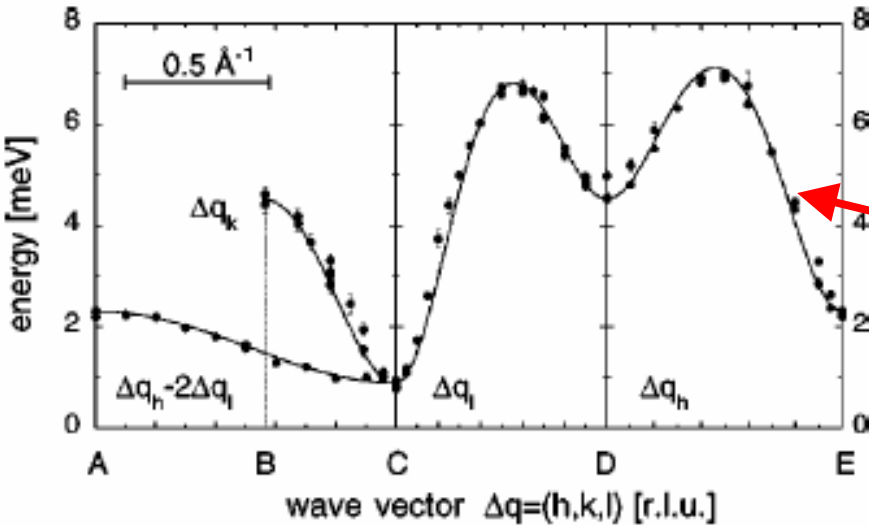
Excitation:  $S=1$  *triplon*  
(*exciton*, spin collective mode)

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

# 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).

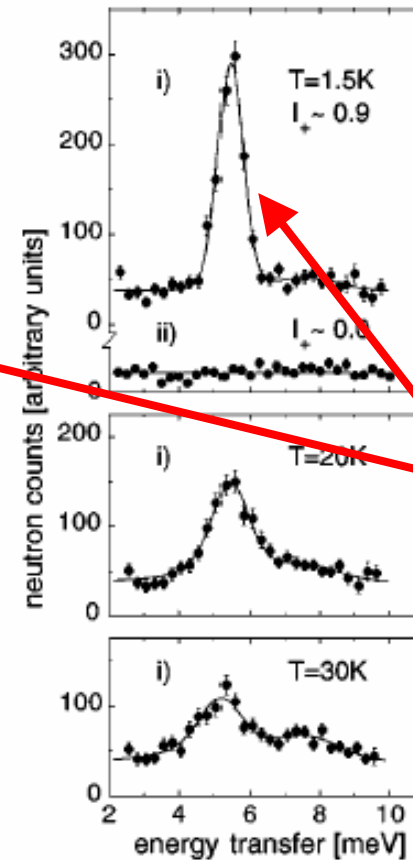


FIG. 1. Measured neutron profiles in the  $a^*c^*$  plane of TlCuCl<sub>3</sub> for  $i=(1.35,0,0)$ ,  $ii=(0,0,3.15)$  [r.l.u.]. The spectrum at  $T=1.5$  K

“triplon”

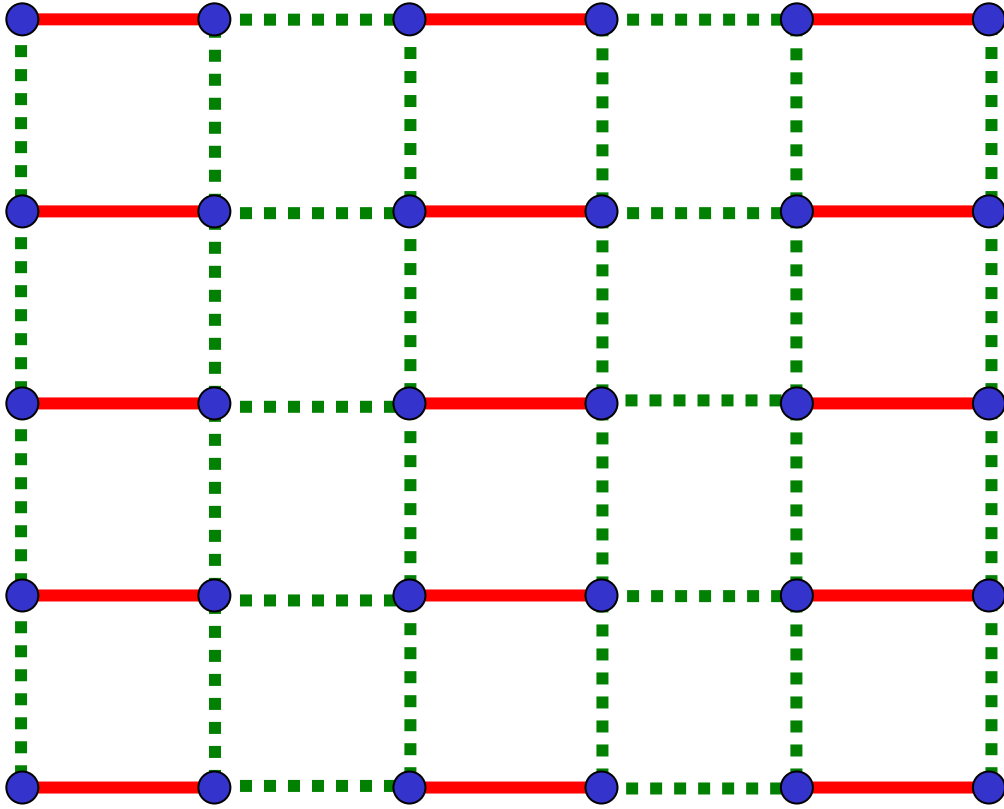
For quasi-one-dimensional systems, the triplon linewidth takes

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)

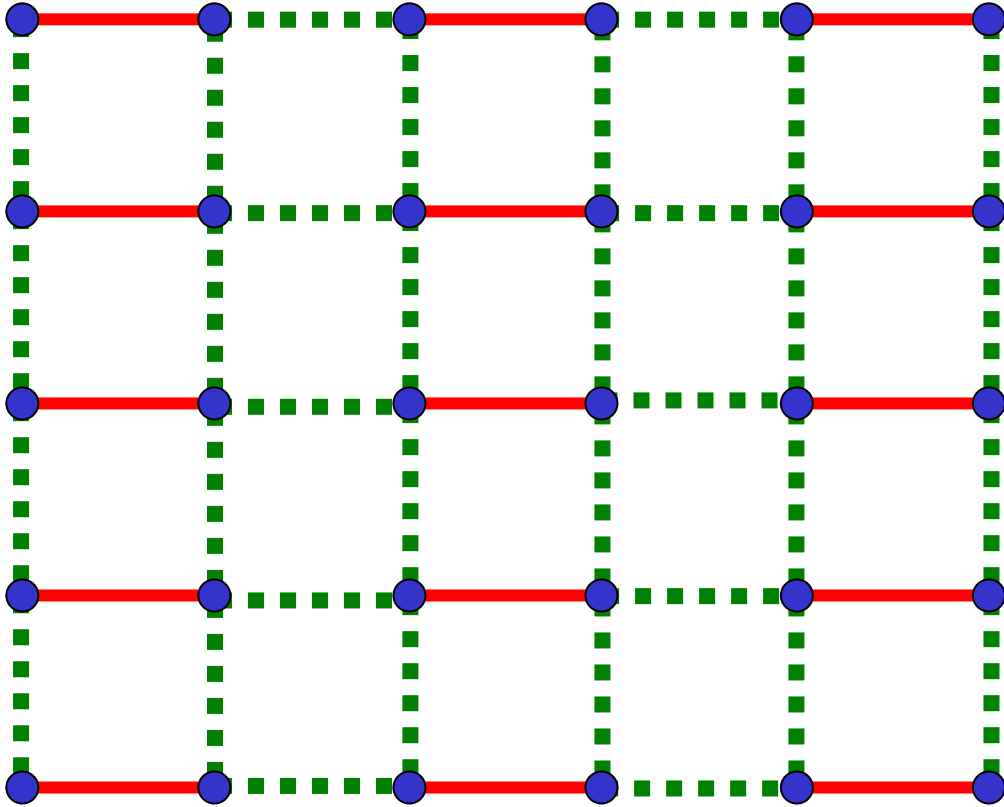
This result is in good agreement with observations in CsNiCl<sub>3</sub> (M. Kenzelmann, R. A. Cowley, W. J. L. Buyers, R. Coldea, M. Enderle, and D. F. McMorrow *Phys. Rev. B* 66, 174412 (2002)) and Y<sub>2</sub>NiBaO<sub>5</sub> (G. Xu, C. Broholm, G. Aeppli, J. F. DiTusa, T. Ito, K. Oka, and H. Takagi,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

# Coupled Dimer Antiferromagnet



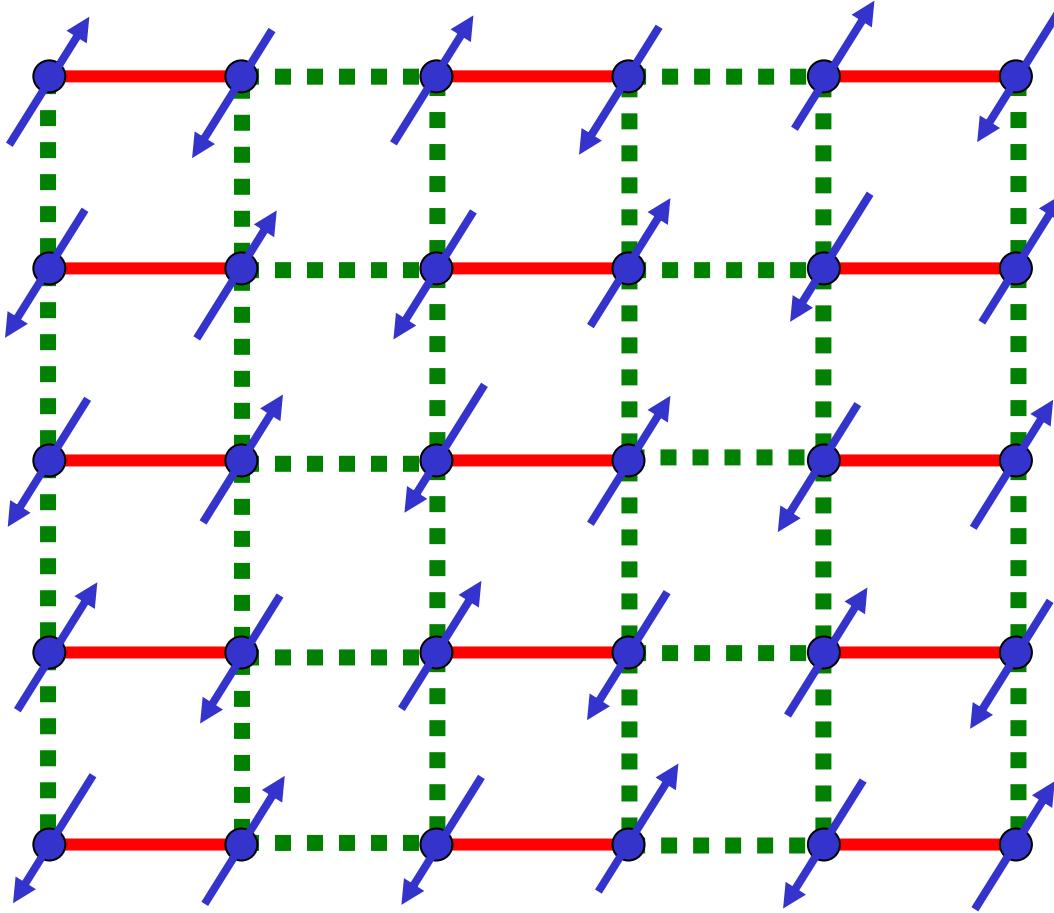
$\lambda$  close to 1

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>

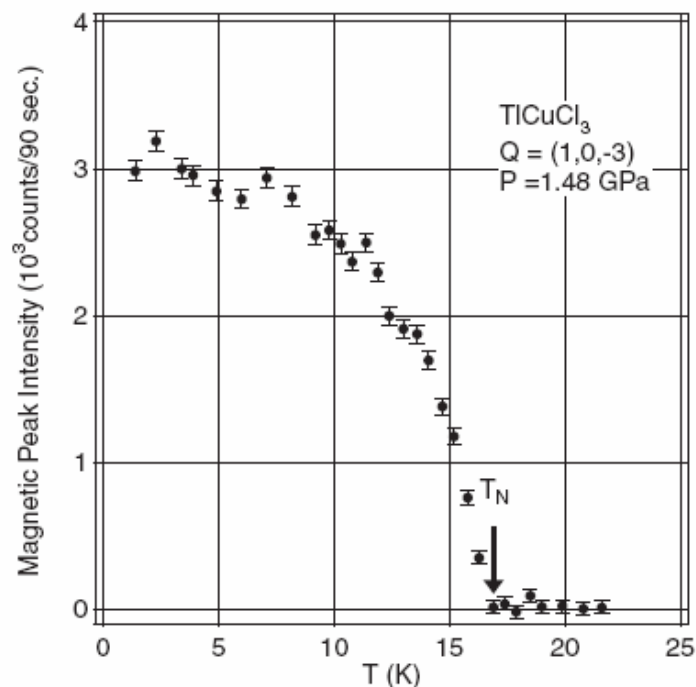
Akira OOSAWA\*, Masashi FUJISAWA<sup>1</sup>, Toyotaka OSAKABE, Kazuhisa KAKURAI and Hidekazu TANAKA<sup>2</sup>

*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)



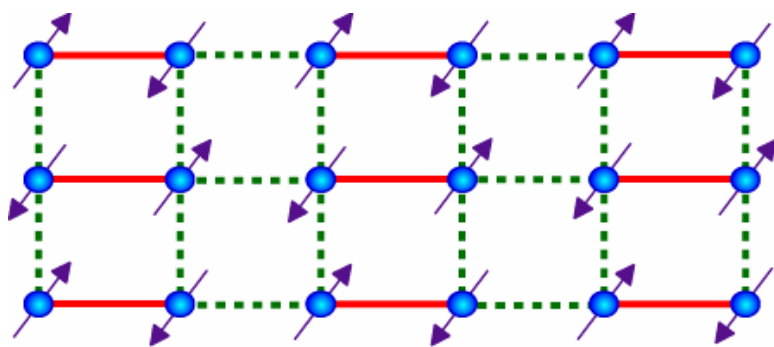
*J. Phys. Soc. Jpn* **72**, 1026 (2003)

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>.

$T=0$

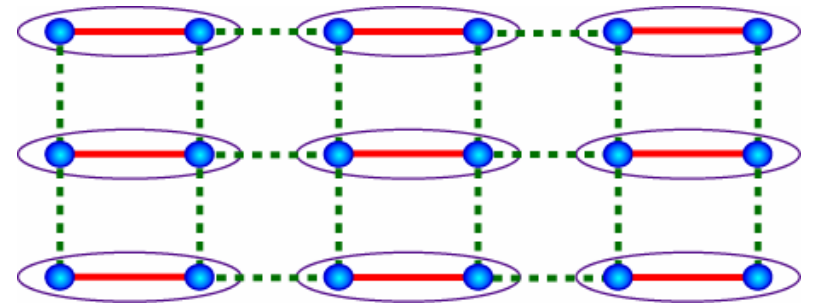
$$\lambda_c = 0.52337(3)$$

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

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

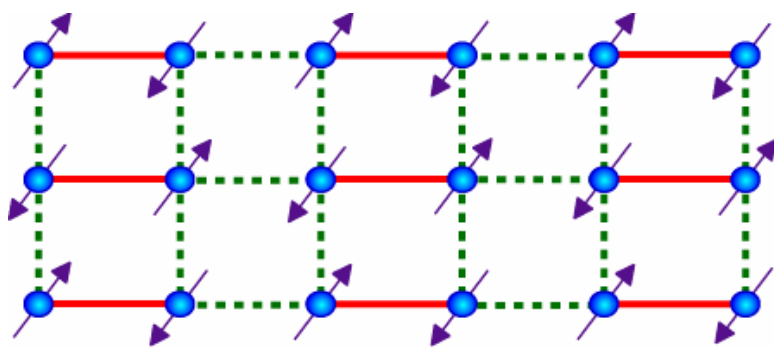


The method of bond operators (S. Sachdev and R.N. Bhatt, *Phys. Rev. B* **41**, 9323 (1990)) provides a quantitative description of spin excitations in  $\text{TlCuCl}_3$  across the quantum phase transition (M. Matsumoto, B. Normand, T.M. Rice, and M. Sigrist, *Phys. Rev. Lett.* **89**, 077203 (2002))

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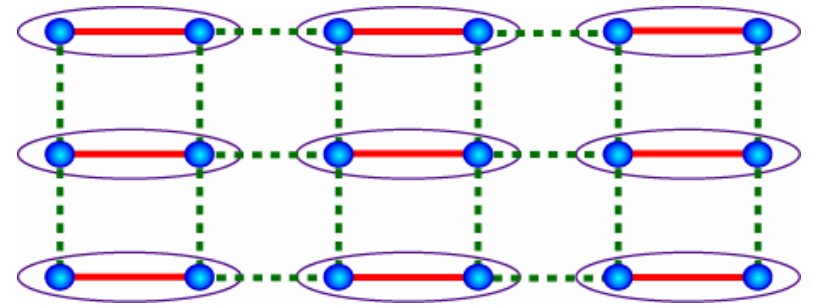
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Néel state

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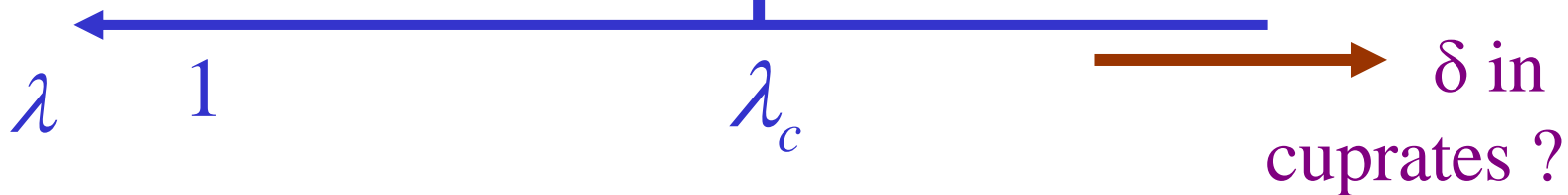


Quantum paramagnet

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

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

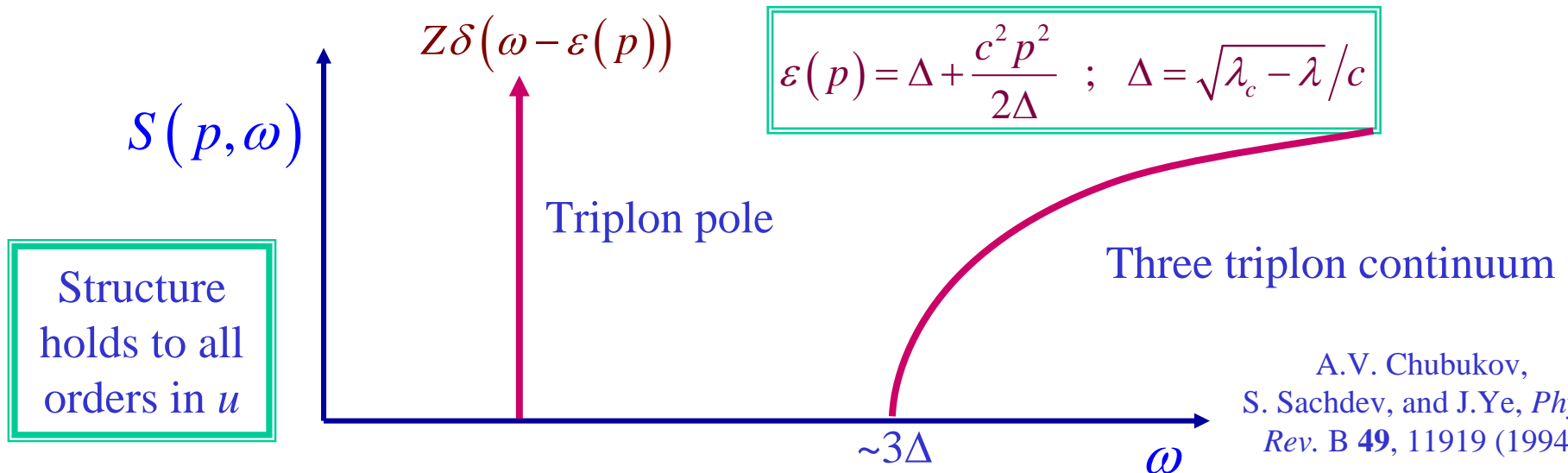
Landau-Ginzburg-Wilson theory: write down an effective action for the antiferromagnetic order parameter  $\vec{\varphi}$  by expanding in powers of  $\vec{\varphi}$  and its spatial and temporal derivatives, while preserving all symmetries of the microscopic Hamiltonian

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

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

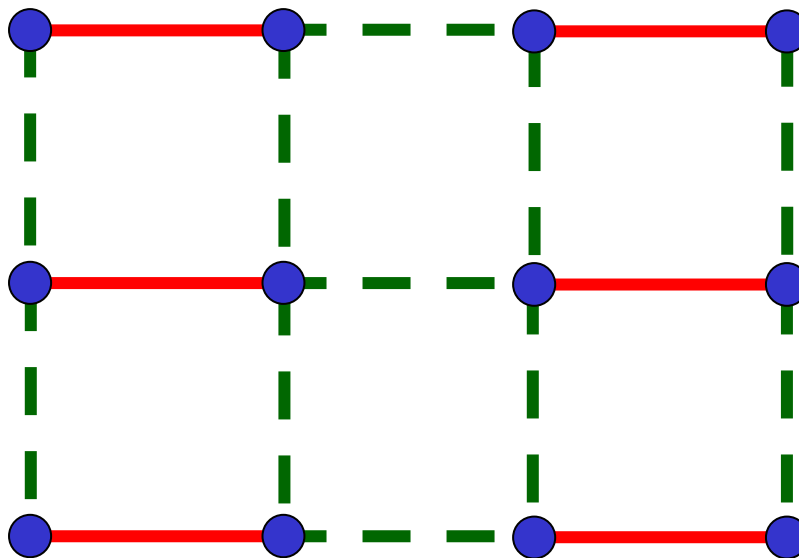
following structure in the dynamic structure factor  $S(p, \omega)$



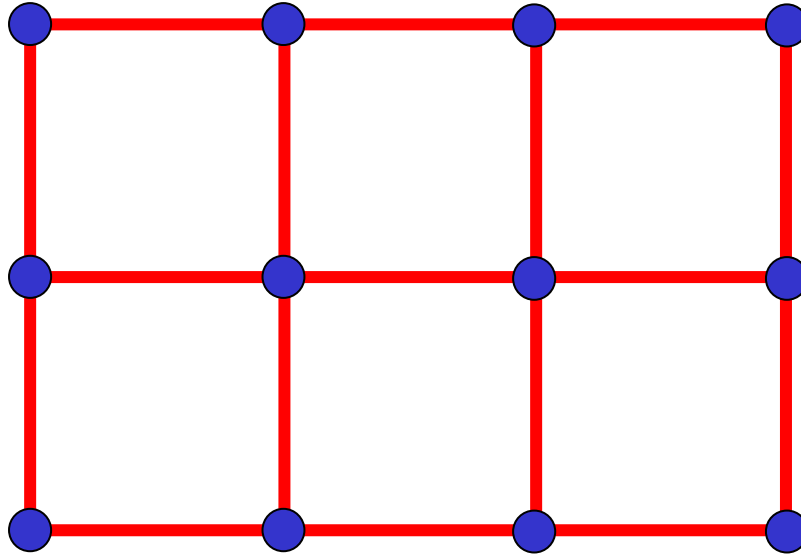
Mott insulators with spin  $S=1/2$  per unit cell:

