

# Quantum phase transitions of correlated electrons and atoms

Subir Sachdev  
*Harvard University*

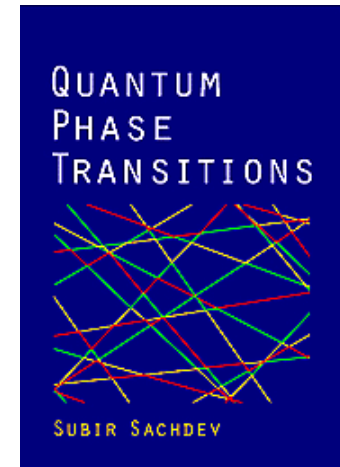
Course at Harvard University:

**Physics 268r**

*Classical and Quantum Phase Transitions.*

MWF 10 in Jefferson 256

First meeting: Feb 1.



*Quantum Phase Transitions*  
Cambridge University Press



# 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

*1. Berry phases and the mapping to a compact  $U(1)$  gauge theory*

*2. Valence-bond-solid (VBS) order in the paramagnet;*

*3. Mapping to hard-core bosons at half-filling*

C. The superfluid-insulator transition of bosons in lattices

*Multiple order parameters in quantum systems*

D. Boson-vortex duality

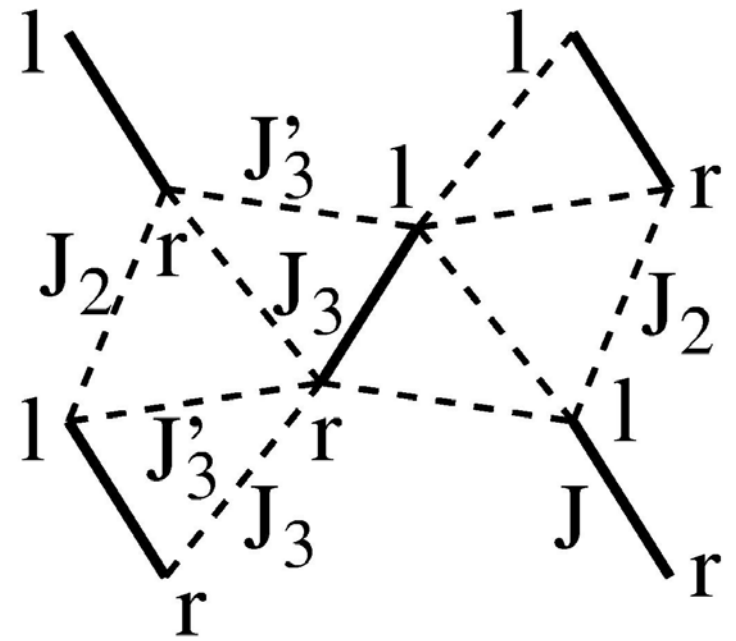
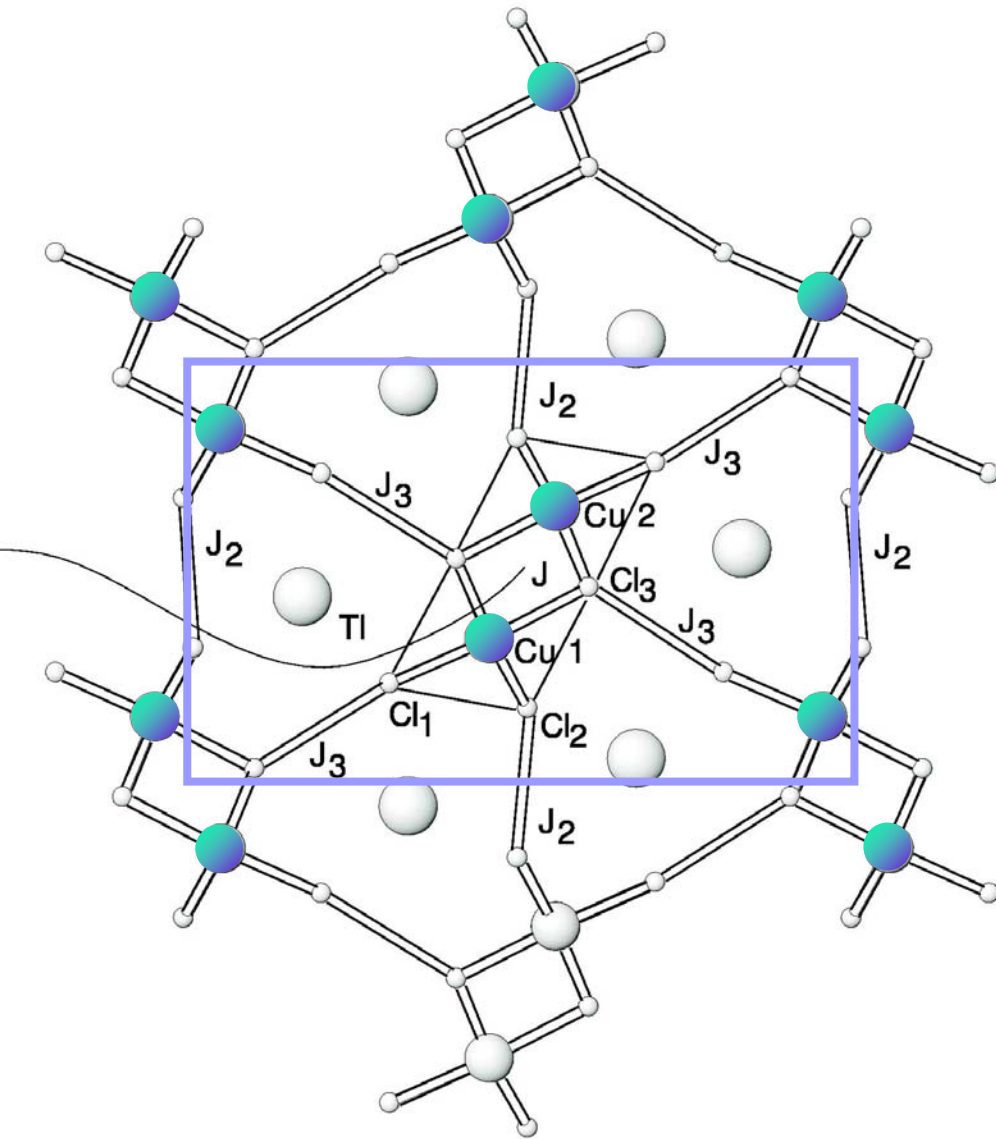
*Breakdown of the LGW paradigm*

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

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

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

# TiCuCl<sub>3</sub>



# Coupled Dimer Antiferromagnet

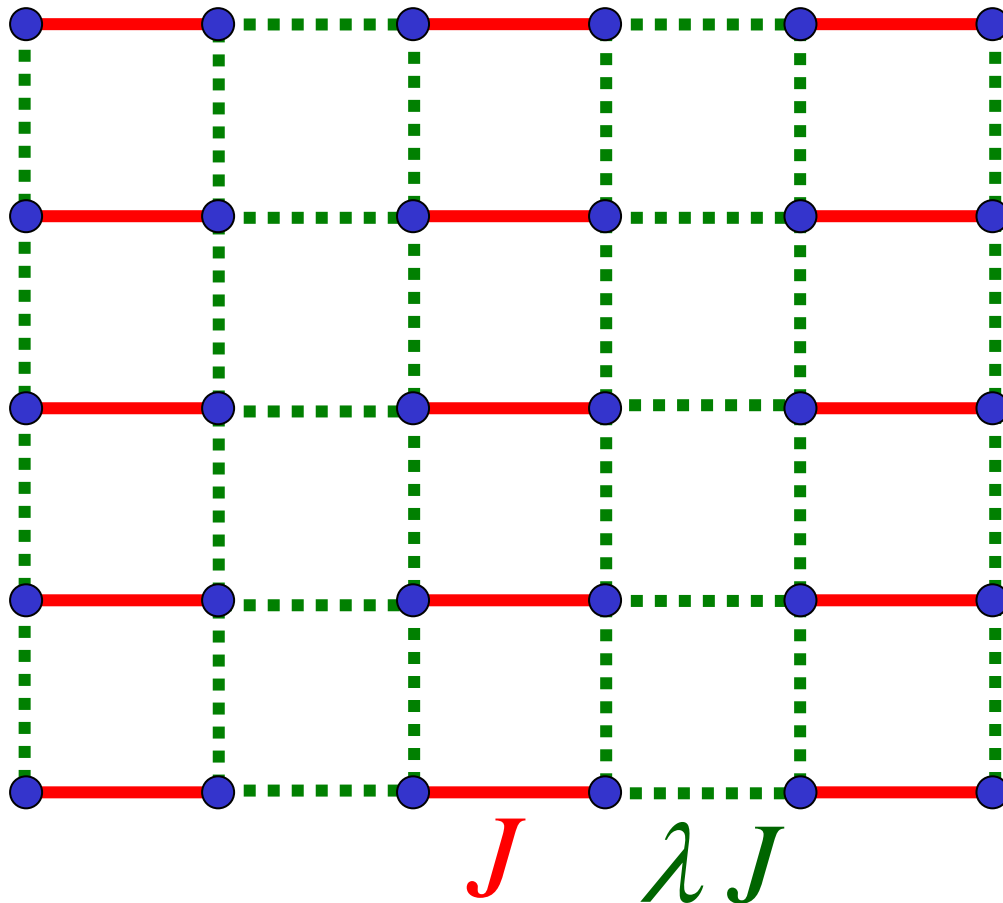
M. P. Gelfand, R. R. P. Singh, and D. A. Huse, *Phys. Rev. B* **40**, 10801-10809 (1989).

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

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

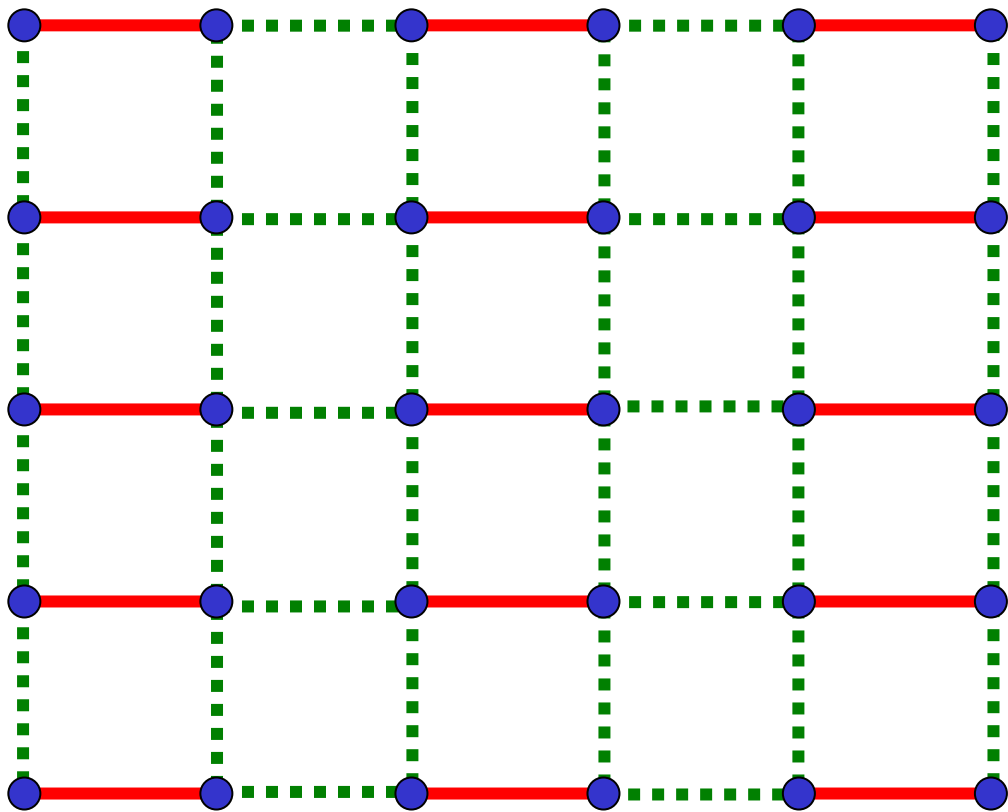
M. Matsumoto, C. Yasuda, S. Todo, and H. Takayama, *Phys. Rev. B* **65**, 014407 (2002).

$S=1/2$  spins on coupled dimers



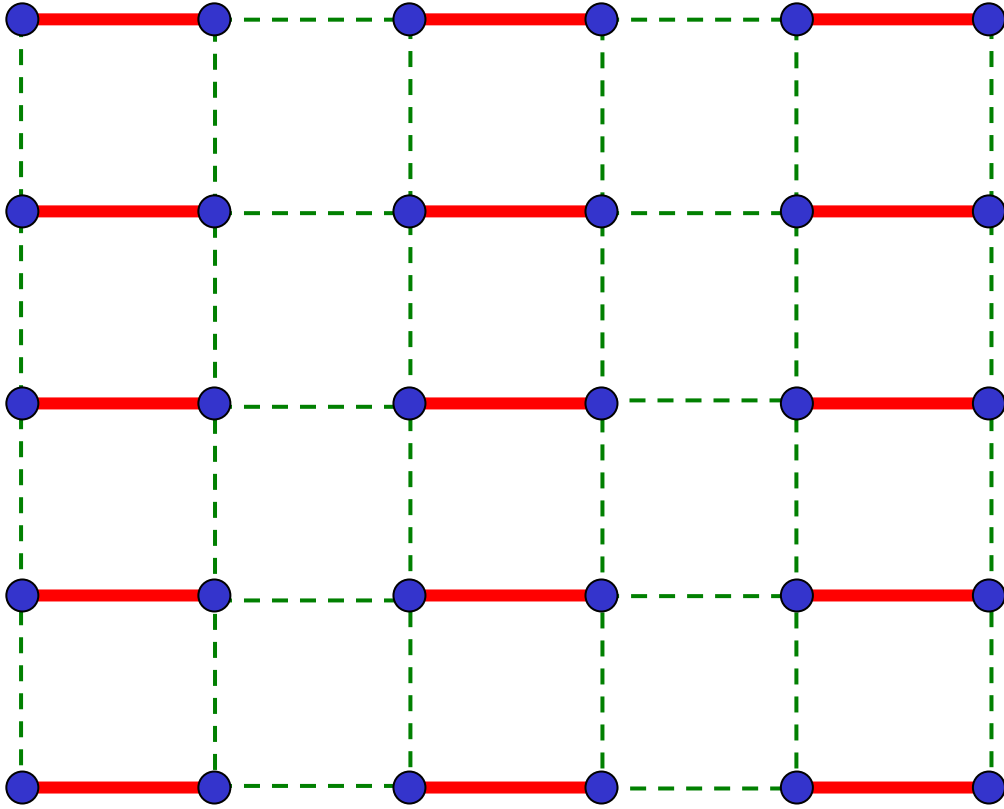
$$H = \sum_{\langle ij \rangle} J_{ij} \vec{S}_i \cdot \vec{S}_j$$

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



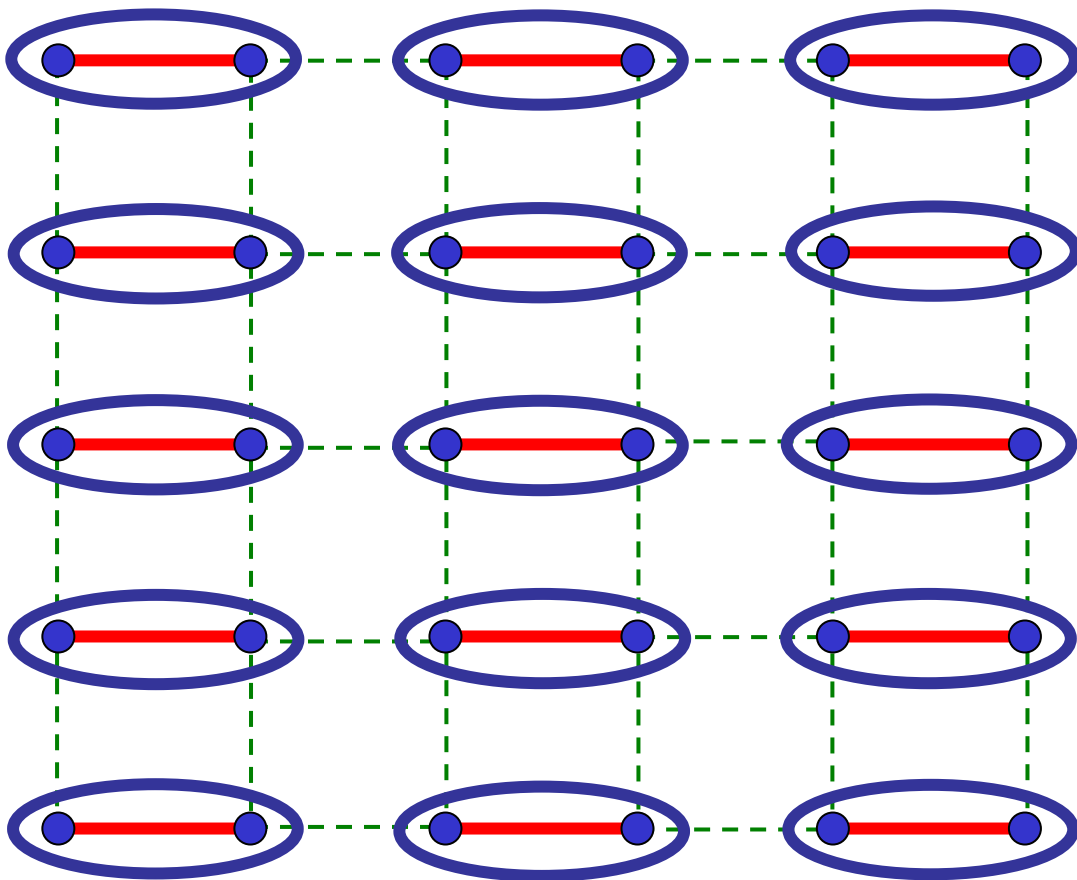
$\lambda$  close to 0

Weakly coupled dimers



$\lambda$  close to 0

Weakly coupled dimers



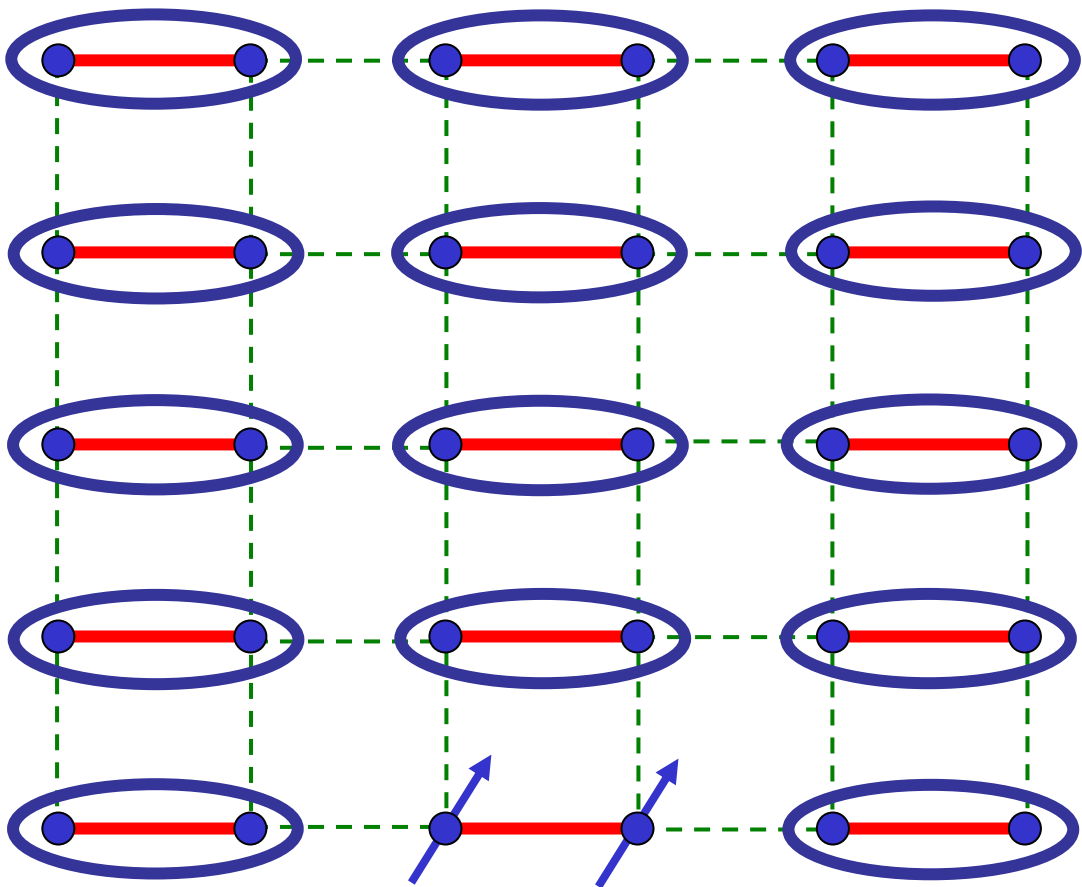
$$\text{Dimer} = \frac{1}{\sqrt{2}} (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$$

Paramagnetic ground state

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

$\lambda$  close to 0

Weakly coupled dimers

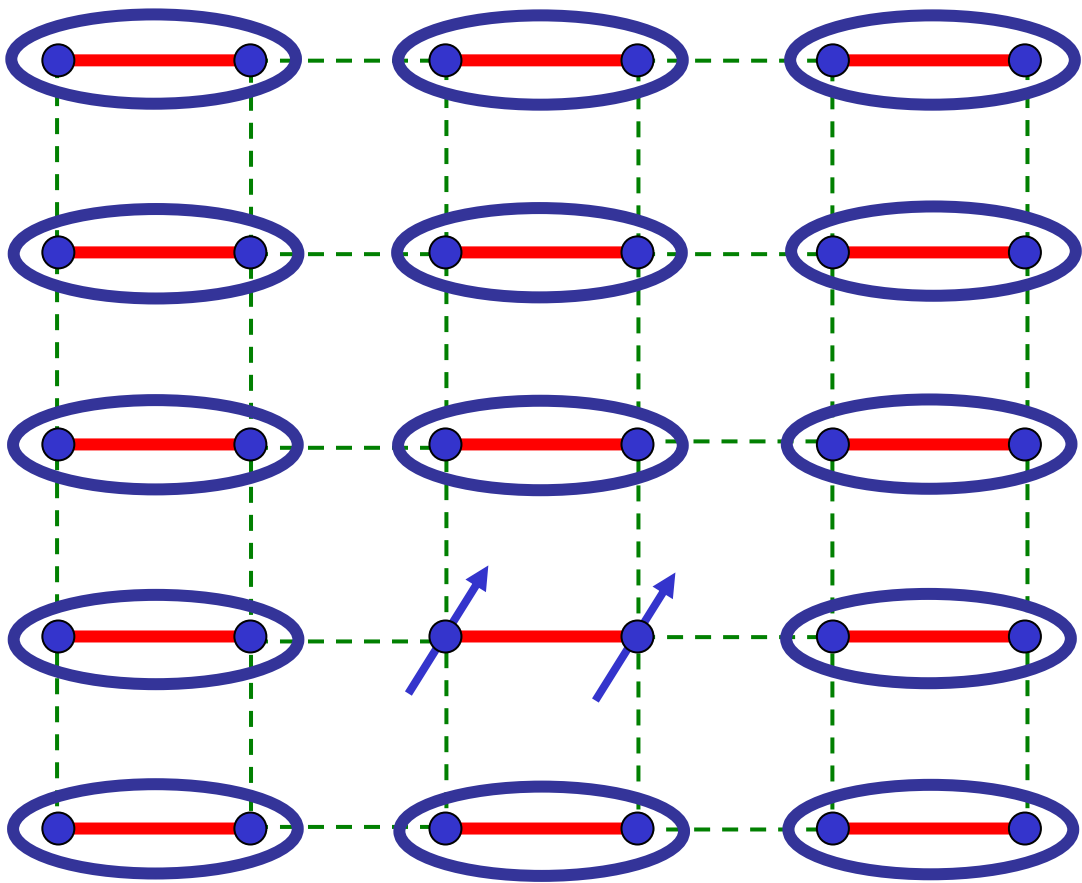


$$\text{dimer} = \frac{1}{\sqrt{2}} (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$$

Excitation:  $S=1$  *triplon*

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Weakly coupled dimers

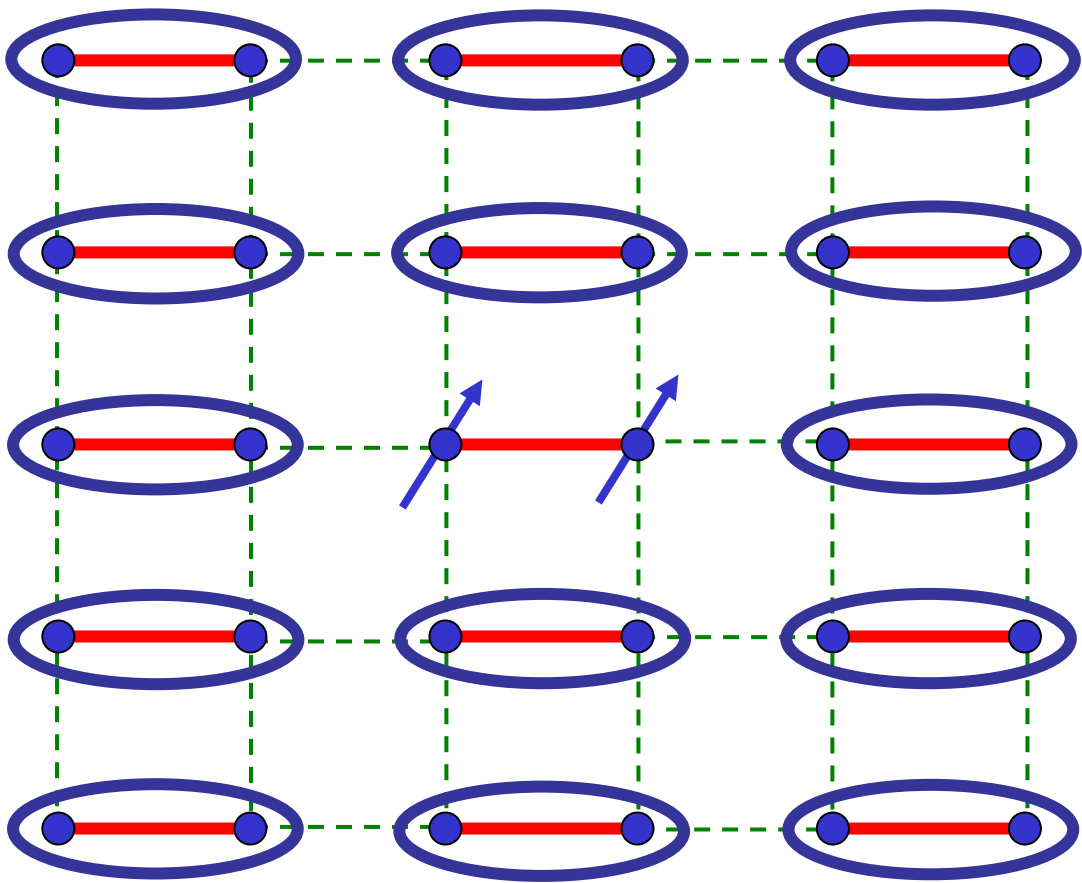


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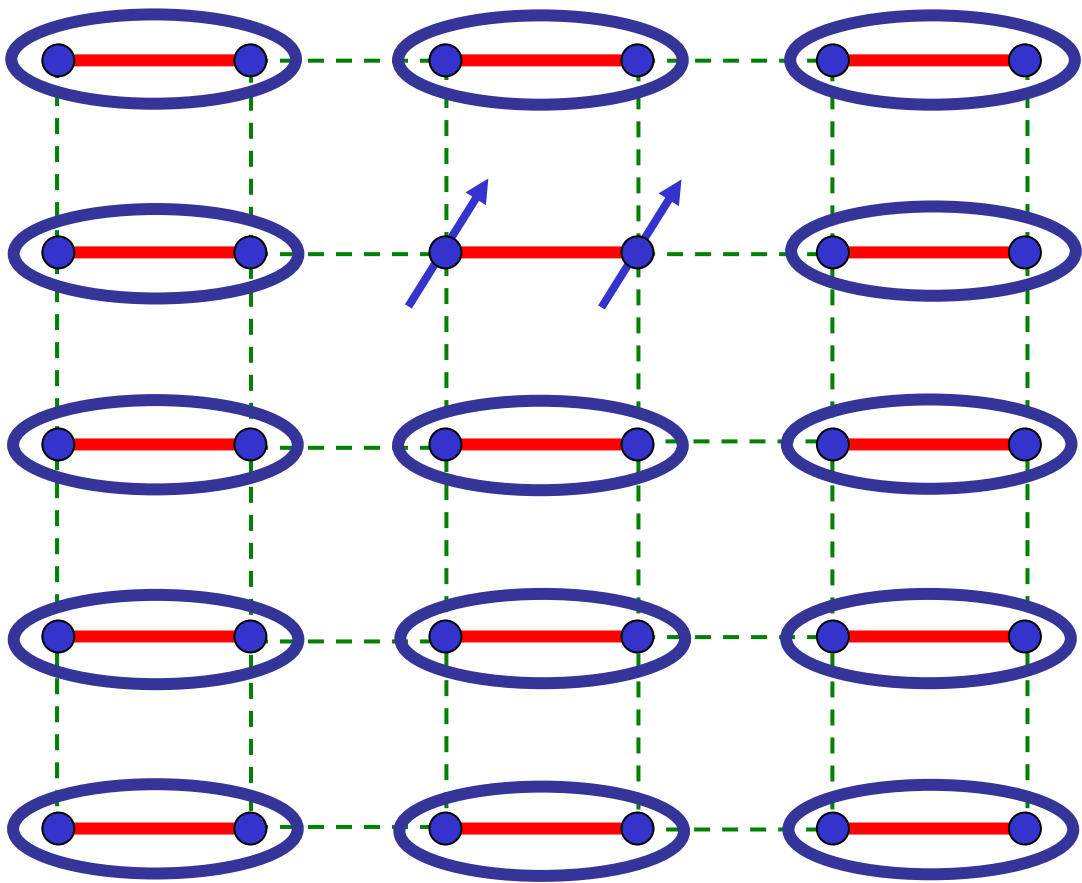


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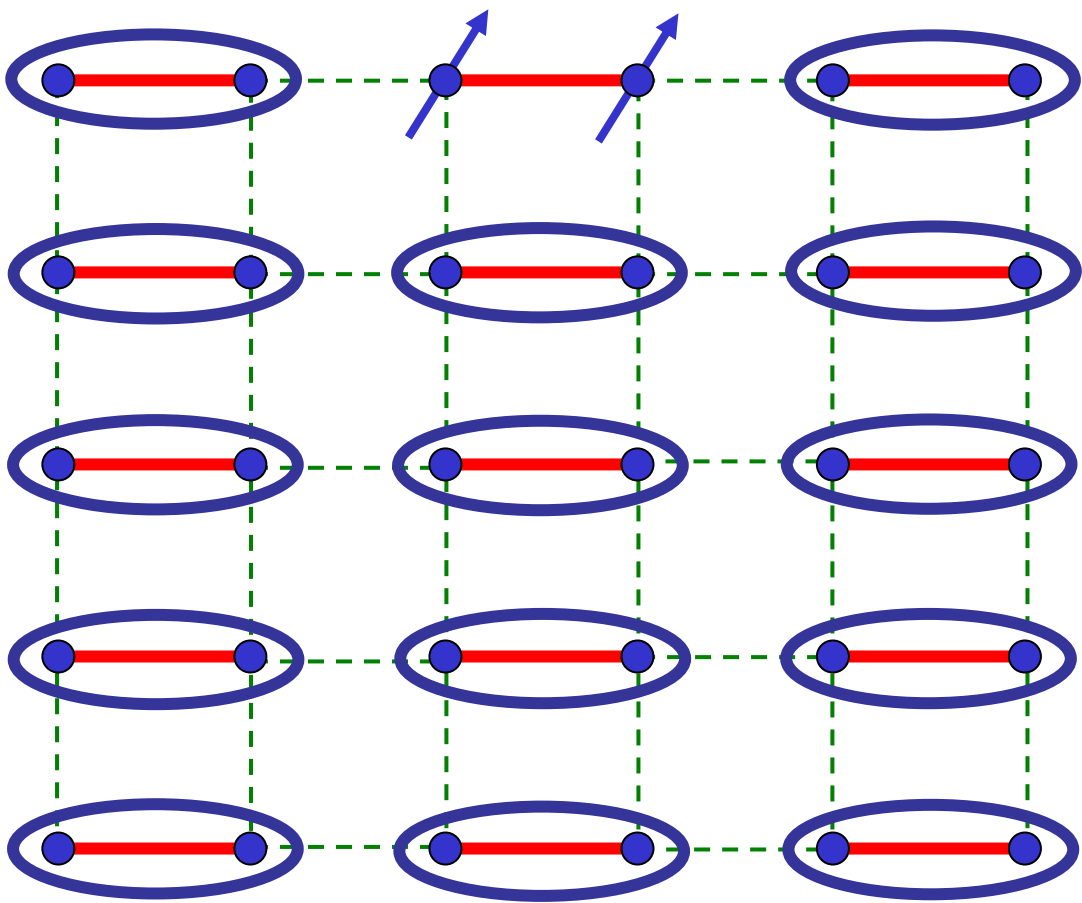