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

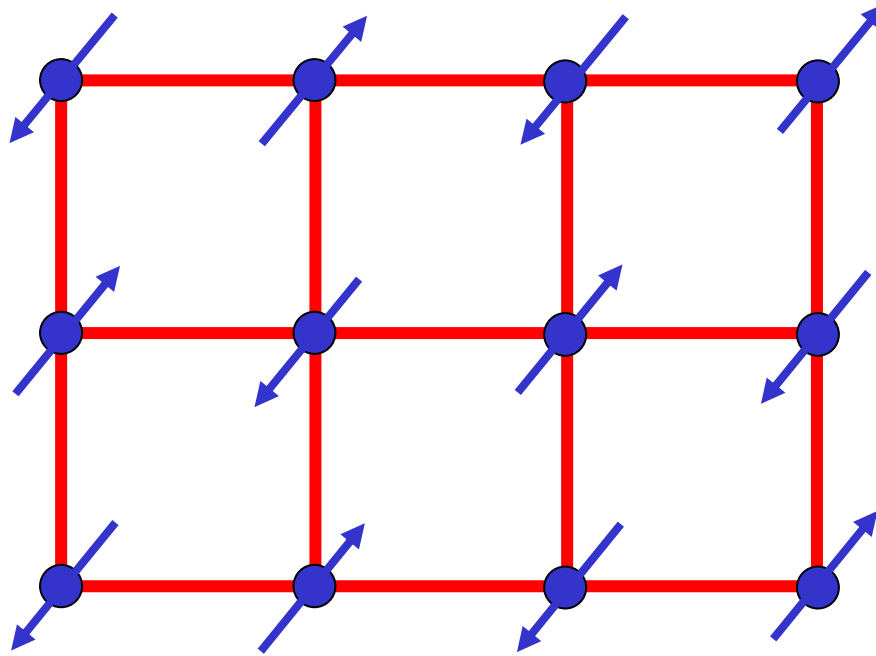
Mott insulator with two  $S=1/2$  spins per unit cell



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

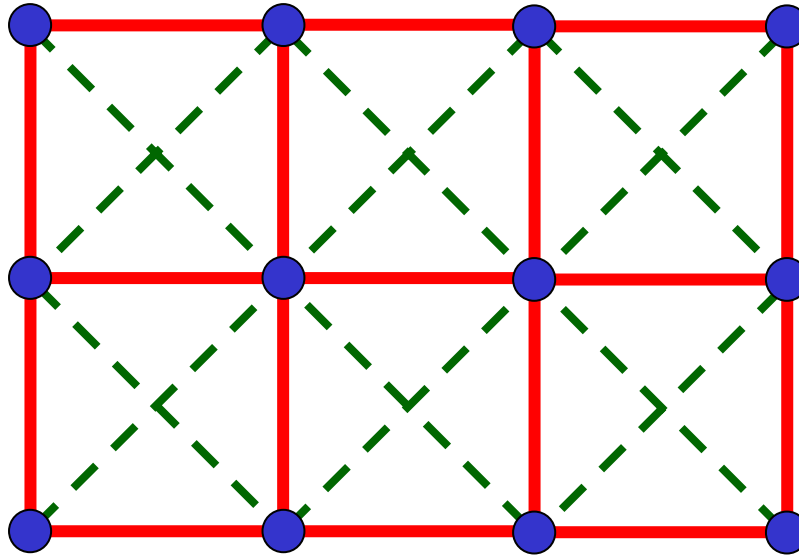


Mott insulator with one  $S=1/2$  spin per unit cell



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

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



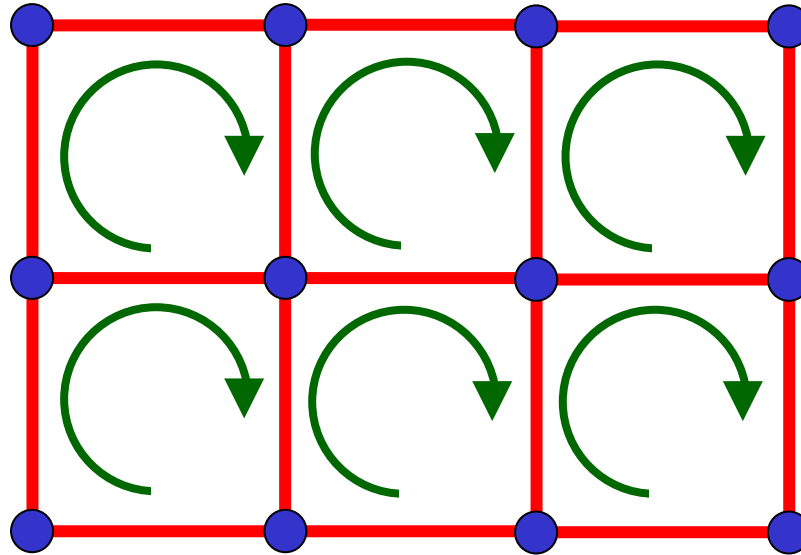
Destroy Neel order by perturbations which preserve full square lattice symmetry *e.g.* second-neighbor or ring exchange.

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



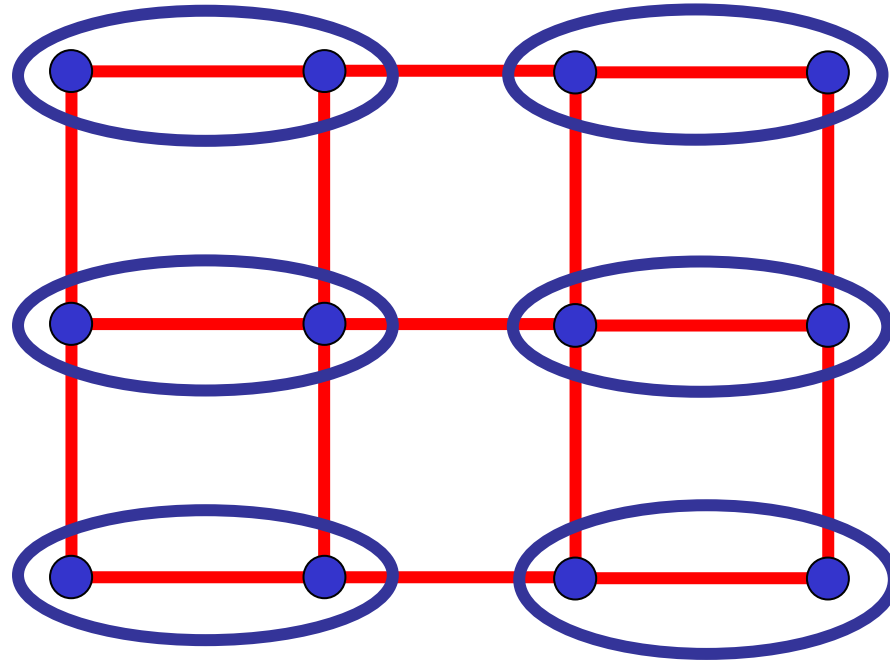
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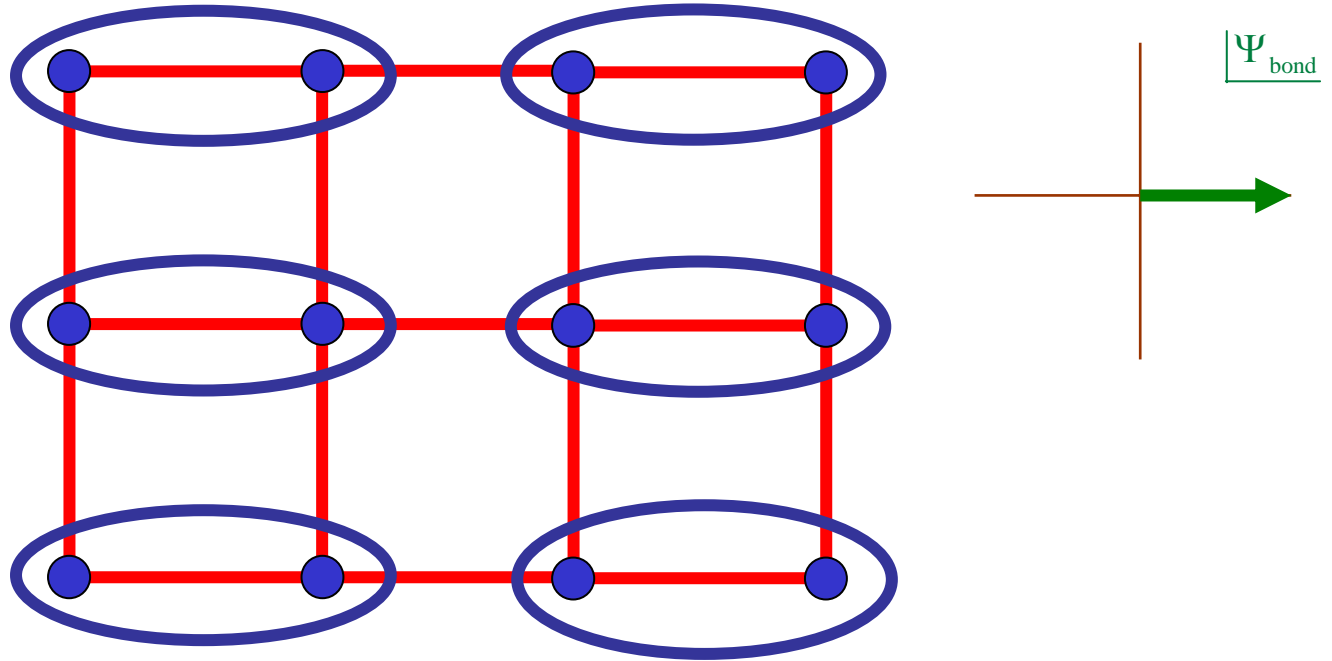
Large  $g \Rightarrow$  paramagnetic ground state with  $\langle \vec{\phi} \rangle = 0$

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



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

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

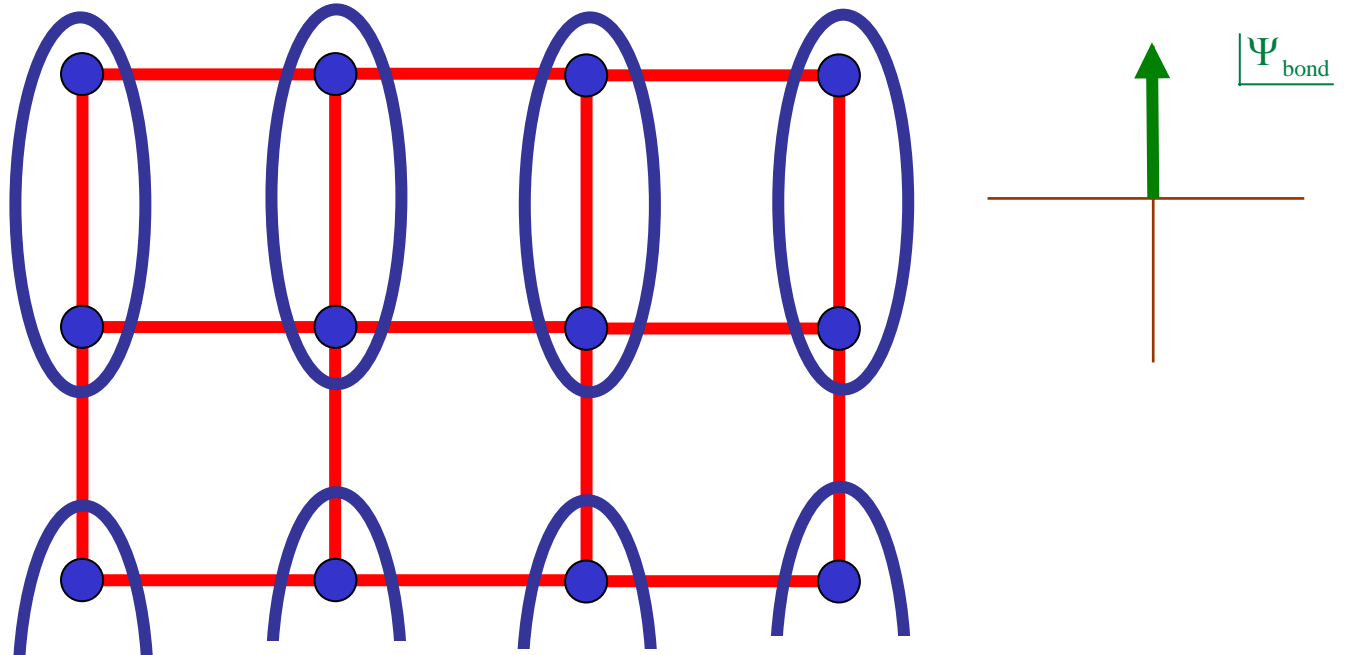


Possible large  $g$  paramagnetic ground state (**Class A**) with  $\langle \vec{\phi} \rangle = 0$

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

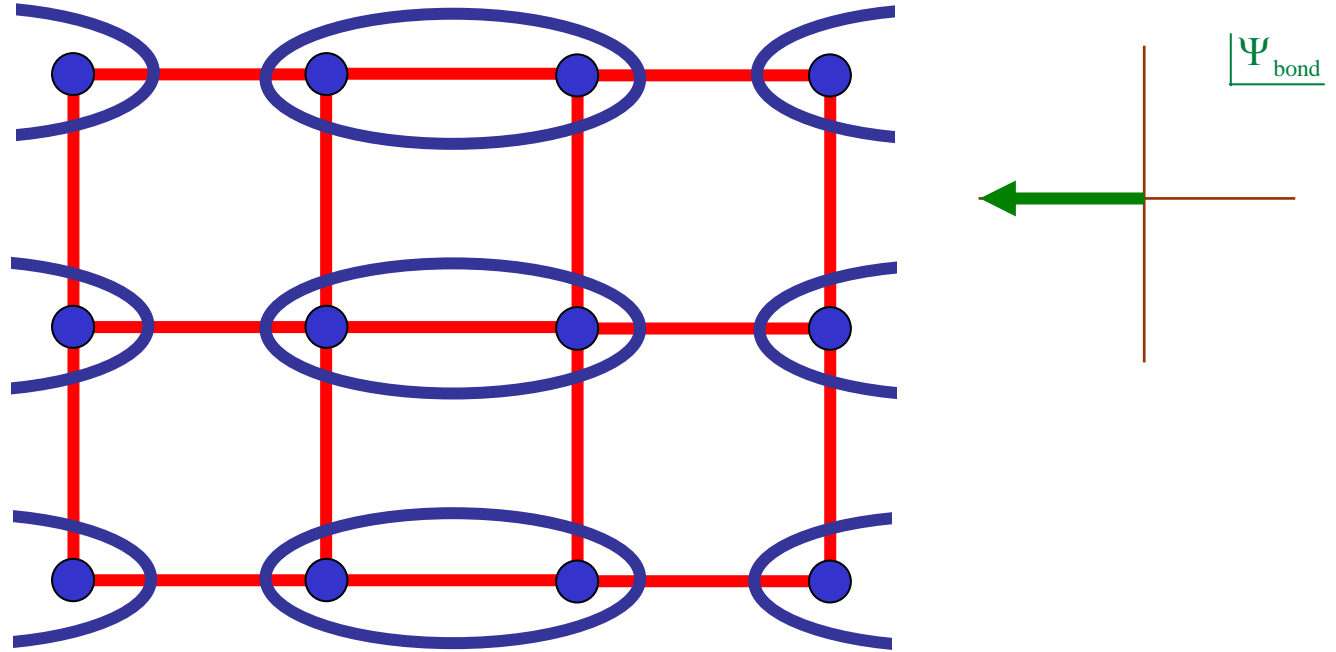


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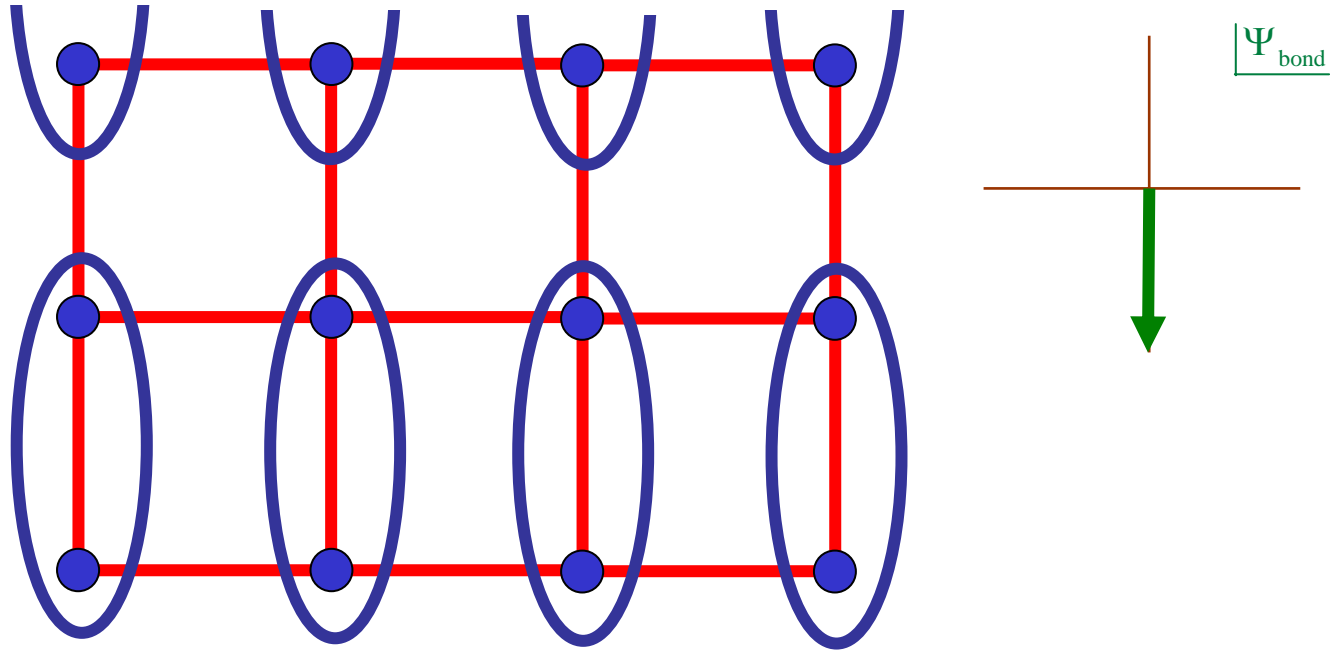


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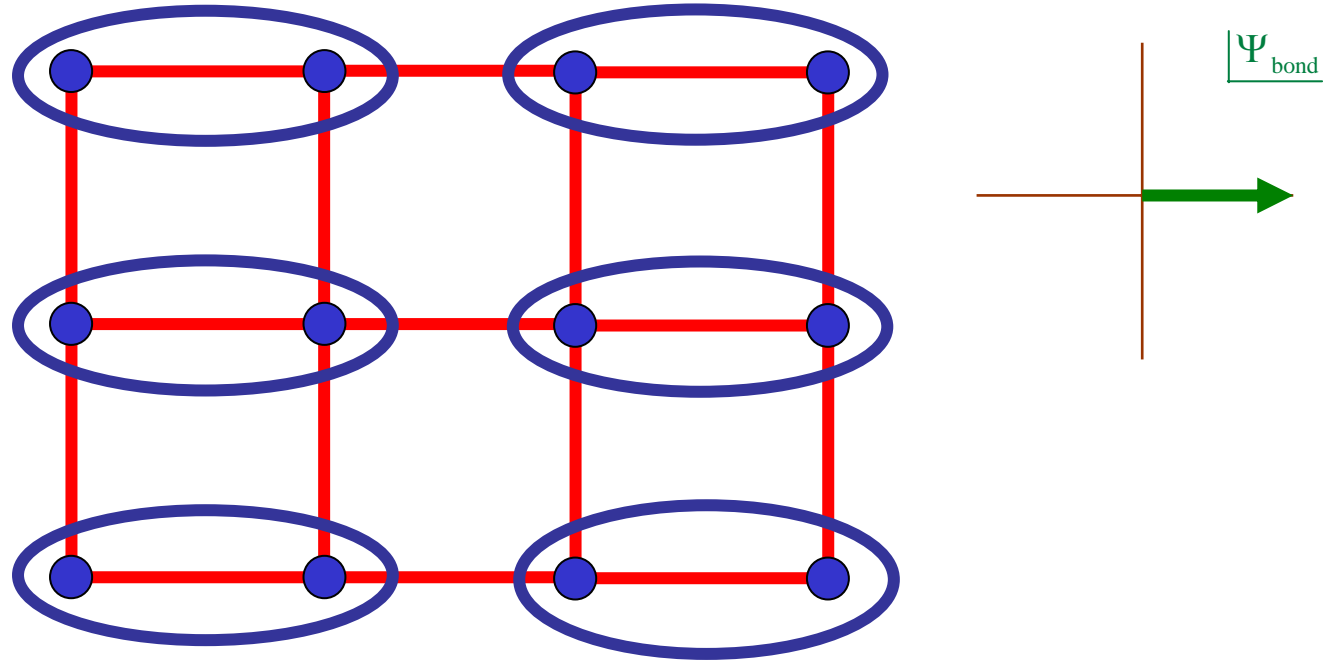


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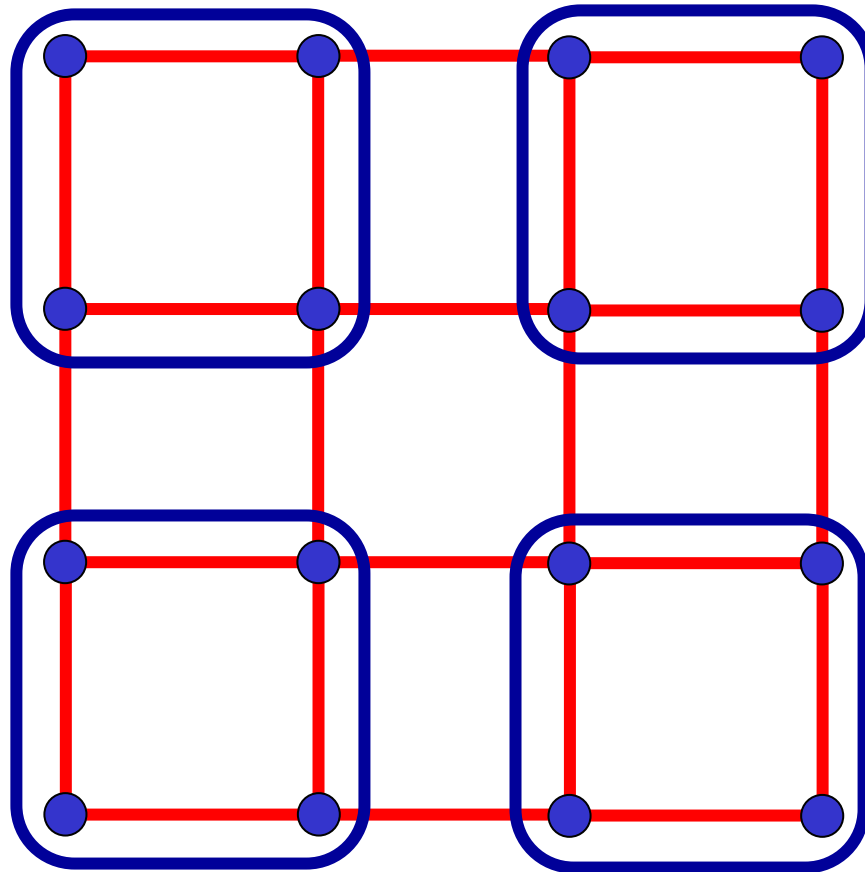