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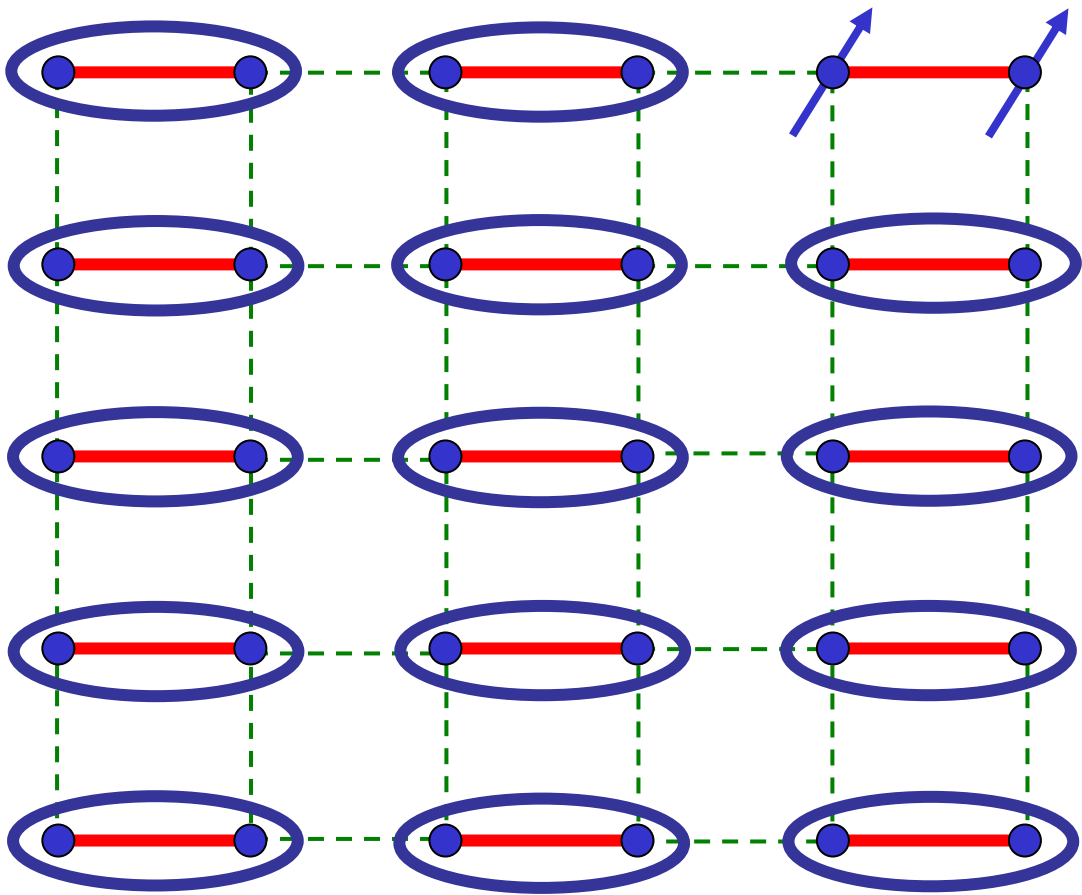


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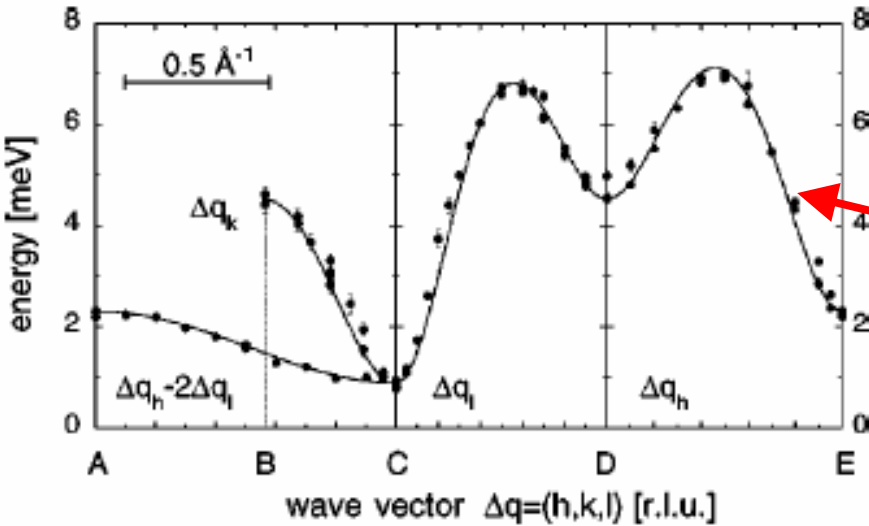
Excitation:  $S=1$  *triplon*  
(*exciton*, spin collective mode)

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).

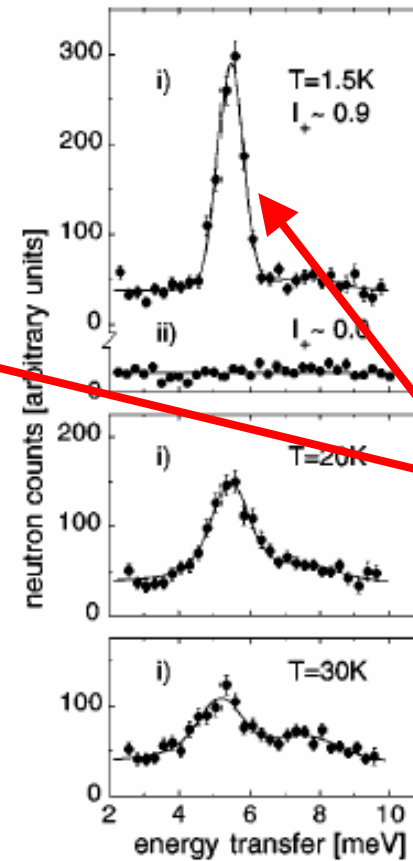


FIG. 1. Measured neutron profiles in the  $a^*c^*$  plane of TlCuCl<sub>3</sub> for  $i=(1.35,0,0)$ ,  $ii=(0,0,3.15)$  [r.l.u.]. The spectrum at  $T=1.5$  K

“triplon”

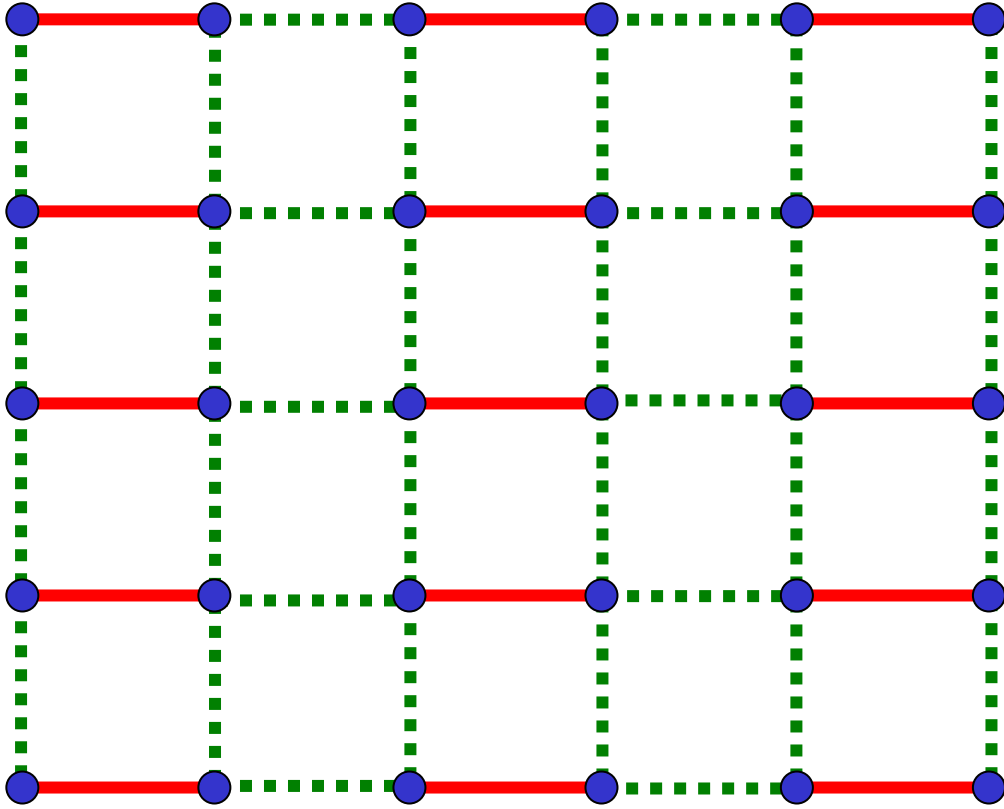
For quasi-one-dimensional systems, the triplon linewidth takes

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)

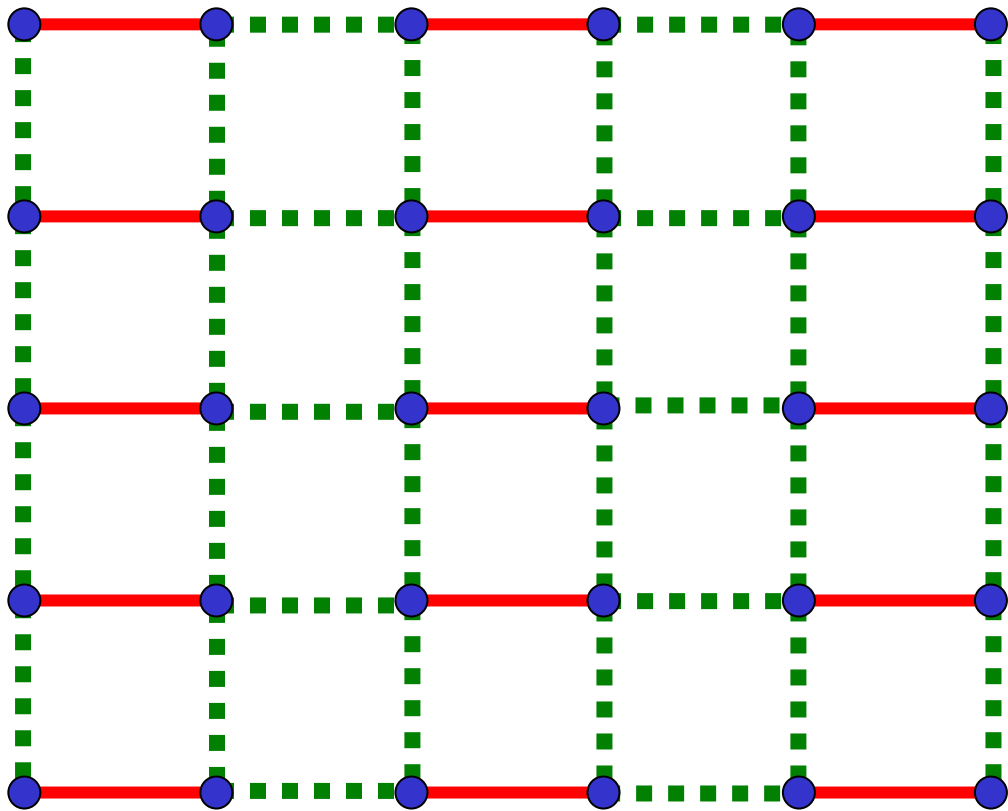
This result is in good agreement with observations in CsNiCl<sub>3</sub> (M. Kenzelmann, R. A. Cowley, W. J. L. Buyers, R. Coldea, M. Enderle, and D. F. McMorrow *Phys. Rev. B* **66**, 174412 (2002)) and Y<sub>2</sub>NiBaO<sub>5</sub> (G. Xu, C. Broholm, G. Aeppli, J. F. DiTusa, T. Ito, K. Oka, and H.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

# Coupled Dimer Antiferromagnet



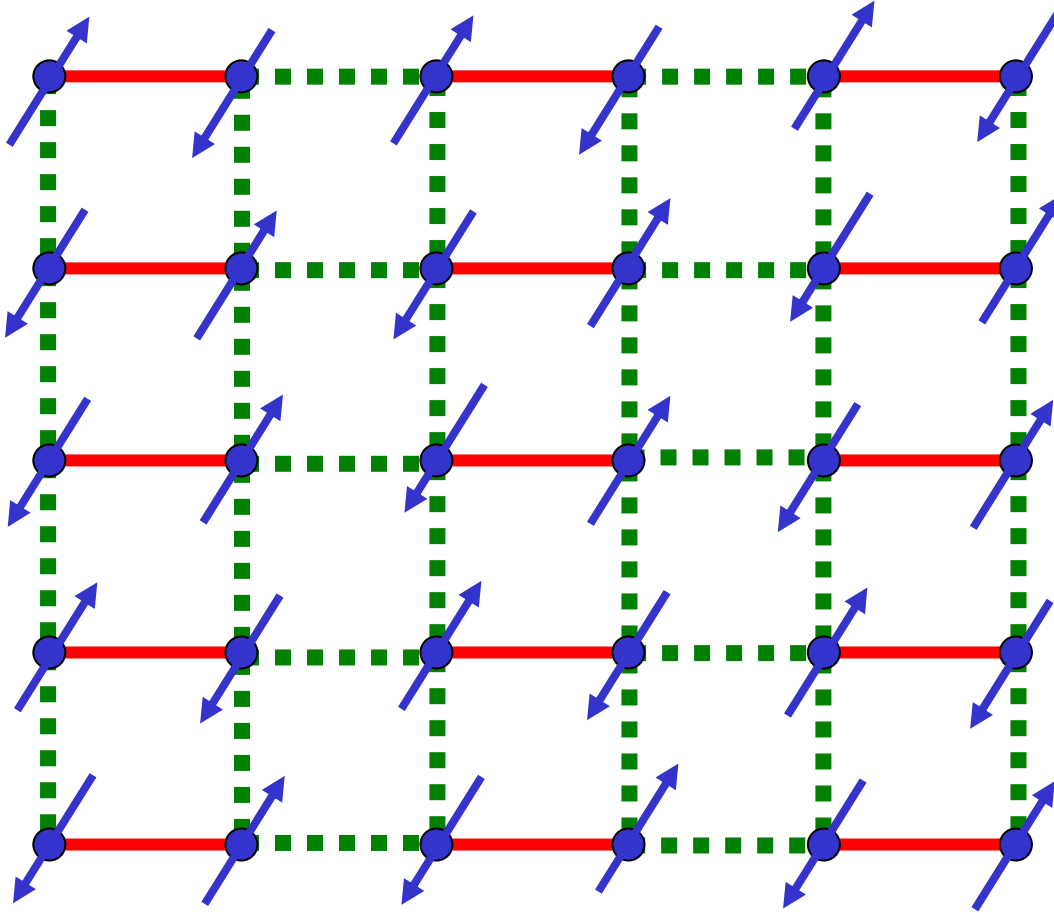
$\lambda$  close to 1

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>

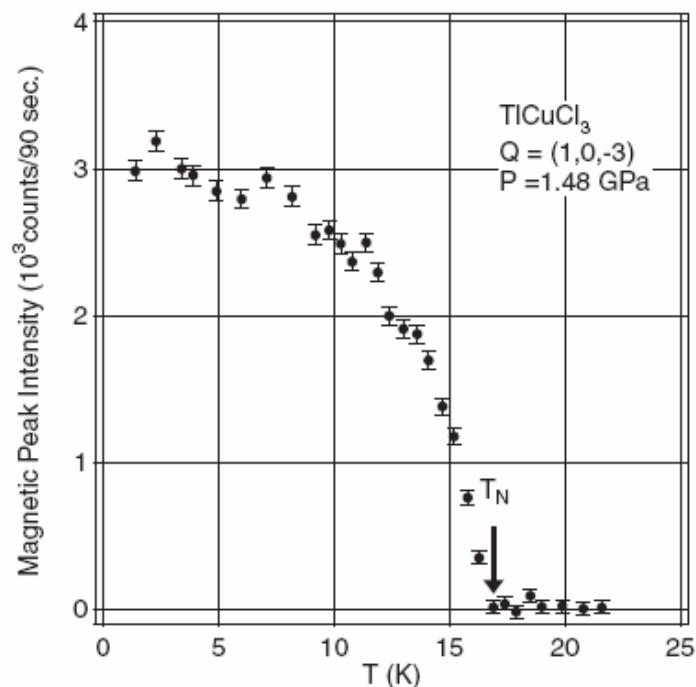
Akira OOSAWA\*, Masashi FUJISAWA<sup>1</sup>, Toyotaka OSAKABE, Kazuhisa KAKURAI and Hidekazu TANAKA<sup>2</sup>

*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)



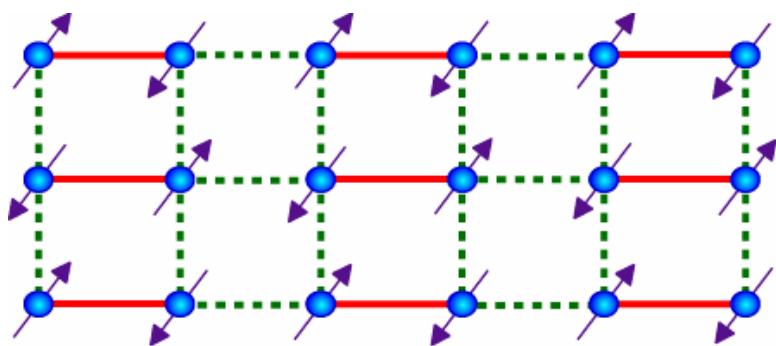
*J. Phys. Soc. Jpn* **72**, 1026 (2003)

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>.

$T=0$

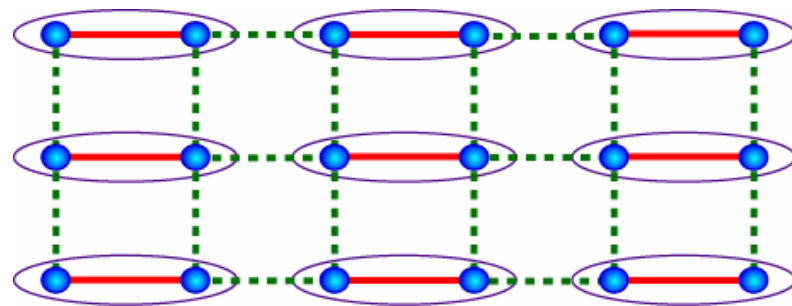
$$\lambda_c = 0.52337(3)$$

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))

# LGW theory for quantum criticality

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

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

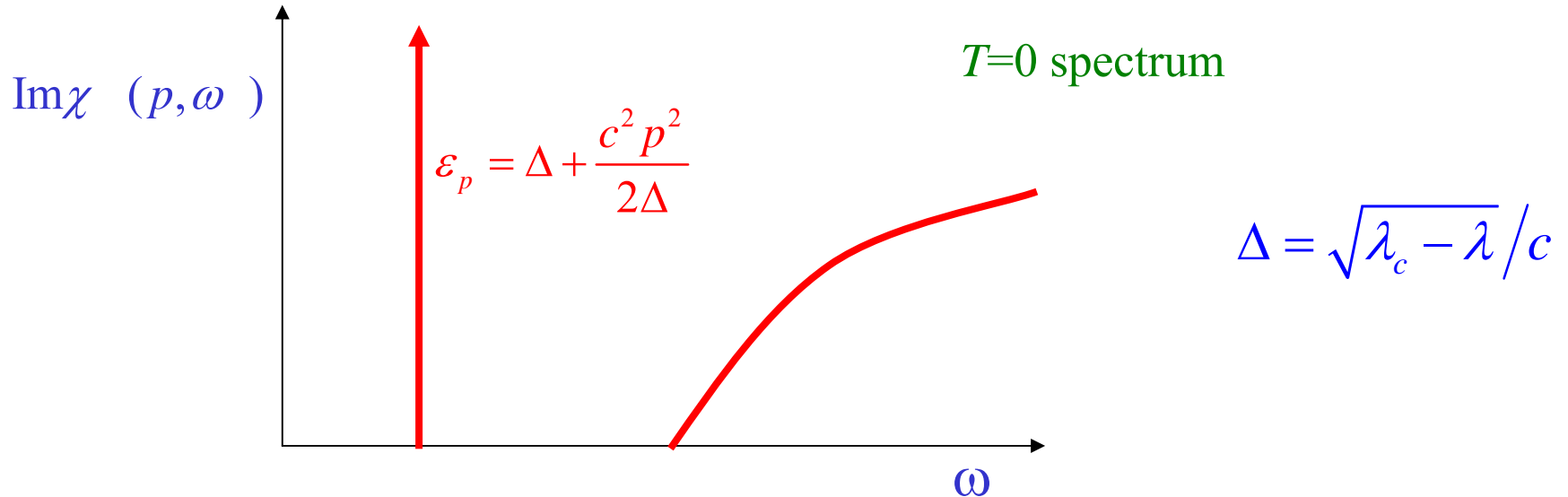
# Quantum field theory for critical point

$\lambda$  close to  $\lambda_c$  : use “soft spin” field

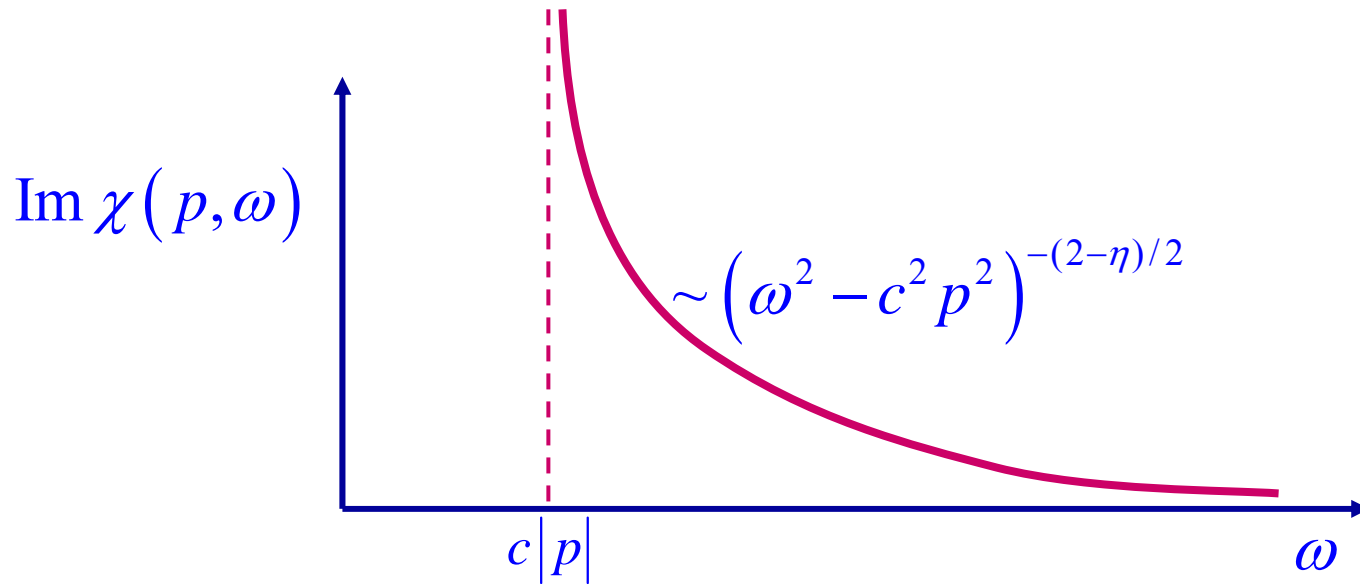
$$\mathcal{S}_b = \int d^2x d\tau \left[ \frac{1}{2} \left( (\nabla_x \phi_\alpha)^2 + c^2 (\partial_\tau \phi_\alpha)^2 + (\lambda_c - \lambda) \phi_\alpha^2 \right) + \frac{u}{4!} (\phi_\alpha^2)^2 \right]$$

$\phi_\alpha \longrightarrow$  3-component antiferromagnetic order parameter

Oscillations of  $\phi_\alpha$  about zero (for  $\lambda < \lambda_c$ )  
 $\longrightarrow$  spin-1 collective mode



Dynamic spectrum at the critical point



No quasiparticles --- dissipative critical continuum

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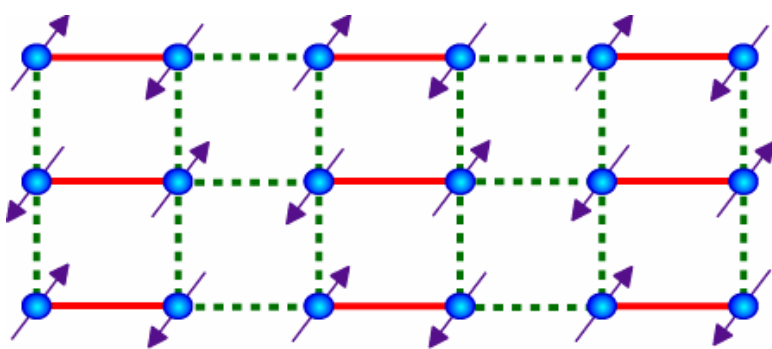
B. Mott insulators with spin  $S=1/2$  per unit cell:

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# Recall: dimerized Mott insulators

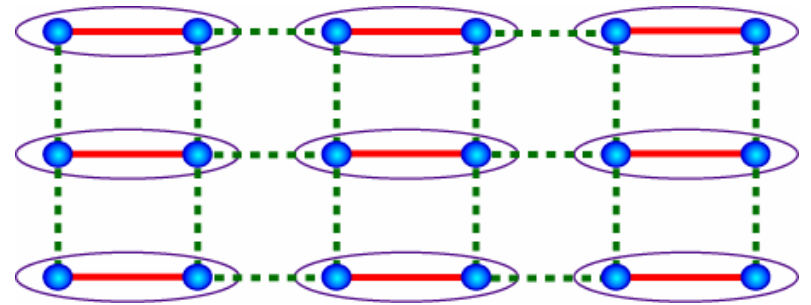
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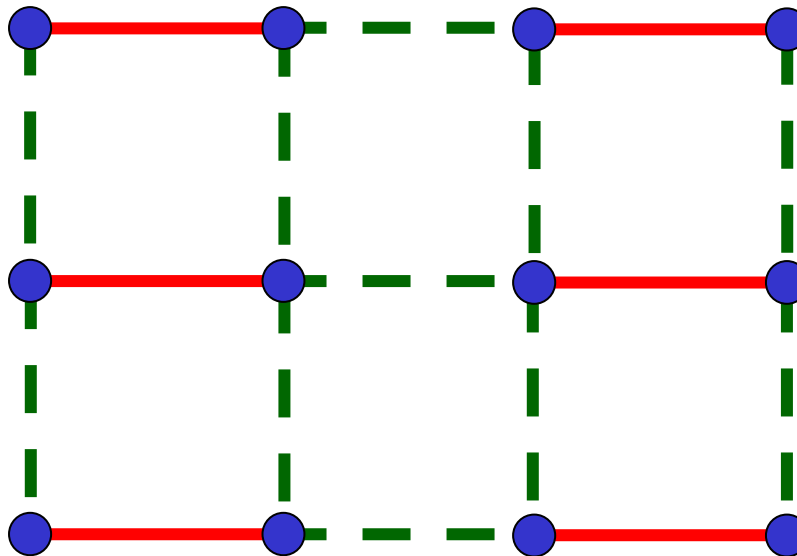


Quantum paramagnet

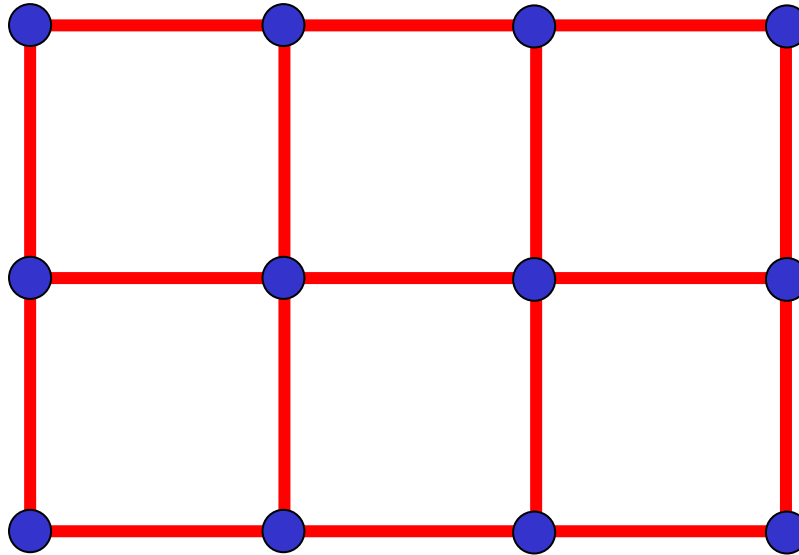
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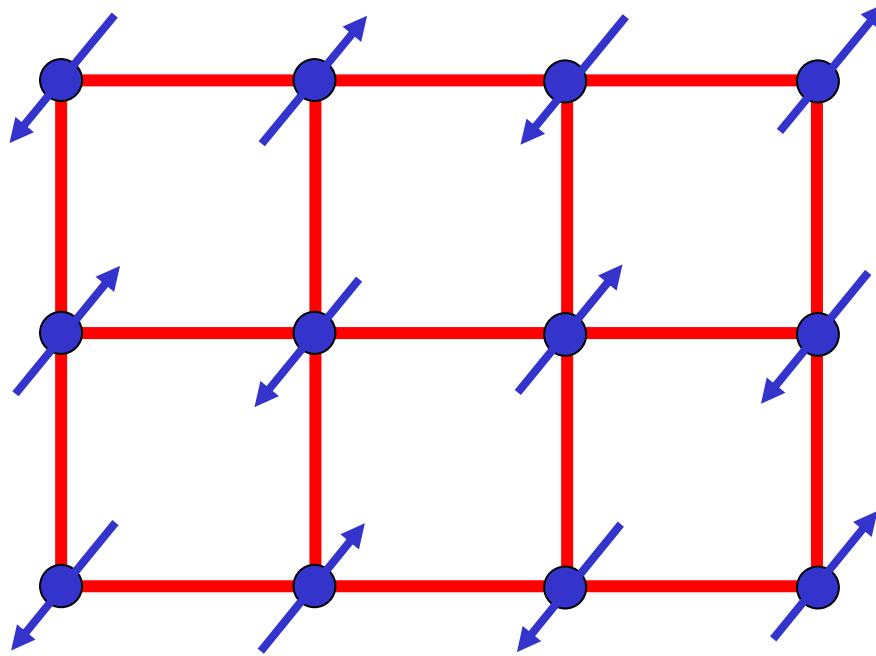
Mott insulator with two  $S=1/2$  spins per unit cell



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

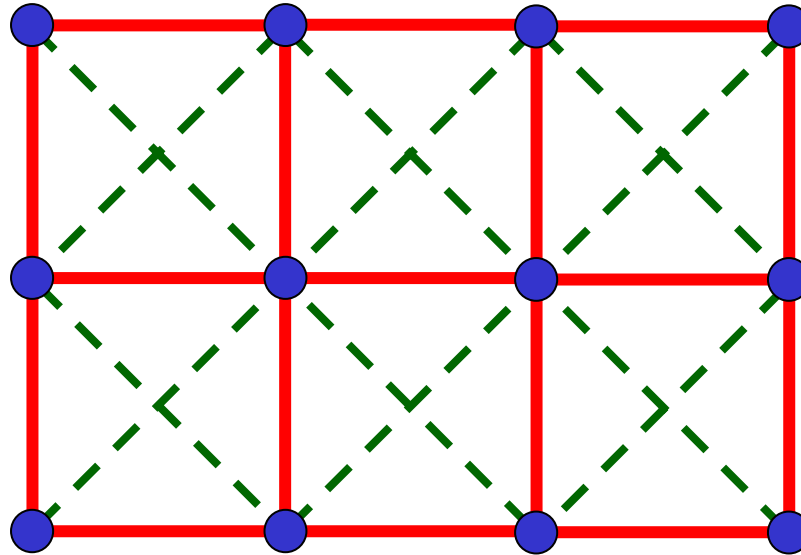


Mott insulator with one  $S=1/2$  spin per unit cell



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

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



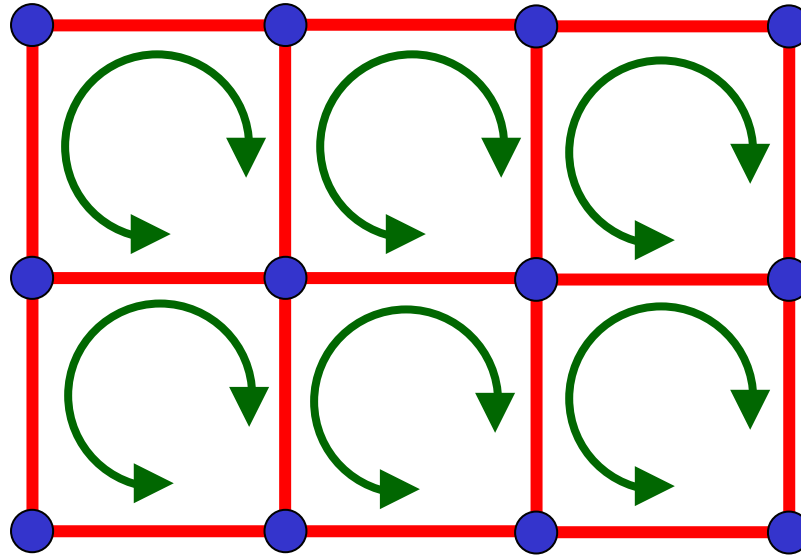
Destroy Neel order by perturbations which preserve full square lattice symmetry *e.g.* second-neighbor or ring exchange.