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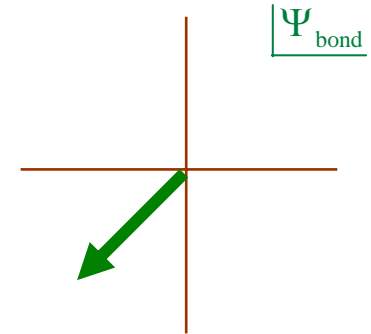
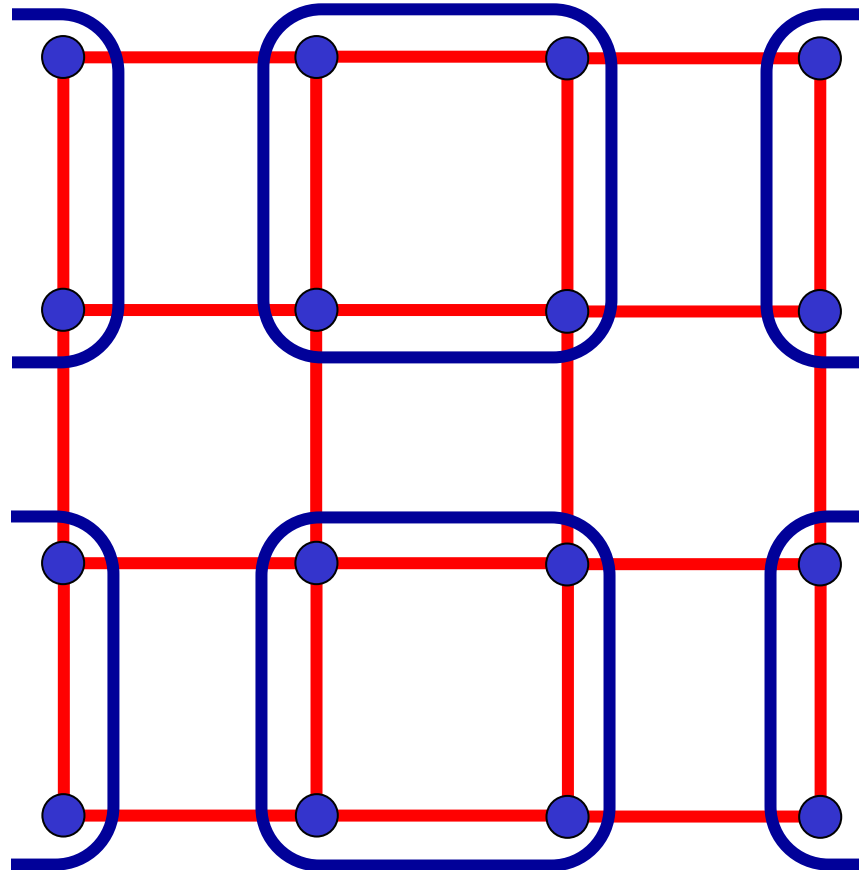


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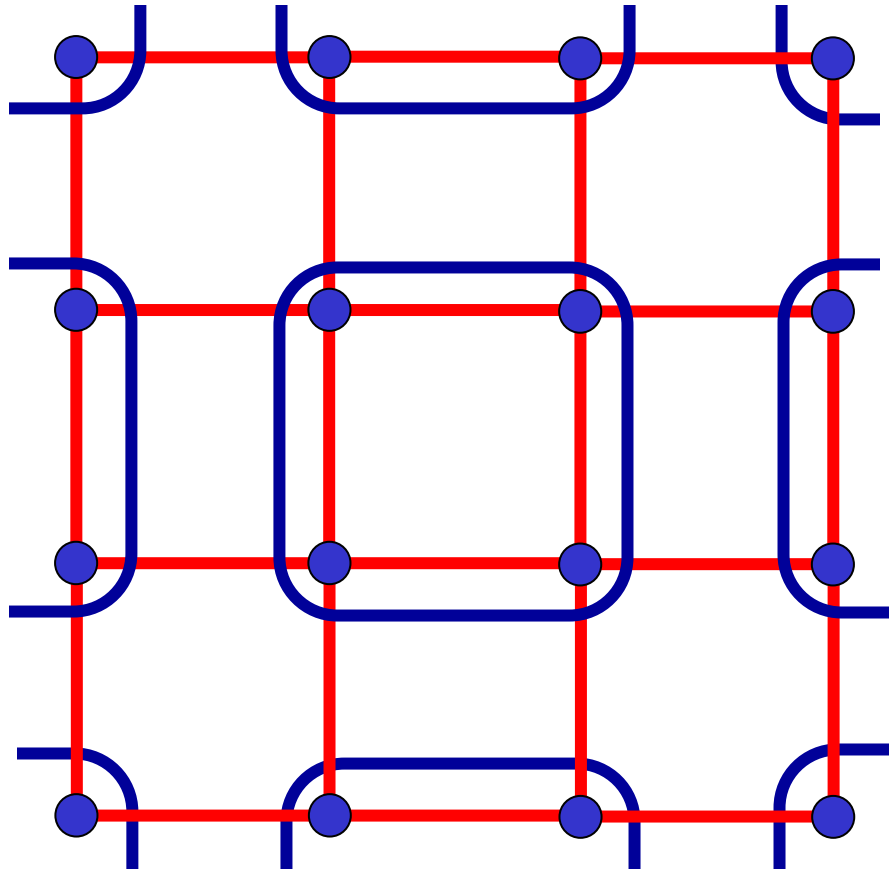


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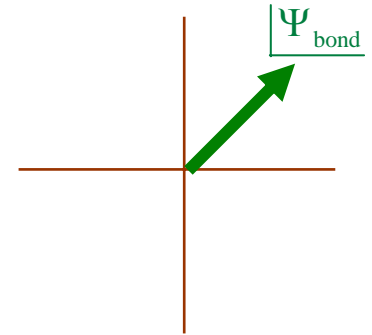
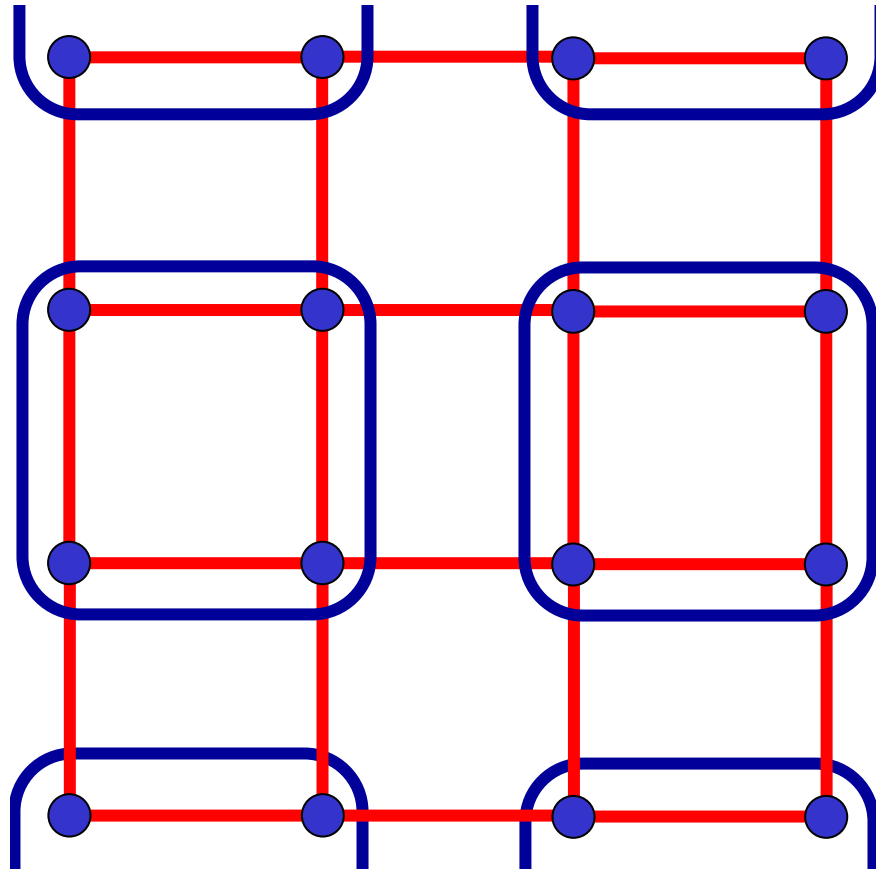


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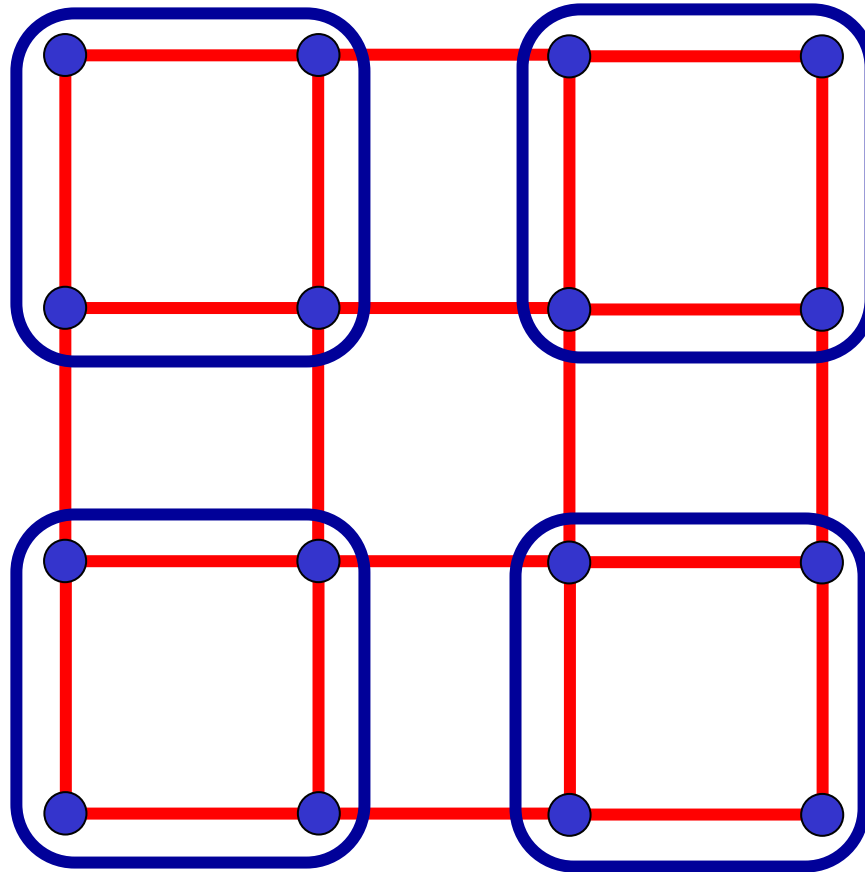


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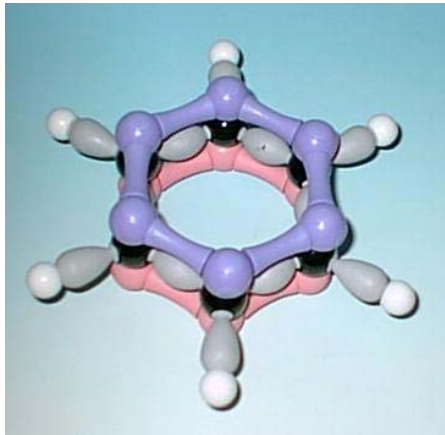
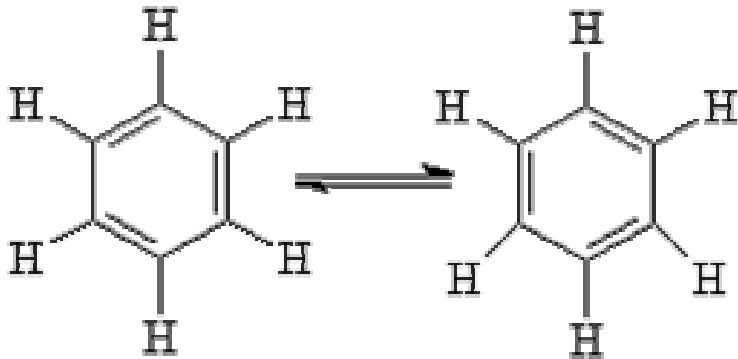


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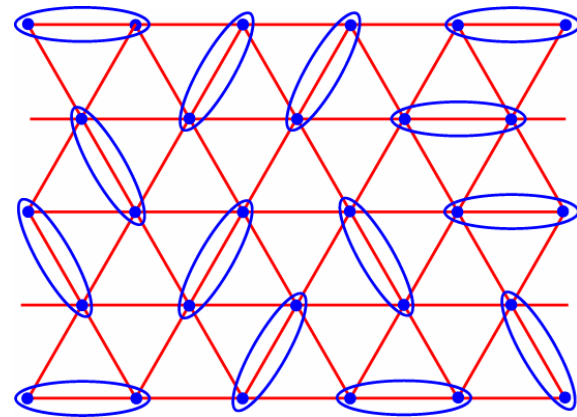
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# Resonating valence bonds



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

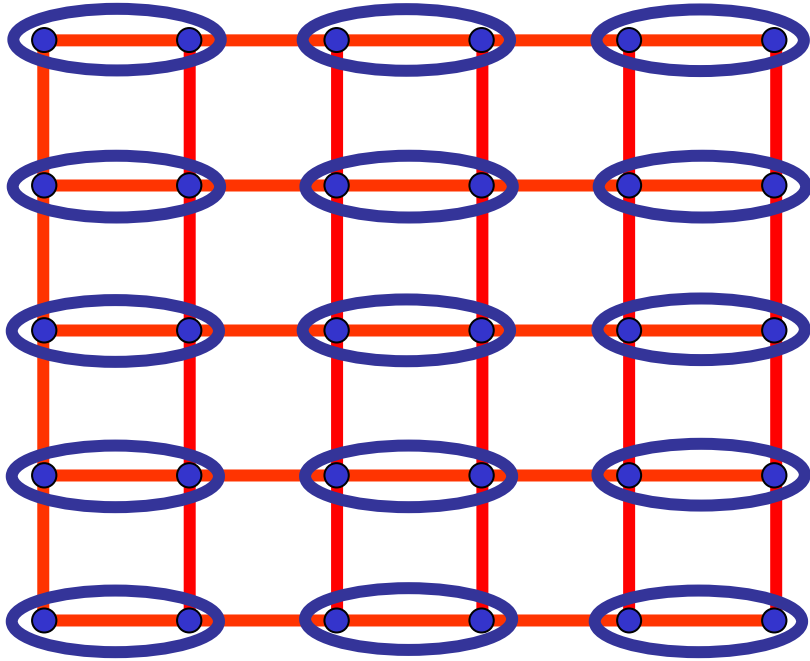
P. Fazekas and P.W. Anderson, *Phil Mag* **30**, 23 (1974); P.W. Anderson 1987

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).

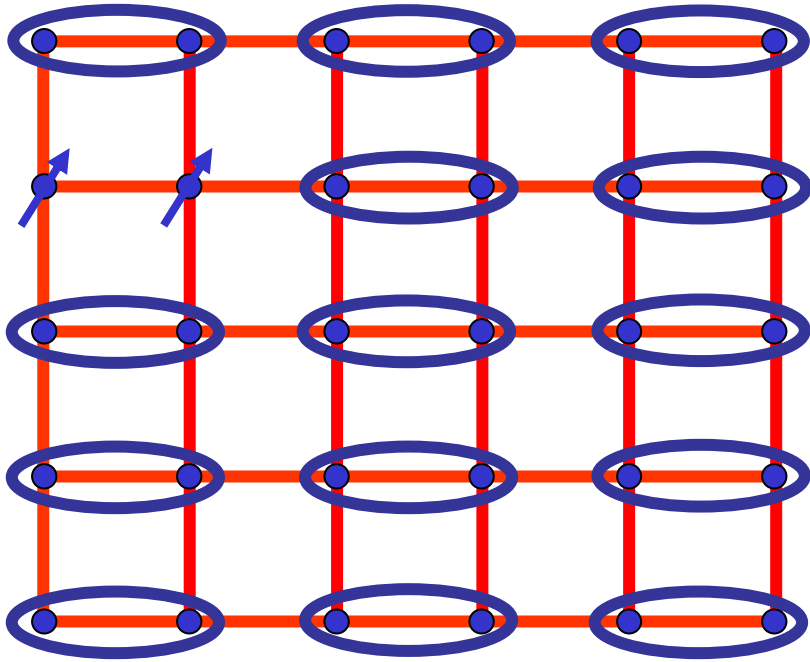
# Excitations of the paramagnet with non-zero spin

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



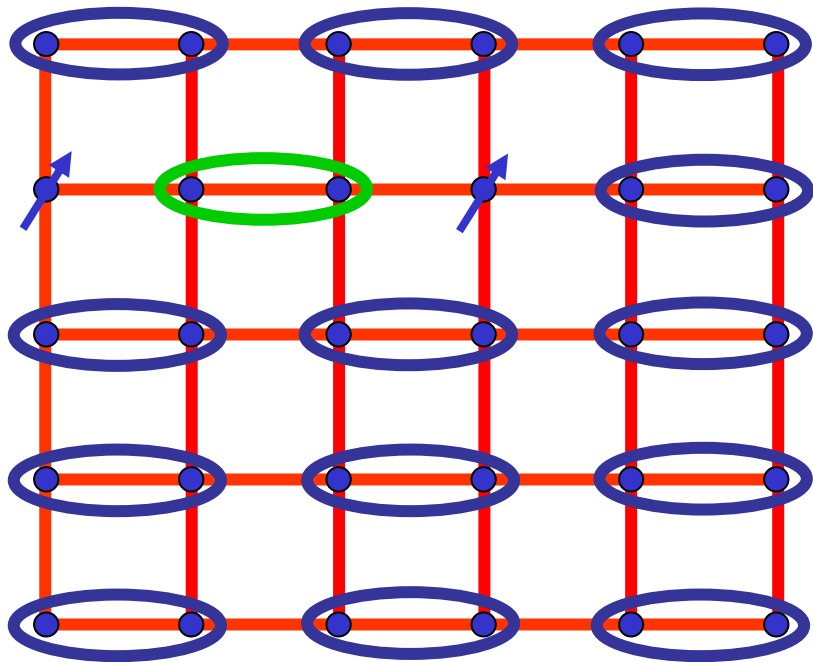
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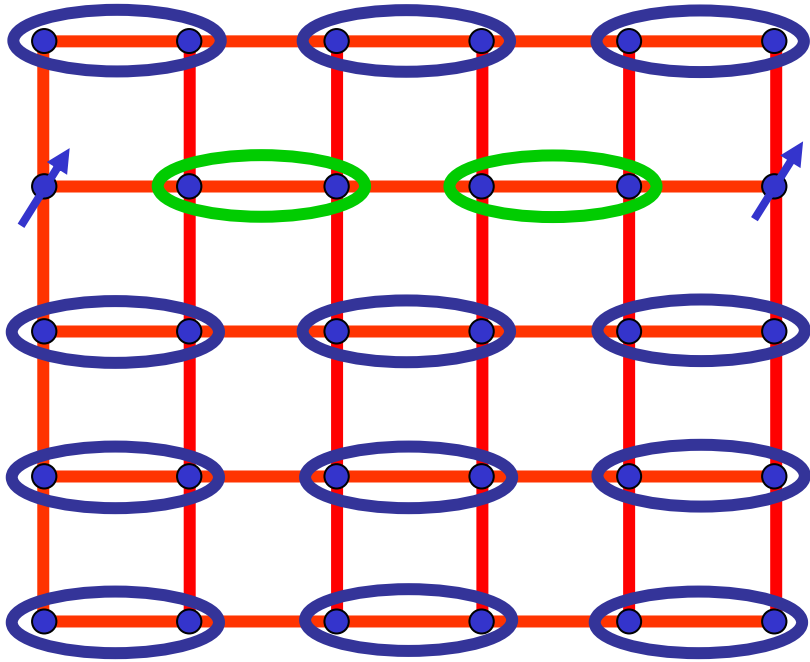
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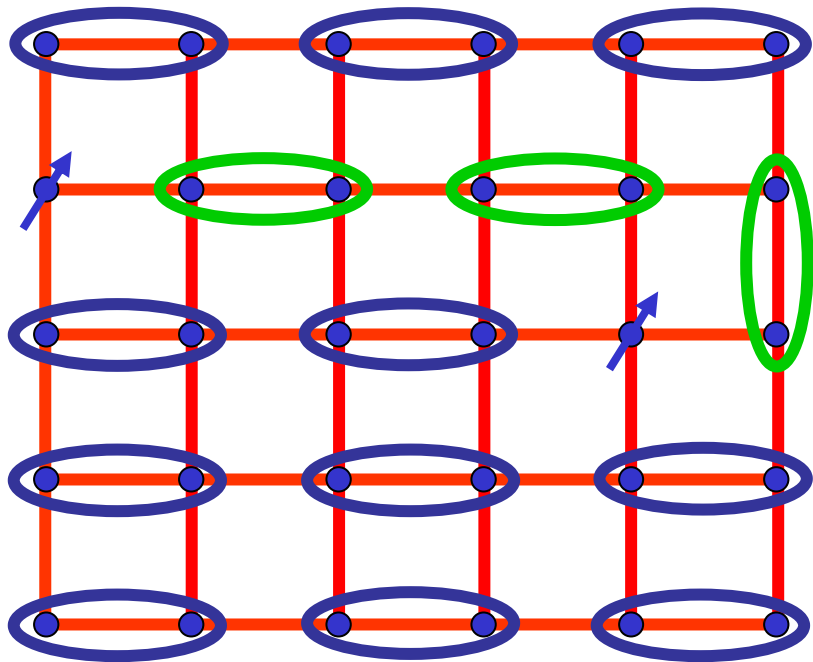
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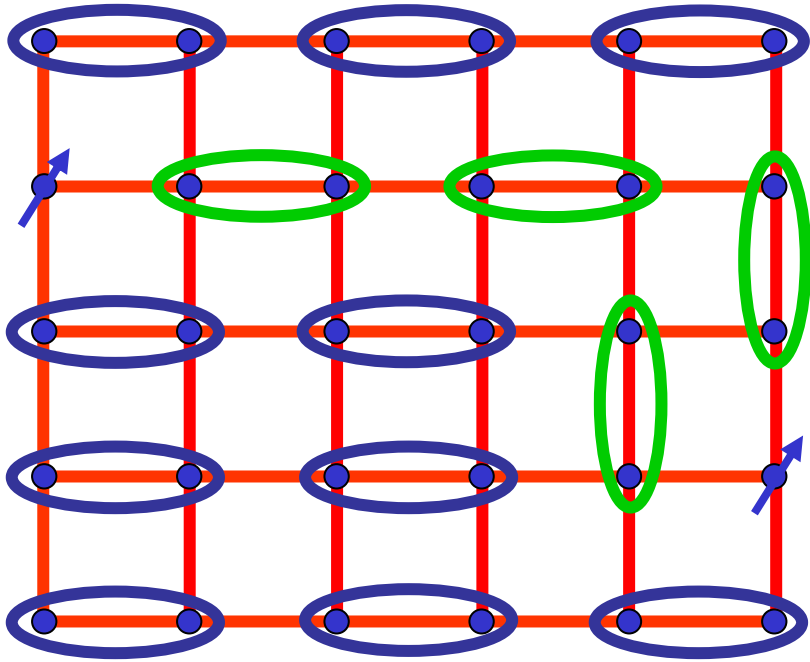
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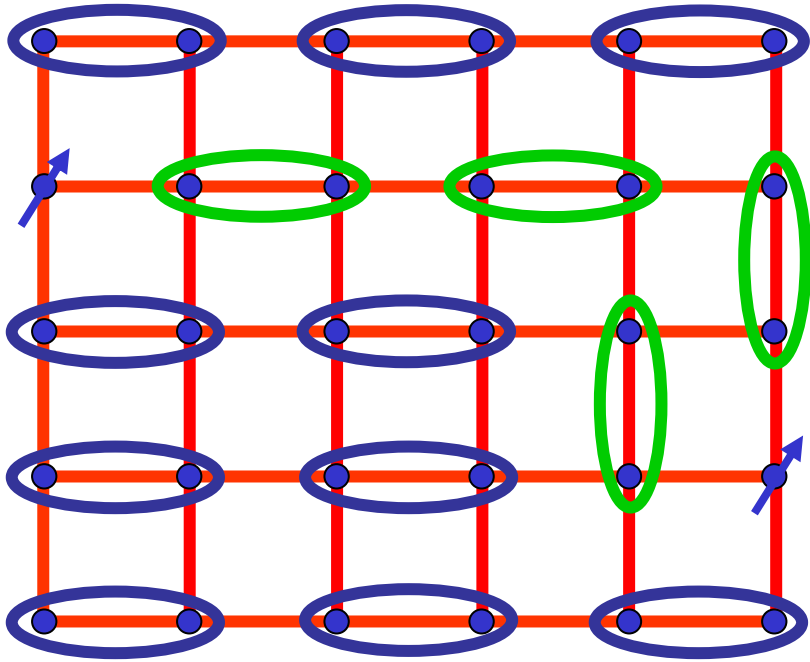