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

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## LGW theory for such a quantum transition

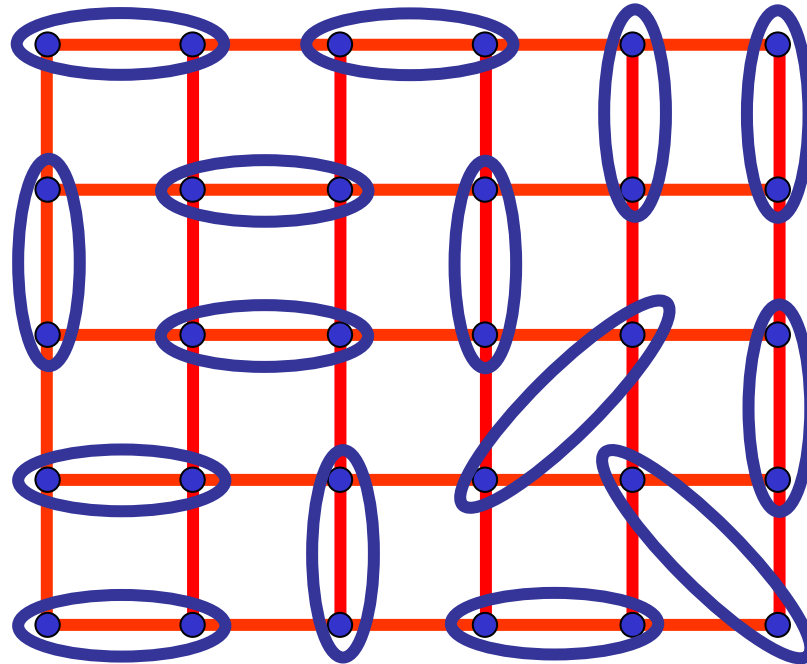
$$S_\phi = \int d^2x d\tau \left[ \frac{1}{2} \left( (\nabla_x \vec{\phi})^2 + \frac{1}{c^2} (\partial_\tau \vec{\phi})^2 + r \vec{\phi}^2 \right) + \frac{u}{4!} (\vec{\phi}^2)^2 \right]$$

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

*The field theory predicts that this state has no broken symmetries and has a stable  $S=1$  quasiparticle excitation (the triplon)*

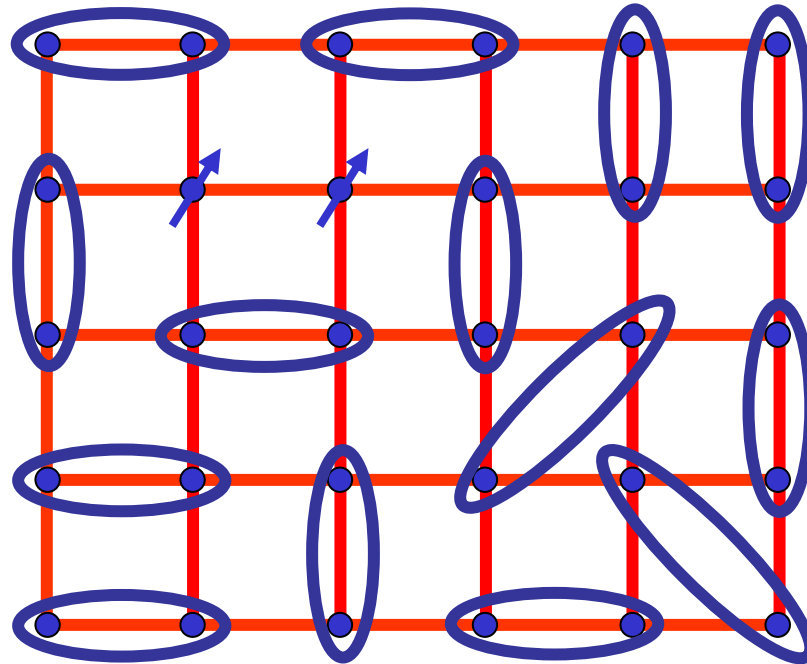
**Problem: there is no state with a gapped, stable**  
 **$S=1$  quasiparticle and no broken symmetries**

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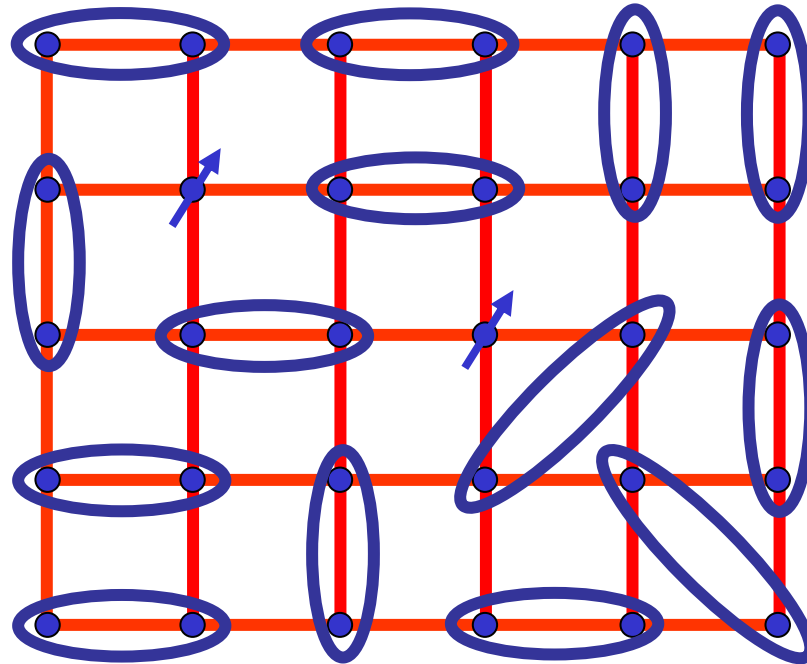
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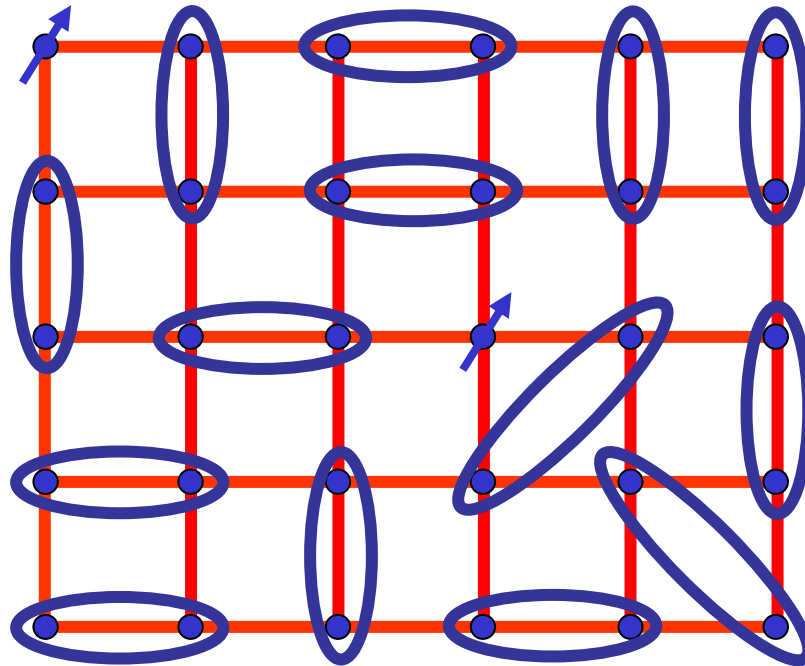
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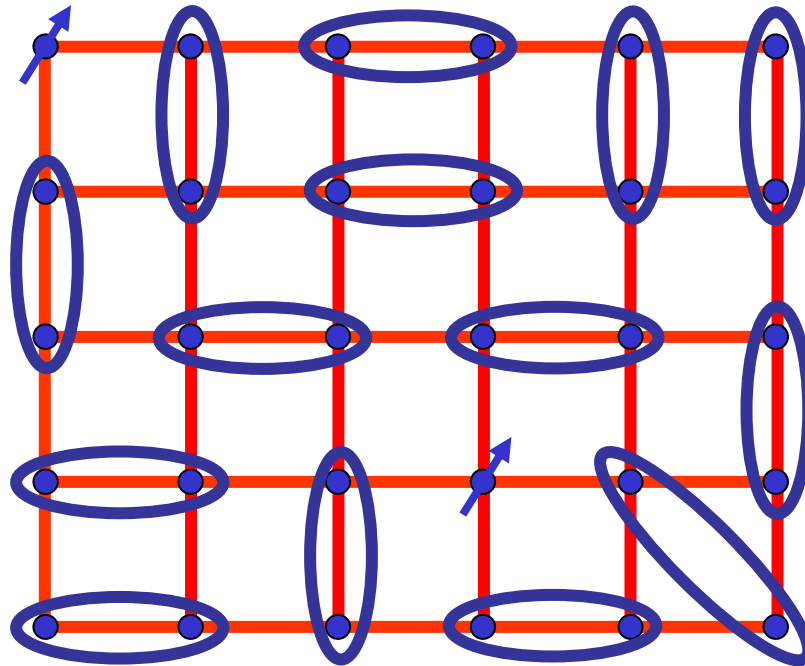
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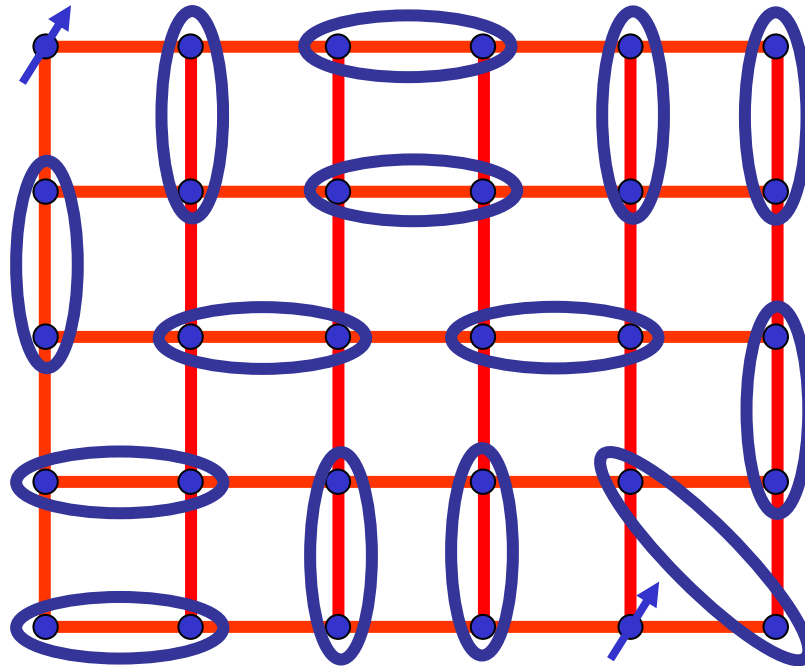
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“Liquid” of valence bonds has fractionalized  $S=1/2$  excitations

# Quantum theory for destruction of Neel order

## Ingredient missing from LGW theory: Spin Berry Phases

### Coherent state path integral for a single spin

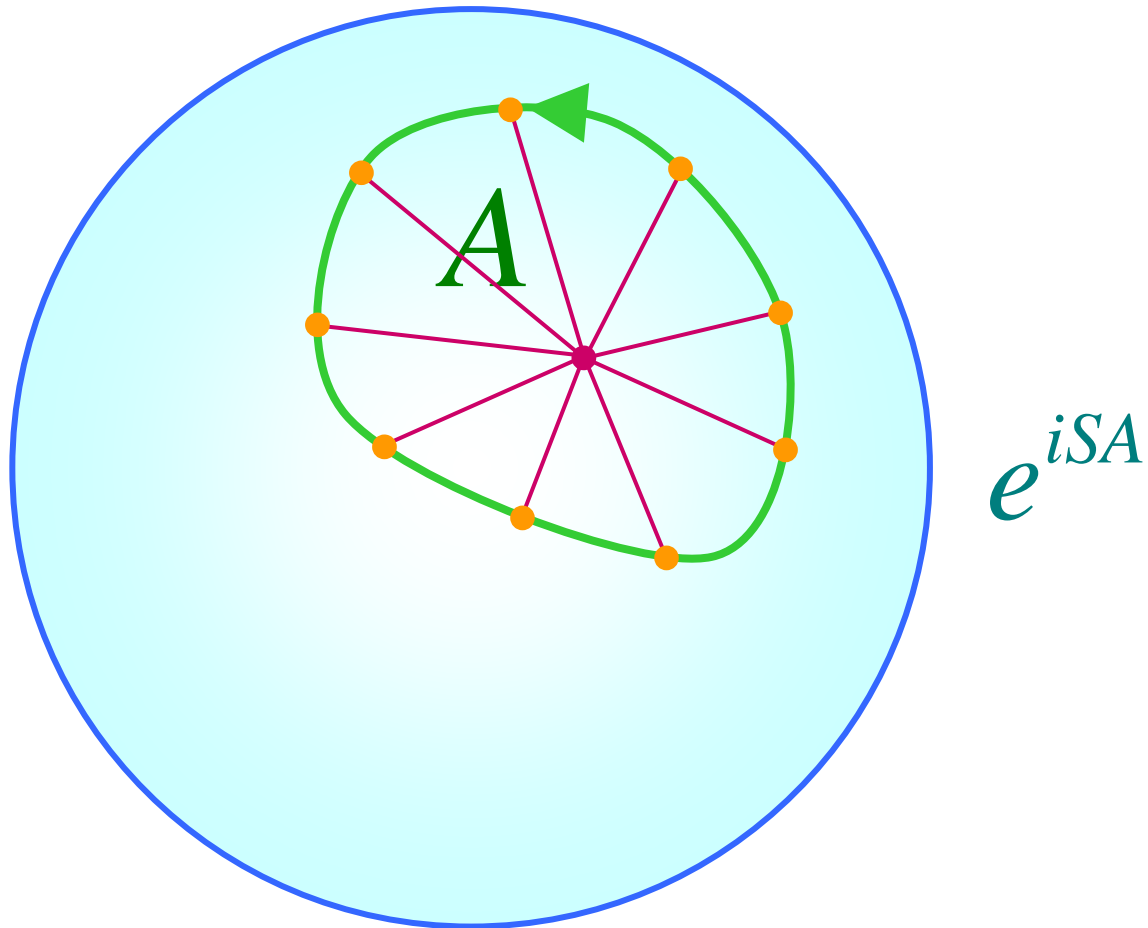
$$\begin{aligned} Z &= \text{Tr} \left( e^{-H[S]/T} \right) \\ &= \int \mathcal{D}N(\tau) \delta(N^2 - 1) \exp \left( -iS \int A_\tau(\tau) d\tau - \int d\tau H [SN(\tau)] \right) \end{aligned}$$

$A_\tau(\tau) d\tau$  = Oriented area of triangle on surface of unit sphere bounded by  $N(\tau)$ ,  $N(\tau + d\tau)$ , and a fixed reference  $N_0$

See Chapter 13 of *Quantum Phase Transitions*, S. Sachdev, Cambridge University Press (1999).

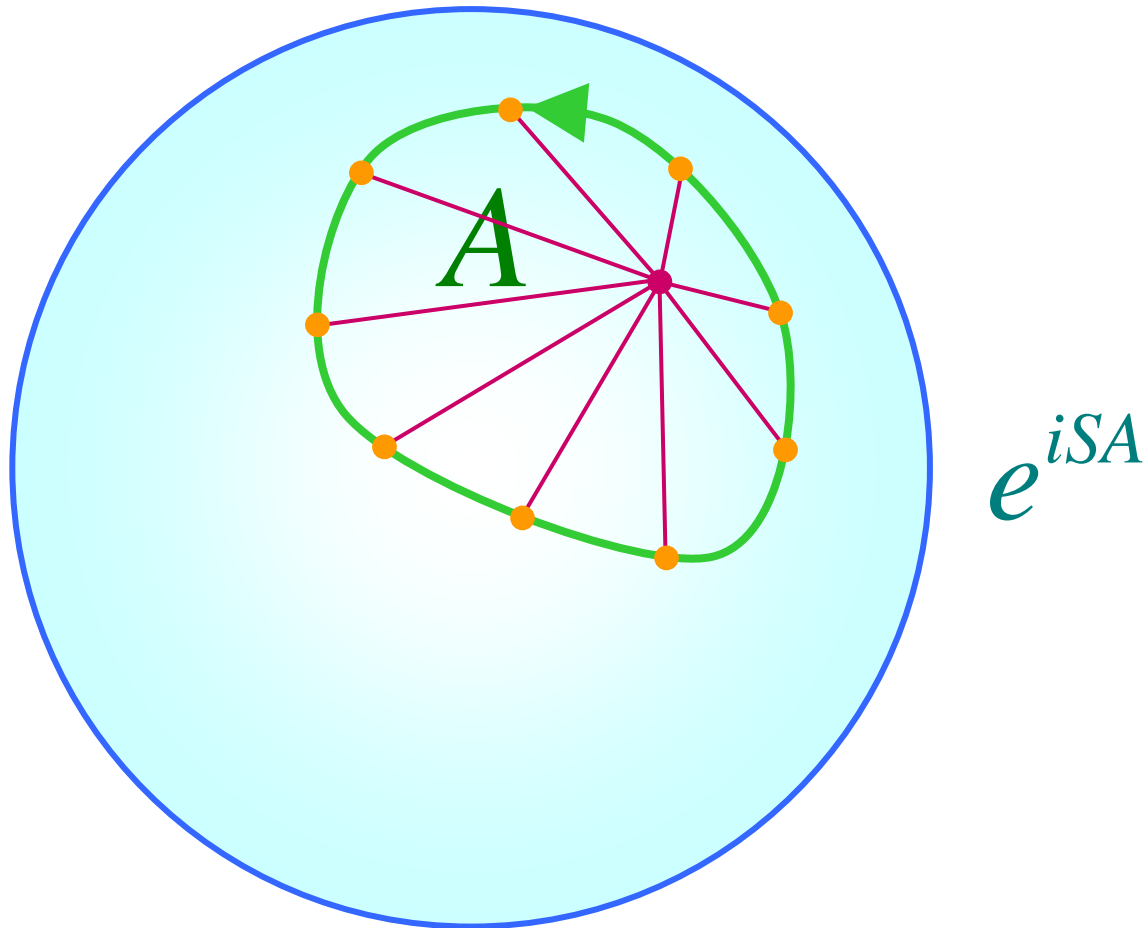
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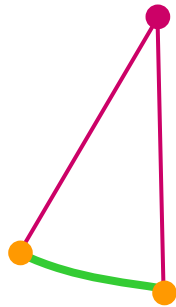


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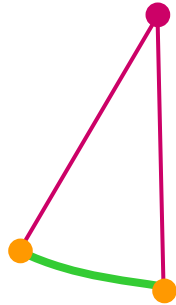


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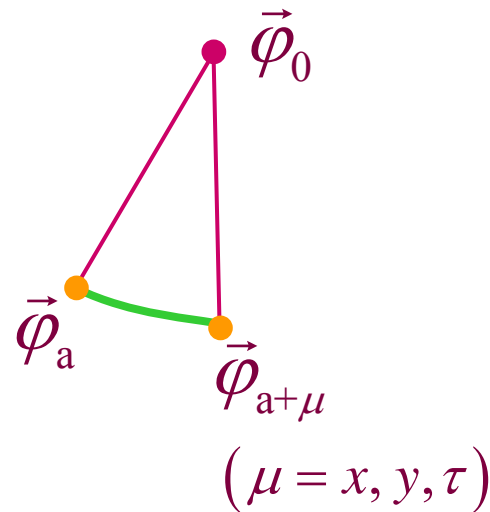
Discretize imaginary time: path integral is over fields on the sites of a cubic lattice of points  $a$



## Quantum theory for destruction of Neel order

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 ;



## Quantum theory for destruction of Neel order

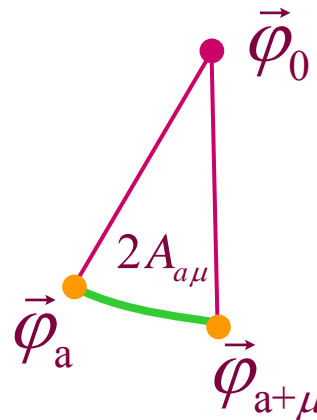
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$A_{a\mu} \rightarrow$  half oriented area of spherical triangle

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



## Quantum theory for destruction of Neel order

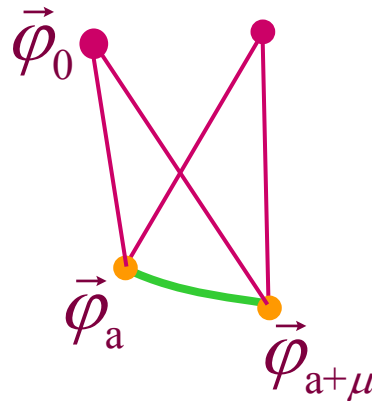
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## Quantum theory for destruction of Neel order

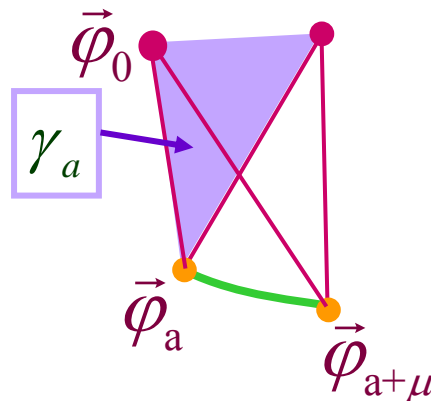
Discretize imaginary time: path integral is over fields on the sites of a cubic lattice of points  $a$

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 ;

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

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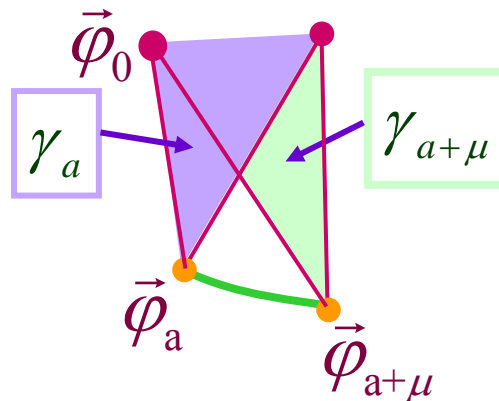
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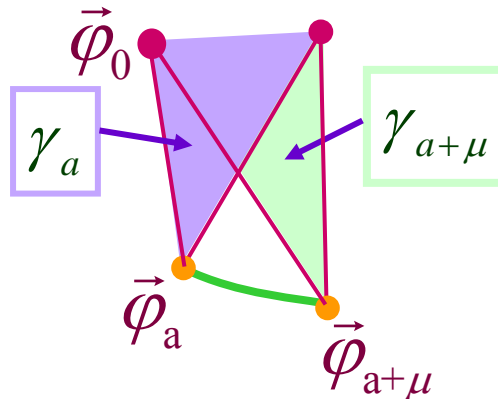
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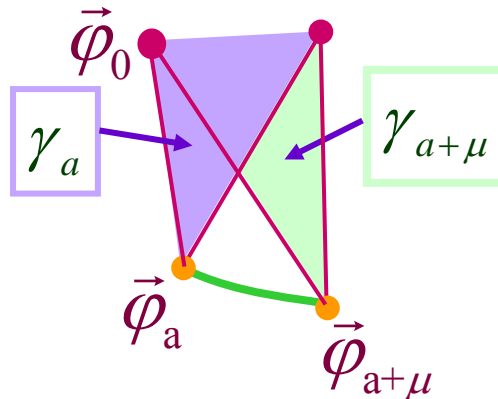
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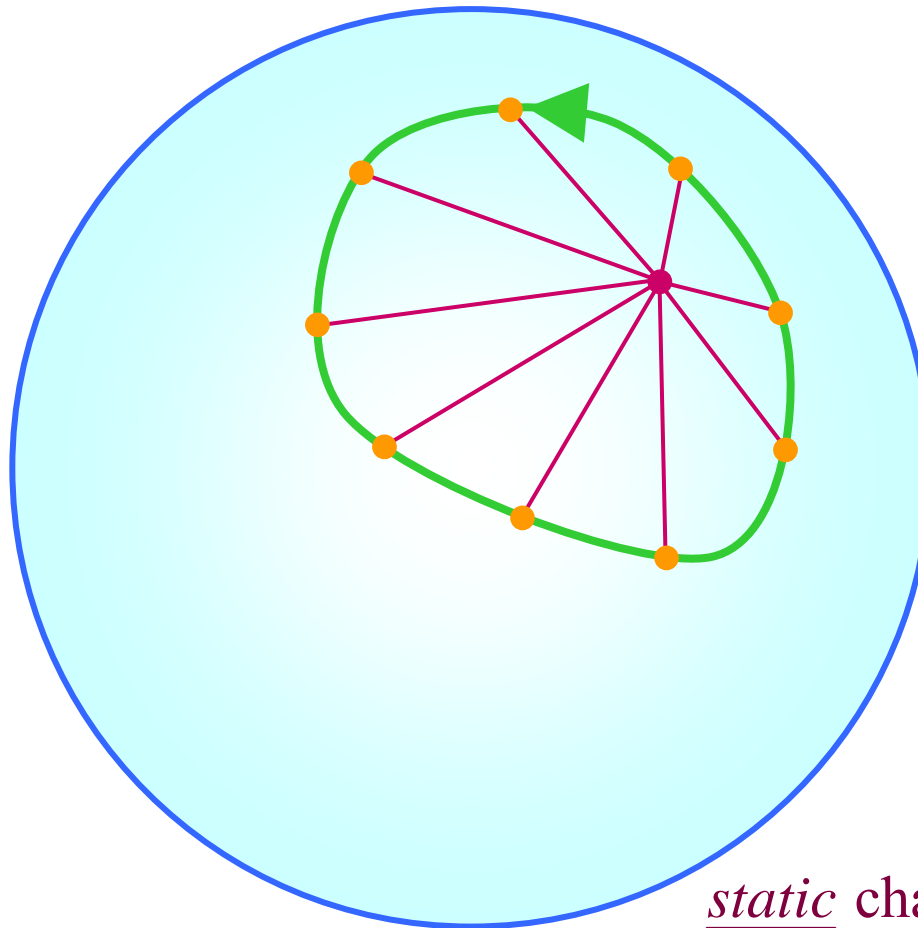
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The area of the triangle is uncertain modulo  $4\pi$ , and the action has to be invariant under  $A_{a\mu} \rightarrow A_{a\mu} + 2\pi$

# 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 gauge theory has valence bond solid (VBS) order in the ground state for all  $e$

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

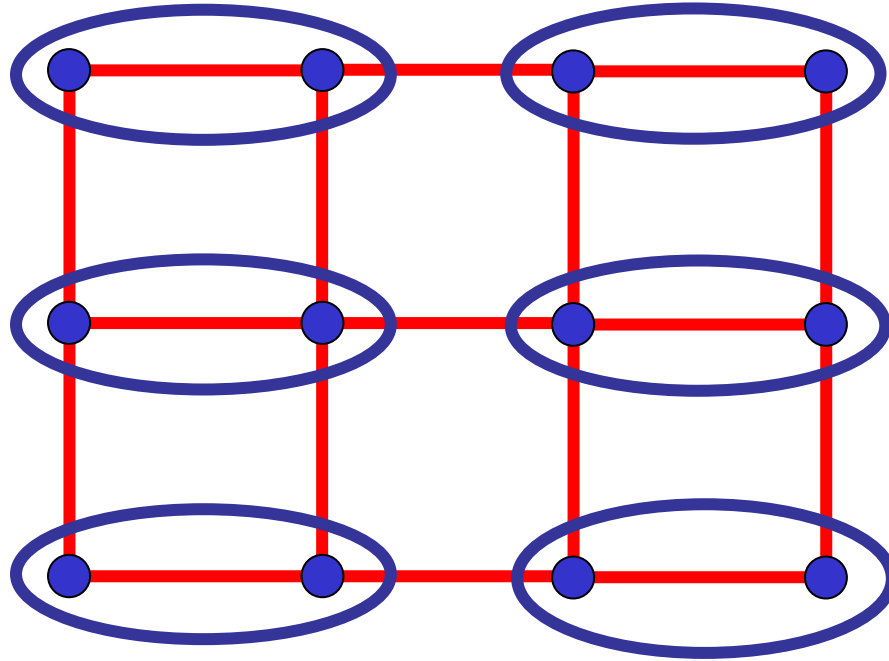
S. Sachdev and R. Jalabert, *Mod. Phys. Lett. B* **4**, 1043 (1990).

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

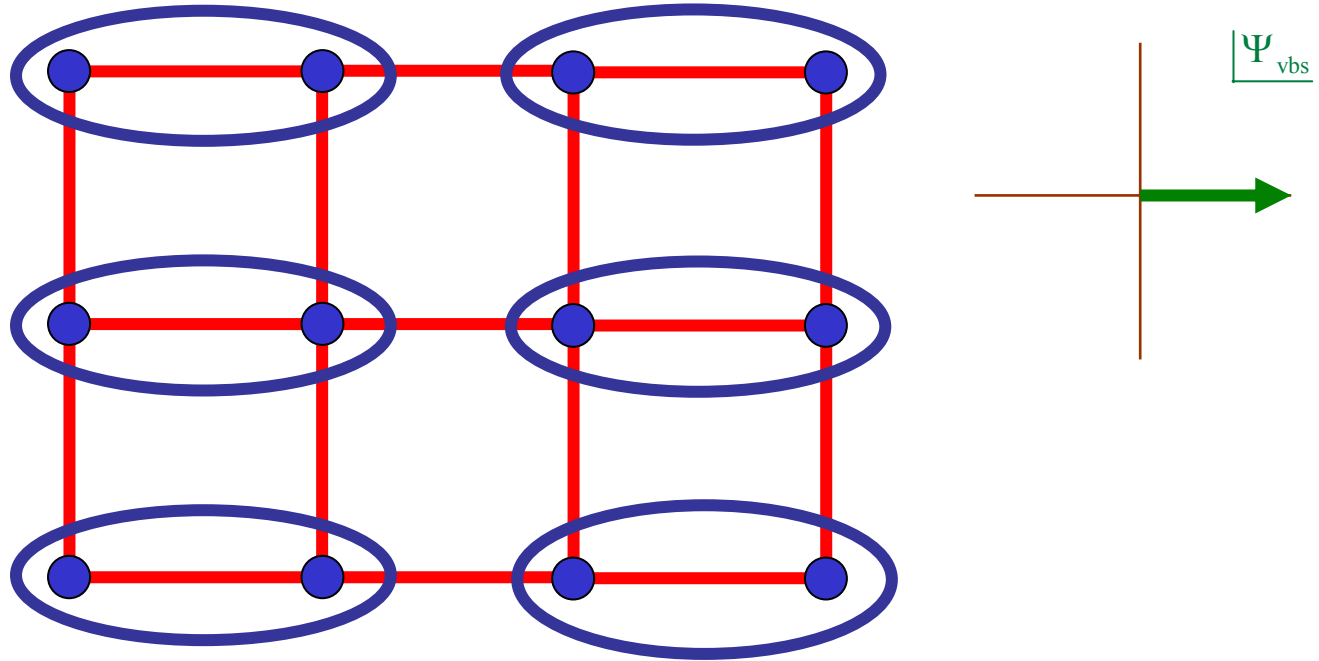
## B. Mott insulators with spin $S=1/2$ per unit cell:

- 1. Berry phases and the mapping to a compact  $U(1)$  gauge theory.*
- 2. Valence bond solid (VBS) order in the paramagnet.*

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



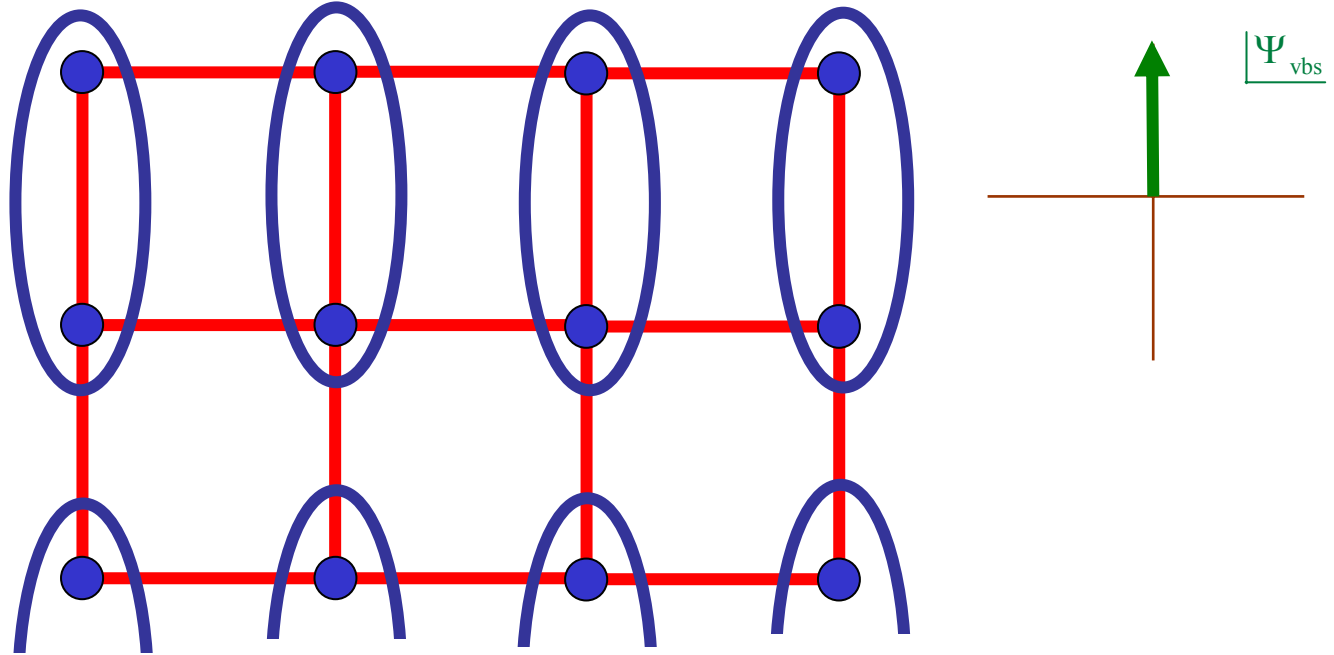
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Such a state breaks the symmetry of rotations by  $n\pi/2$  about lattice sites,  
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$$\Psi_{\text{vbs}}(i) = \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j e^{i \arctan(\mathbf{r}_j - \mathbf{r}_i)}$$

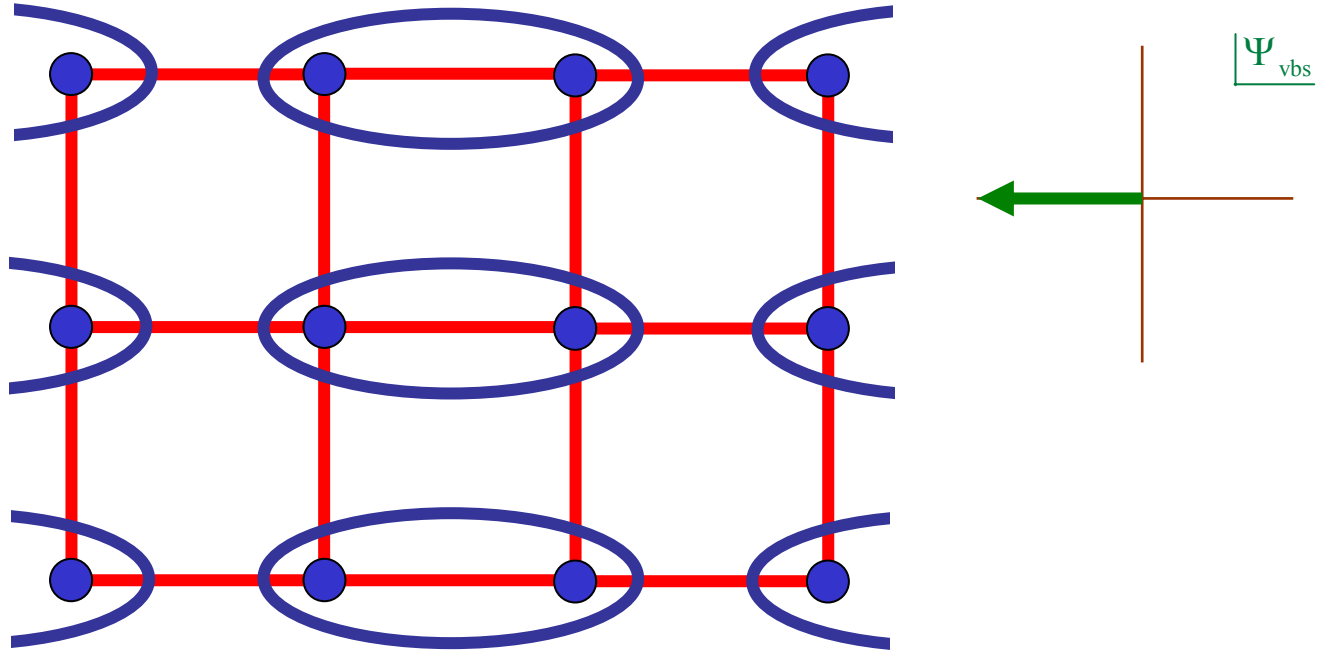
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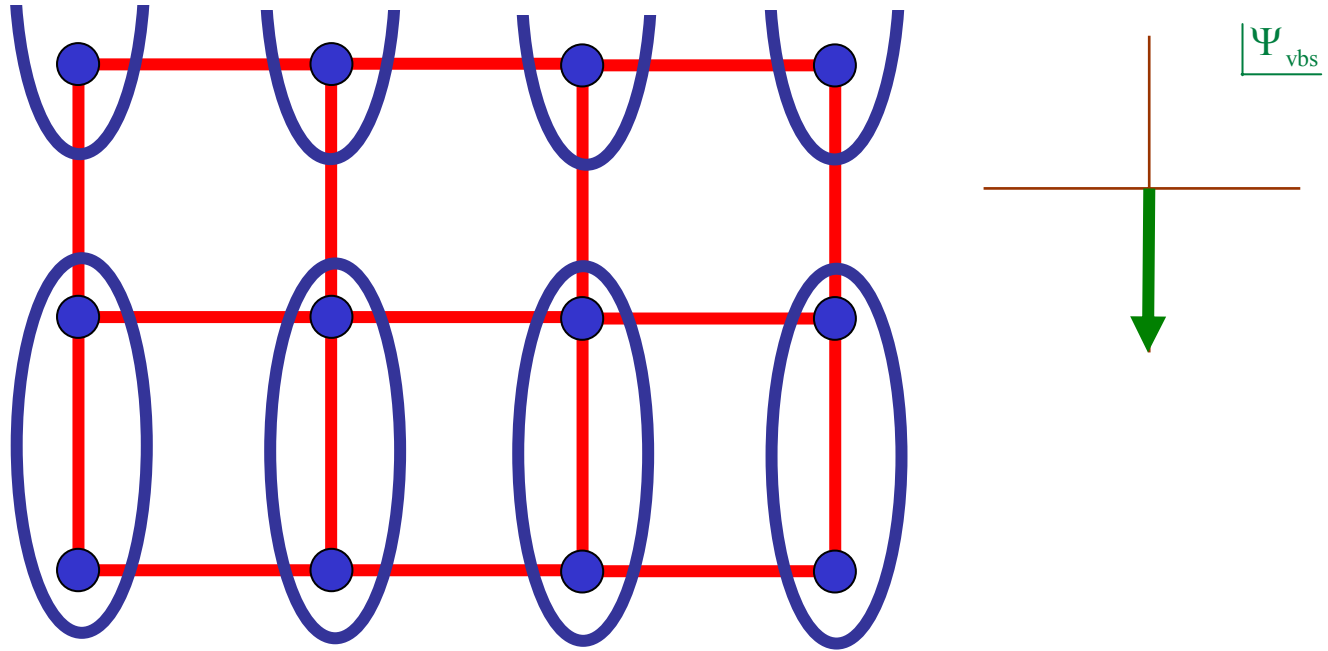
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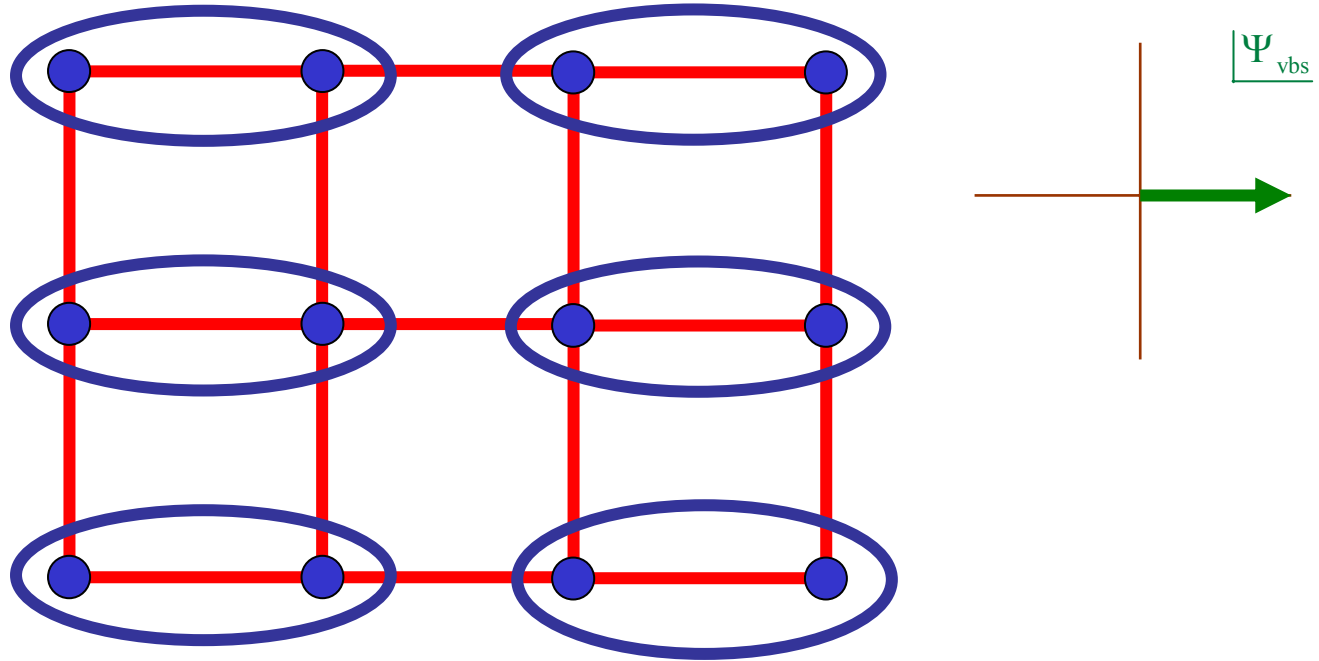
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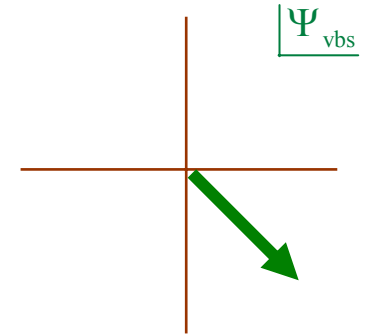
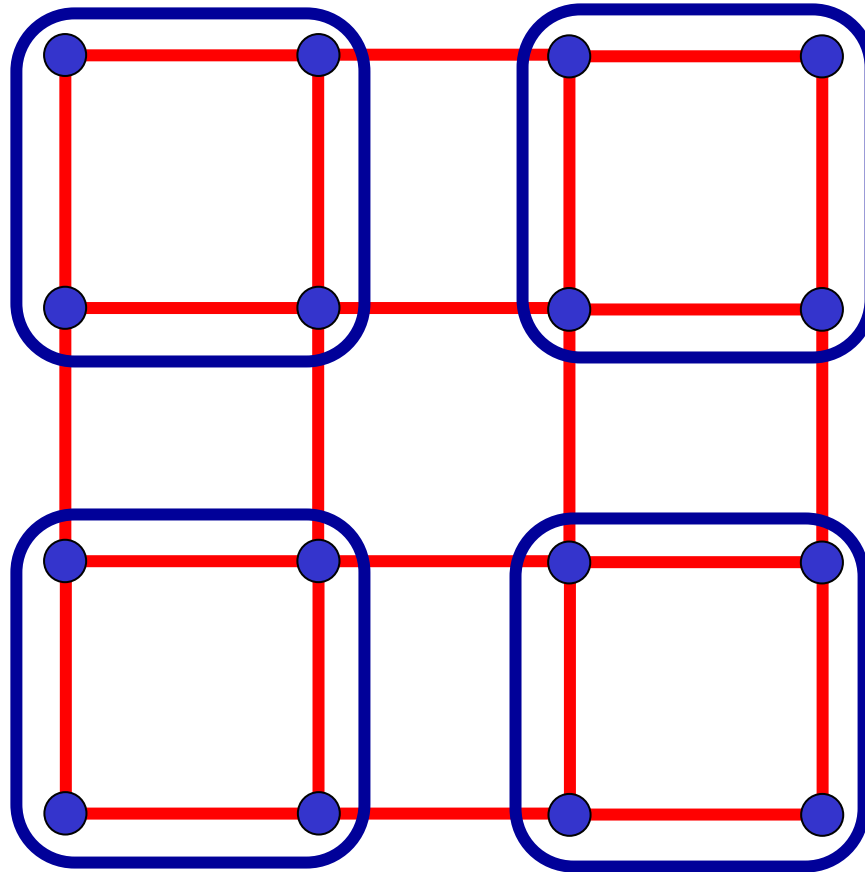
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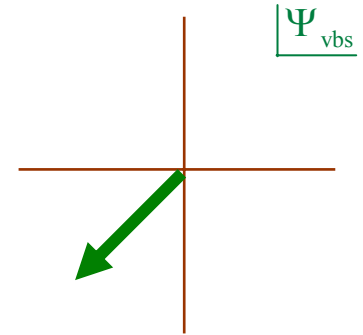
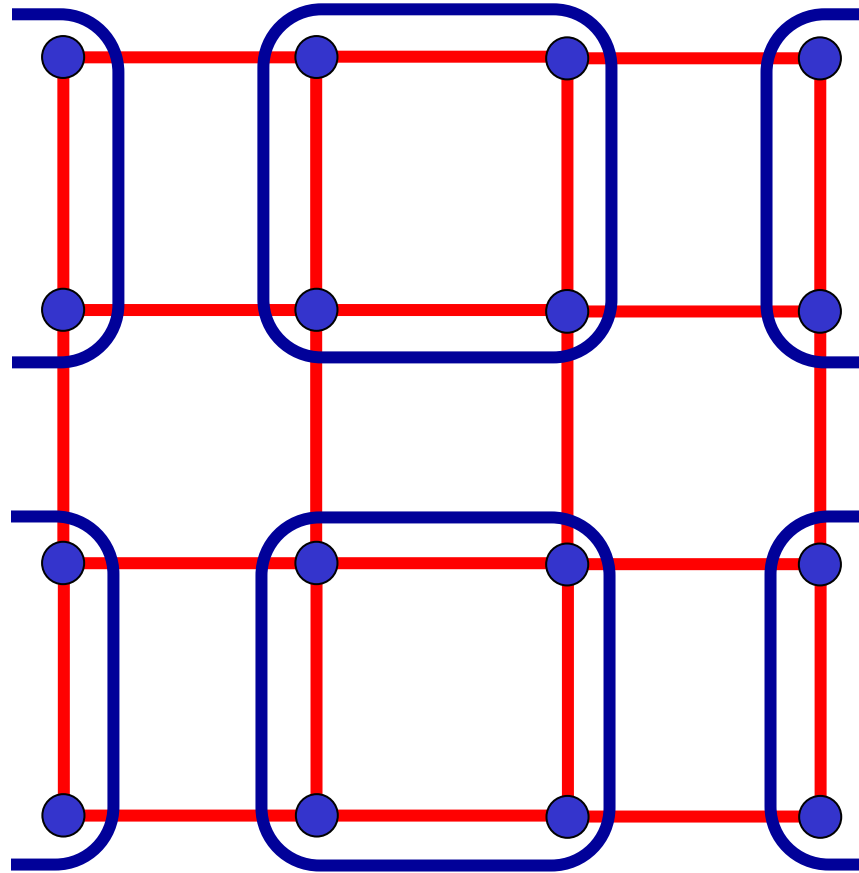
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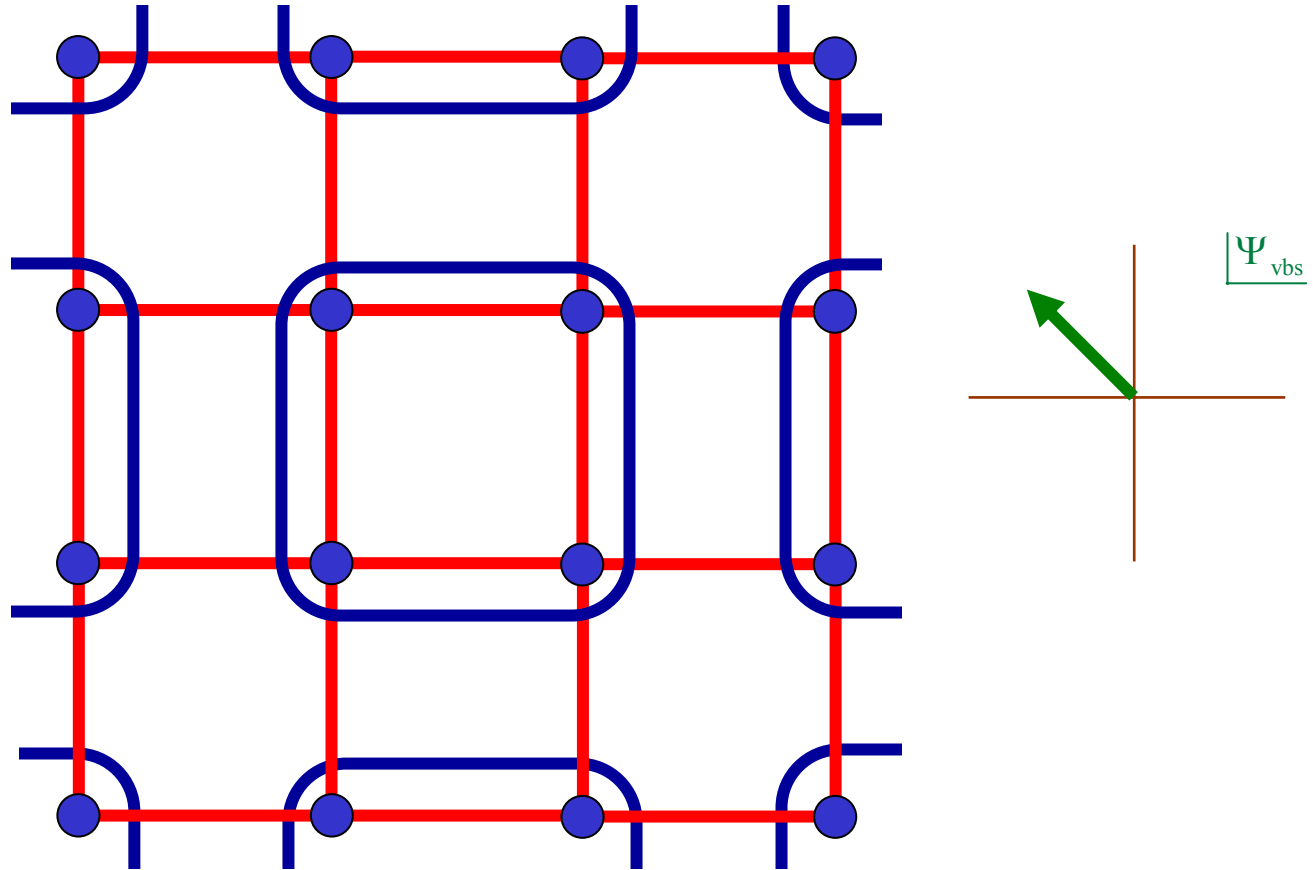
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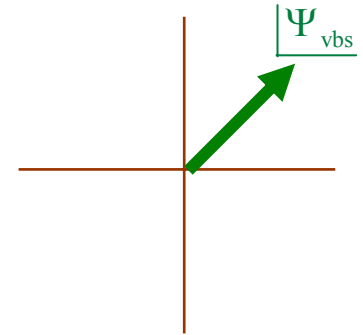
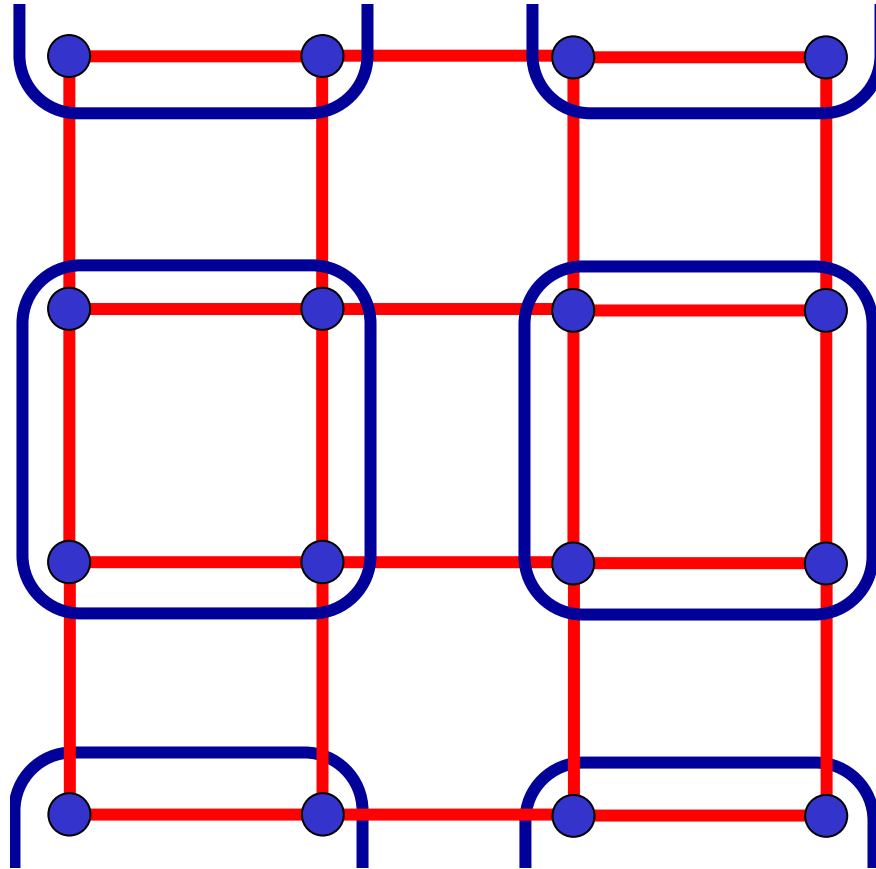
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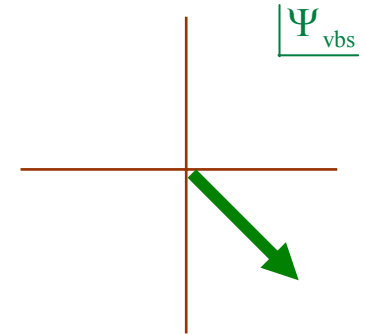
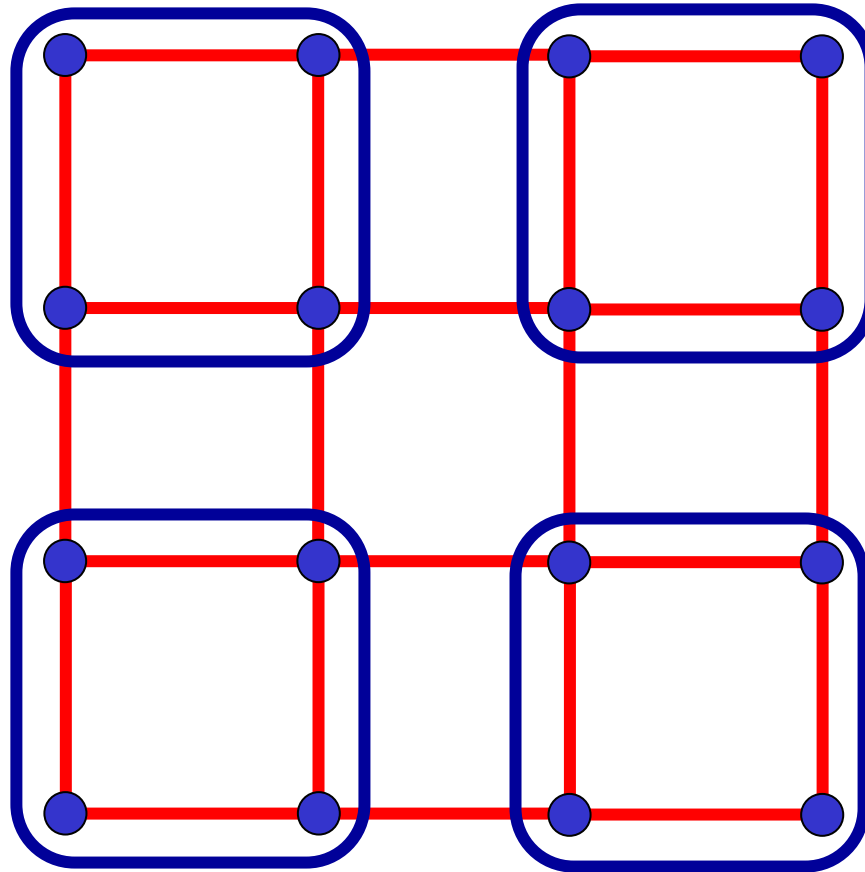
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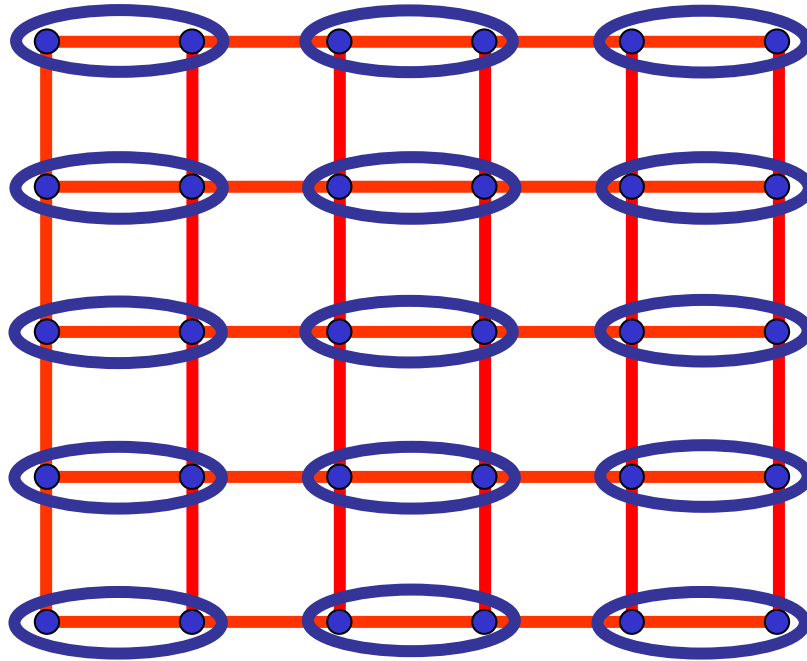