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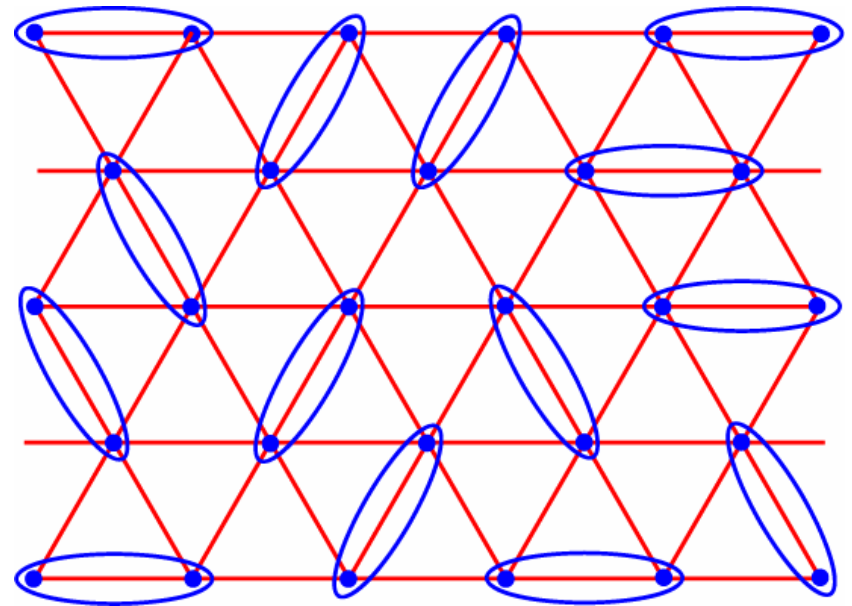
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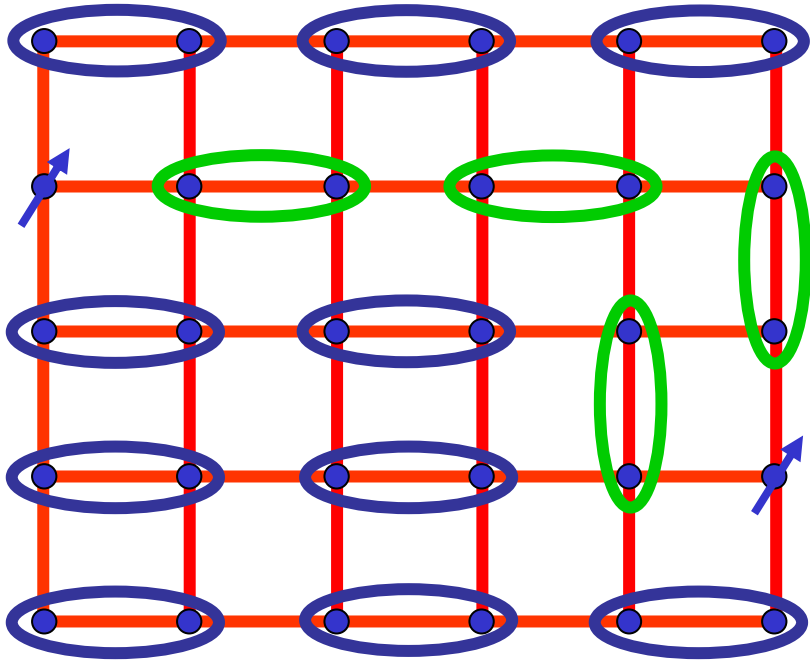
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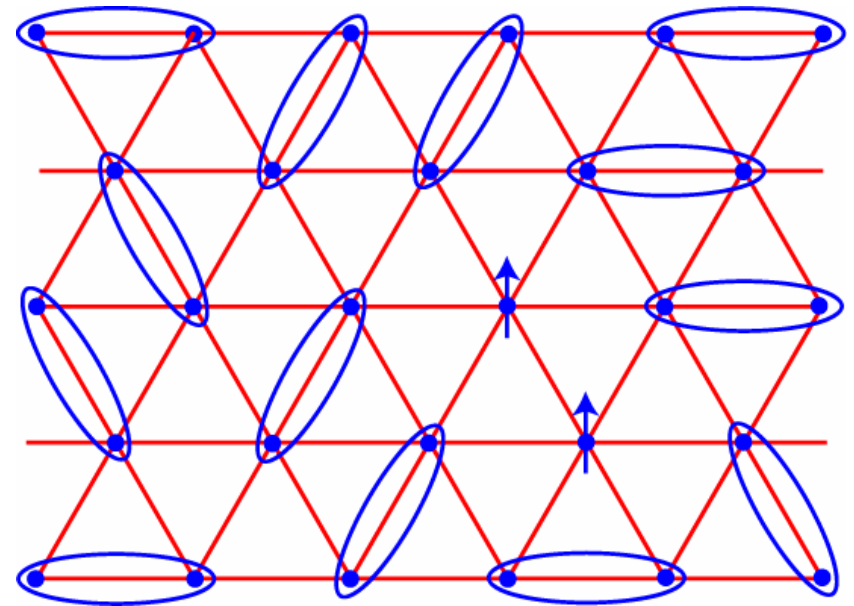
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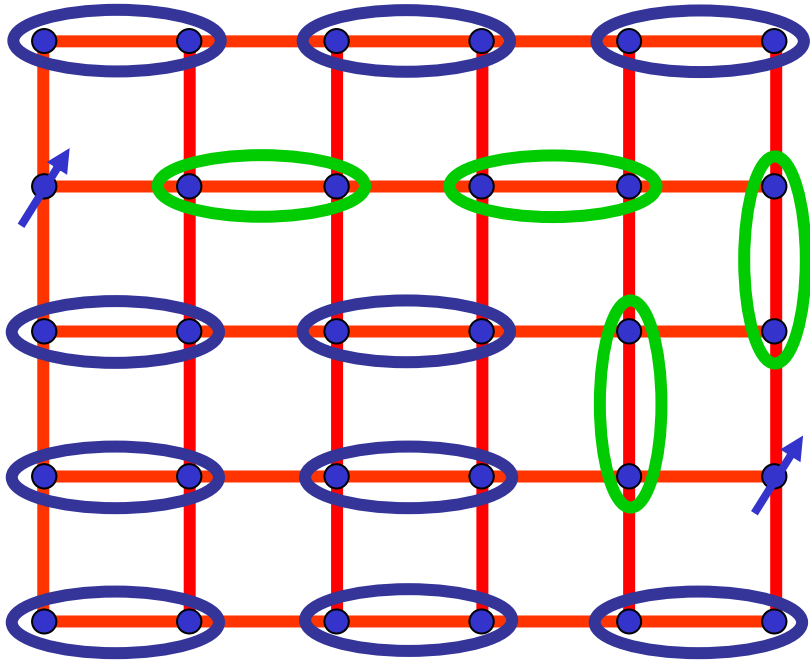
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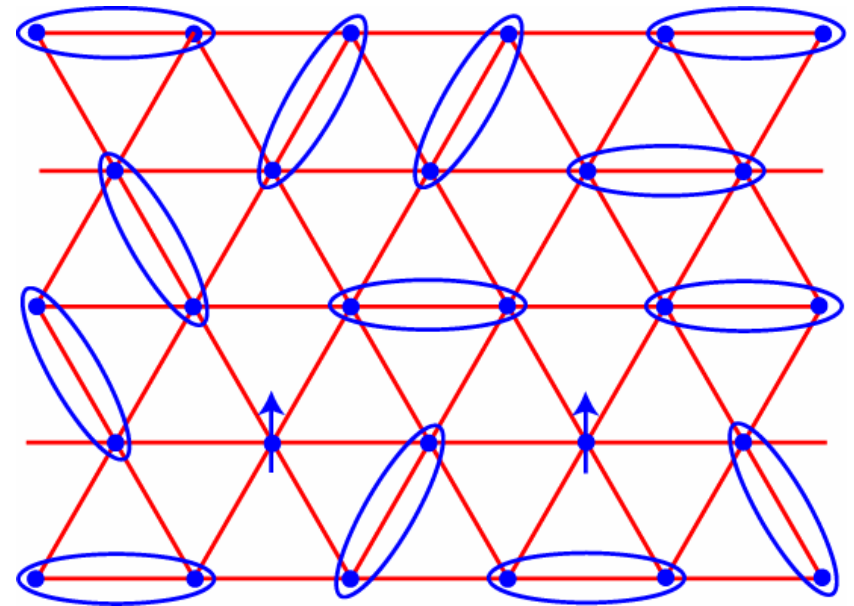
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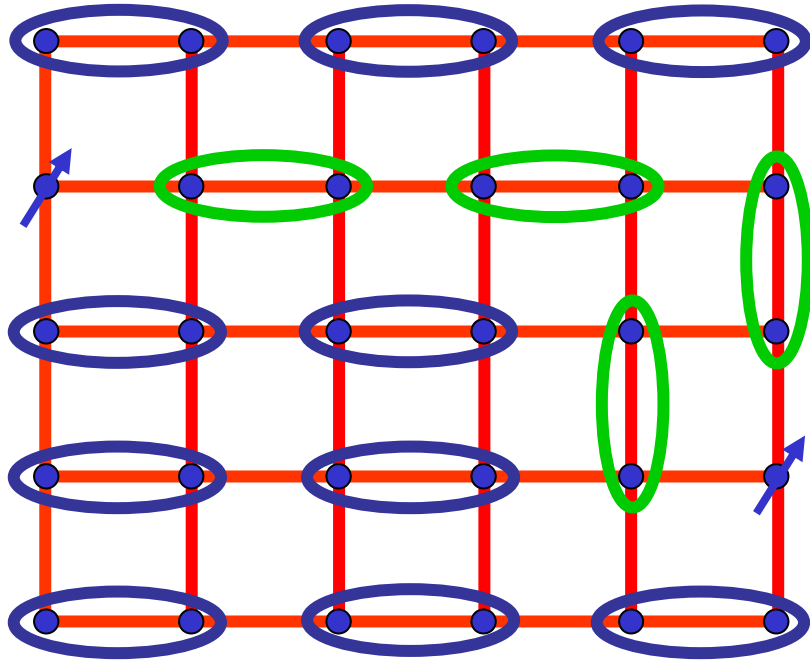
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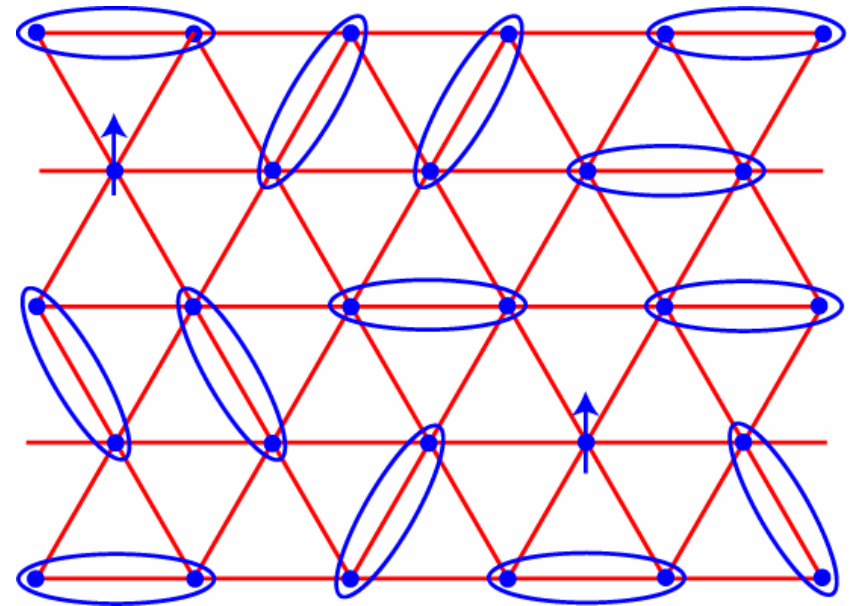
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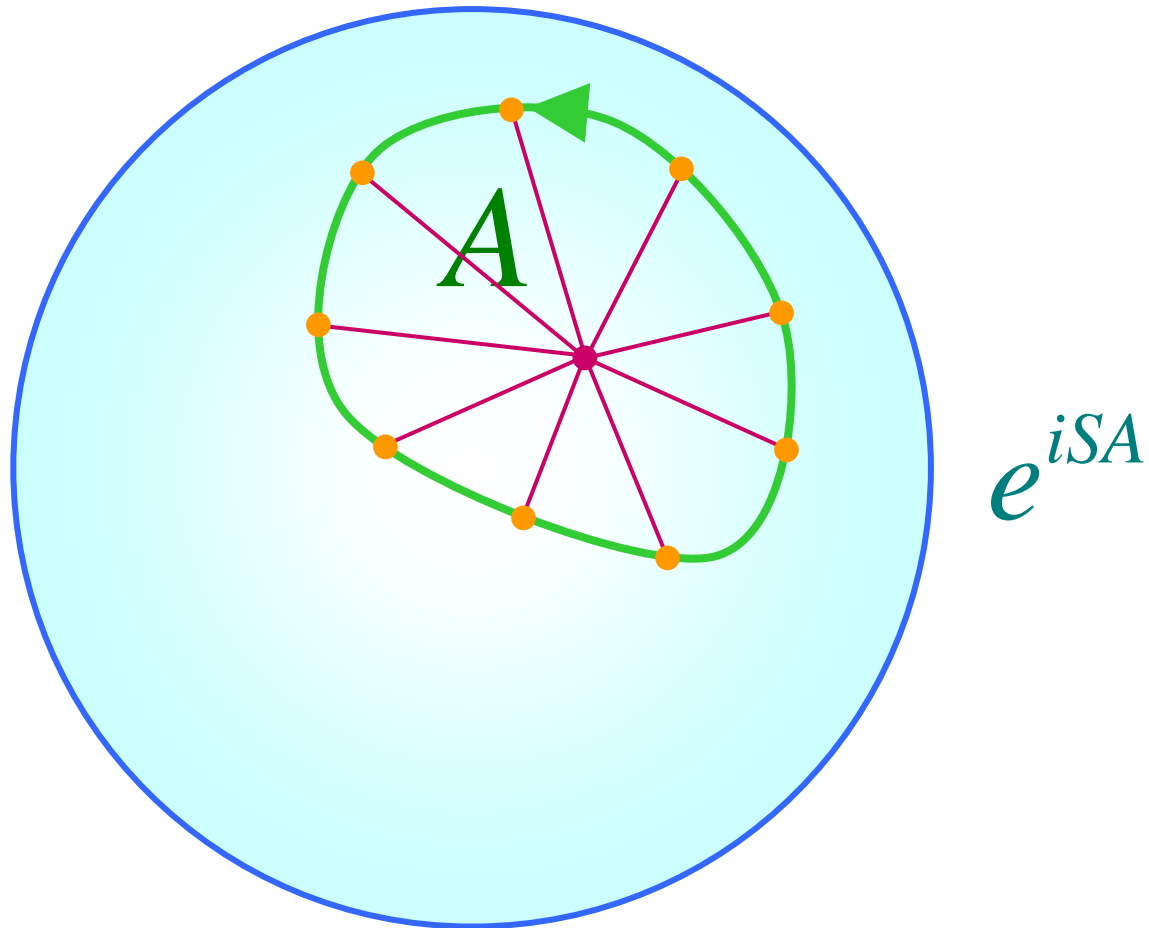
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$S=1/2$  *spinons* can  
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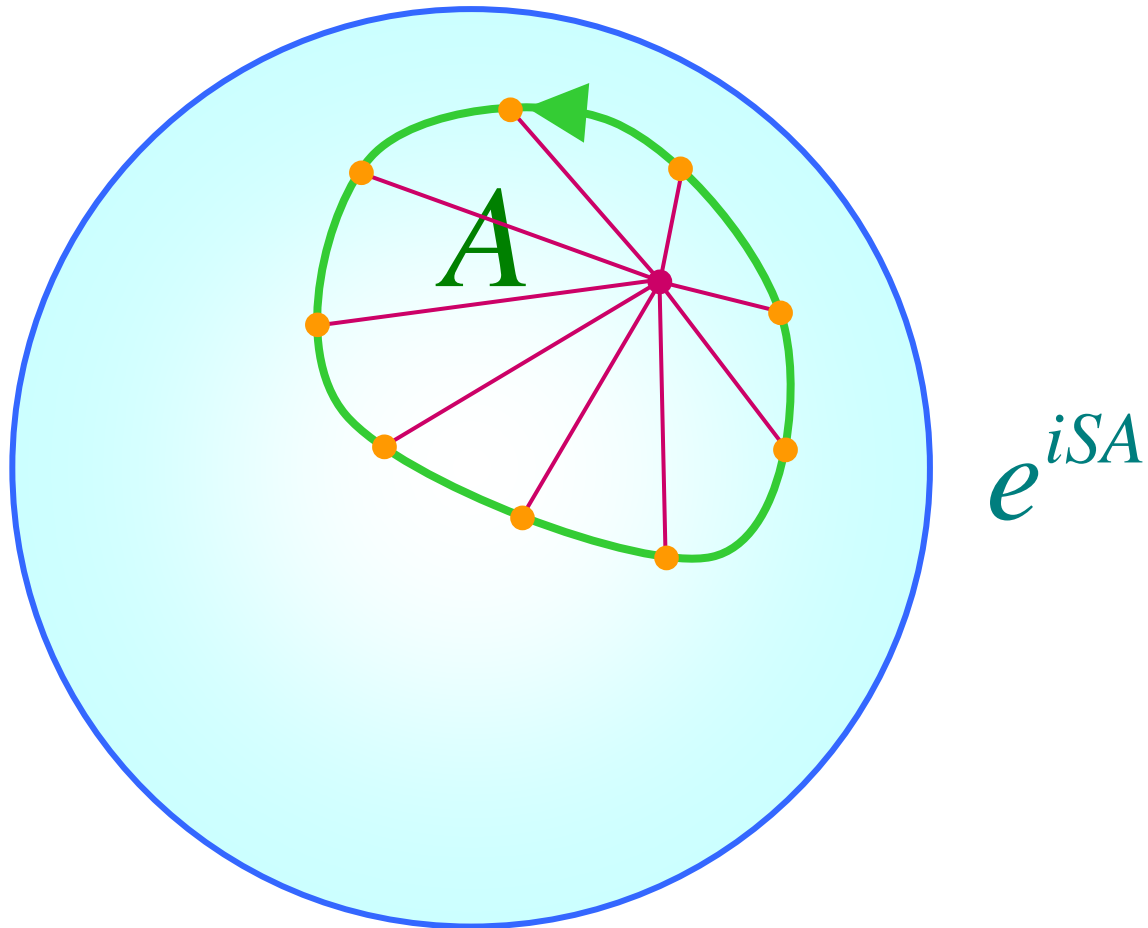
# Quantum theory for destruction of Neel order

## Ingredient missing from LGW theory: Spin Berry Phases

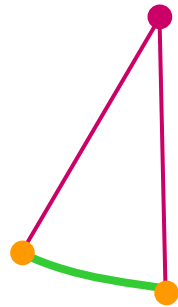


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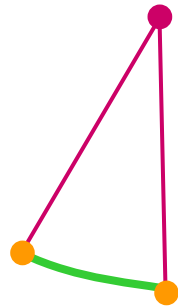


# Quantum theory for destruction of Neel order



## Quantum theory for destruction of Neel order

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

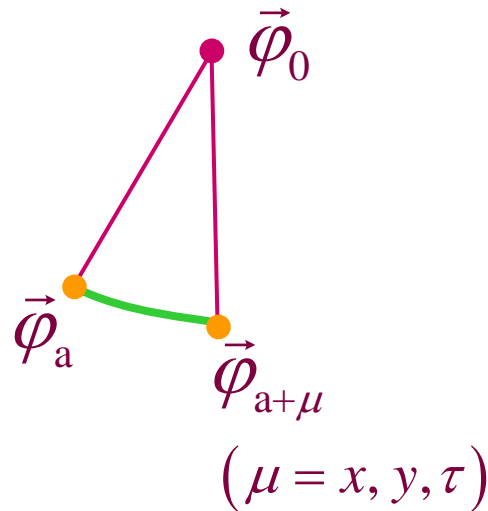


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Discretize imaginary time: path integral is over fields on the sites of a cubic lattice of points  $a$

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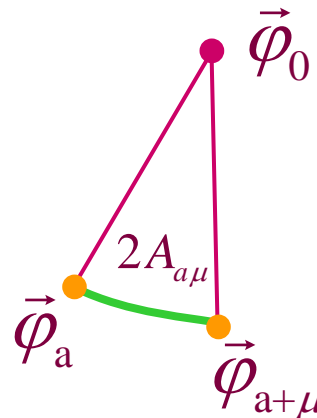
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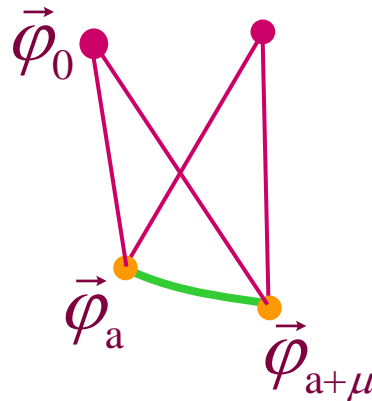
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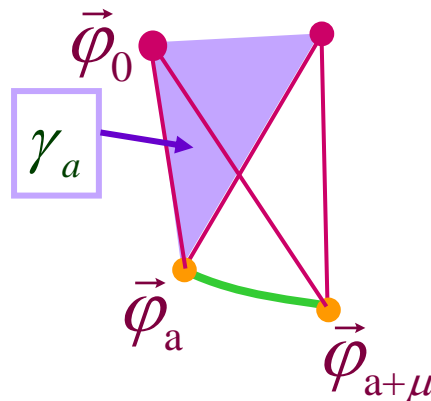
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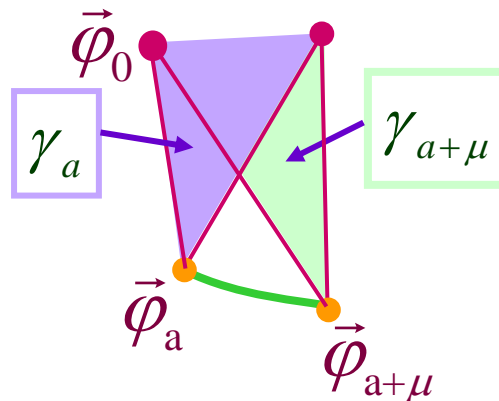
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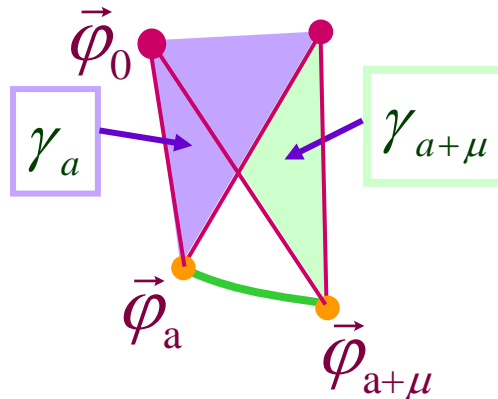
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Change in choice of  $\vec{\varphi}_0$  is like a “gauge transformation”



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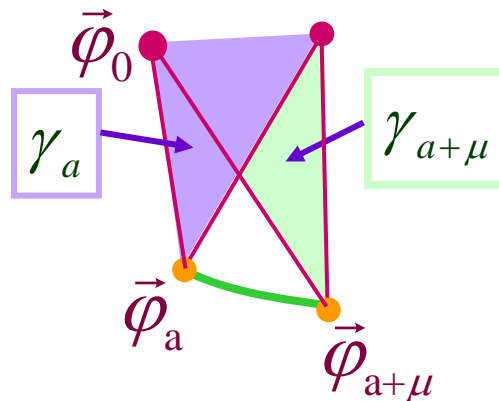
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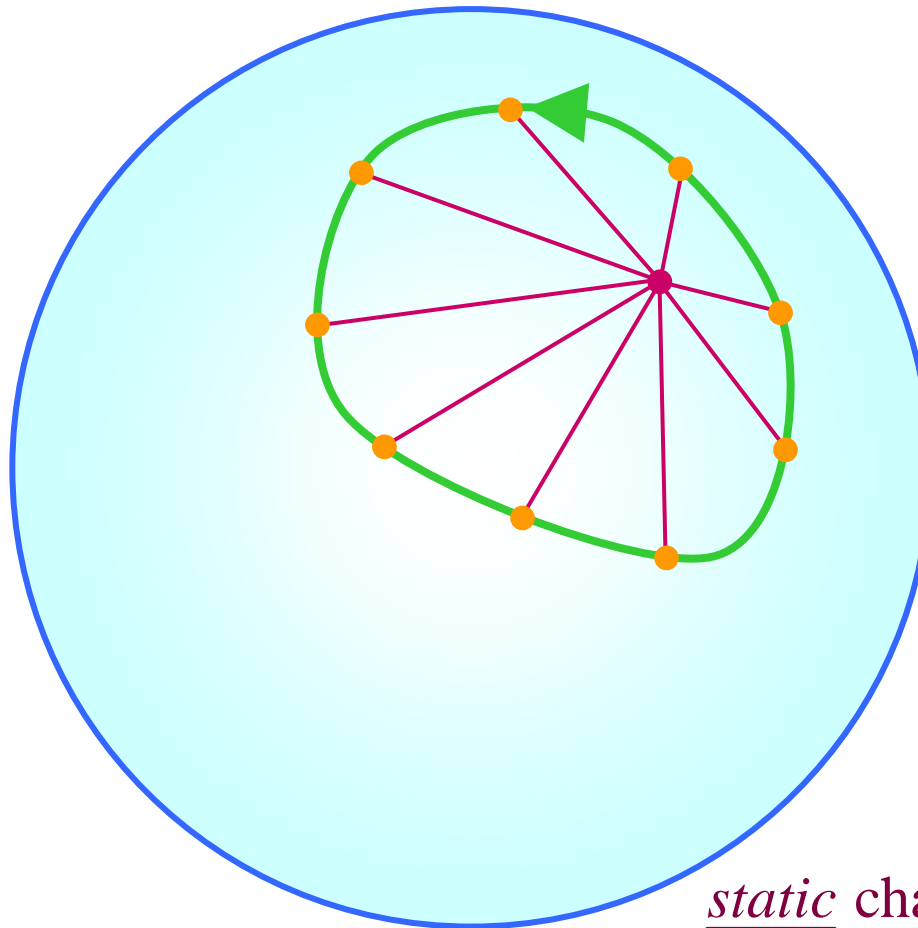
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The area of the triangle is uncertain modulo  $4\pi$ , and the action has to be invariant under  $A_{a\mu} \rightarrow A_{a\mu} + 2\pi$

# 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.

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

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.

Analysis by a duality mapping shows that this theory is *always* in a phase with  $\langle \Psi_{\text{bond}} \rangle \neq 0$  (Class A paramagnet).

The gauge theory is in a *confining* phase (spinons are confined and only  $S=1$  triplons propagate).

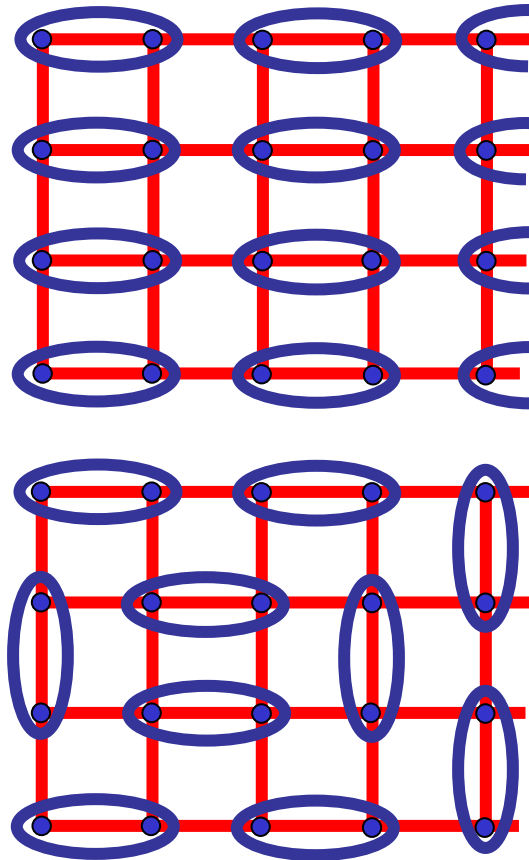
Proliferation of monopoles in the presence of Berry phases.

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

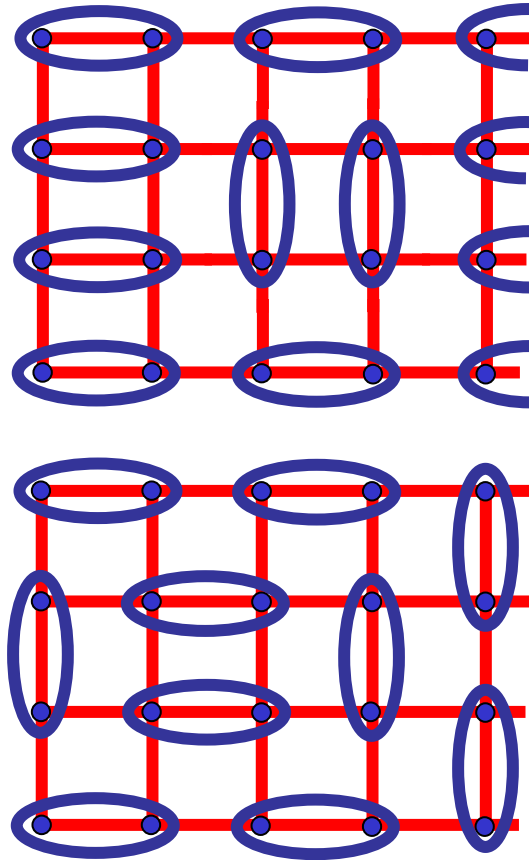
S. Sachdev and R. Jalabert, *Mod. Phys. Lett. B* **4**, 1043 (1990).

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

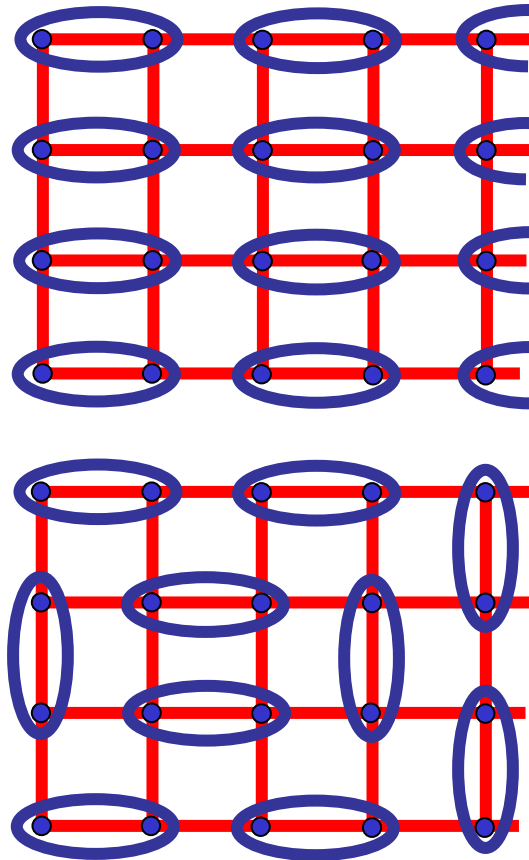
# Ordering by quantum fluctuations



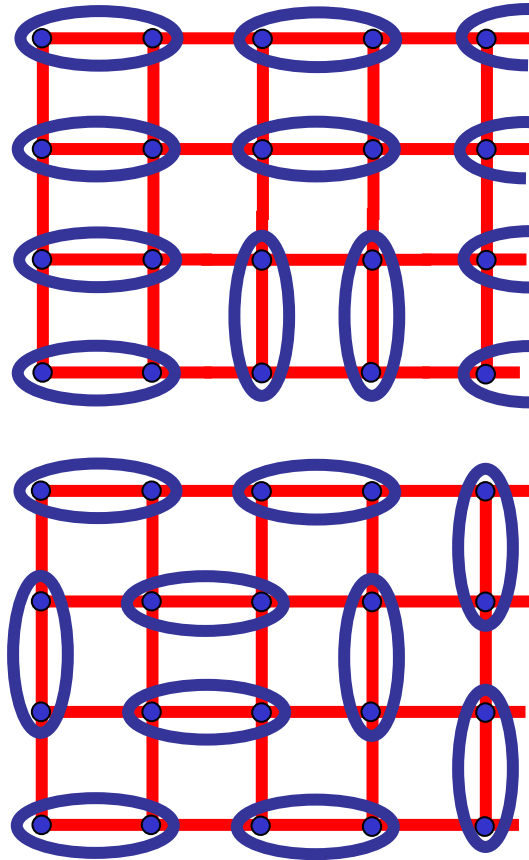
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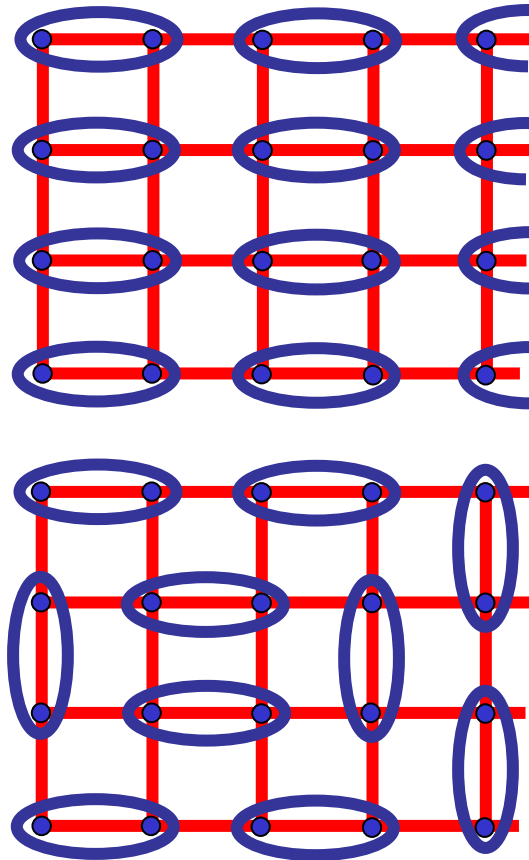
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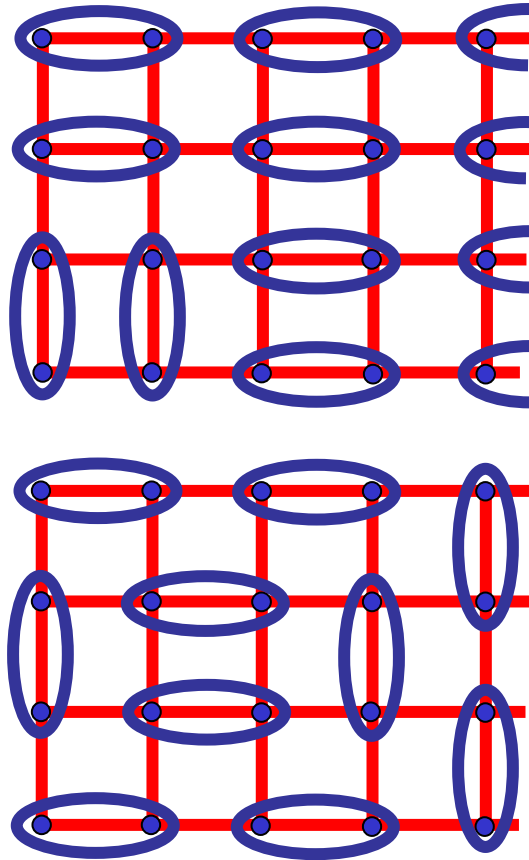
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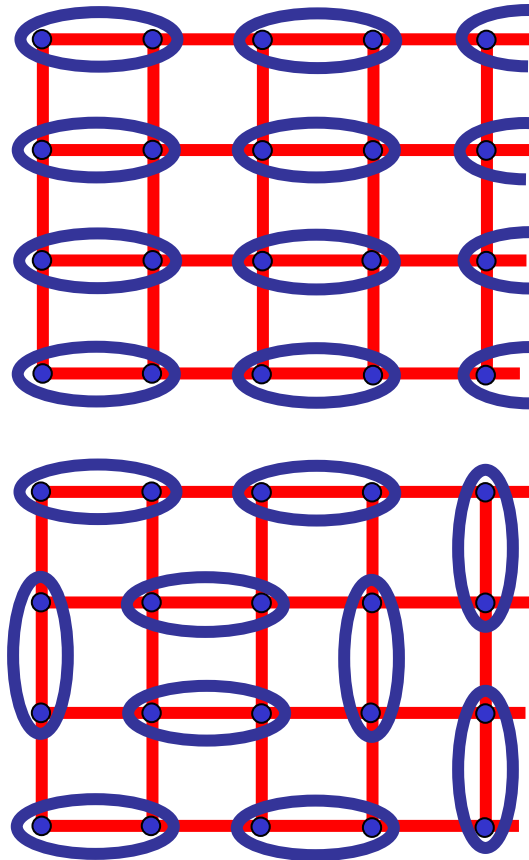
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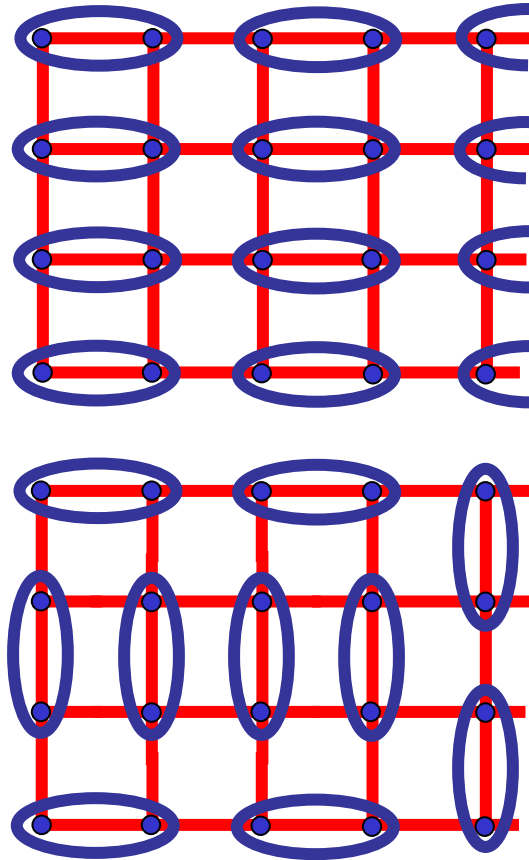
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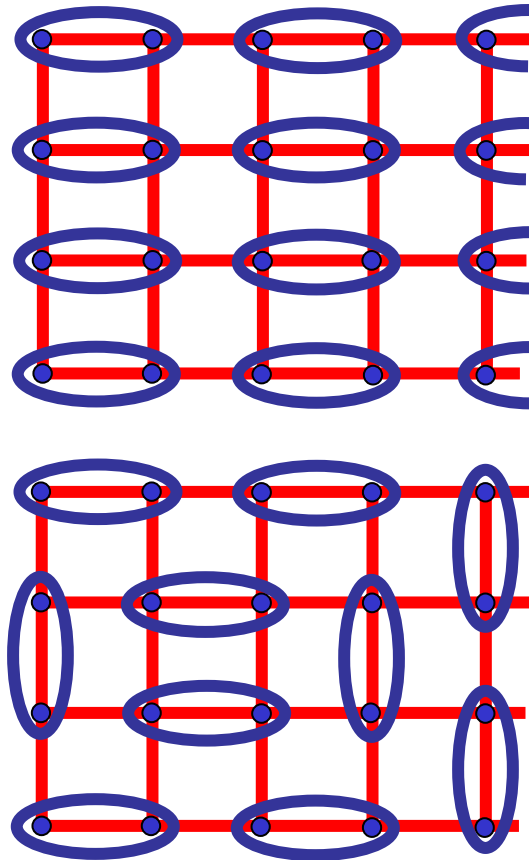
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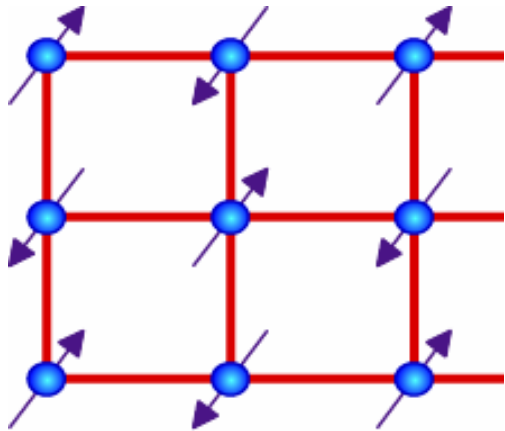
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# Ordering by quantum fluctuations

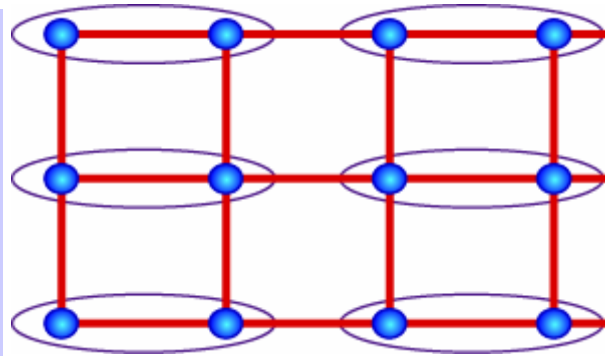


$$Z = \prod_a \int d\vec{\varphi}_a \delta(\vec{\varphi}_a^2 - 1) \exp\left(\frac{1}{g} \sum_{a,\mu} \vec{\varphi}_a \cdot \vec{\varphi}_{a+\mu} + i \sum_a \eta_a A_{a\tau}\right)$$

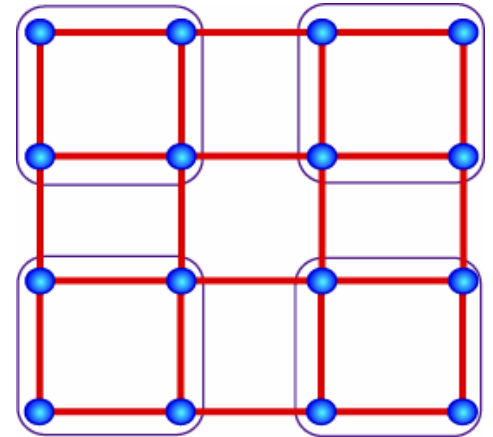


Neel order

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



or



Bond order

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

Not present in

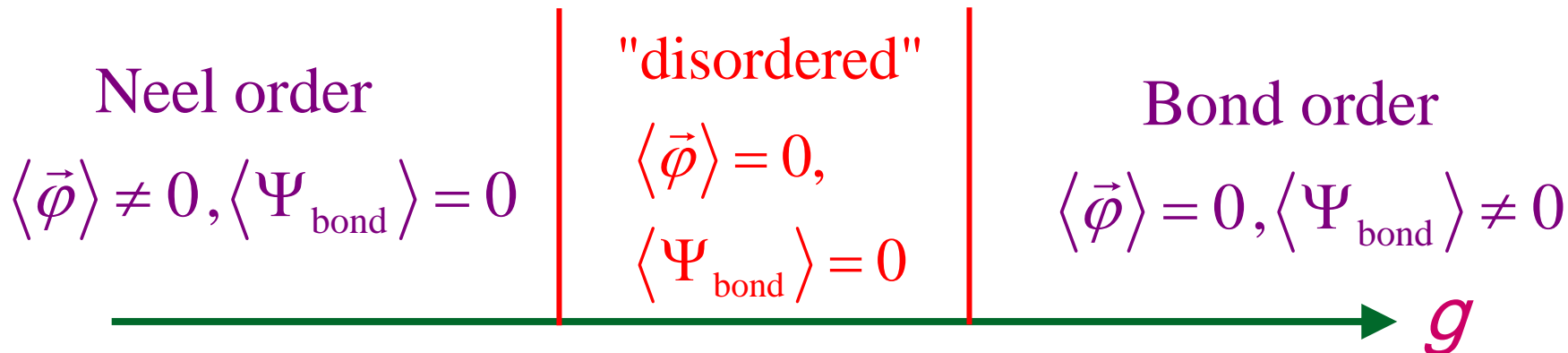
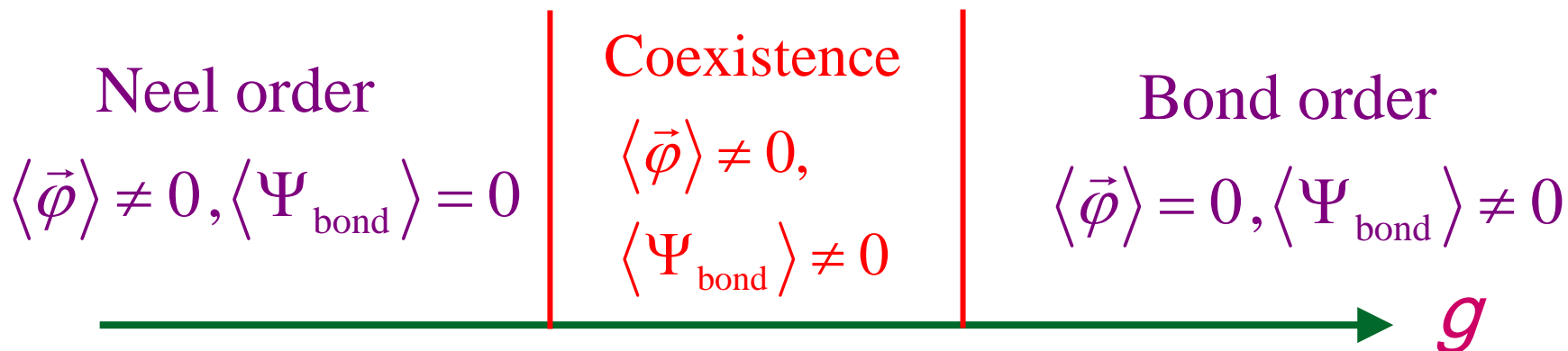
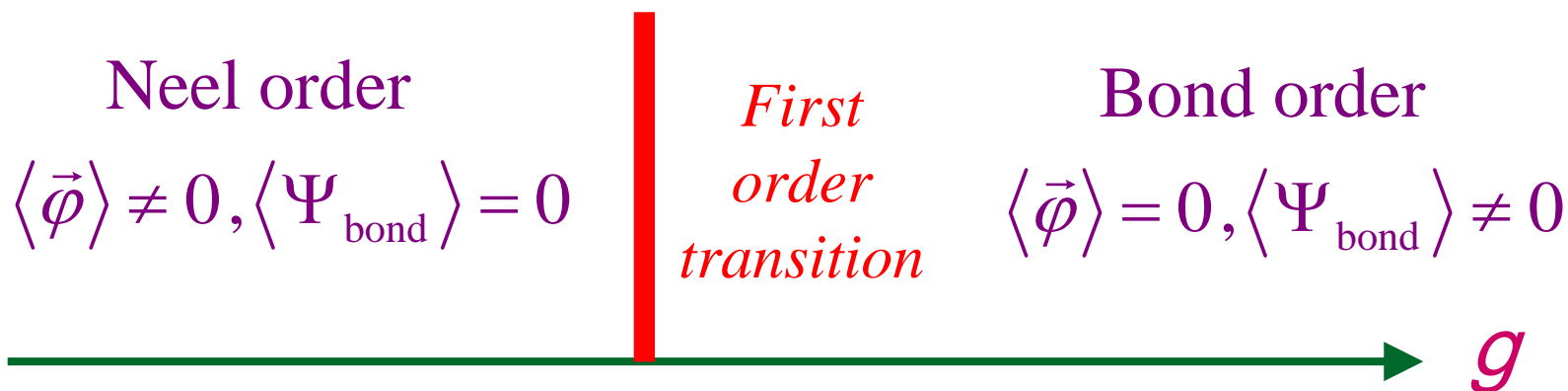
LGW theory

of  $\vec{\varphi}$  order

0

$g$

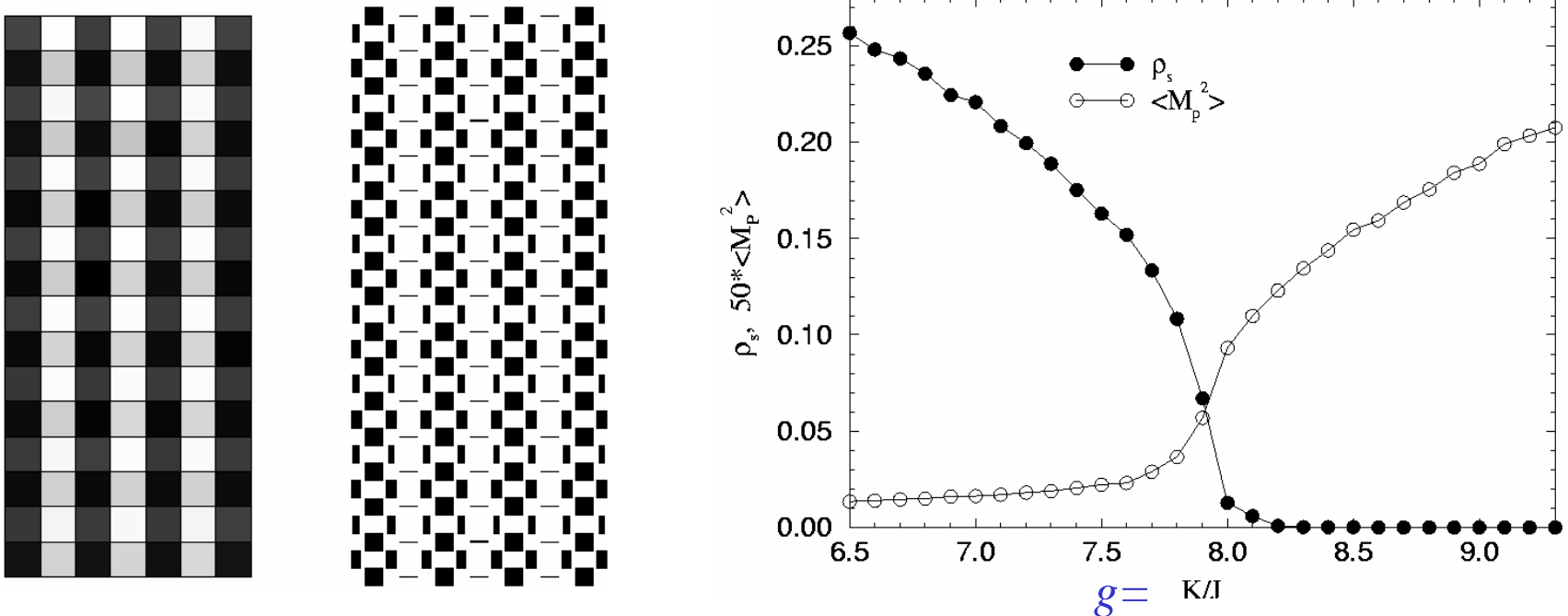
# Naïve approach: add bond order parameter to LGW theory “by hand”