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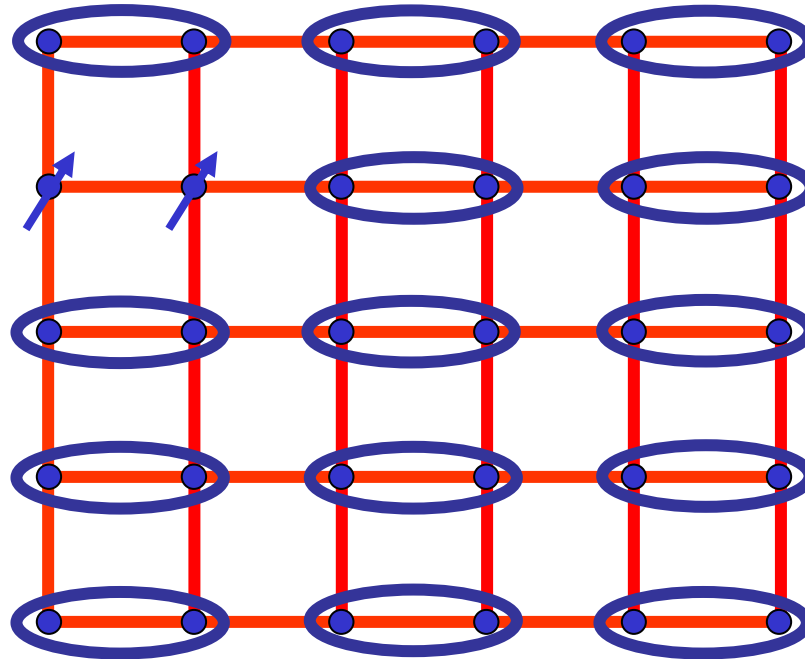
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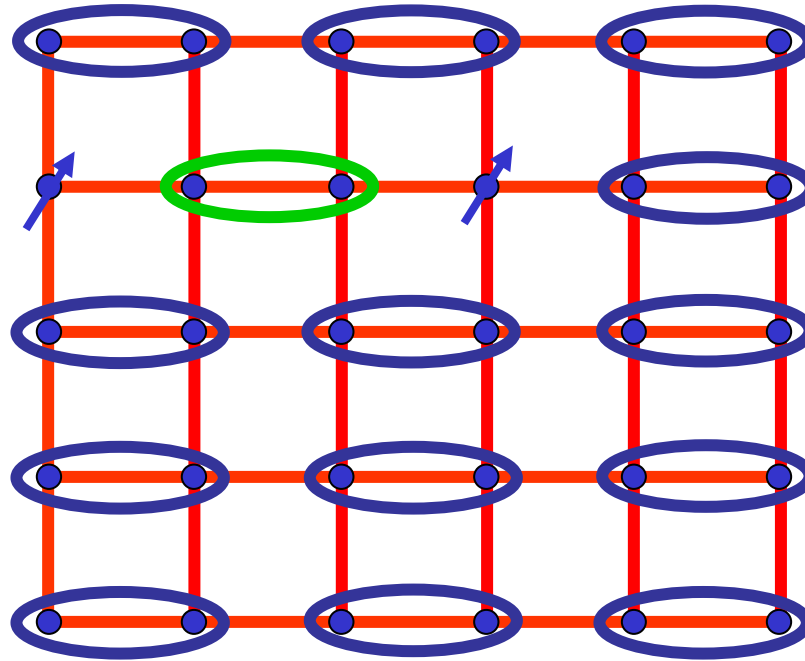
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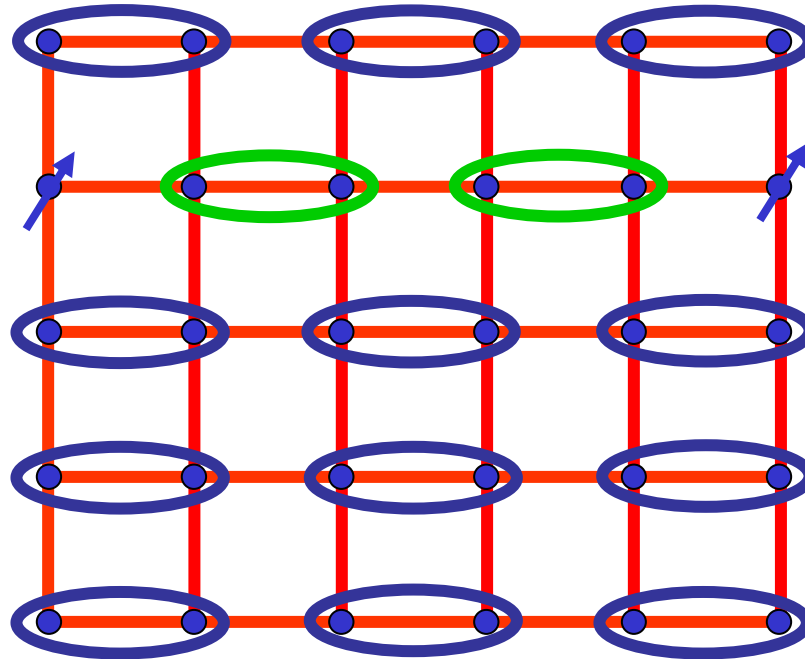
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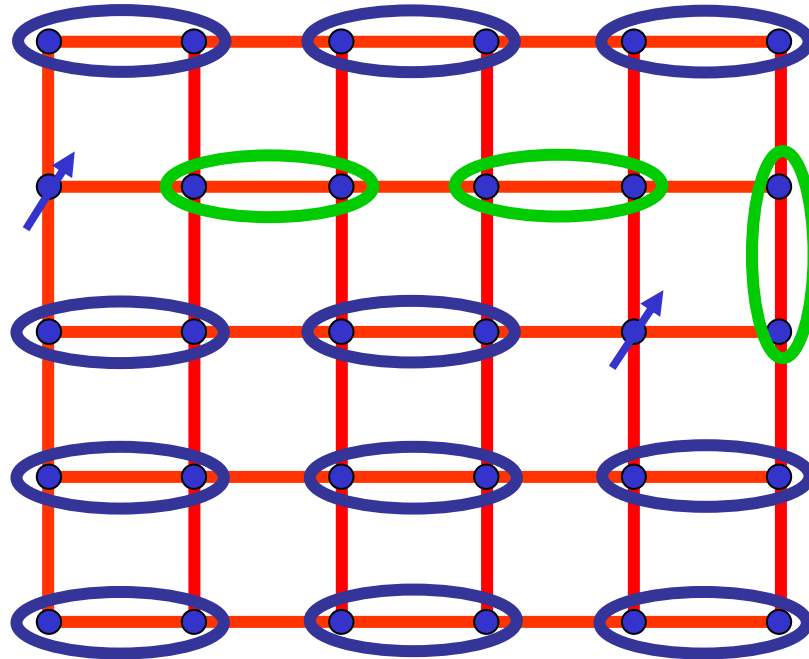
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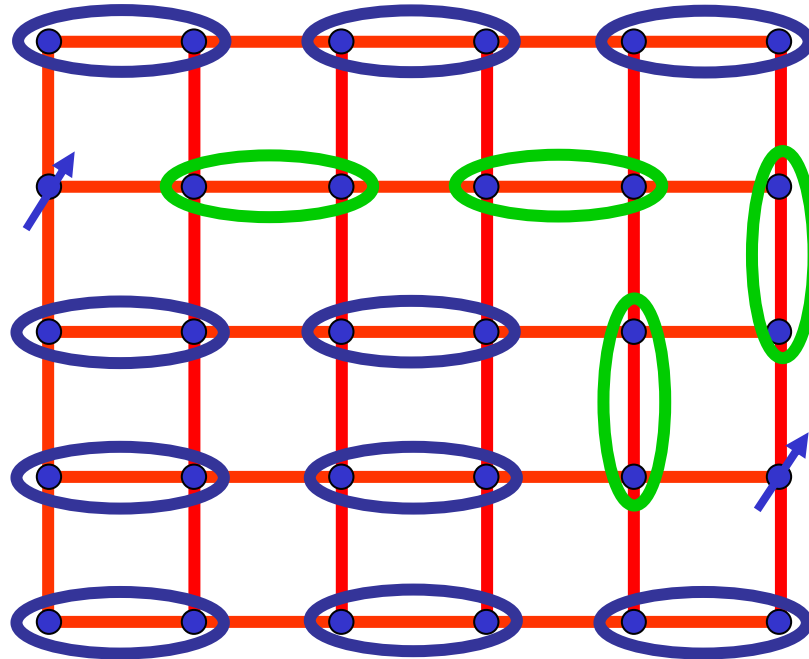
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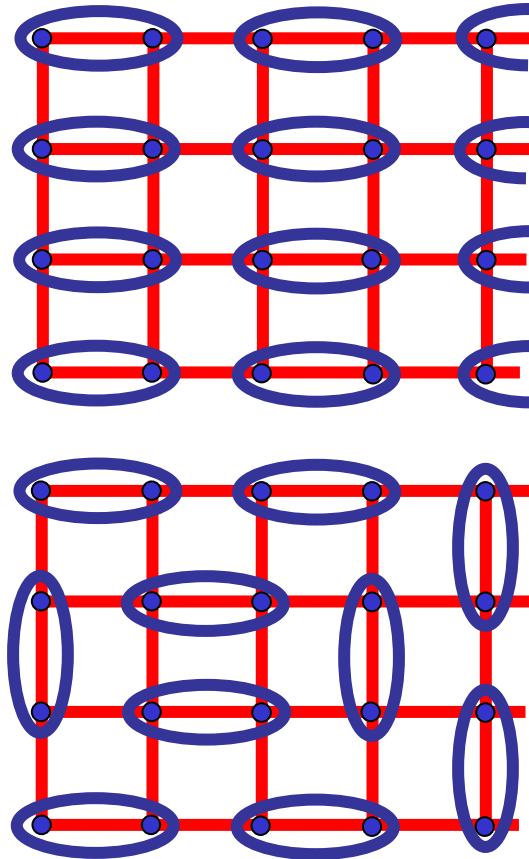


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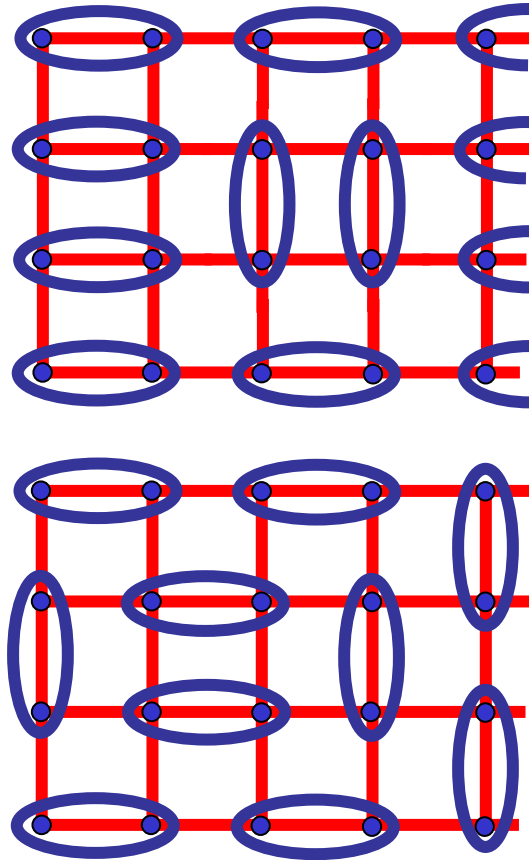
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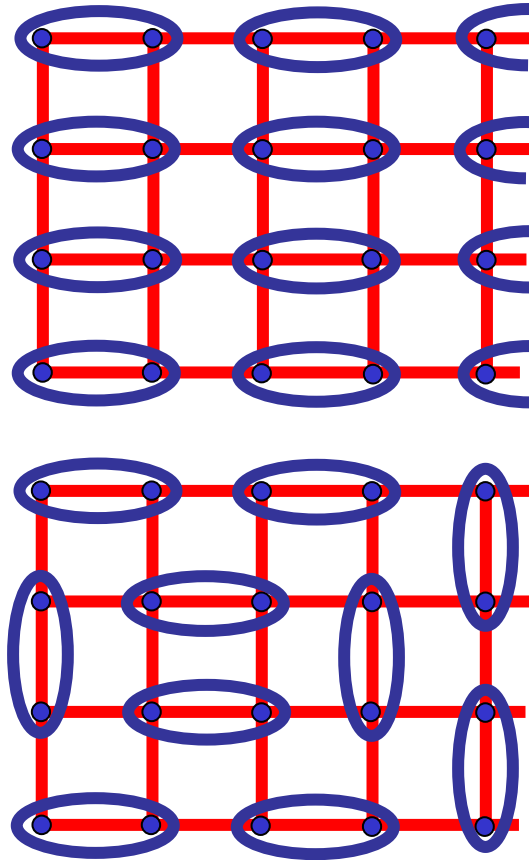
# Ordering by quantum fluctuations



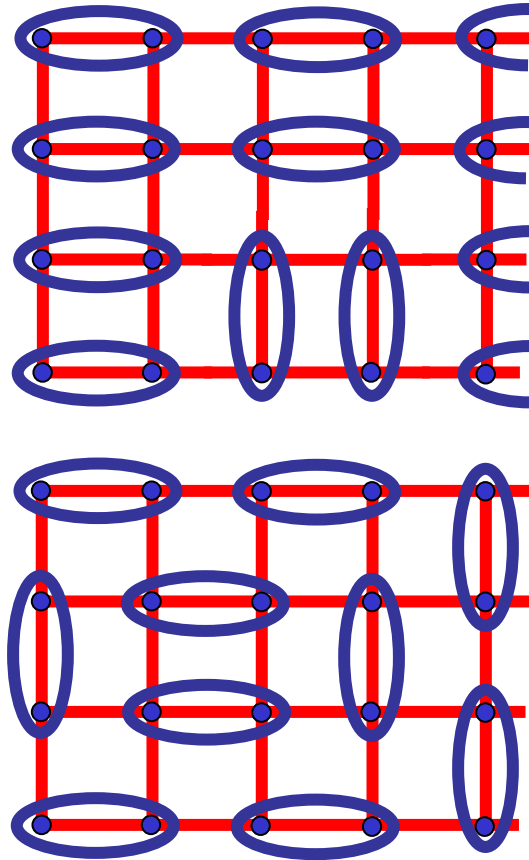
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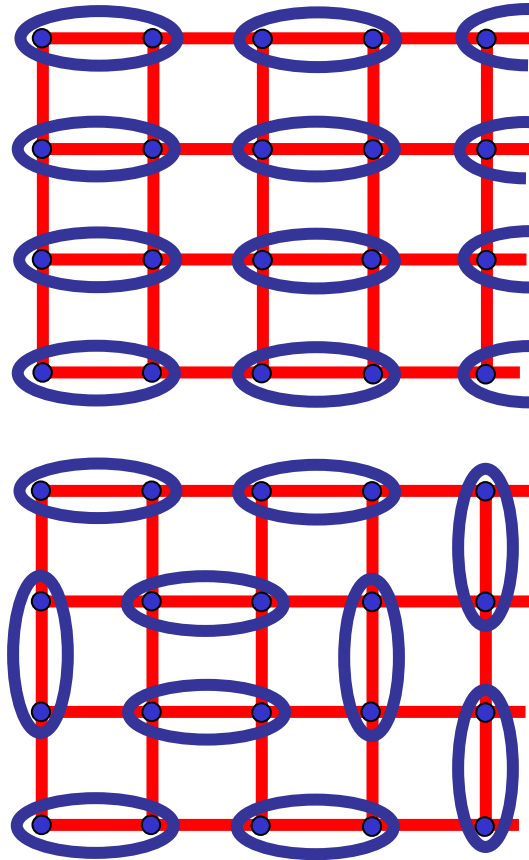
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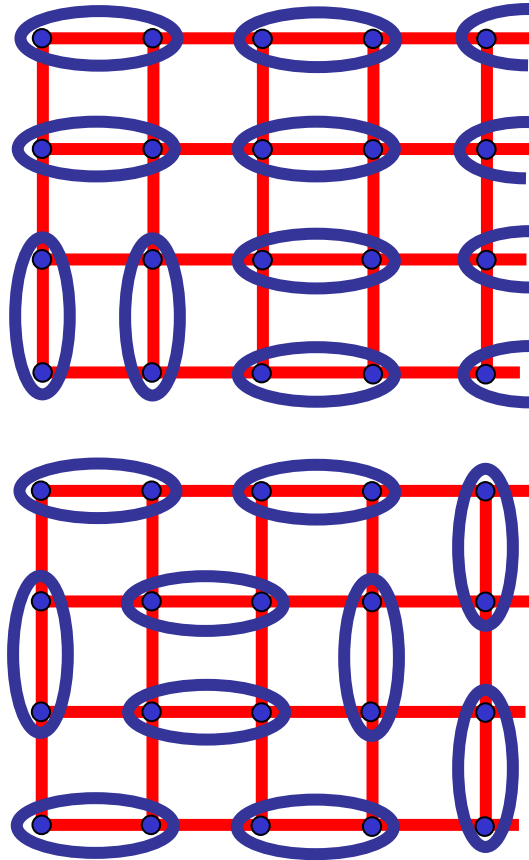
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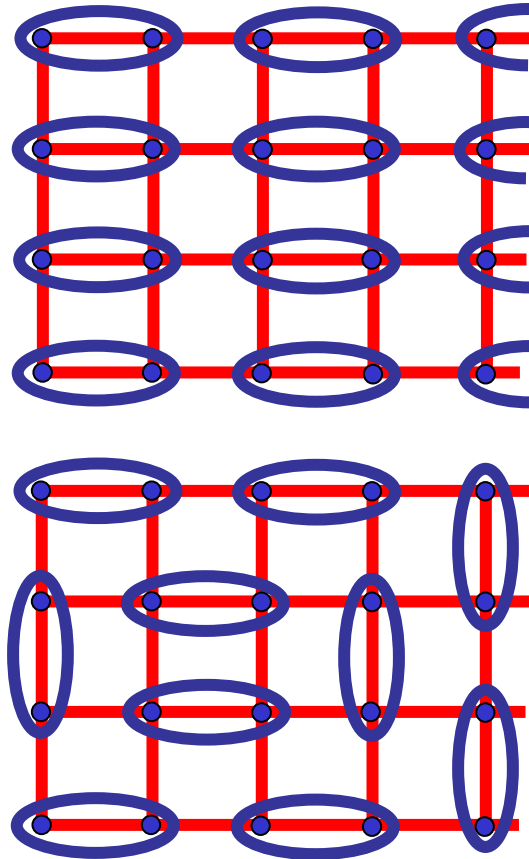
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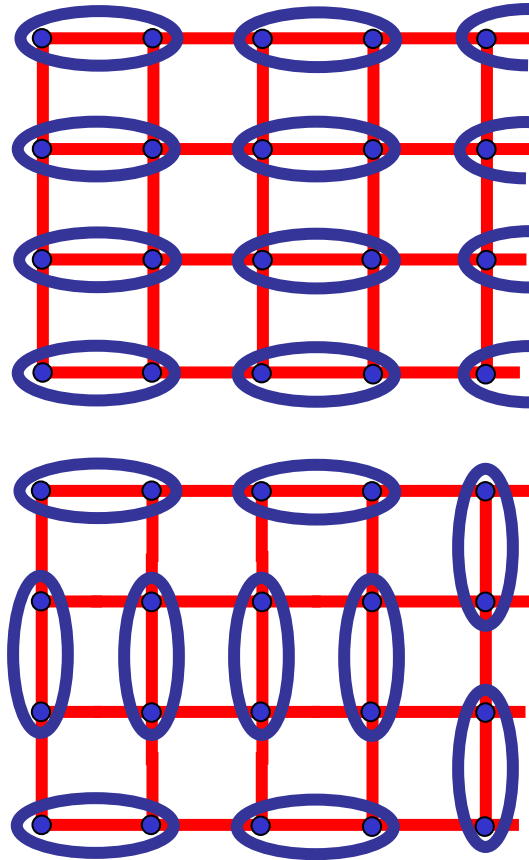
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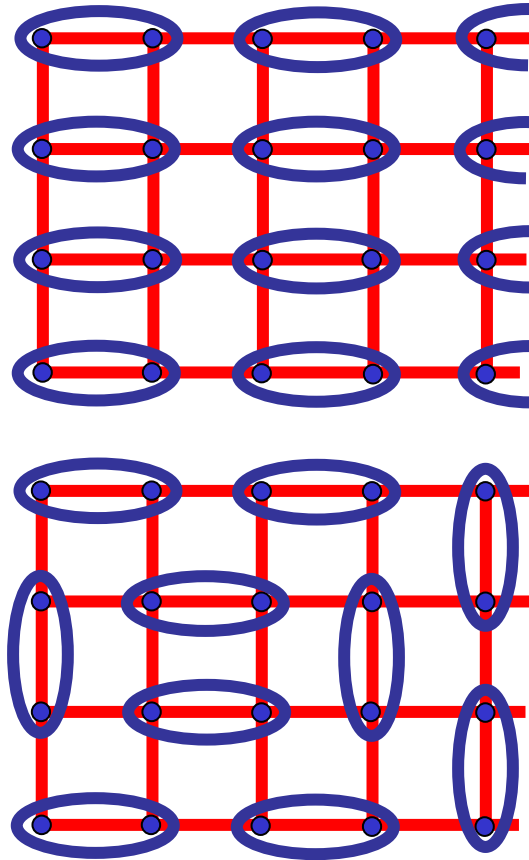
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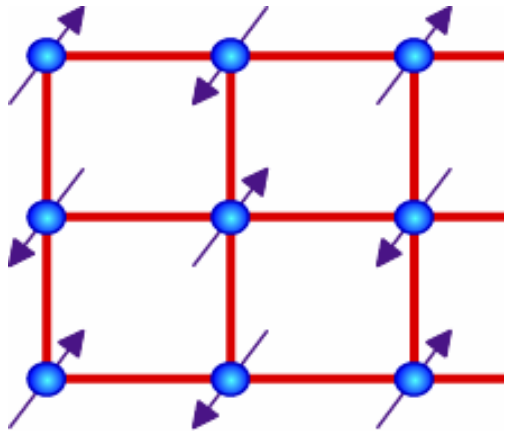
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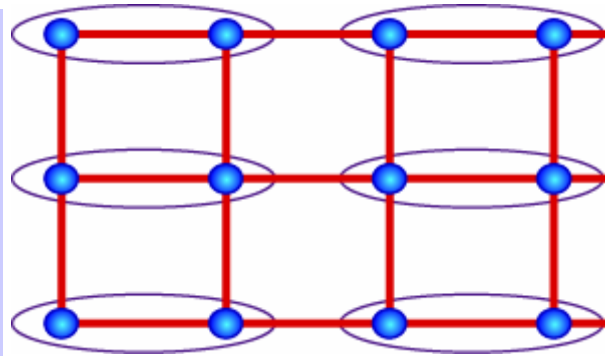
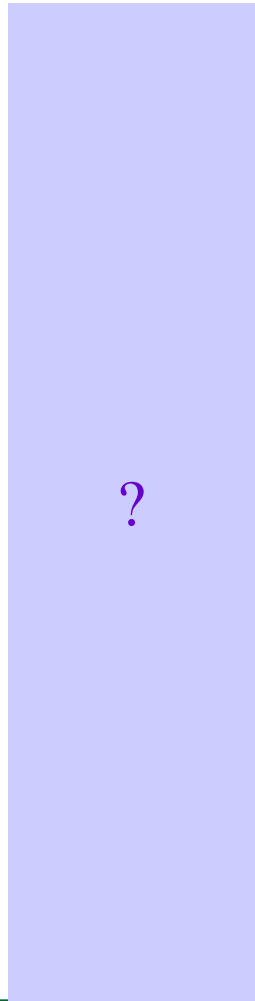


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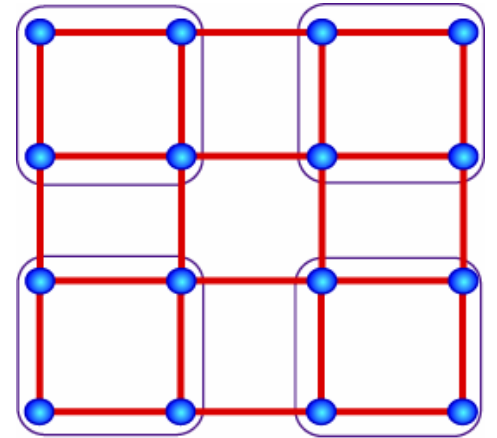


Neel order

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



or



Bond order

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

Not present in

LGW theory

of  $\vec{\varphi}$  order

0

$g$

# LGW theory of multiple order parameters

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

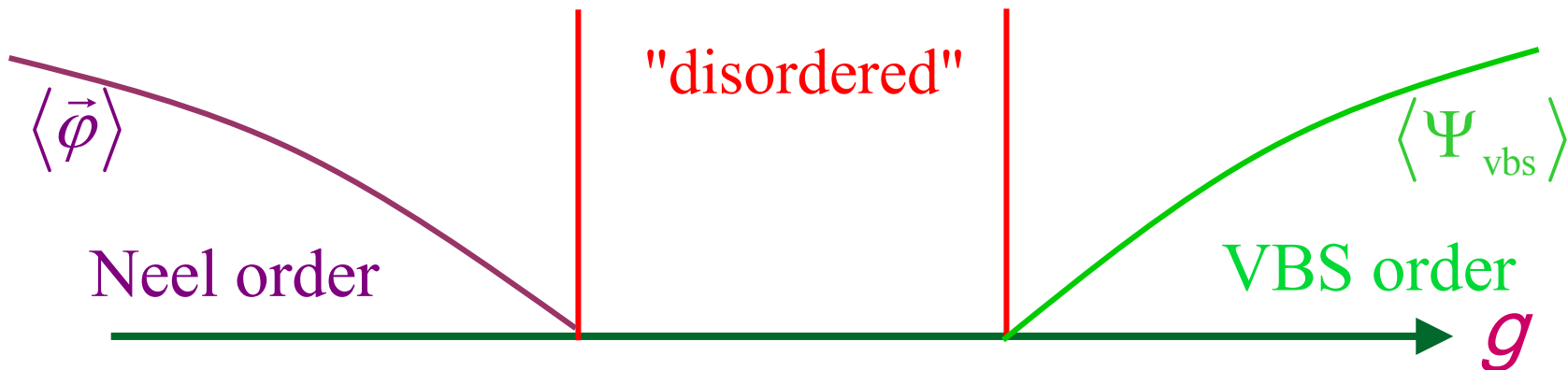
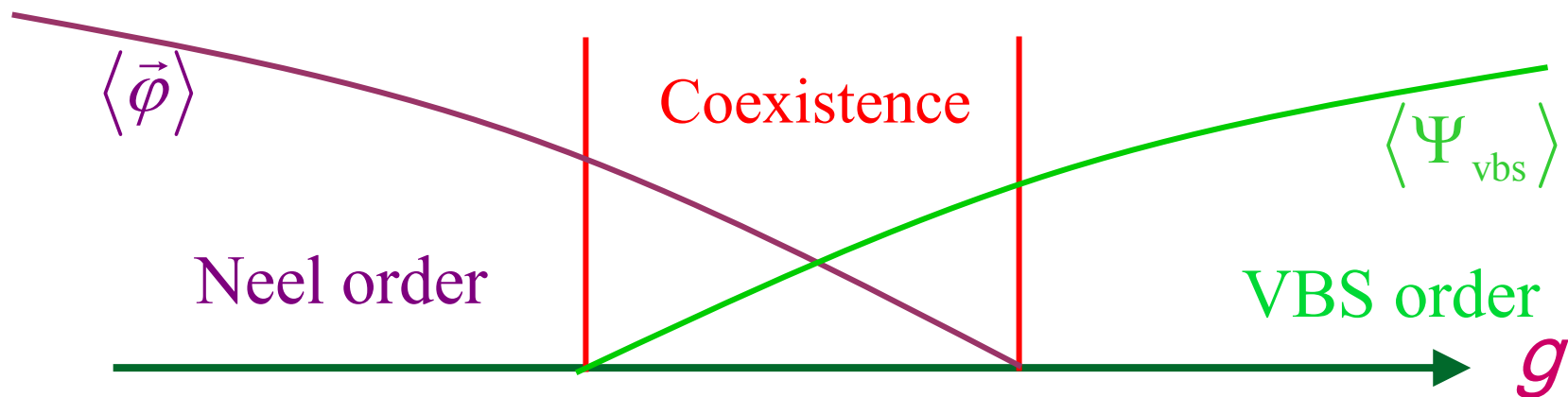
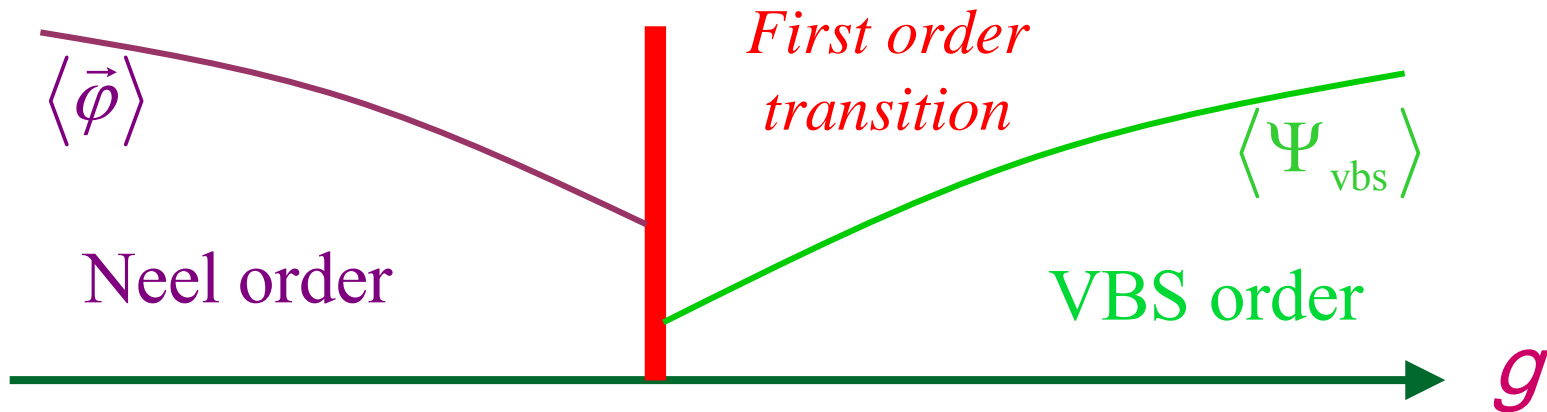
$$F_{\text{vbs}} [\Psi_{\text{vbs}}] = r_1 |\Psi_{\text{vbs}}|^2 + u_1 |\Psi_{\text{vbs}}|^4 + \dots$$

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

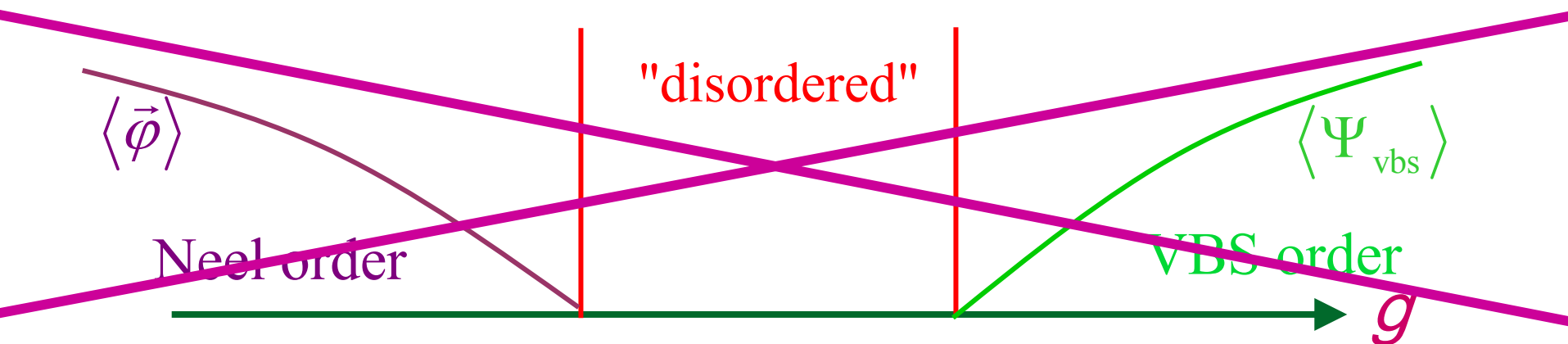
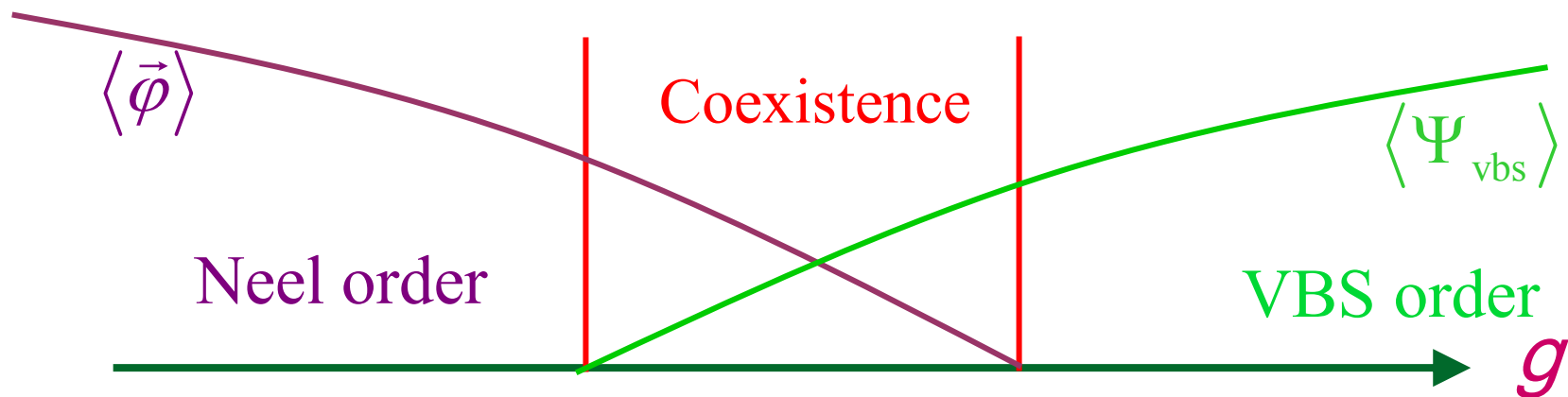
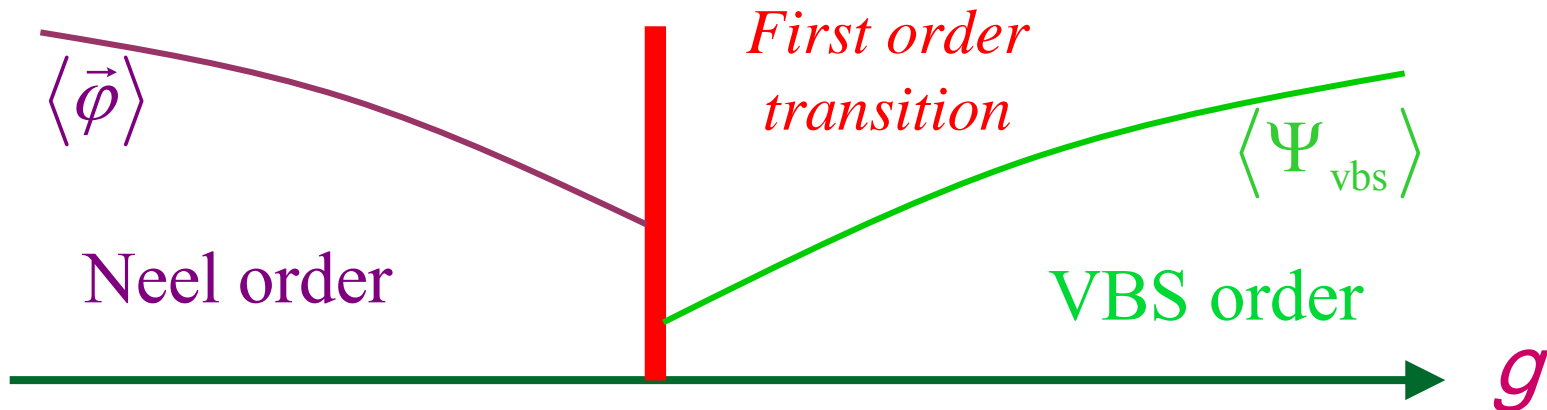
$$F_{\text{int}} = v |\Psi_{\text{vbs}}|^2 |\vec{\varphi}|^2 + \dots$$

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

# LGW theory of multiple order parameters



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

- 1. Berry phases and the mapping to a compact  $U(1)$  gauge theory.*
- 2. Valence bond solid (VBS) order in the paramagnet.*
- 3. Mapping to hard-core bosons at half-filling.*

At each site, identify the states  $|\uparrow\rangle$ ,  $|\downarrow\rangle$ , with the occupation number of a hard-core boson:

$$\begin{aligned}|\downarrow\rangle &= |0\rangle \\ |\uparrow\rangle &= b^\dagger|0\rangle\end{aligned}$$