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

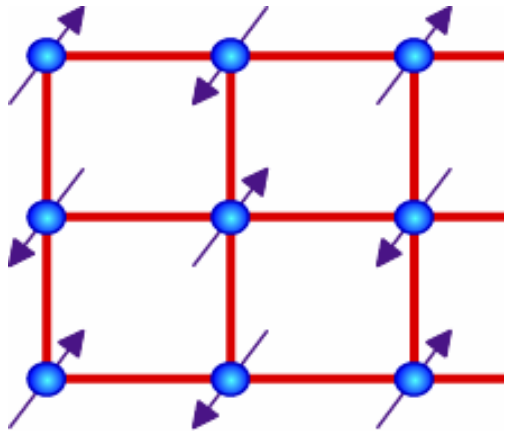
A. W. Sandvik, S. Daul, R. R. P. Singh, and D. J. Scalapino, *Phys. Rev. Lett.* **89**, 247201 (2002)

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



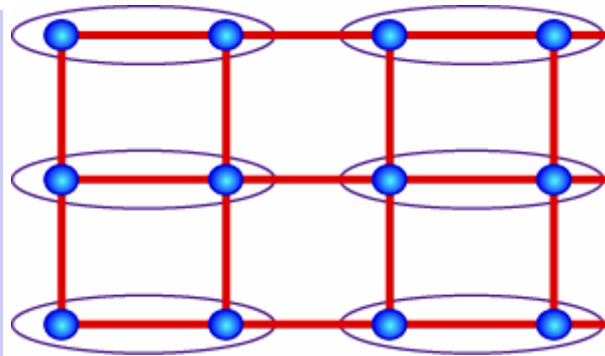
$$H = 2J \sum_{\langle ij \rangle} (S_i^x S_j^x + S_i^y S_j^y) - K \sum_{\langle ijkl \rangle \square} (S_i^+ S_j^- S_k^+ S_l^- + S_i^- S_j^+ S_k^- S_l^+)$$

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

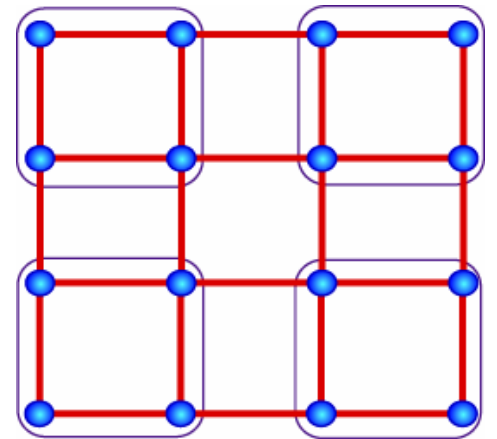


Neel order

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



or



Bond order

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

Not present in

LGW theory

of  $\vec{\varphi}$  order

0

$g$

# 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).

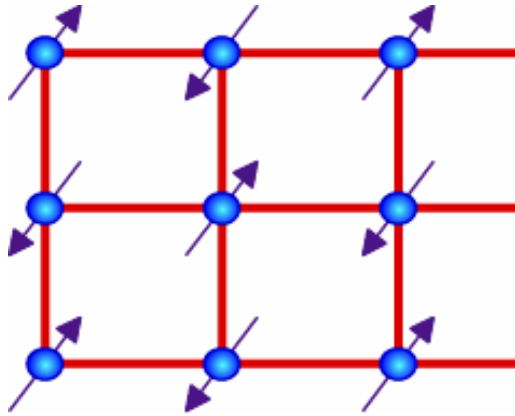
- $S=1/2$  spinons  $z_\alpha$ , with  $\vec{\varphi} \sim z_\alpha^* \vec{\sigma}_{\alpha\beta} z_\beta$ , are globally propagating degrees of freedom.

*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.

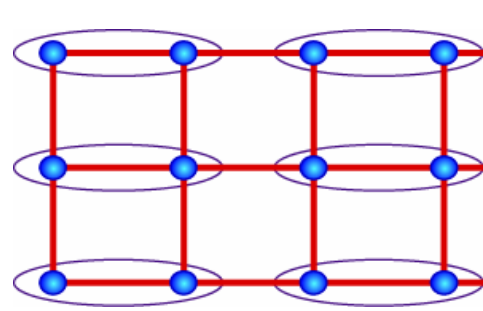
T. Senthil, A. Vishwanath, L. Balents, S. Sachdev and M.P.A. Fisher, *Science* **303**, 1490 (2004).

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

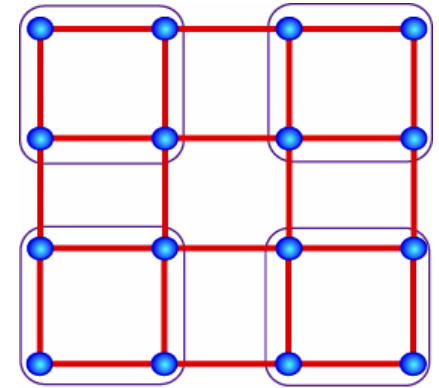


Neel order

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



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



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*

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.*

Cuprate superconductors:  
*Competing orders and recent experiments*

# Minimal LGW phase diagram with $\vec{\phi}$ and $\Psi_{\text{BCS}}$

Quantum phase transitions

Paramagnetic  
Mott Insulator

$$\langle \vec{\phi} \rangle = 0, \langle \Psi_{\text{BCS}} \rangle = 0$$

$$\langle \vec{\phi} \rangle \neq 0, \langle \Psi_{\text{BCS}} \rangle = 0$$

Magnetic  
Mott Insulator

Superconductor

$$\langle \vec{\phi} \rangle = 0, \langle \Psi_{\text{BCS}} \rangle \neq 0$$

$$\langle \vec{\phi} \rangle \neq 0, \langle \Psi_{\text{BCS}} \rangle \neq 0$$

Magnetic  
Superconductor

High temperature  
superconductor



# Minimal LGW phase diagram with $\vec{\phi}$ and $\Psi_{\text{BCS}}$

High temperature  
superconductor



Quantum phase  
transitions

Paramagnetic  
Mott Insulator

$$\langle \vec{\phi} \rangle = 0, \langle \Psi_{\text{BCS}} \rangle = 0$$

Superconductor

$$\langle \vec{\phi} \rangle = 0, \langle \Psi_{\text{BCS}} \rangle \neq 0$$

$$\langle \vec{\phi} \rangle \neq 0, \langle \Psi_{\text{BCS}} \rangle = 0$$

Magnetic  
Mott Insulator

$$\langle \vec{\phi} \rangle \neq 0, \langle \Psi_{\text{BCS}} \rangle \neq 0$$

Magnetic  
Superconductor



Spin density wave order  $K \neq (\pi, \pi)$   
Spirals.....Shraiman, Siggia  
Stripes.....Zaanen, Kivelson.....

Quantum phase  
transitions

Paramagnetic  
Mott Insulator

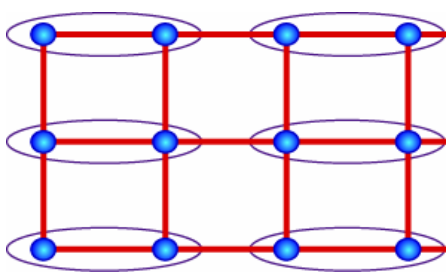
$$\langle \vec{\phi} \rangle = 0, \quad \langle \Psi_{\text{BCS}} \rangle = 0$$

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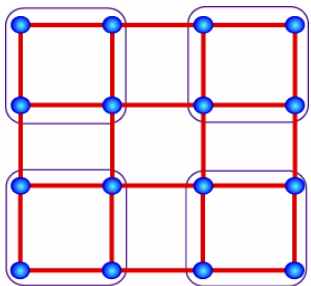
$$\langle \vec{\phi} \rangle \neq 0, \quad \langle \Psi_{\text{BCS}} \rangle = 0$$

Magnetic  
Mott Insulator

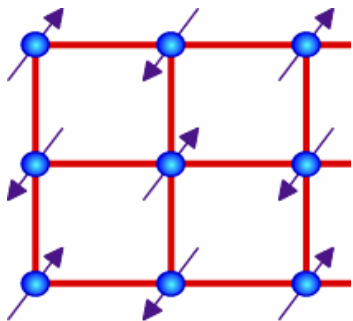




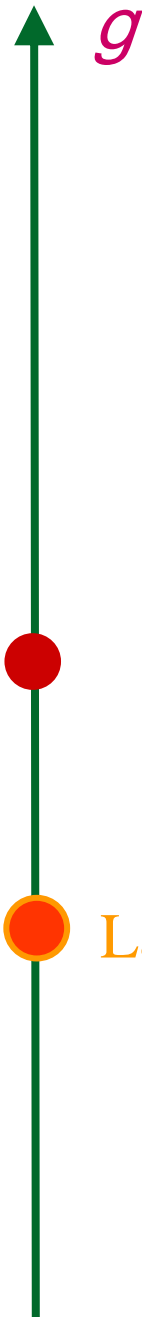
or



Bond order



Neel order



Quantum phase transitions

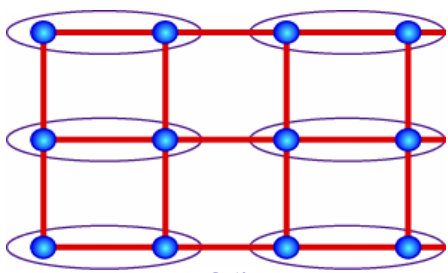
Paramagnetic  
Mott Insulator

$$\langle \vec{\phi} \rangle = 0, \quad \langle \Psi_{\text{BCS}} \rangle = 0$$

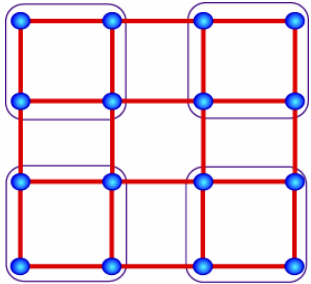
$$\langle \vec{\phi} \rangle \neq 0, \quad \langle \Psi_{\text{BCS}} \rangle = 0$$

Magnetic  
Mott Insulator

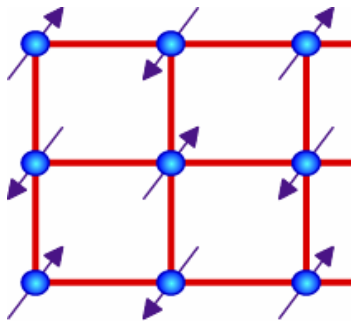




or



Bond order



Neel order



$g$

Localized holes

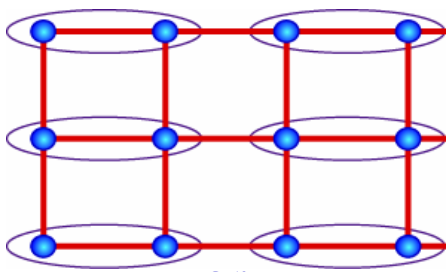


$\text{La}_2\text{CuO}_4$

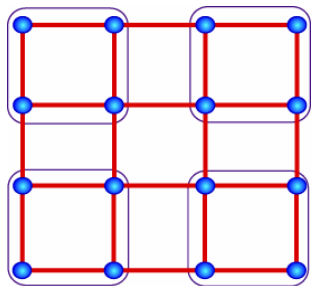
Large  $N$  limit of a theory with  $\text{Sp}(2N)$  symmetry: yields existence of bond order and  $d$ -wave superconductivity

S. Sachdev and N. Read, *Int. J. Mod. Phys. B* **5**, 219 (1991); M. Vojta and S. Sachdev, *Phys. Rev. Lett.* **83**, 3916 (1999); M. Vojta, *Phys. Rev. B* **66**, 104505 (2002).

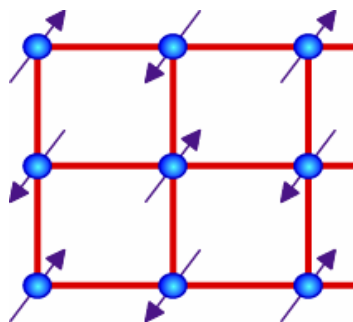
Hole density  $\delta$



OR



Bond order



Neel order

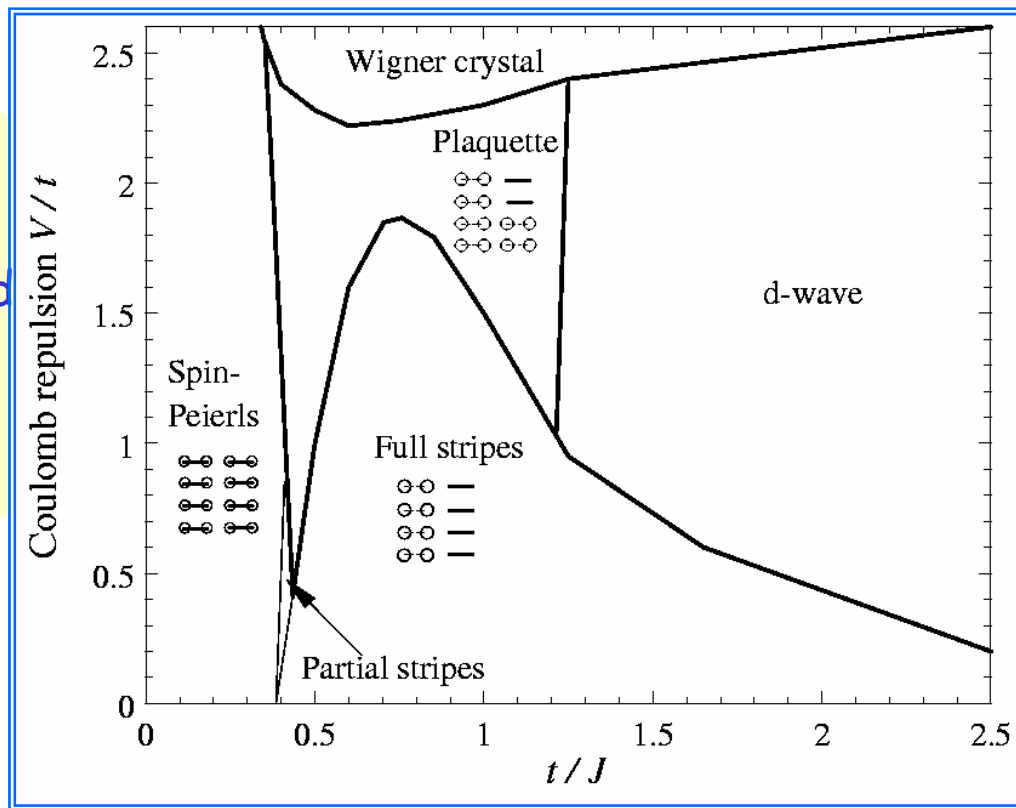
$g$

Localized holes



$\text{La}_2\text{CuO}_4$

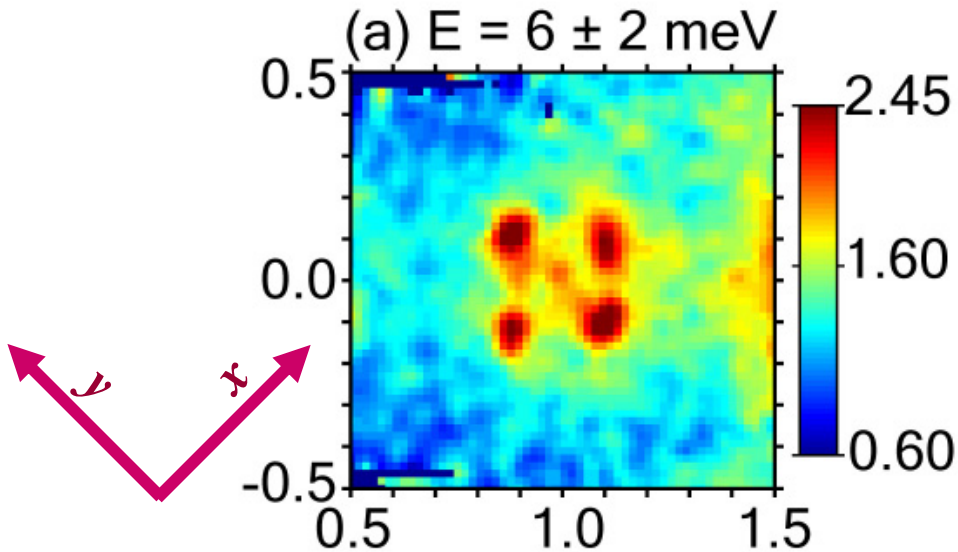
Magnetic, bond and super-conducting order



Hole density  $\delta$

# Neutron scattering measurements of $\text{La}_{15/8}\text{Ba}_{1/8}\text{CuO}_4$ (Zurich oxide)

J. M. Tranquada, H. Woo, T. G. Perring, H. Goka, G. D. Gu,  
G. Xu, M. Fujita, and K. Yamada, cond-mat/0401621

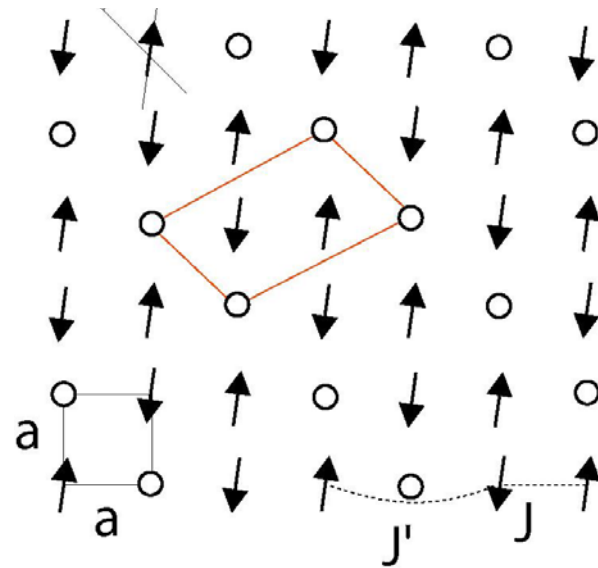


Scattering off spin density wave order with

$$\langle \vec{S}_i \rangle = \vec{N} \cos(\mathbf{Q} \cdot \mathbf{r}_i + \alpha)$$

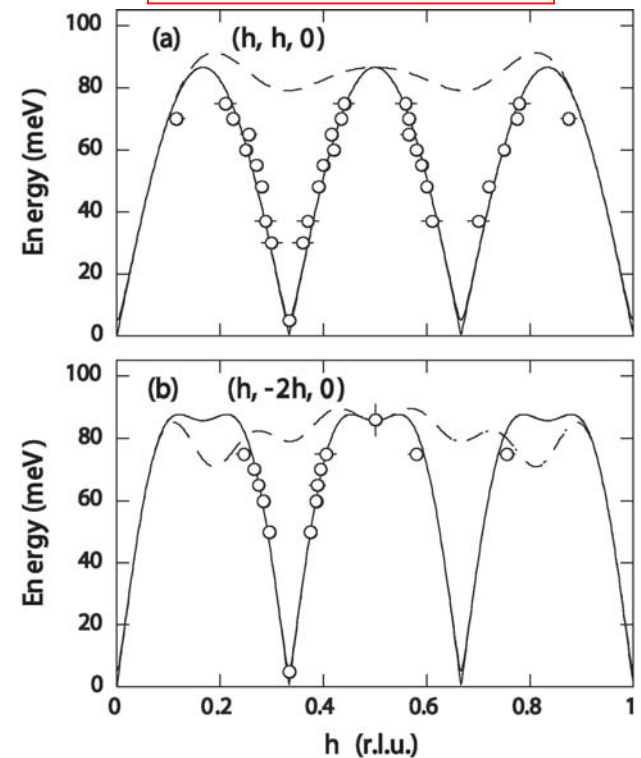
$$\mathbf{Q} = 2\pi \left( \frac{1}{2}, \frac{1}{2} \pm \frac{1}{8} \right) \text{ and } 2\pi \left( \frac{1}{2} \pm \frac{1}{8}, \frac{1}{2} \right)$$

At higher energies, semiclassical theory predicts  
that peaks lead to spin-wave ("light") cones.



Ni has  $S = 1$ ;  $\mathbf{Q} = 2\pi \left( \frac{1}{2} \pm \frac{1}{6}, \frac{1}{2} \pm \frac{1}{6} \right)$

A. T. Boothroyd, D. Prabhakaran, P. G. Freeman, S.J.S. Lister, M. Enderle, A. Hiess, and J. Kulda, *Phys. Rev. B* **67**, 100407 (2003).