Then the spin operators map as follows

$$\begin{aligned}S_z &= b^\dagger b - 1/2 \\ S_+ &= b^\dagger \\ S_- &= b\end{aligned}$$

# 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

*1. Berry phases and the mapping to a compact  $U(1)$  gauge theory*

*2. Valence-bond-solid (VBS) order in the paramagnet;*

*3. Mapping to hard-core bosons at half-filling*

C. The superfluid-insulator transition of bosons in lattices

*Multiple order parameters in quantum systems*

D. Boson-vortex duality

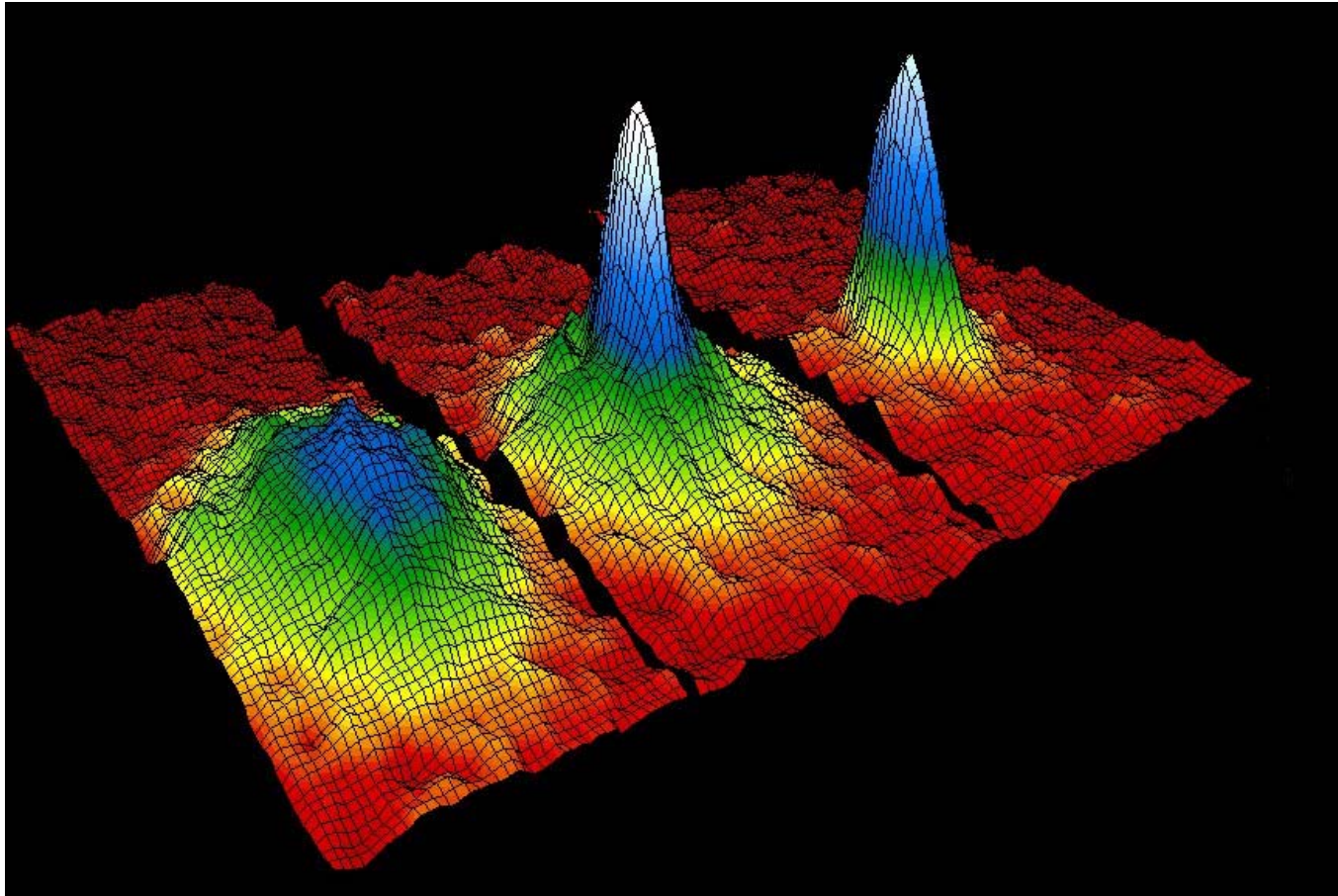
*Breakdown of the LGW paradigm*

## B. Superfluid-insulator transition

### *1. Bosons in a lattice at integer filling*

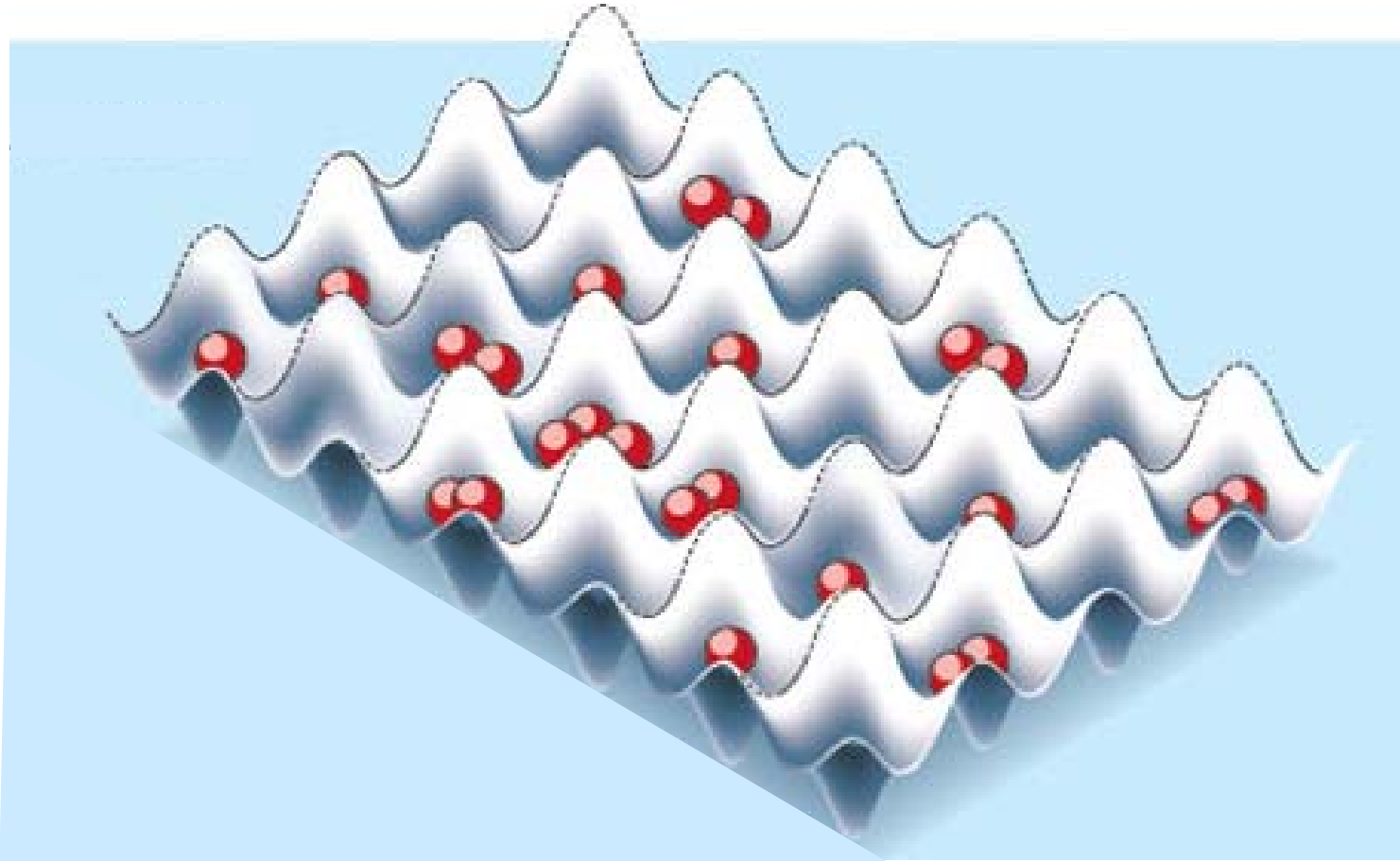
## Bose condensation

Velocity distribution function of ultracold  $^{87}\text{Rb}$  atoms

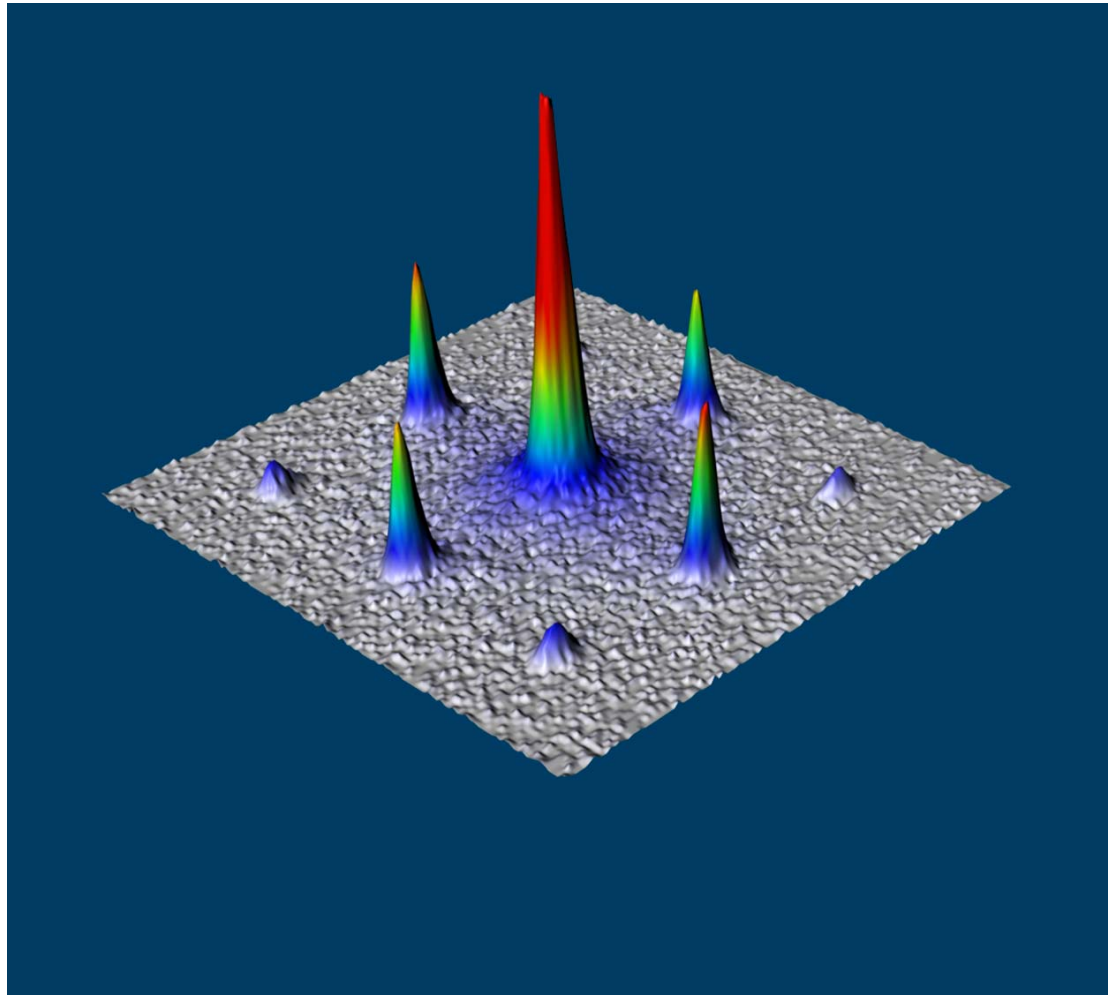


M. H. Anderson, J. R. Ensher, M. R. Matthews, C. E. Wieman  
and E. A. Cornell, *Science* **269**, 198 (1995)

Apply a periodic potential (standing laser beams)  
to trapped ultracold bosons ( $^{87}\text{Rb}$ )

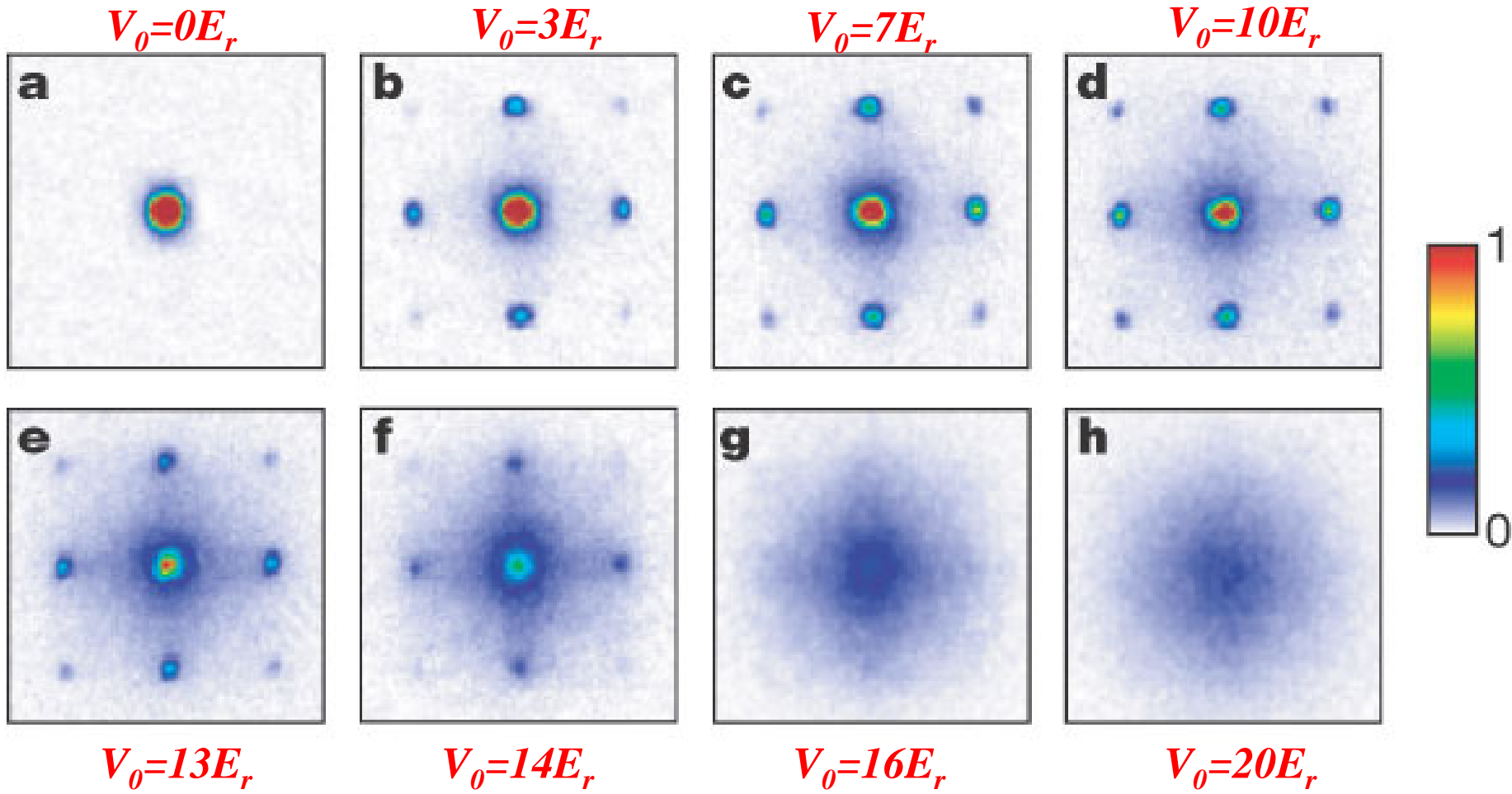
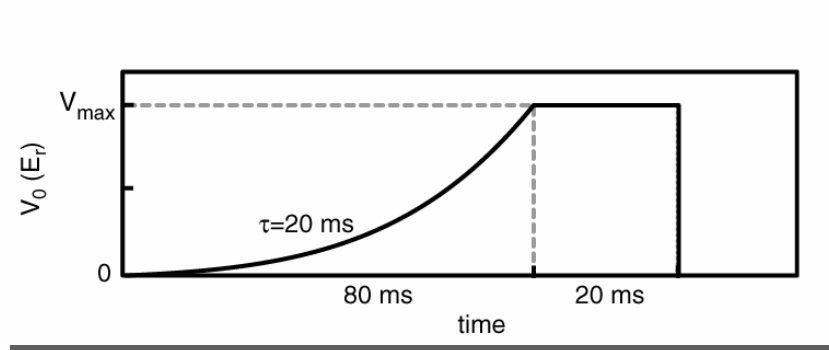


# Momentum distribution function of bosons



Bragg reflections of condensate at reciprocal lattice vectors

# Superfluid-insulator quantum phase transition at $T=0$



# Bosons at filling fraction $f = 1$

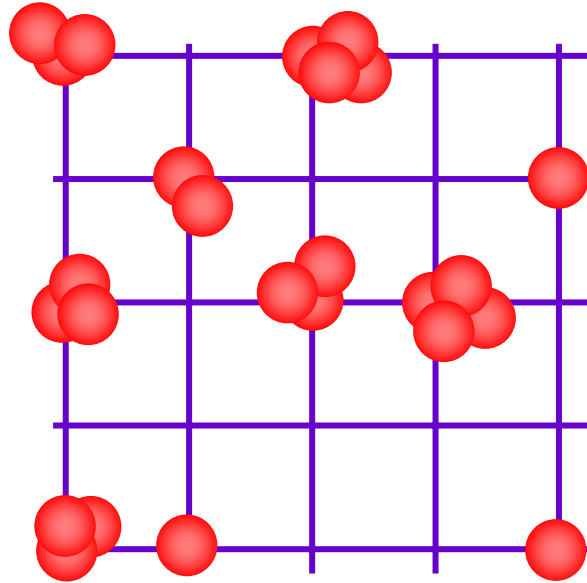
Weak interactions:  
superfluidity

**a** Superfluid state

**b** Insulating state

Strong interactions:  
Mott insulator which  
preserves all lattice  
symmetries

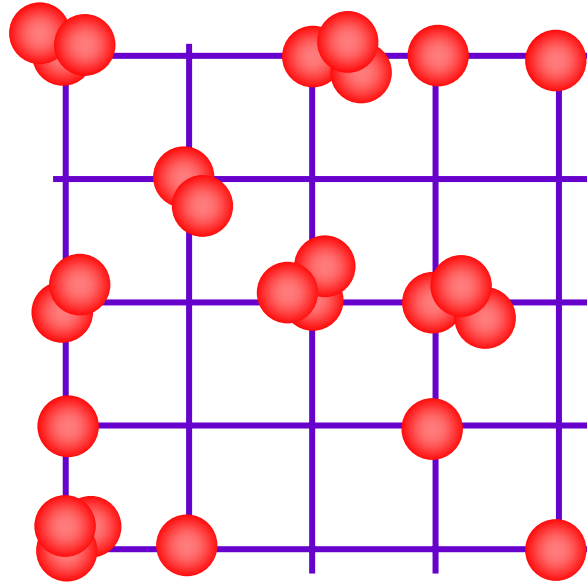
# Bosons at filling fraction $f = 1$



$$\langle \Psi \rangle \neq 0$$

Weak interactions: superfluidity

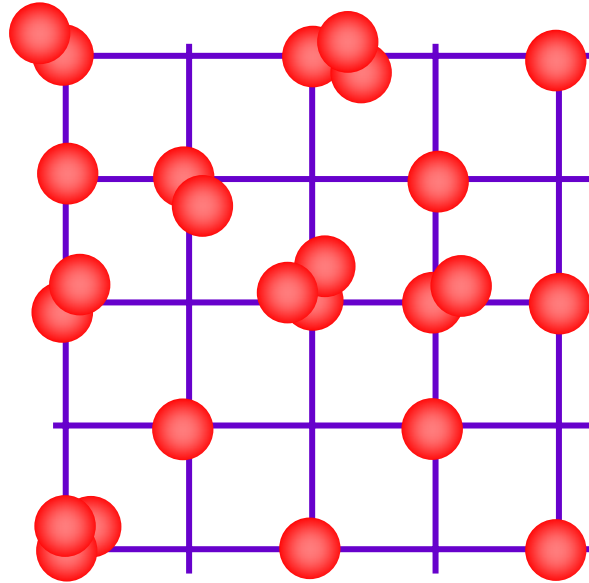
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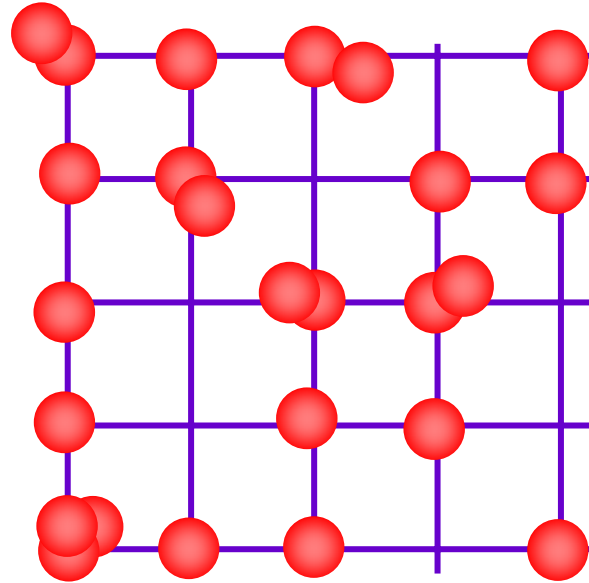
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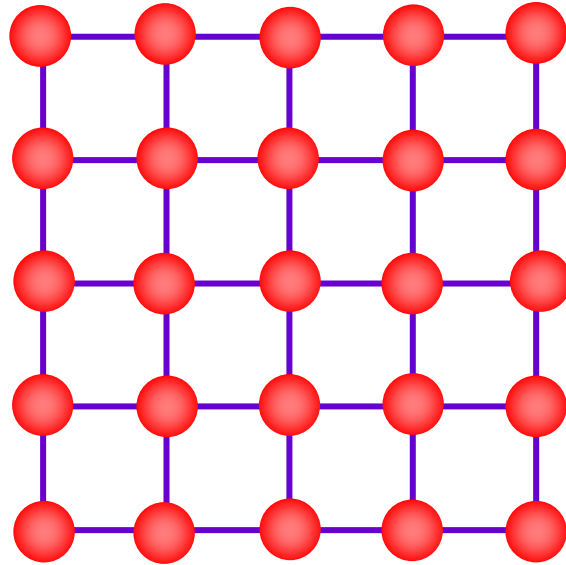
# Bosons at filling fraction $f = 1$



$$\langle \Psi \rangle \neq 0$$

Weak interactions: superfluidity

# Bosons at filling fraction $f = 1$



$$\langle \Psi \rangle = 0$$

Strong interactions: insulator

# The Superfluid-Insulator transition

## Boson Hubbard model

Degrees of freedom: Bosons,  $b_j^\dagger$ , hopping between the sites,  $j$ , of a lattice, with short-range repulsive interactions.

$$H = -t \sum_{\langle ij \rangle} b_i^\dagger b_j - \mu \sum_j n_j + \frac{U}{2} \sum_j n_j (n_j - 1) + \dots$$

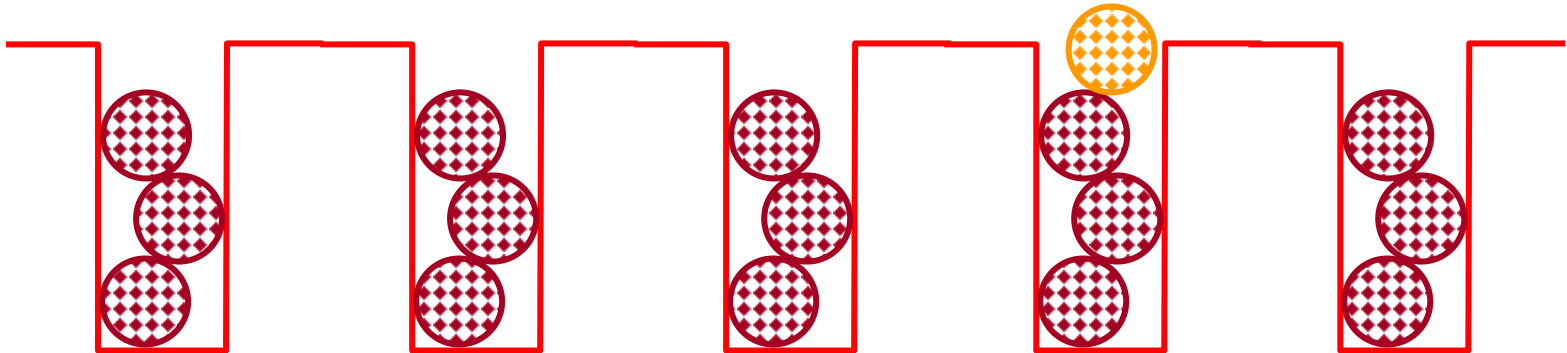
$$n_j \equiv b_j^\dagger b_j$$

M.P.A. Fisher, P.B. Weichmann,  
G. Grinstein, and D.S. Fisher  
*Phys. Rev. B* **40**, 546 (1989).

For small  $U/t$ , ground state is a superfluid BEC with  
superfluid density  $\approx$  density of bosons

## What is the ground state for large $U/t$ ?

Typically, the ground state remains a superfluid, but with  
superfluid density  $\ll$  density of bosons

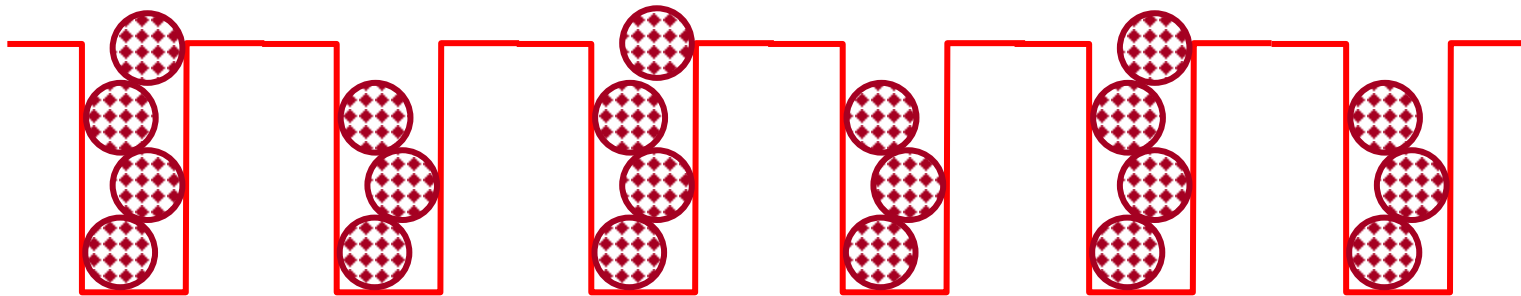
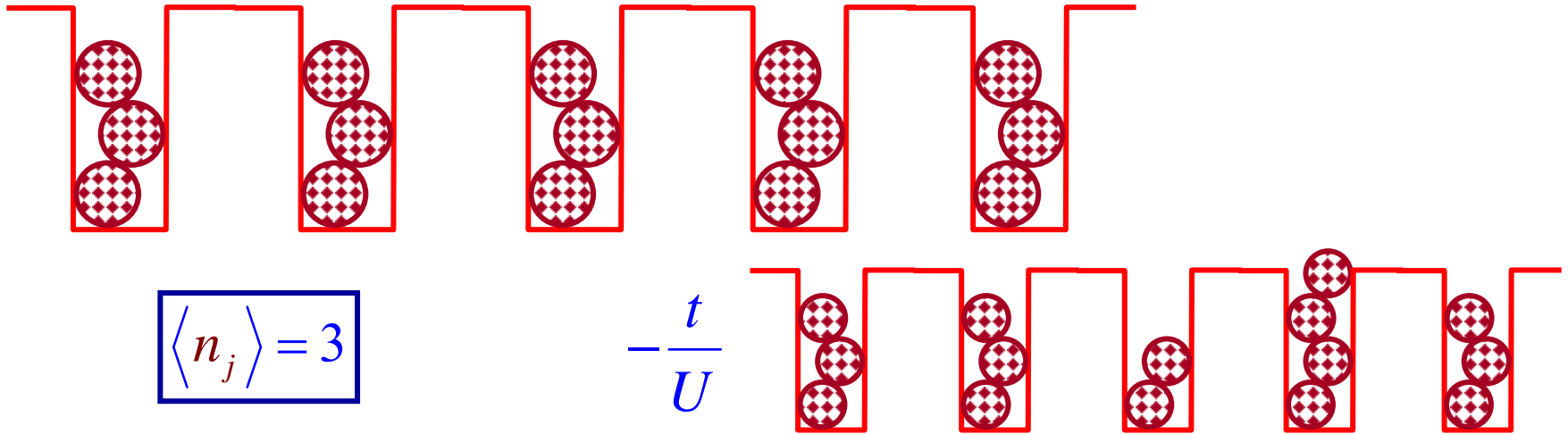


The superfluid density evolves smoothly from large values at small  $U/t$ , to small values at large  $U/t$ , and there is no quantum phase transition at any intermediate value of  $U/t$ .

(In systems with Galilean invariance and at zero temperature, superfluid density=density of bosons always, independent of the strength of the interactions)

# What is the ground state for large $U/t$ ?

Incompressible, insulating ground states, with zero superfluid density, appear at special commensurate densities



$$\langle n_j \rangle = 7/2$$

Ground state has “density wave” order, which spontaneously breaks lattice symmetries

## LGW theory of the superfluid insulator transition

- Identify order parameter  $\Psi(x, \tau) \sim b_j^\dagger$
- Symmetries:

$$\text{Gauge invariance:} \quad \Psi \rightarrow \Psi e^{i\theta}$$

$$\text{Time reversal} \quad \tau \rightarrow -\tau \quad ; \quad \Psi \rightarrow \Psi^*$$

$$\text{Spatial inversion} \quad x \rightarrow -x$$

- Write down most general Lagrangian consistent with symmetries

$$\mathcal{Z} = \int \mathcal{D}\Psi(x, \tau) \exp \left( - \int d^d x \int d\tau \mathcal{L}[\Psi] \right)$$
$$\mathcal{L}[\Psi] = K \Psi^* \frac{\partial \Psi}{\partial \tau} + |\partial_\tau \Psi|^2 + c^2 |\nabla_x \Psi|^2 + r |\Psi|^2 + \frac{u}{2} |\Psi|^4 + \dots$$

- Identify phases at  $r \gg 0$  and  $r \ll 0$  with the insulator and the superfluid respectively.
- For  $K \neq 0$ , the particle and hole excitations have different energies.

- Gauge-invariance of the underlying boson Hamiltonian shows that

$$K = -\frac{\partial r}{\partial \mu}$$

- In mean-field theory, the ground state energy,  $E$ , across the superfluid-insulator transition has the non-analytic term

$$E = E_0 - \frac{r^2}{2u}\theta(-r)$$

(Beyond mean-field theory, the non-analytic term is  $E \sim r^{(d+z)\nu}$ ).

- Because the density of bosons  $= -\partial E/\partial \mu$ , this implies a change in the boson density across the transition *unless*  $\partial r/\partial \mu = 0$
- A superfluid-insulator transition at fixed boson density must have.

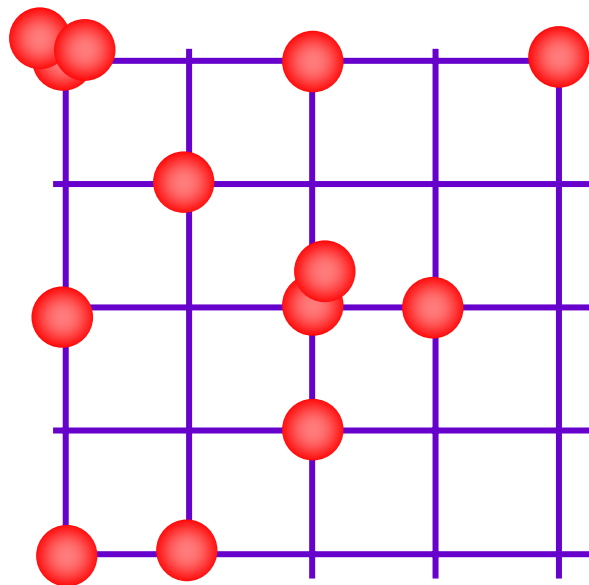
$$K = 0$$

## B. Superfluid-insulator transition

### *2. Bosons in a lattice at fractional filling*

L. Balents, L. Bartosch, A. Burkov, S. Sachdev, K. Sengupta,  
*Physical Review B* **71**, 144508 and 144509 (2005),  
cond-mat/0502002, and cond-mat/0504692.

## Bosons at filling fraction $f = 1/2$



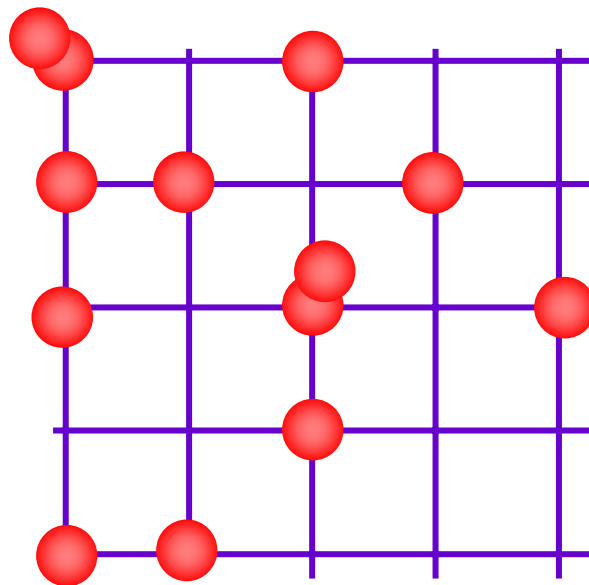
$$\langle \Psi \rangle \neq 0$$

Weak interactions: superfluidity

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

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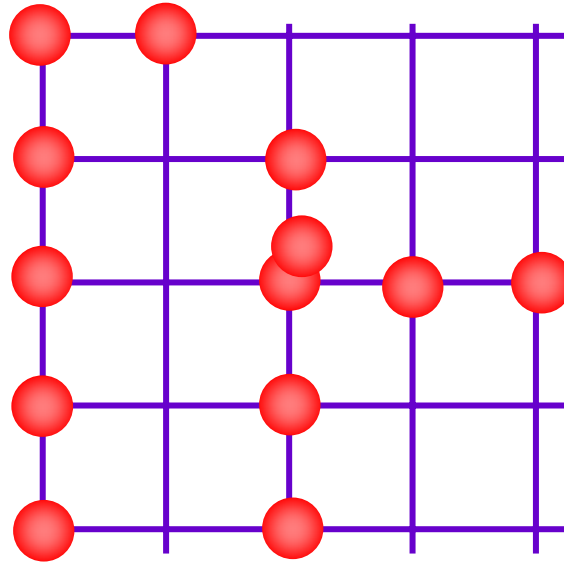
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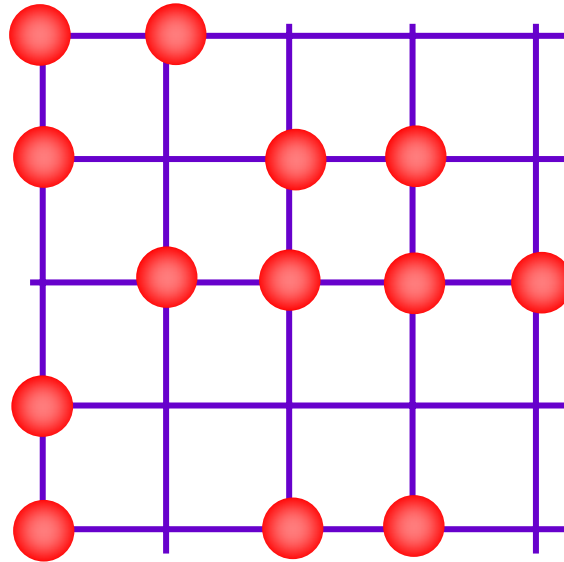
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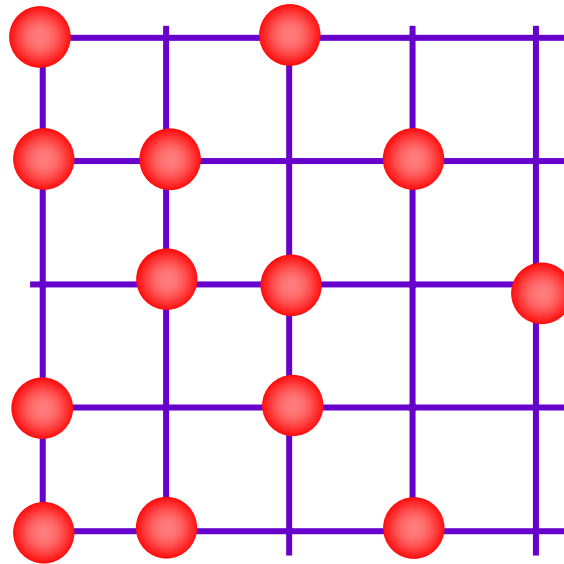
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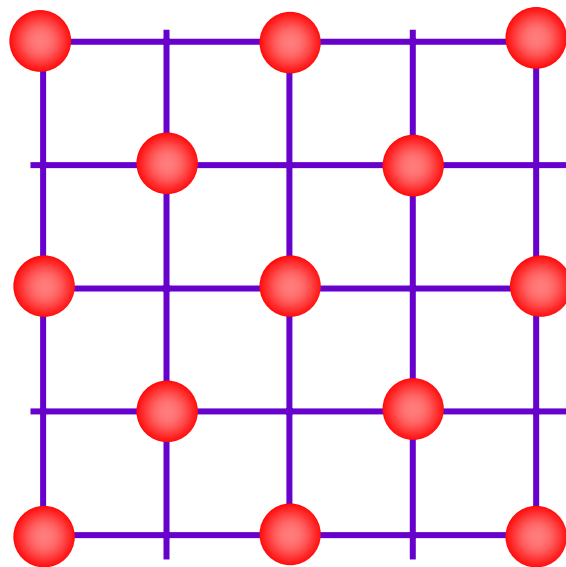
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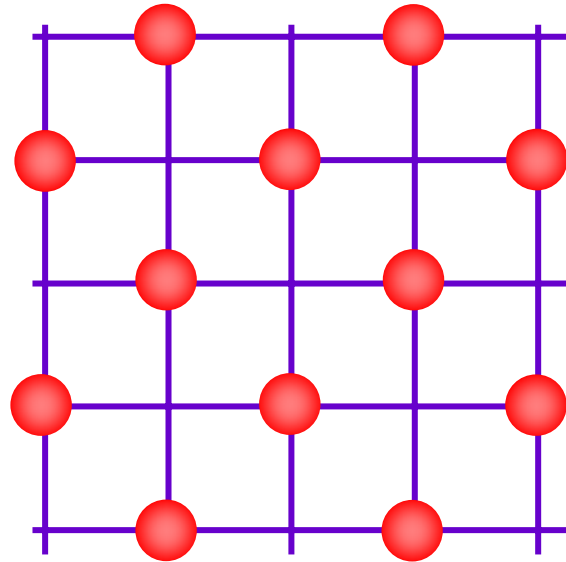
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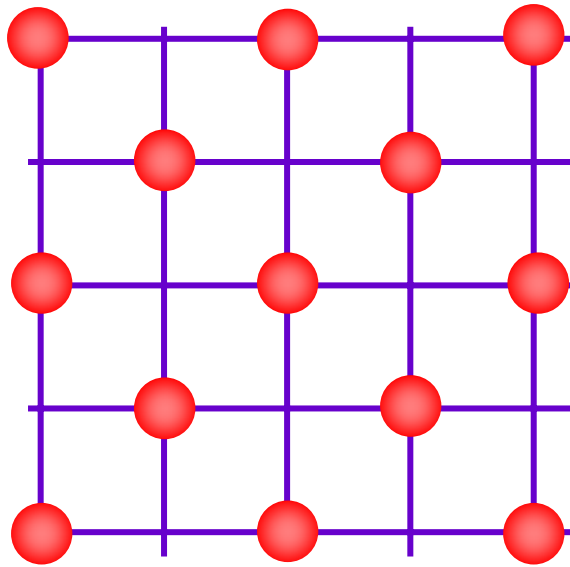
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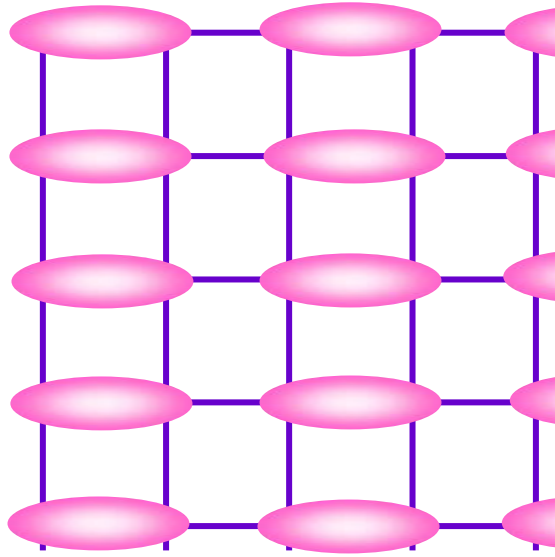
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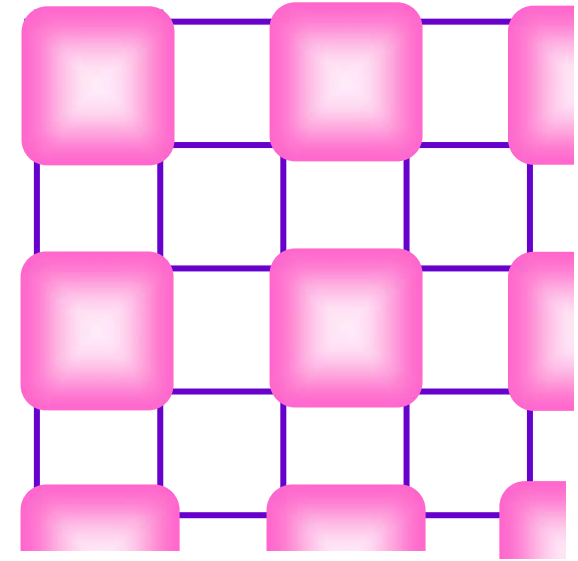
# Insulating phases of bosons at filling fraction $f = 1/2$



Charge density wave (CDW) order



Valence bond solid (VBS) order



Valence bond solid (VBS) order

$$\text{pink oval} = \frac{1}{\sqrt{2}} \left( \text{red sphere} - \text{bond} + \text{bond} - \text{bond} + \text{red sphere} \right)$$

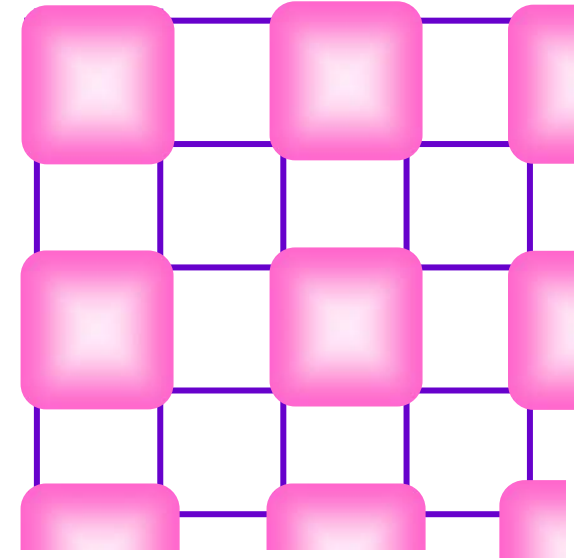
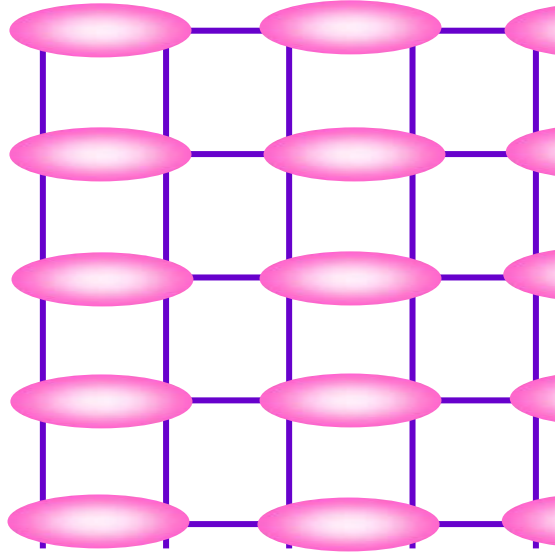
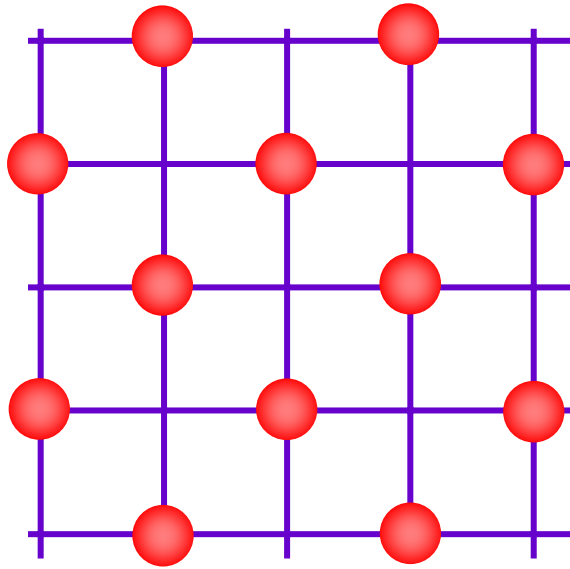
Can define a common CDW/VBS order using a generalized "density"  $\rho(\mathbf{r}) = \sum_{\mathbf{Q}} \rho_{\mathbf{Q}} e^{i\mathbf{Q} \cdot \mathbf{r}}$

All insulators have  $\langle \Psi \rangle = 0$  and  $\langle \rho_{\mathbf{Q}} \rangle \neq 0$  for certain  $\mathbf{Q}$

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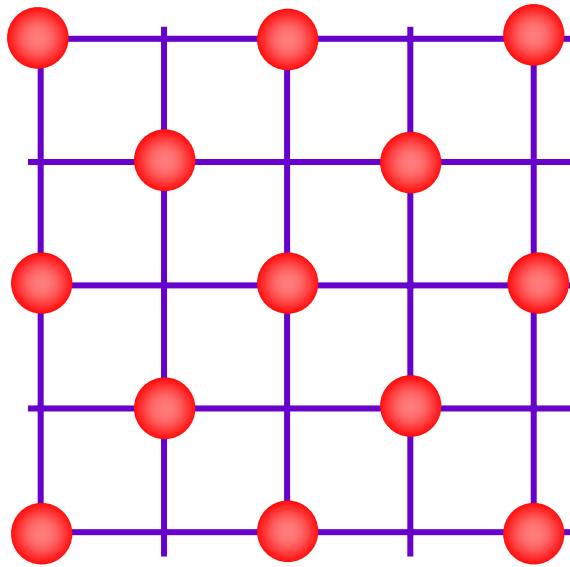
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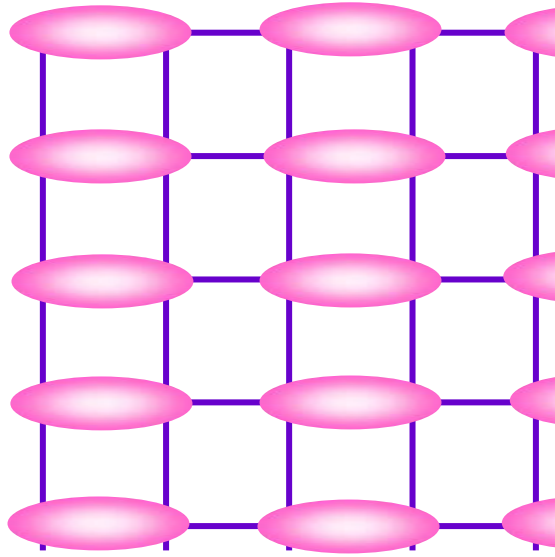
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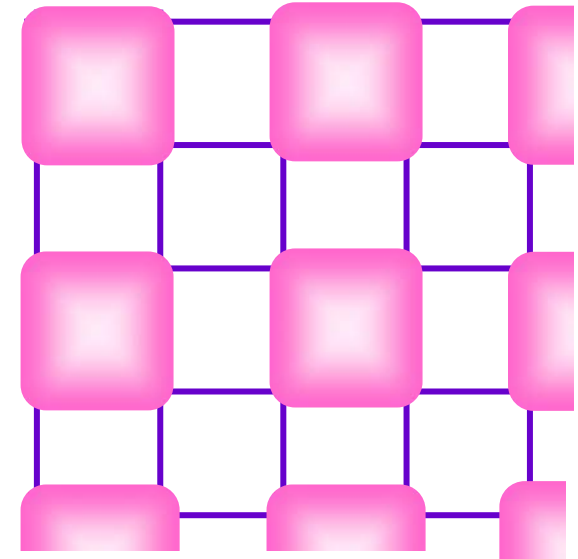
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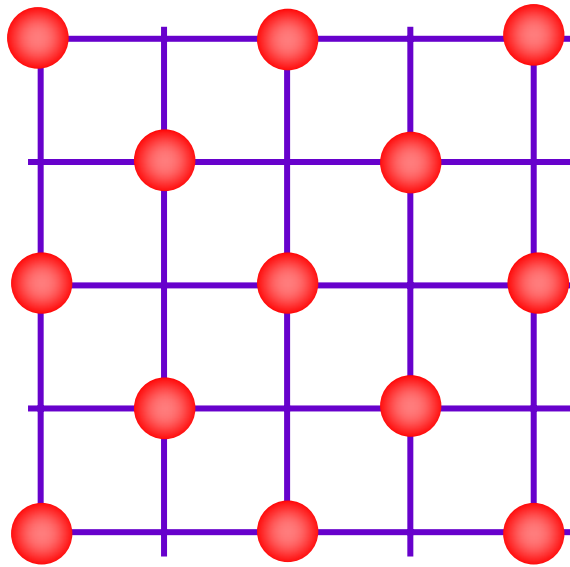
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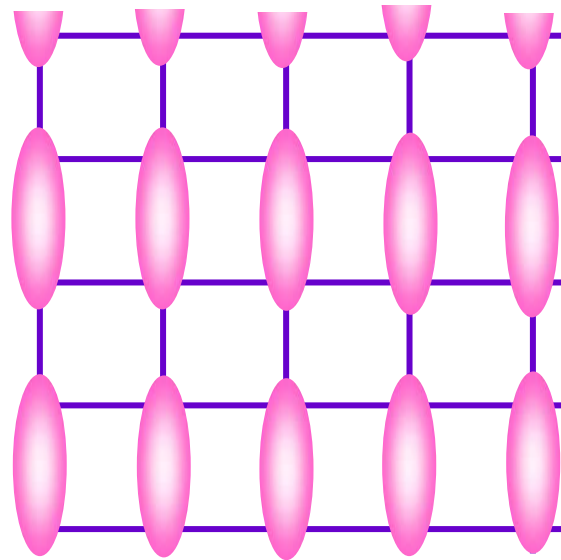
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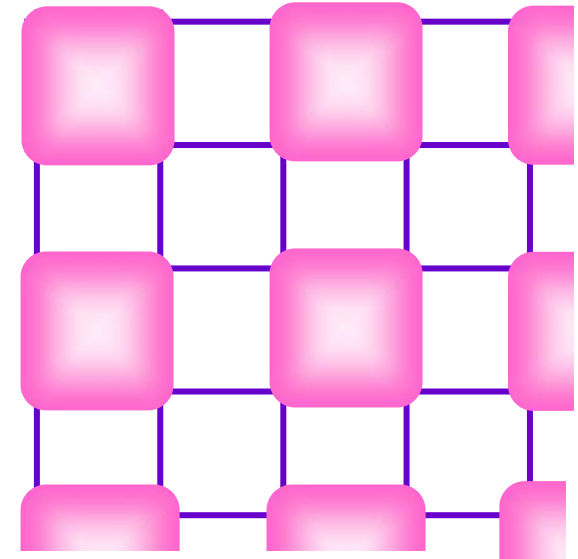
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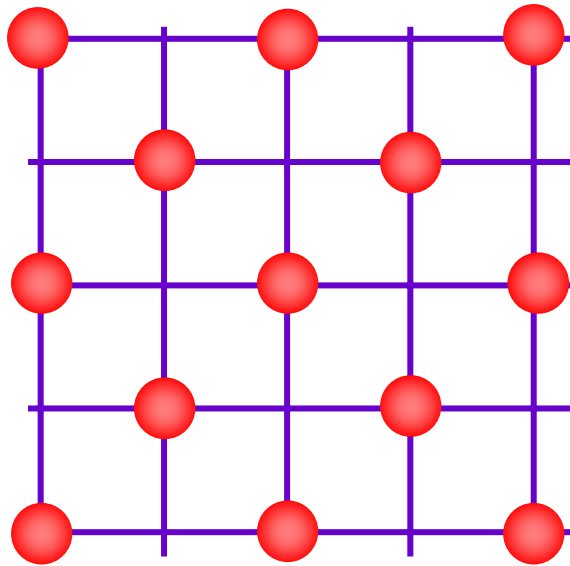
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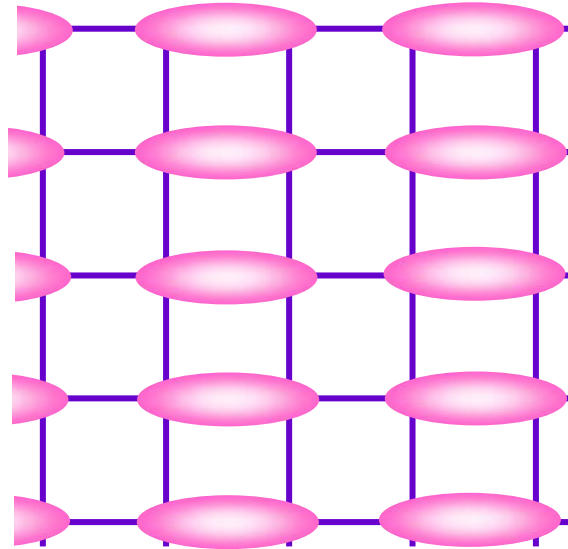
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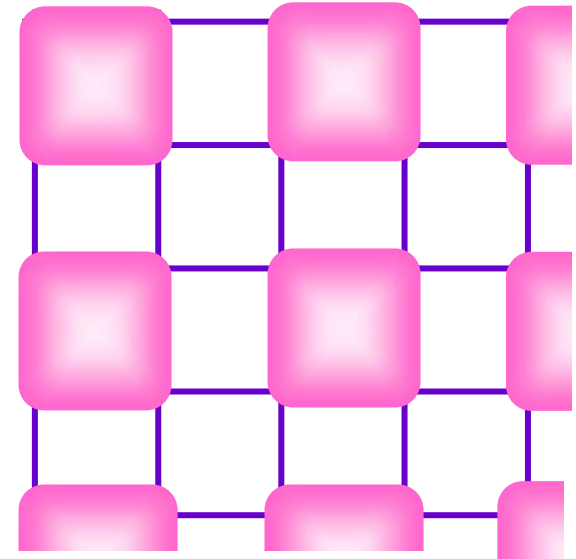
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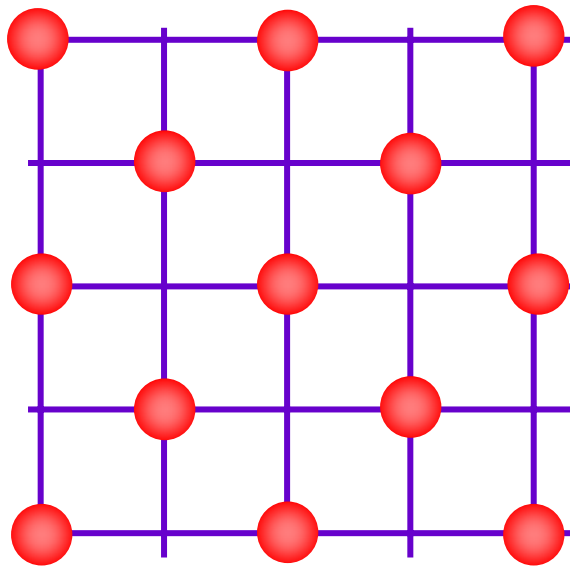
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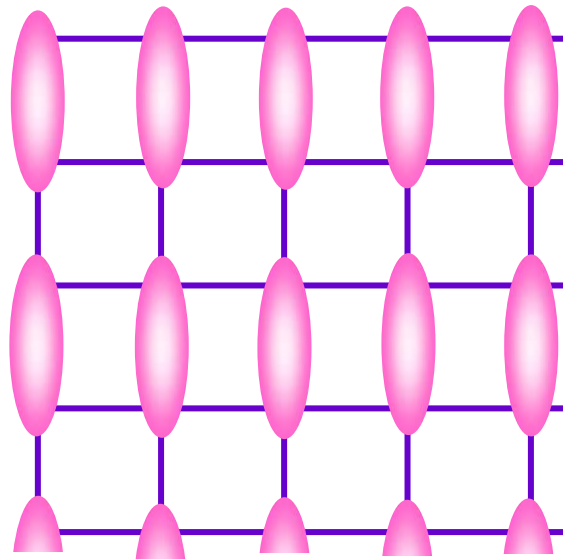
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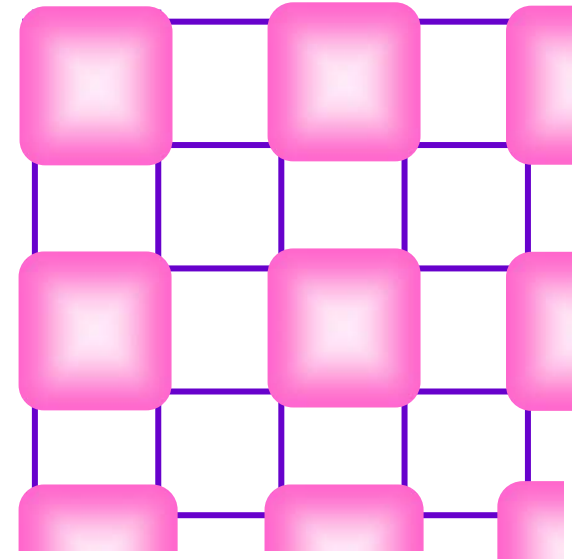
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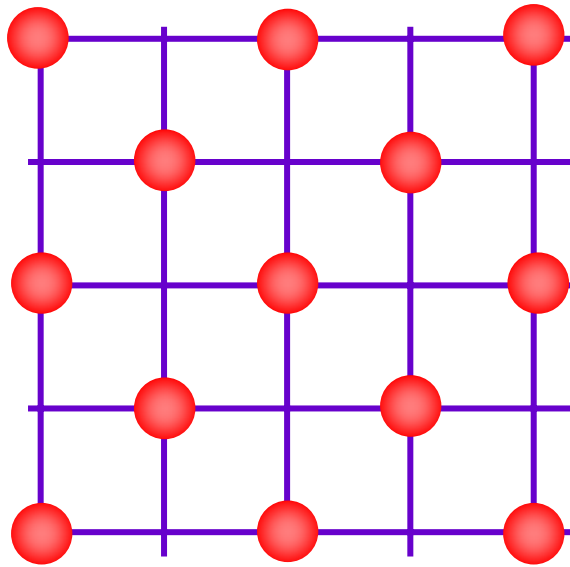
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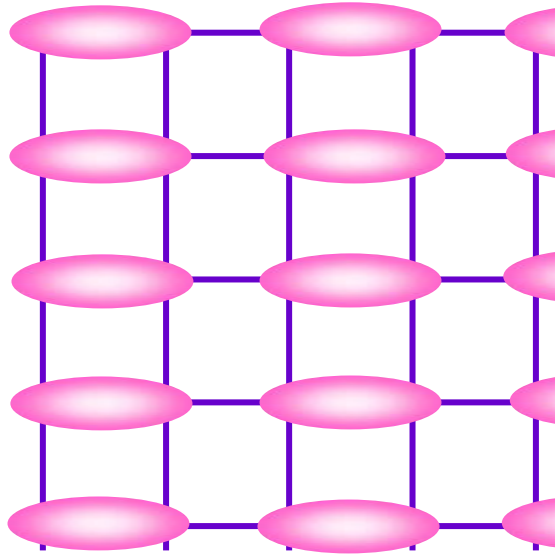
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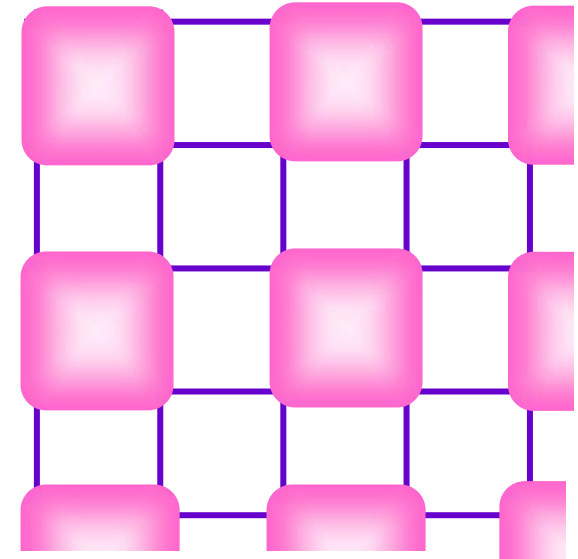
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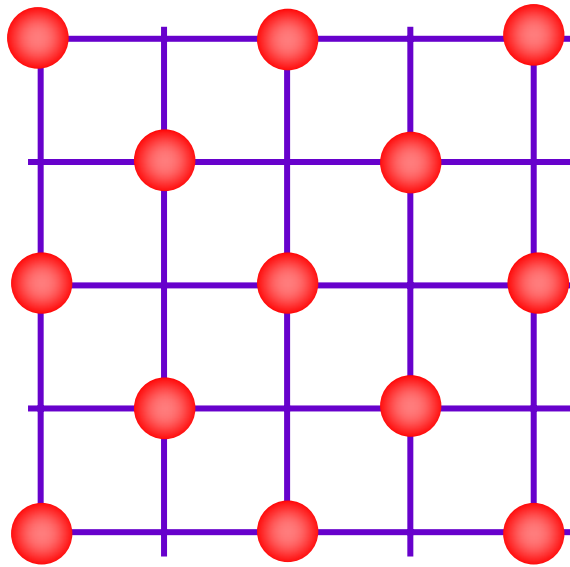
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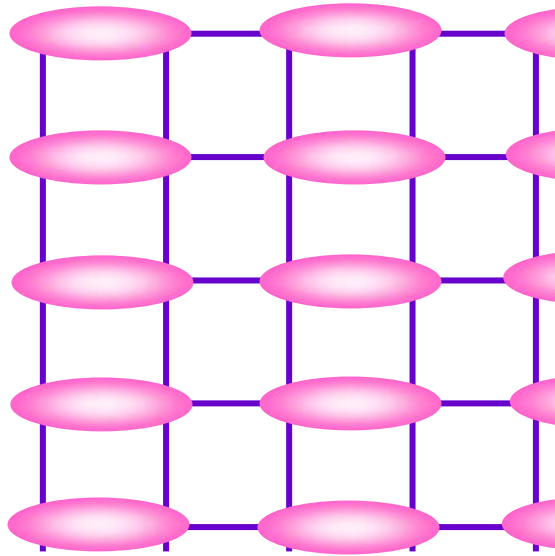
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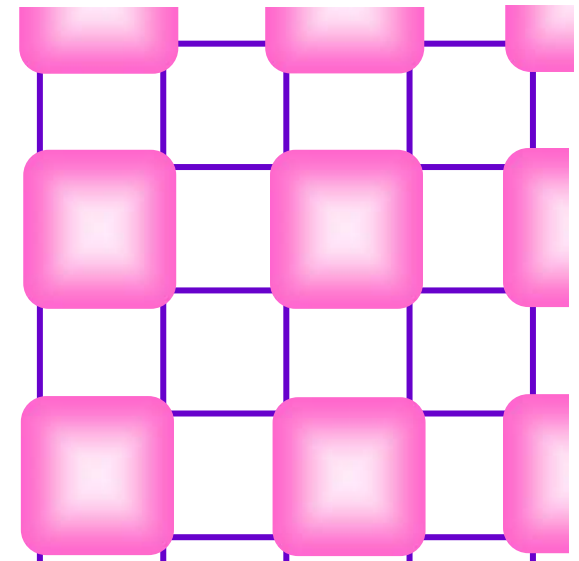
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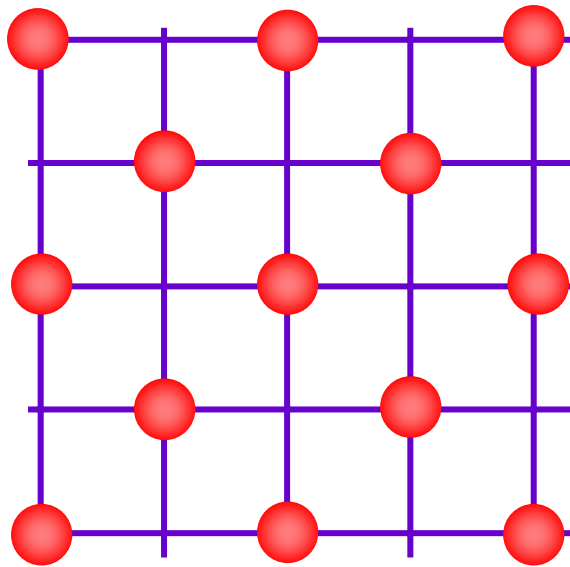
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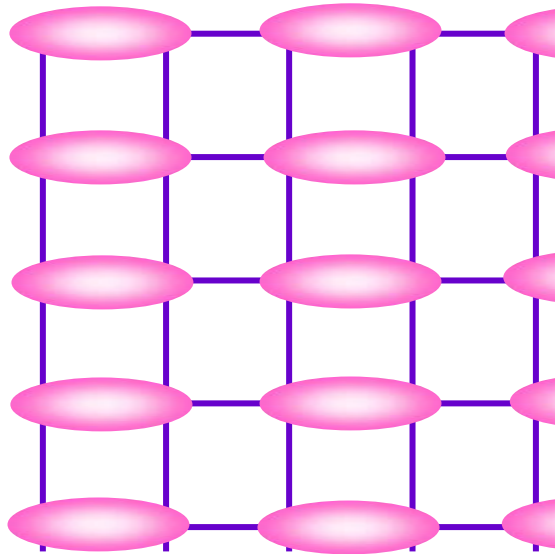
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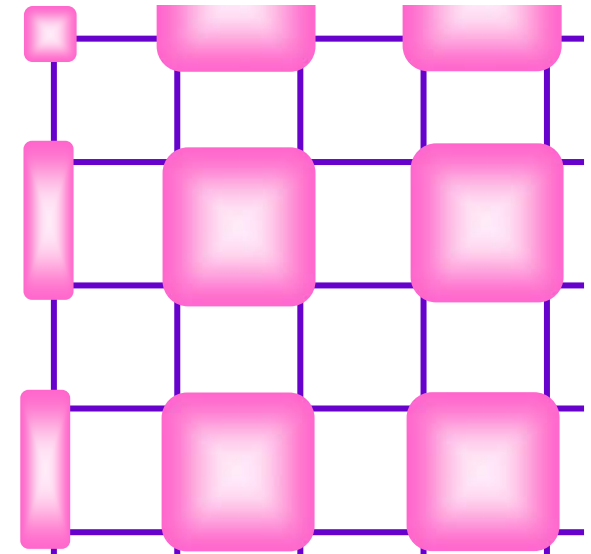
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Charge density wave (CDW) order