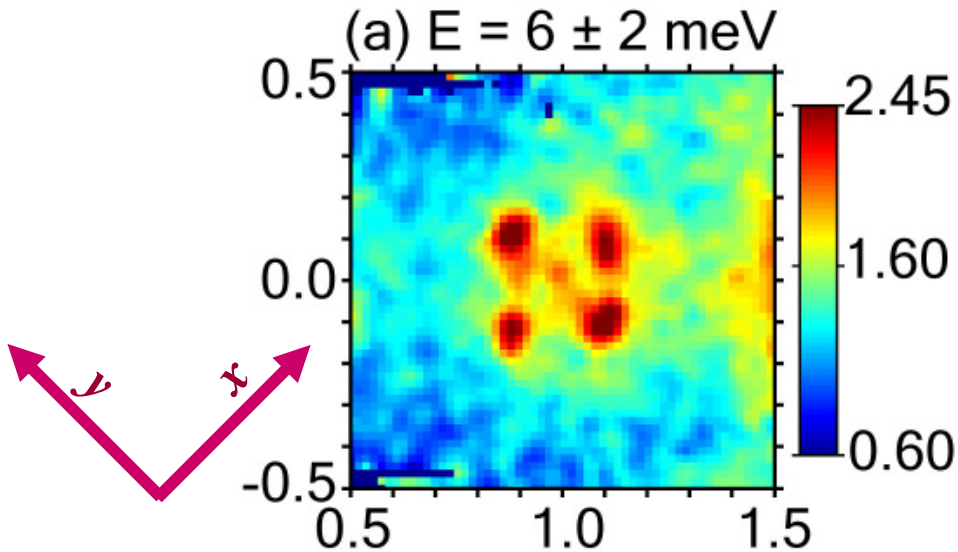


Spin waves:  $J=15$  meV,  $J'=7.5$  meV

A. T. Boothroyd, D. Prabhakaran, P. G. Freeman, S.J.S. Lister, M. Enderle, A. Hiess, and J. Kulda, *Phys. Rev. B* **67**, 100407 (2003).

# Neutron scattering measurements of $\text{La}_{15/8}\text{Ba}_{1/8}\text{CuO}_4$ (Zurich oxide)

J. M. Tranquada, H. Woo, T. G. Perring, H. Goka, G. D. Gu,  
G. Xu, M. Fujita, and K. Yamada, cond-mat/0401621

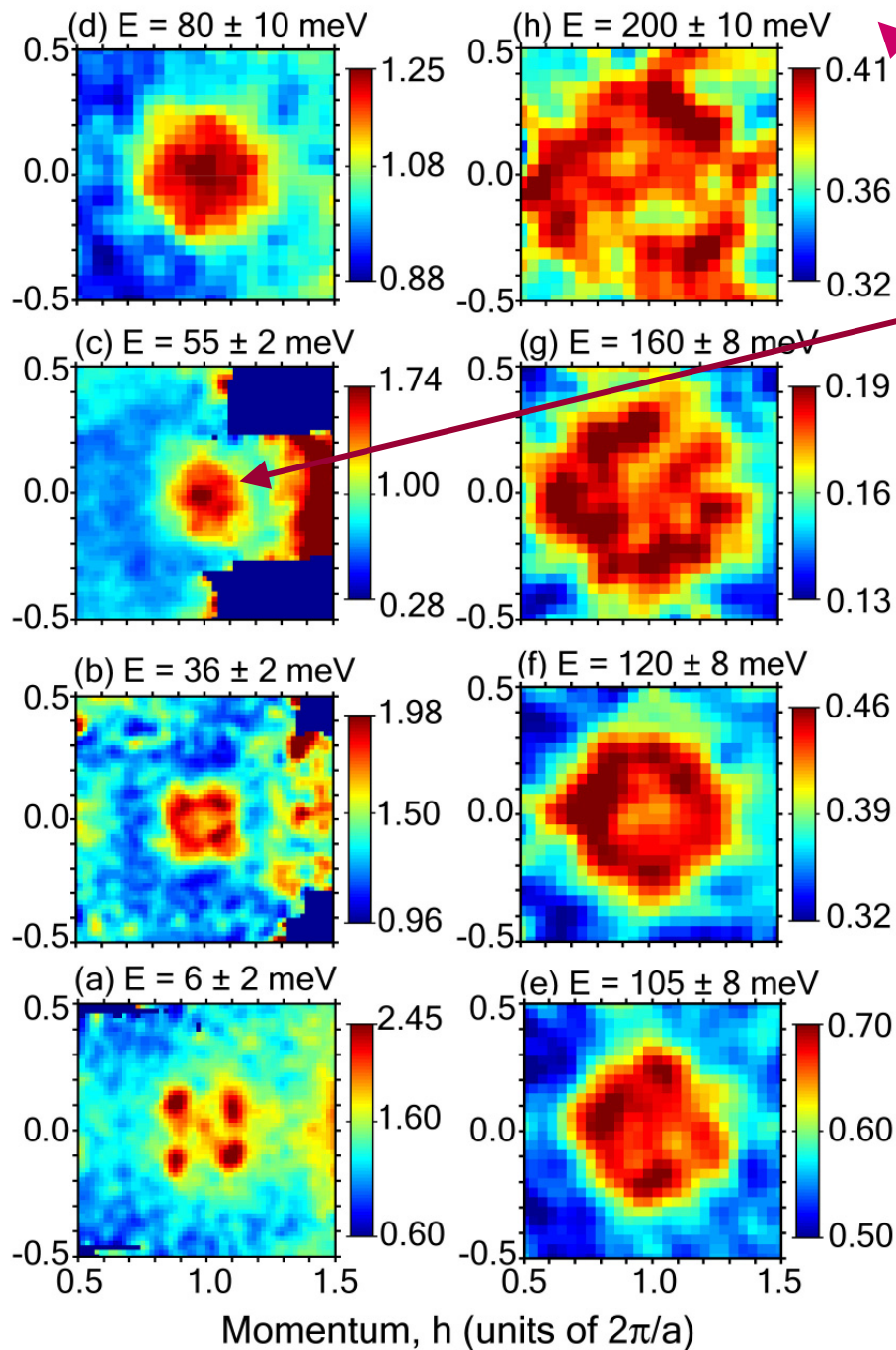


Scattering off spin density wave order with

$$\langle \vec{S}_i \rangle = \vec{N} \cos(\mathbf{Q} \cdot \mathbf{r}_i + \alpha)$$

$$\mathbf{Q} = 2\pi \left( \frac{1}{2}, \frac{1}{2} \pm \frac{1}{8} \right) \text{ and } 2\pi \left( \frac{1}{2} \pm \frac{1}{8}, \frac{1}{2} \right)$$

At higher energies, semiclassical theory predicts that peaks lead to spin-wave ("light") cones.

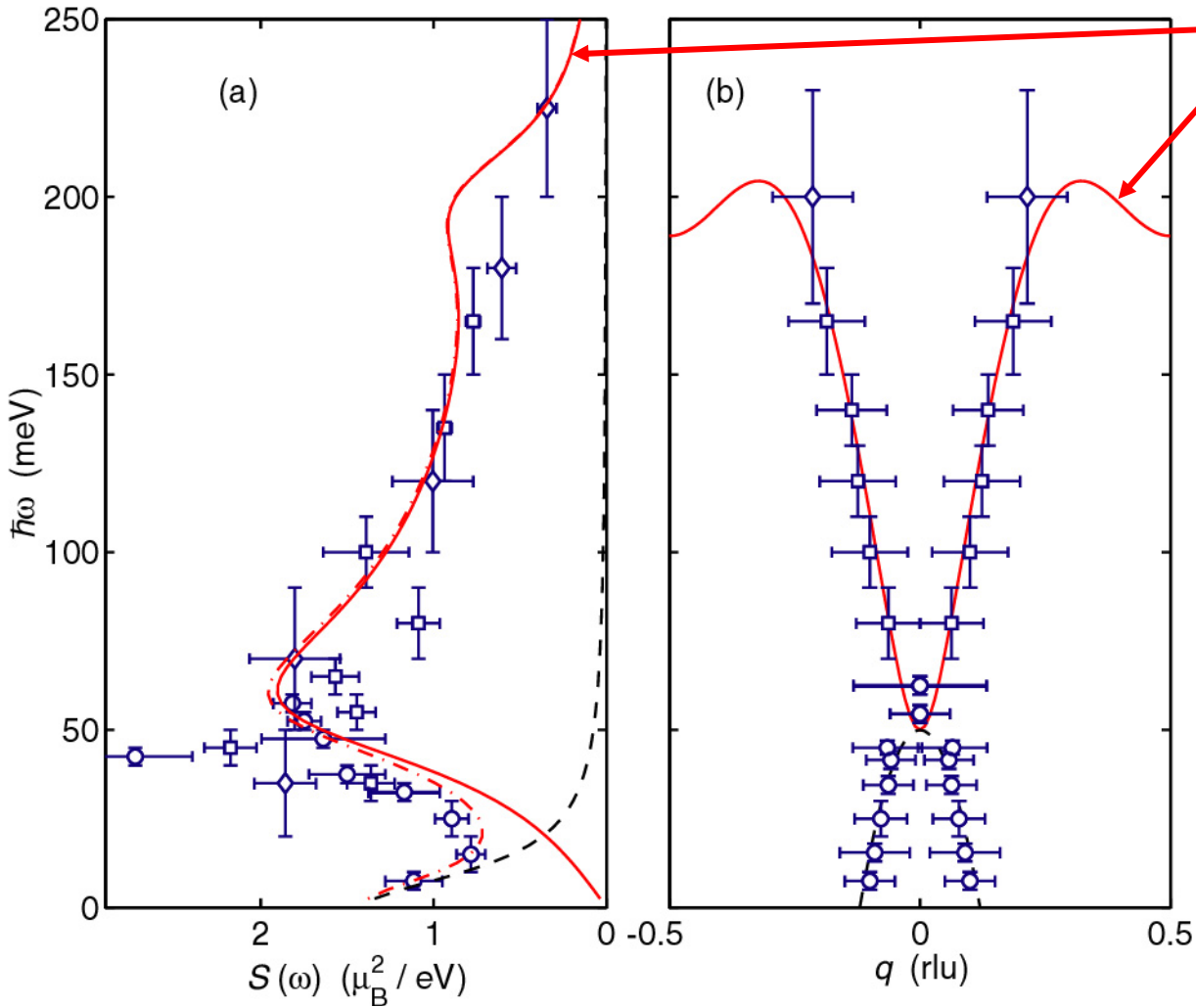


“Resonance peak”

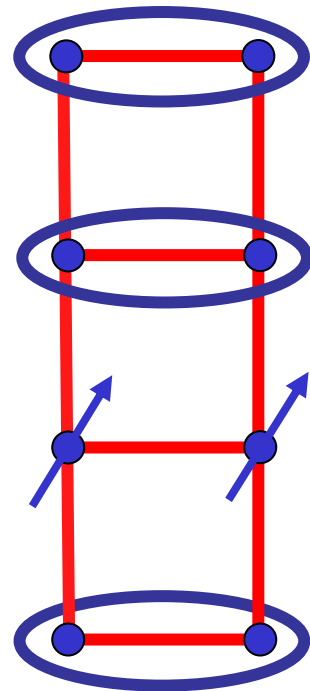
Observations in  $\text{La}_{15/8}\text{Ba}_{1/8}\text{CuO}_4$  are very different and do not obey spin-wave model.

Similar spectra are seen in most hole-doped cuprates.

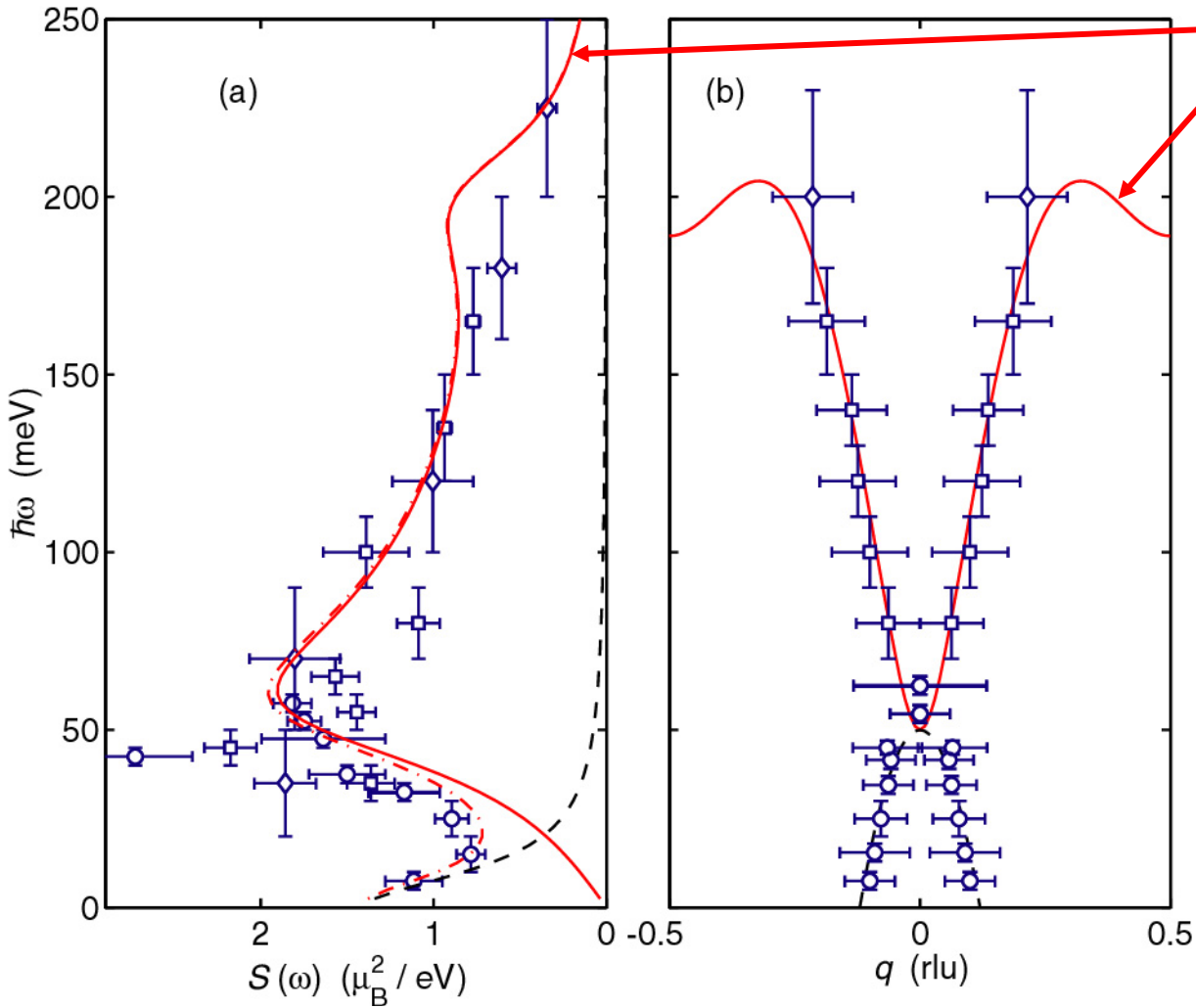
J. M. Tranquada, H. Woo, T. G. Perring, H. Goka, G. D. Gu, G. Xu, M. Fujita, and K. Yamada, cond-mat/0401621



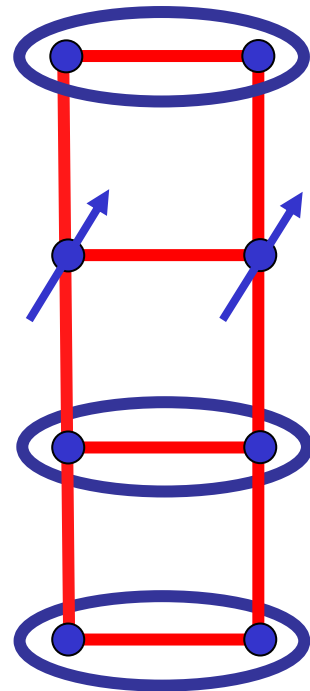
Red lines: triplon excitation of a 2 leg ladder with exchange  $J=100$  meV



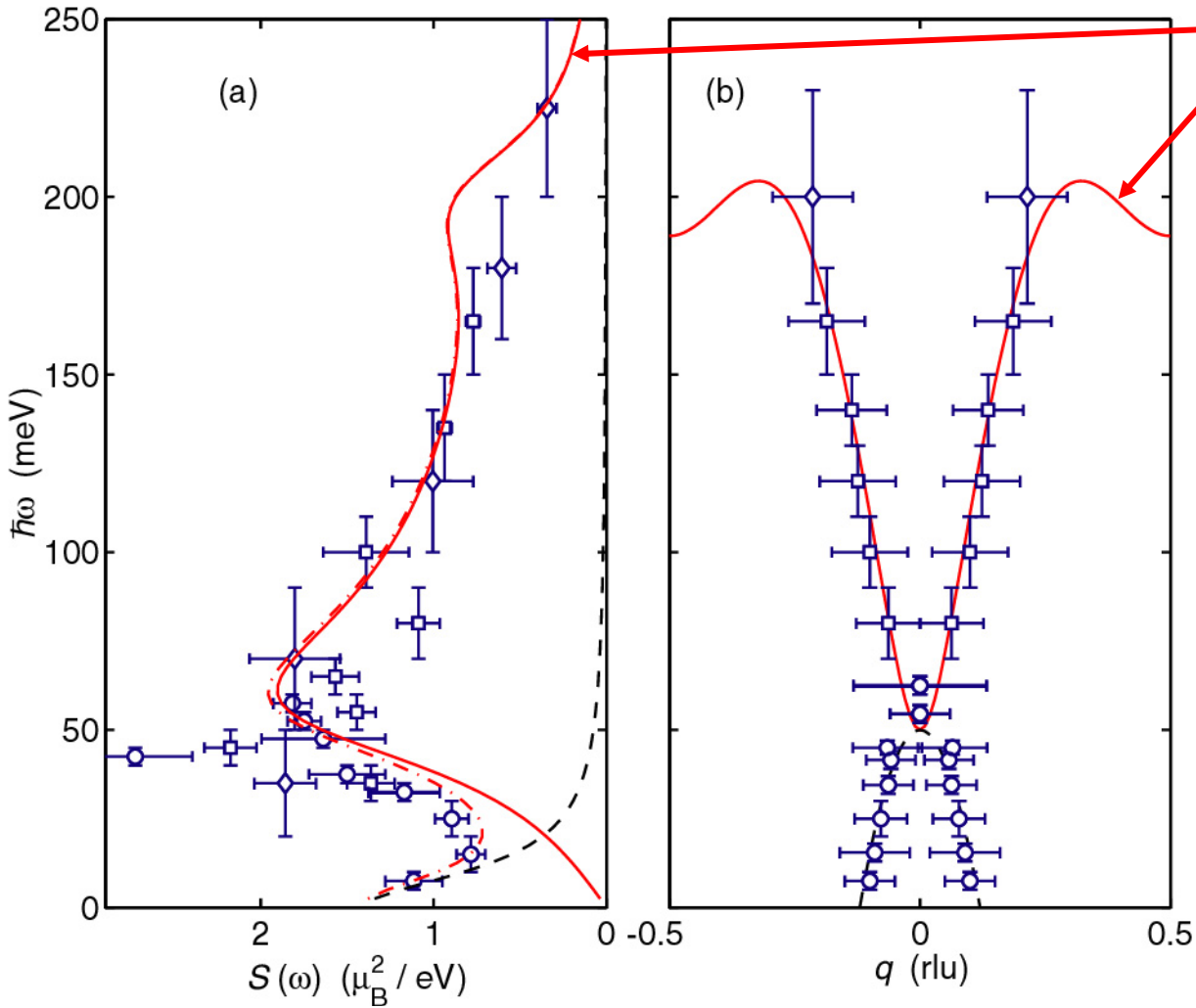
J. M. Tranquada, H. Woo, T. G. Perring, H. Goka, G. D. Gu, G. Xu, M. Fujita, and K. Yamada, cond-mat/0401621



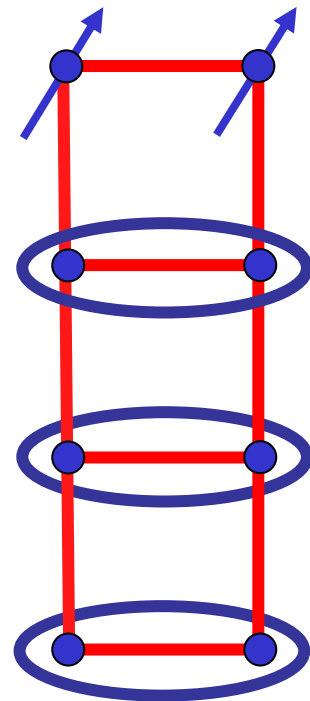
Red lines: triplon excitation of a 2 leg ladder with exchange  $J=100$  meV



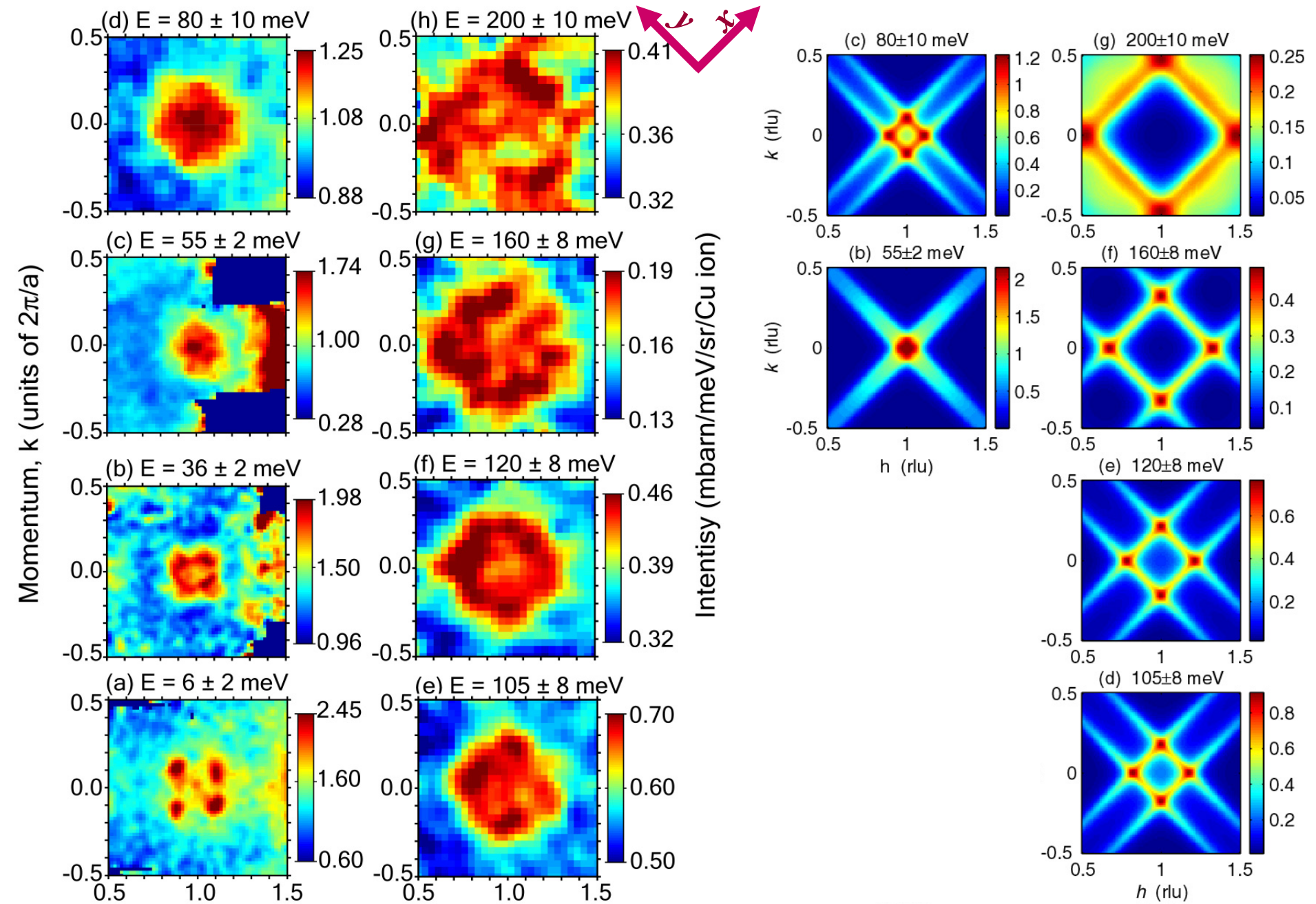
J. M. Tranquada, H. Woo, T. G. Perring, H. Goka, G. D. Gu, G. Xu, M. Fujita, and K. Yamada, cond-mat/0401621



Red lines: triplon excitation of a 2 leg ladder with exchange  $J=100$  meV



J. M. Tranquada, H. Woo, T. G. Perring, H. Goka, G. D. Gu, G. Xu, M. Fujita, and K. Yamada, cond-mat/0401621



## Proposals of

- M. Vojta and T. Ulbricht, cond-mat/0402377
- G.S. Uhrig, K.P. Schmidt, and M. Grüninger, cond-mat/0402659
- M. Vojta and S. Sachdev, to appear.

Magnetic excitations display a crossover from *spin-waves* (at low energies) to *triplons* (at high energies), and main features can be described by proximity to a magnetic quantum phase transition in the presence of period 4, *static*, bond order.

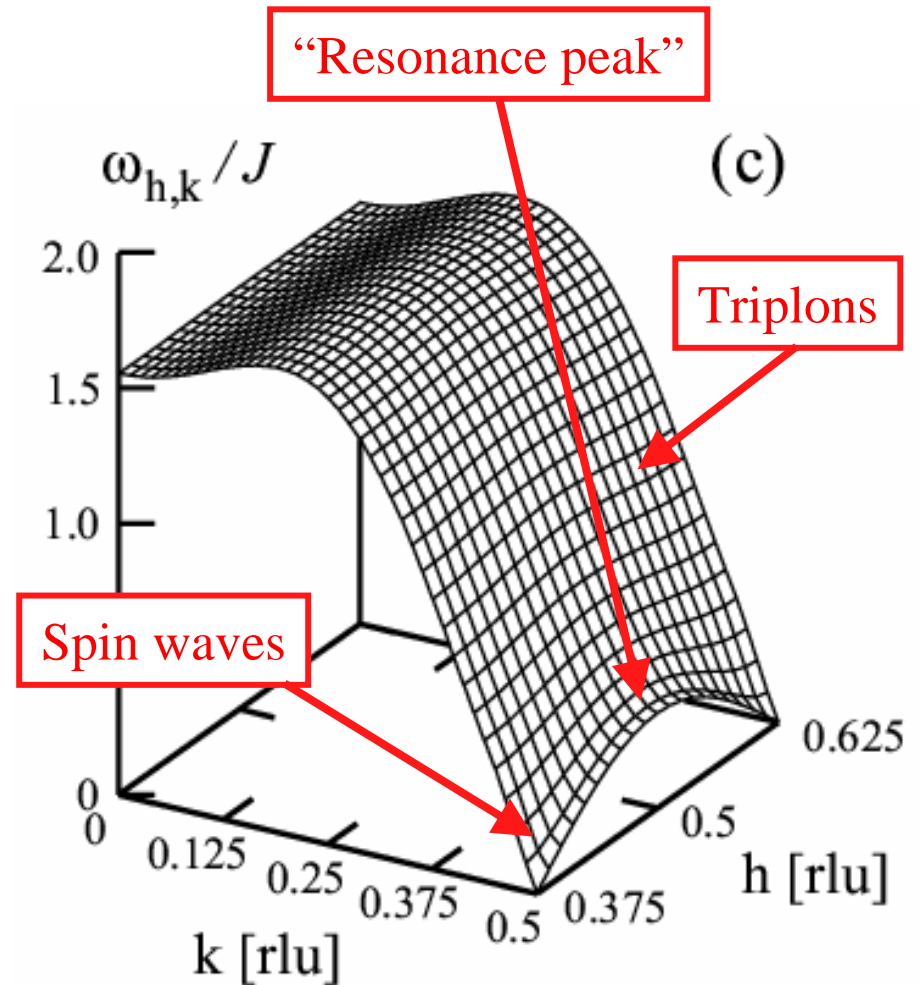
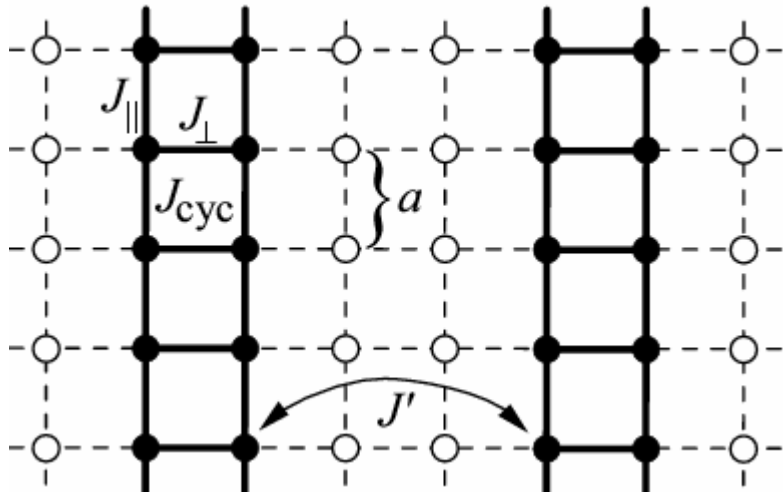
LGW action for magnetic order parameter  $\vec{\varphi}_i = e^{i\mathbf{K}\cdot\mathbf{r}_i} \vec{S}_i$  ( $\mathbf{K} = (\pi, \pi)$ ):

$$S_\varphi = \int d\tau \sum_i \left\{ \frac{1}{2} \left( c^2 (\partial_\tau \vec{\varphi}_i)^2 + (g - g_c) \vec{\varphi}_i^2 \right) + \frac{u}{4!} (\vec{\varphi}_i^2)^2 \right\}$$

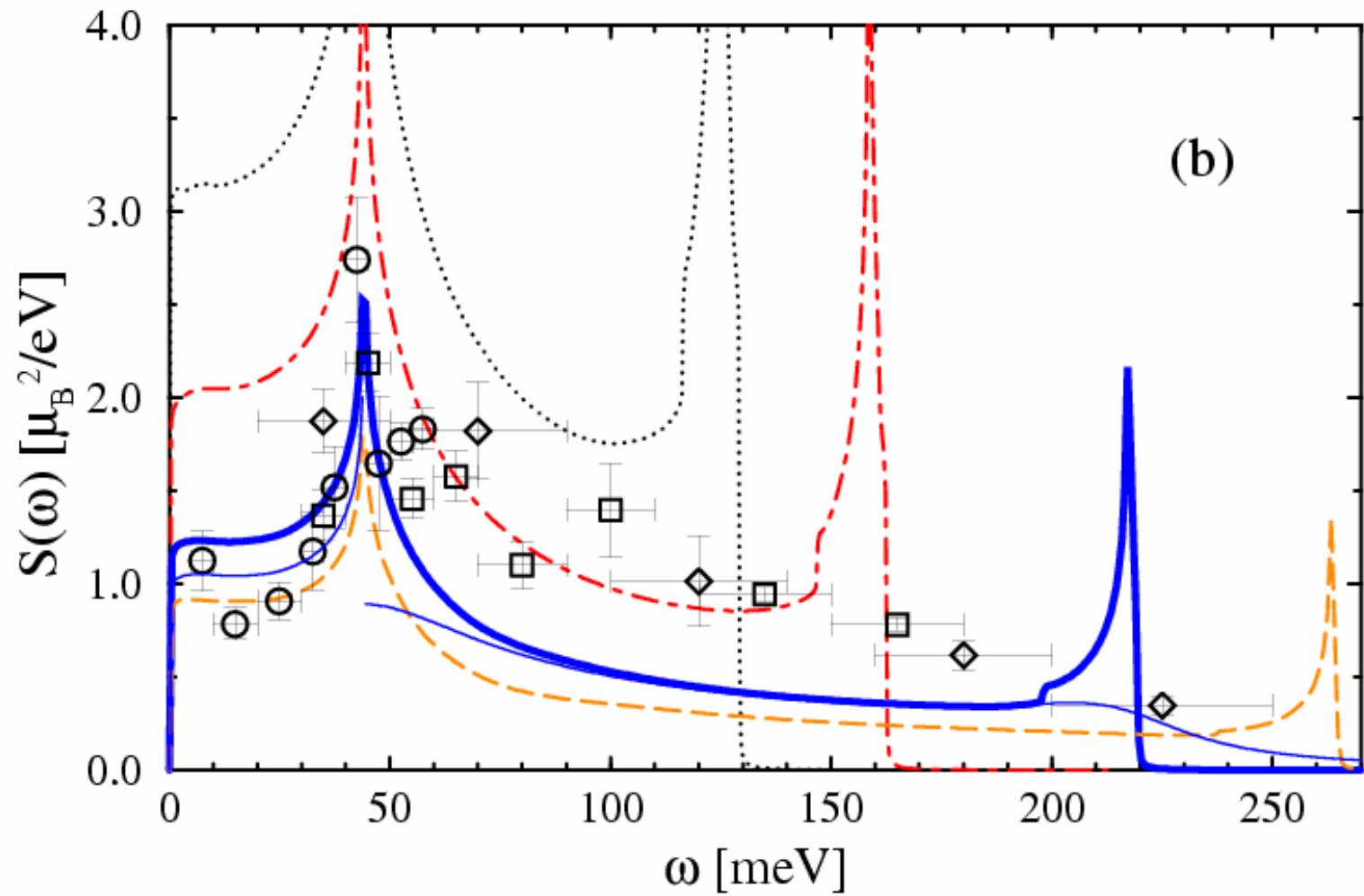
$$+ \int d\tau \sum_{\langle ij \rangle} \left\{ (\vec{\varphi}_i - \vec{\varphi}_j)^2 - P(i, j) \vec{\varphi}_i \cdot \vec{\varphi}_j \right\}$$

$$P(i, j) = \Psi_{\text{bond}} e^{i\mathbf{Q}\cdot(\mathbf{r}_i + \mathbf{r}_j)} + \text{c.c.}$$

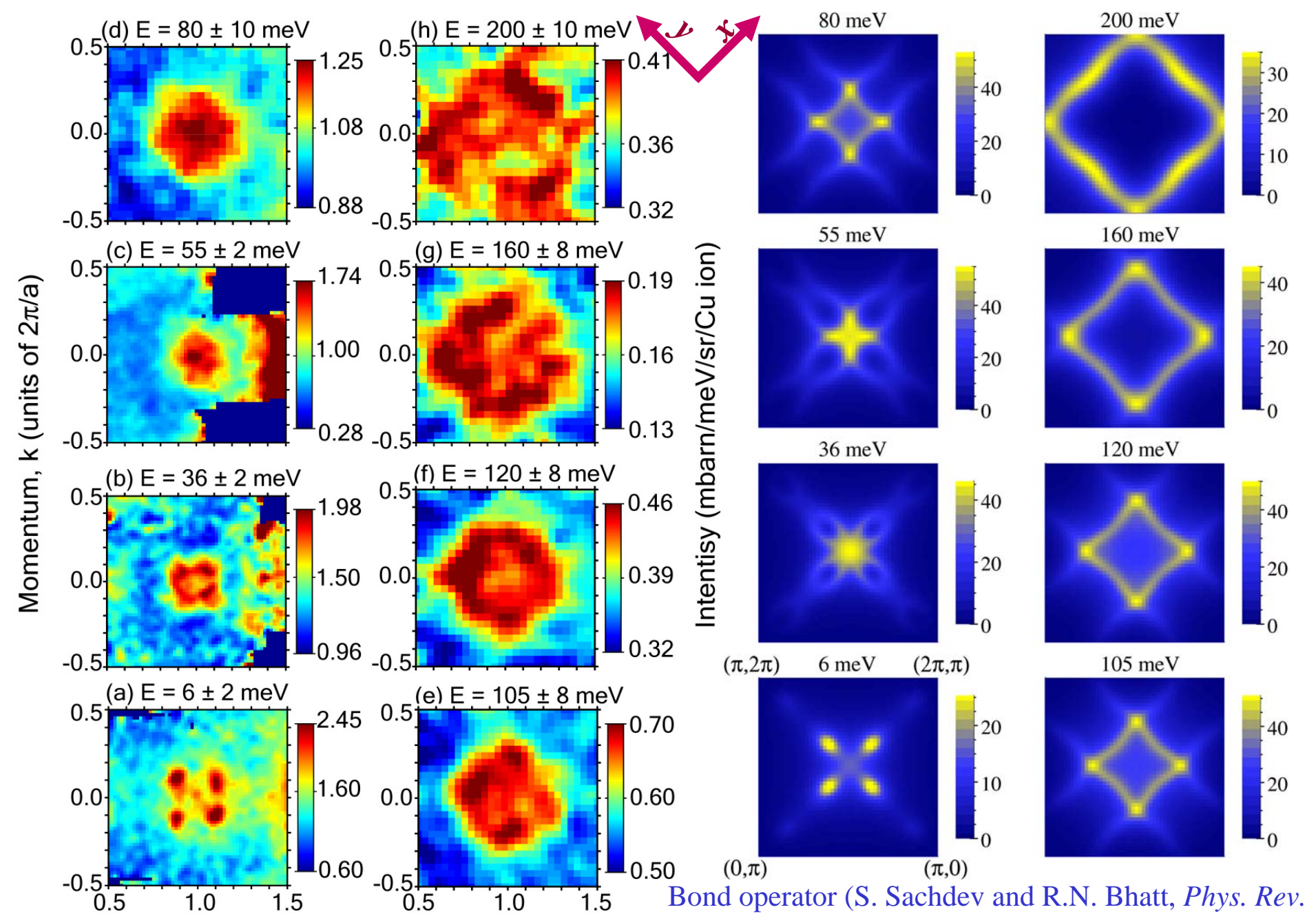
# Possible simple microscopic model of bond order



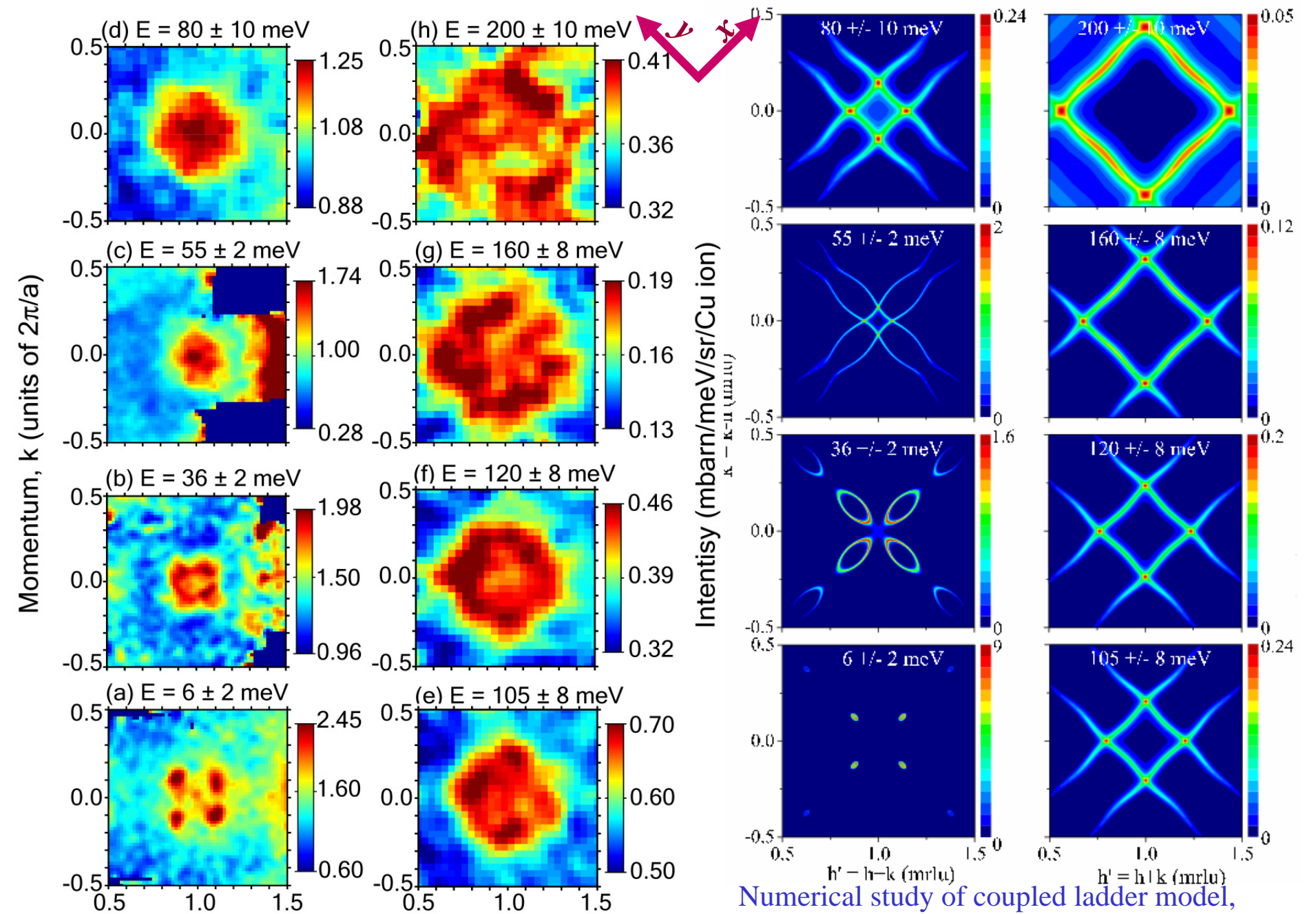
G.S. Uhrig, K.P. Schmidt, and  
M. Grüninger, cond-mat/0402659



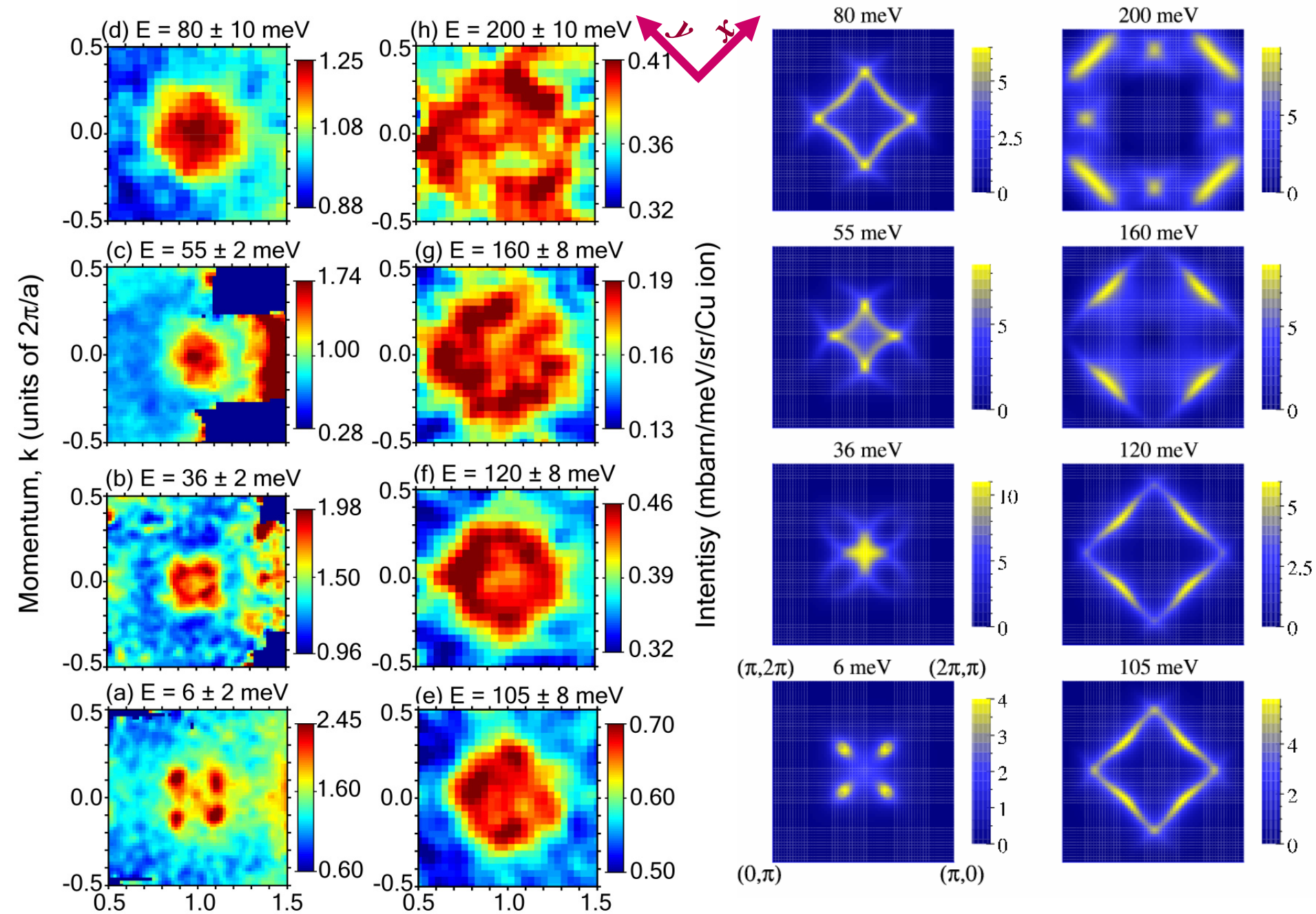
G.S. Uhrig, K.P. Schmidt, and  
M. Grüninger, cond-mat/0402659



Bond operator (S. Sachdev and R.N. Bhatt, *Phys. Rev. B* 41, 9323 (1990)) theory of coupled-ladder model,  
M. Vojta and T. Ulbricht, cond-mat/0402377



Numerical study of coupled ladder model,  
 G.S. Uhrig, K.P. Schmidt, and M. Grüninger,  
 cond-mat/0402659



## Conclusions

I. Theory of quantum phase transitions between magnetically ordered and paramagnetic states of Mott insulators:

*A. Dimerized Mott insulators:* Landau-Ginzburg-Wilson theory of fluctuating magnetic order parameter.

*B.  $S=1/2$  square lattice:* Berry phases induce bond order, and LGW theory breaks down. Critical theory is expressed in terms of emergent fractionalized modes, and the *order parameters are secondary.*

# Conclusions

## II. Competing spin-density-wave/bond/superconducting orders in the hole-doped cuprates.

- Main features of spectrum of excitations in LBCO modeled by LGW theory of quantum critical fluctuations in the presence of static bond order across a wide energy range.
- Predicted magnetic field dependence of spin-density-wave order observed by neutron scattering in LSCO. E. Demler, S. Sachdev, and Y. Zhang, *Phys.Rev. Lett.* **87**, 067202 (2001); B. Lake *et al. Nature*, **415**, 299 (2002); B. Khaykovich *et al. Phys. Rev. B* **66**, 014528 (2002).
- Predicted pinned bond order in vortex halo consistent with STM observations in BSCCO. K. Park and S. Sachdev *Phys. Rev. B* **64**, 184510 (2001); Y. Zhang, E. Demler and S. Sachdev, *Phys. Rev. B* **66**, 094501 (2002); J.E. Hoffman *et al. Science* **295**, 466 (2002).
- Energy dependence of LDOS modulations in BSCCO best modeled by modulations in bond variables. M. Vojta, *Phys. Rev. B* **66**, 104505 (2002); D. Podolsky, E. Demler, K. Damle, and B.I. Halperin, *Phys. Rev. B* **67**, 094514 (2003); C. Howald, H. Eisaki, N. Kaneko, and A. Kapitulnik, *Phys. Rev. B* **67**, 014533 (2003).

## Conclusions

III. Breakdown of LGW theory of quantum phase transitions with magnetic/bond/superconducting orders in doped Mott insulators ?