Valence bond solid (VBS) order



Valence bond solid (VBS) order

$$\text{pink oval} = \frac{1}{\sqrt{2}} \left( \text{red sphere} - \text{red sphere} + \text{red sphere} - \text{red sphere} \right)$$

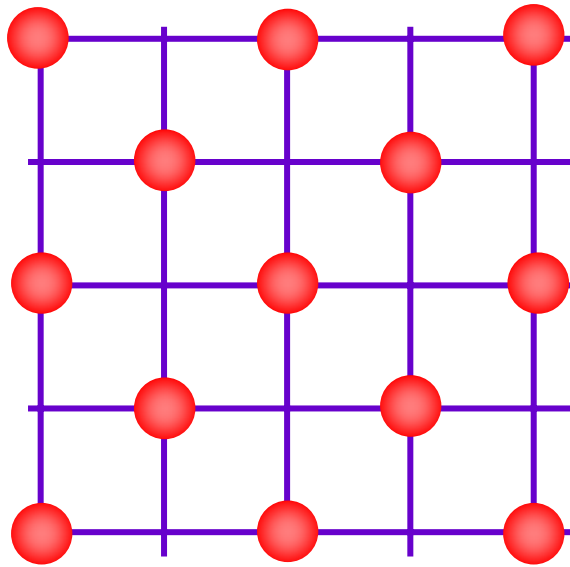
Can define a common CDW/VBS order using a generalized "density"  $\rho(\mathbf{r}) = \sum_{\mathbf{Q}} \rho_{\mathbf{Q}} e^{i\mathbf{Q} \cdot \mathbf{r}}$

All insulators have  $\langle \Psi \rangle = 0$  and  $\langle \rho_{\mathbf{Q}} \rangle \neq 0$  for certain  $\mathbf{Q}$

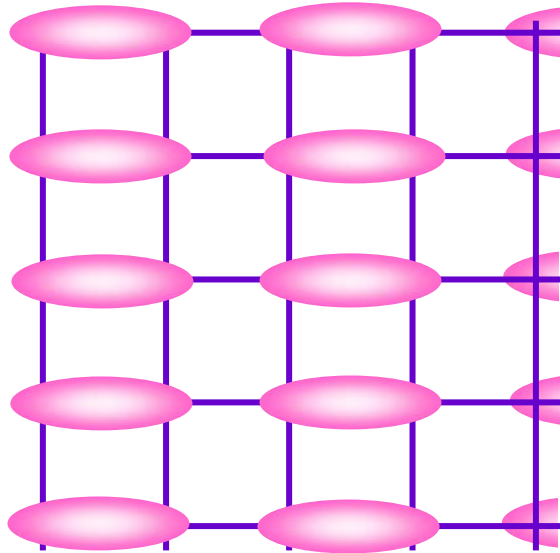
C. Lannert, M.P.A. Fisher, and T. Senthil, *Phys. Rev. B* **63**, 134510 (2001)

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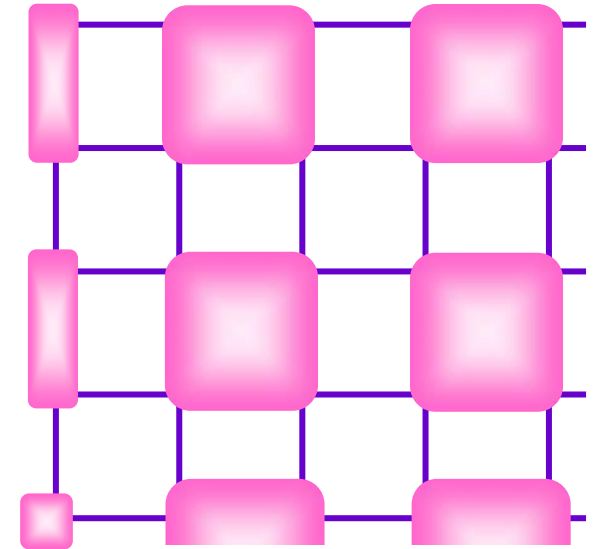
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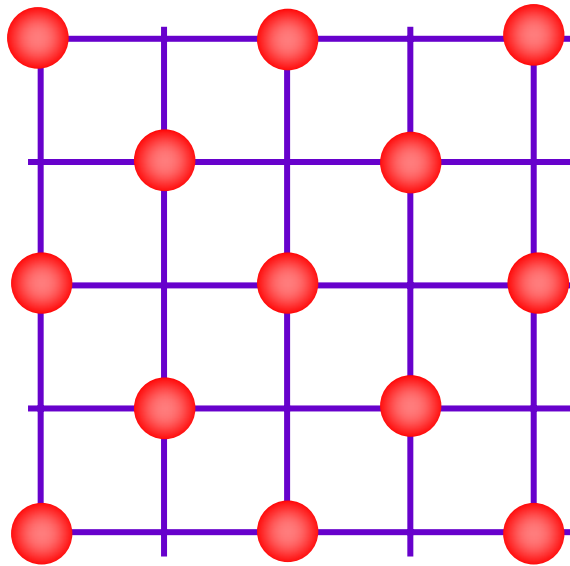
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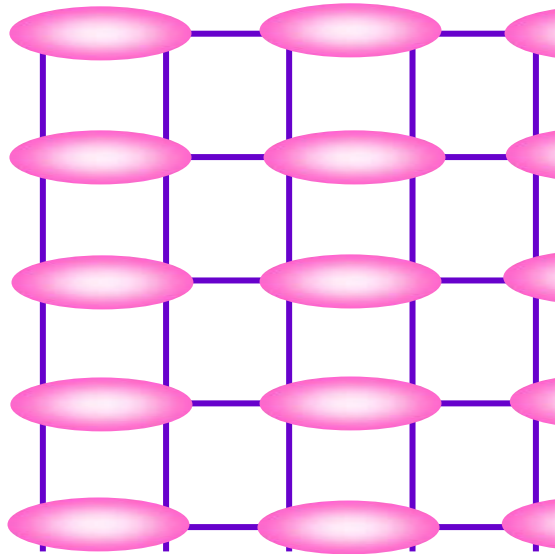
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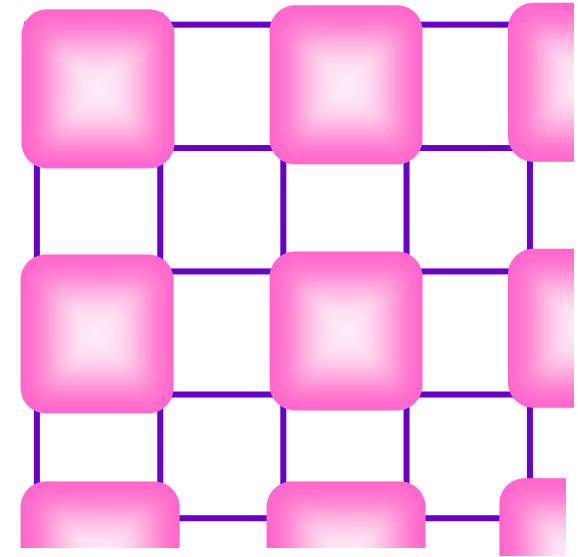
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Ginzburg-Landau-Wilson approach to multiple order parameters:

$$F = F_{sc} [\Psi_{sc}] + F_{\text{charge}} [\rho_Q] + F_{\text{int}}$$

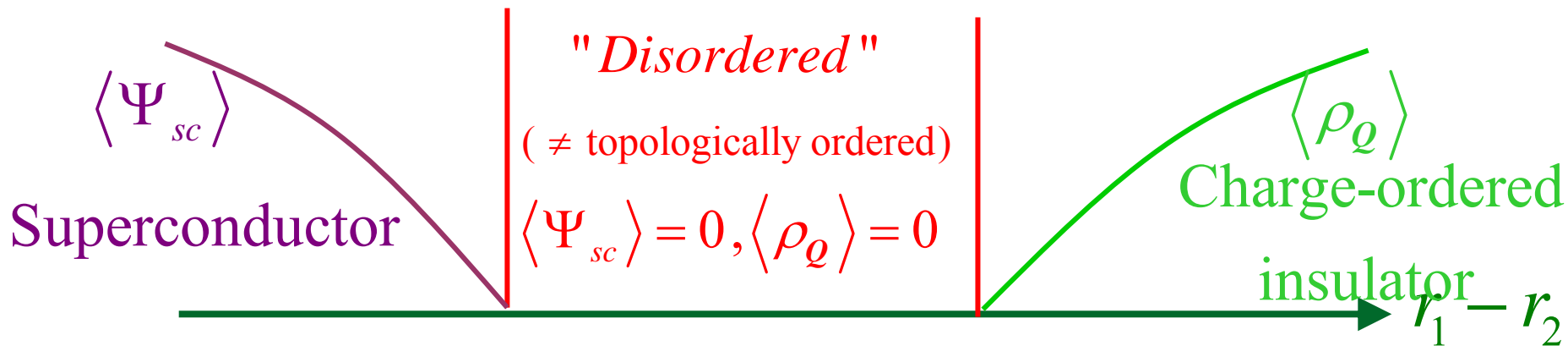
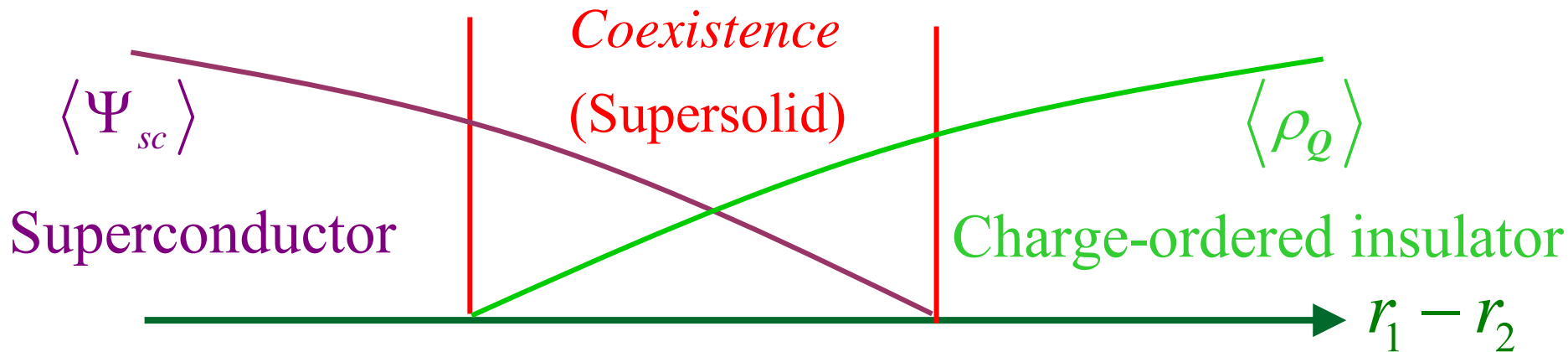
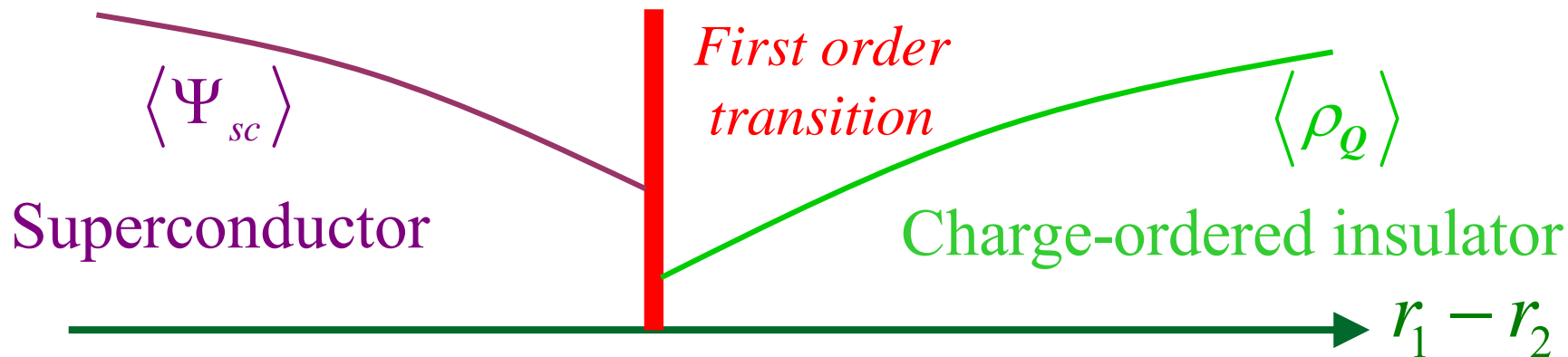
$$F_{sc} [\Psi_{sc}] = r_1 |\Psi_{sc}|^2 + u_1 |\Psi_{sc}|^4 + \dots$$

$$F_{\text{charge}} [\rho_Q] = r_2 |\rho_Q|^2 + u_2 |\rho_Q|^4 + \dots$$

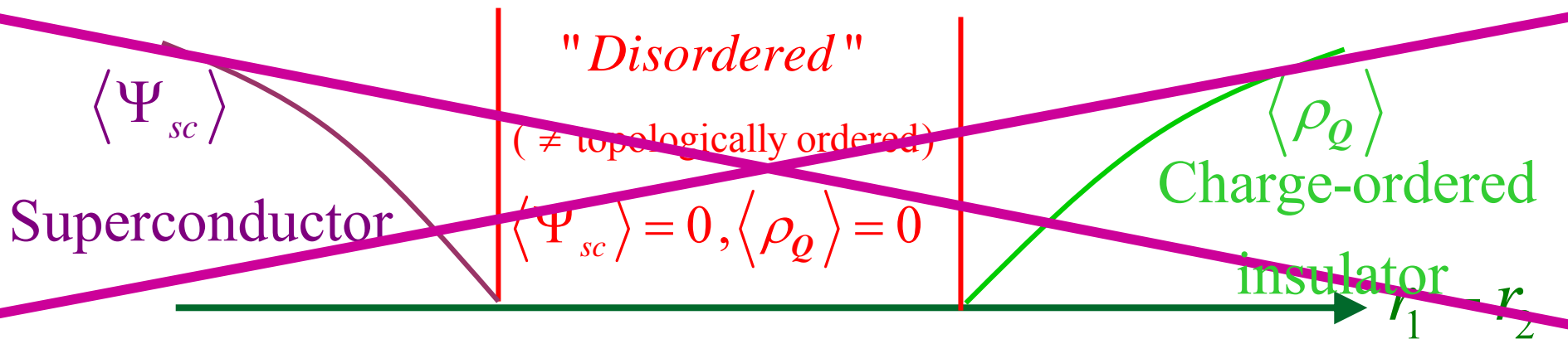
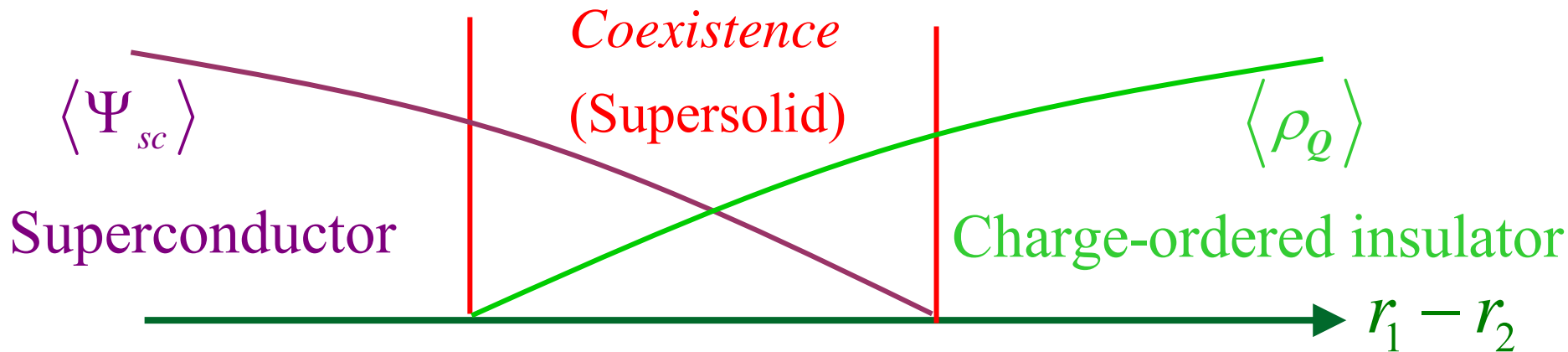
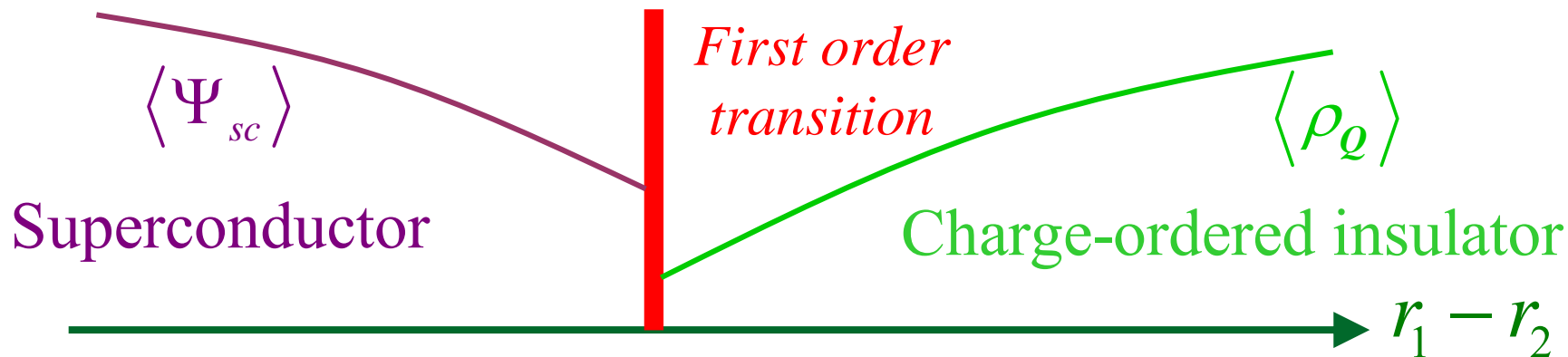
$$F_{\text{int}} = v |\Psi_{sc}|^2 |\rho_Q|^2 + \dots$$

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

# Predictions of LGW theory



# Predictions of LGW theory



# 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

*1. Berry phases and the mapping to a compact  $U(1)$  gauge theory*

*2. Valence-bond-solid (VBS) order in the paramagnet;*

*3. Mapping to hard-core bosons at half-filling*

C. The superfluid-insulator transition of bosons in lattices

*Multiple order parameters in quantum systems*

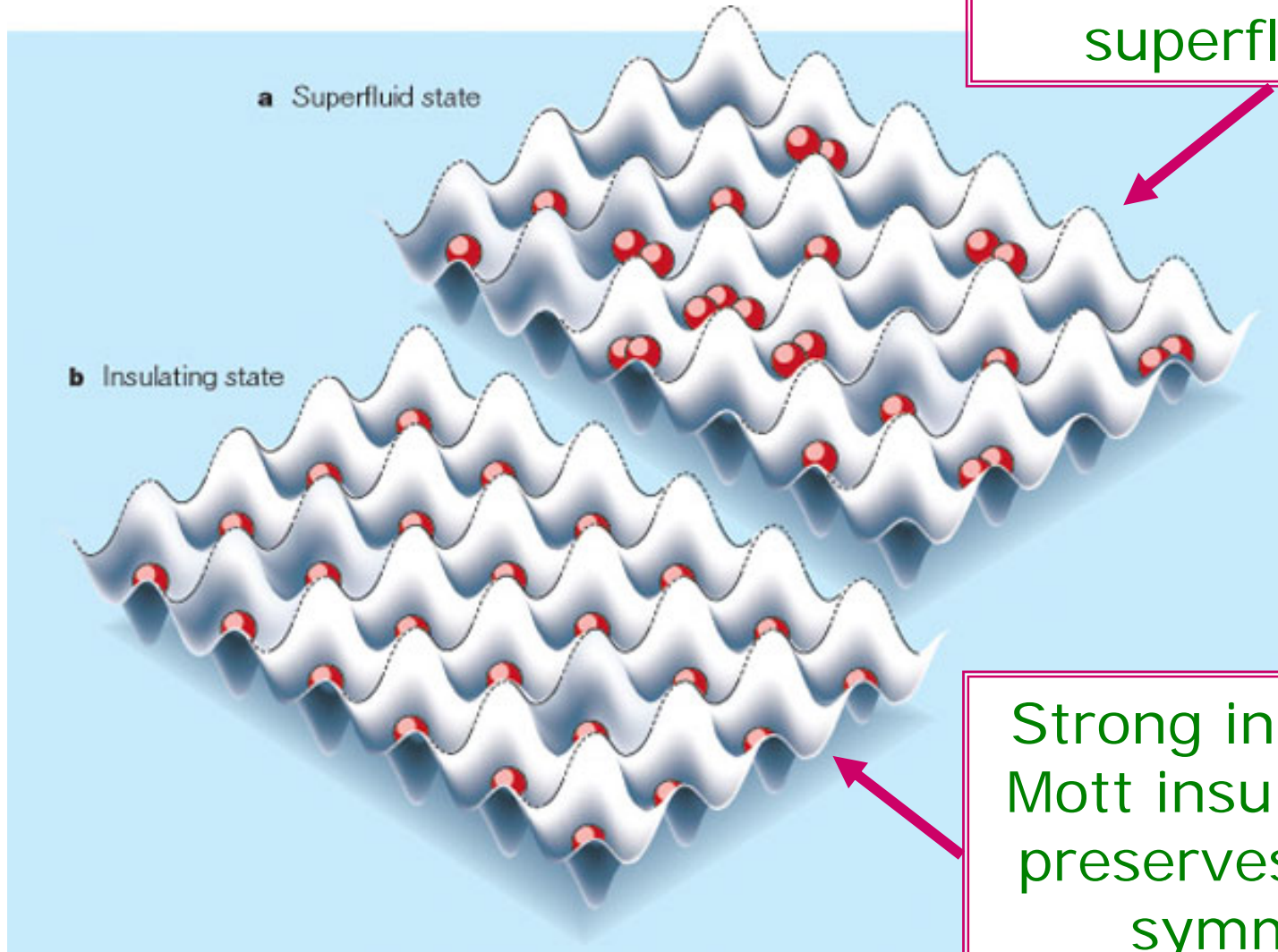
D. Boson-vortex duality

*Breakdown of the LGW paradigm*

## D. Boson-vortex duality

### *1. Bosons in a lattice at integer filling*

# Bosons at density $f = 1$

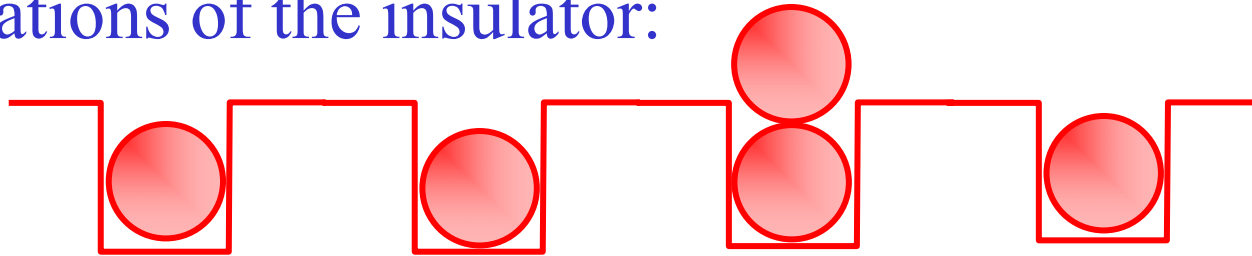


Weak interactions:  
superfluidity

Strong interactions:  
Mott insulator which  
preserves all lattice  
symmetries

# Approaching the transition from the insulator ( $f=1$ )

Excitations of the insulator:



Particles  $\sim \psi^\dagger$



Holes  $\sim \psi$

Density of particles = density of holes  $\Rightarrow$

“relativistic” field theory for  $\psi$ :

$$\mathcal{S} = \int d^2r d\tau \left[ |\partial_\tau \psi|^2 + |\nabla_r \psi|^2 + s|\psi|^2 + \frac{u}{2}|\psi|^4 \right]$$

Insulator  $\Leftrightarrow \langle \psi \rangle = 0$

Superfluid  $\Leftrightarrow \langle \psi \rangle \neq 0$

# Approaching the transition from the superfluid ( $f=1$ )

## Excitations of the superfluid: (A) **Spin waves**

With  $\psi \sim e^{i\theta}$ , action for spin waves is

$$\mathcal{S}_{sw} = \frac{\rho_s}{2} \int d^3x (\partial_\mu \theta)^2$$

**Dual form:** After a Hubbard-Stratonovich transformation, write

$$\mathcal{S}_{sw} = \int d^3x \left[ \frac{1}{2\rho_s} J_\mu^2 + iJ_\mu \partial_\mu \theta \right]$$

Integrating over  $\theta$  yields  $\partial_\mu J_\mu = 0$ . Solve, by writing

$$J_\mu = \epsilon_{\mu\nu\lambda} \partial_\nu A_\lambda$$

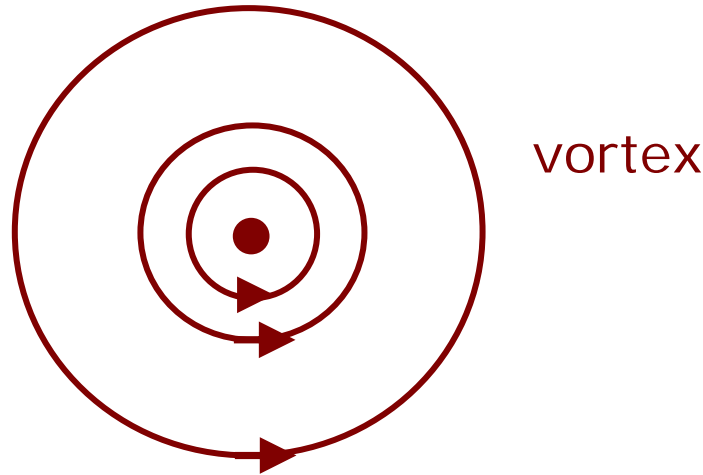
leading to

$$\mathcal{S}_{sw} = \int d^3x \left[ \frac{1}{2\rho_s} (\epsilon_{\mu\nu\lambda} \partial_\nu A_\lambda)^2 \right]$$

**Spin waves are dual to a U(1) gauge theory in 2+1 dimensions**

# Approaching the transition from the superfluid ( $f=1$ )

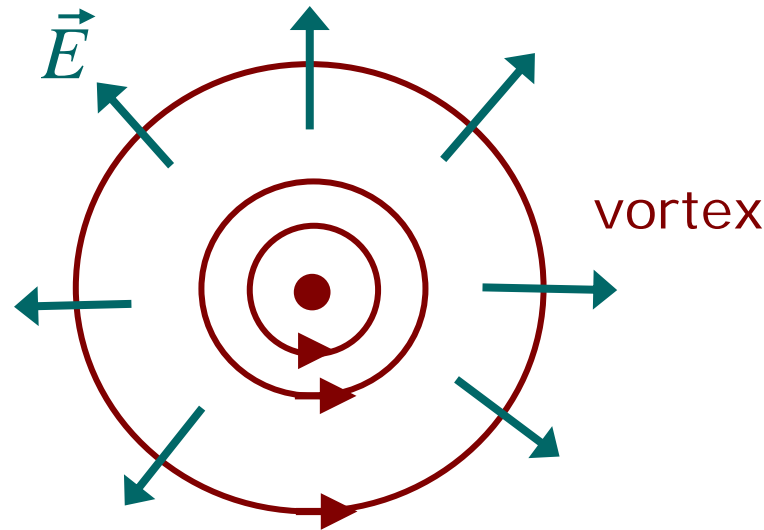
## Excitations of the superfluid: (B) **Vortices**



A vortex is a point-like object. We can therefore define a local field operator,  $\varphi$ , which annihilates a vortex.

# Approaching the transition from the superfluid ( $f=1$ )

## Excitations of the superfluid: (B) **Vortices**



A vortex is a point-like object. We can therefore define a local field operator,  $\varphi$ , which annihilates a vortex.

Each vortex is the source of an 'electric field'  $\vec{E}$  associated with the U(1) gauge field  $A_\mu$ .

Consequently,  $\varphi$  carries +1 U(1) gauge charge.

## Approaching the transition from the superfluid ( $f=1$ )

### Excitations of the superfluid: **Spin wave and vortices**

$\varphi$ : vortex annihilation operator.

$\epsilon_{\mu\nu\lambda}\partial_\nu A_\lambda$ : boson current  $\sim i\psi^*\partial_\mu\psi - i\partial_\mu\psi^*\psi$ .

Density of vortices = density of antivortices  $\Rightarrow$   
“relativistic” field theory for  $\varphi$ :

$$\mathcal{S}_{\text{dual}} = \int d^3x \left[ |(\partial_\mu - iA_\mu)\varphi|^2 + \tilde{s}|\varphi|^2 + \frac{\tilde{u}}{2}|\varphi|^4 + \frac{1}{2\rho_s}(\epsilon_{\mu\nu\lambda}\partial_\nu A_\lambda)^2 \right]$$

Superfluid  $\Leftrightarrow \langle \varphi \rangle = 0$

Insulator  $\Leftrightarrow \langle \varphi \rangle \neq 0$

# Dual theories of the superfluid-insulator transition ( $f=1$ )

## Excitations of the superfluid: **Spin wave and vortices**

Using the boson quasiparticle excitations of the insulator  $\sim \psi$

$$\mathcal{S} = \int d^2r d\tau \left[ |\partial_\tau \psi|^2 + |\nabla_r \psi|^2 + s|\psi|^2 + \frac{u}{2}|\psi|^4 \right]$$

$$\text{Insulator} \Leftrightarrow \langle \psi \rangle = 0$$

$$\text{Superfluid} \Leftrightarrow \langle \psi \rangle \neq 0$$

is dual to

Using the vortex quasiparticle excitations of the superfluid  $\sim \varphi$

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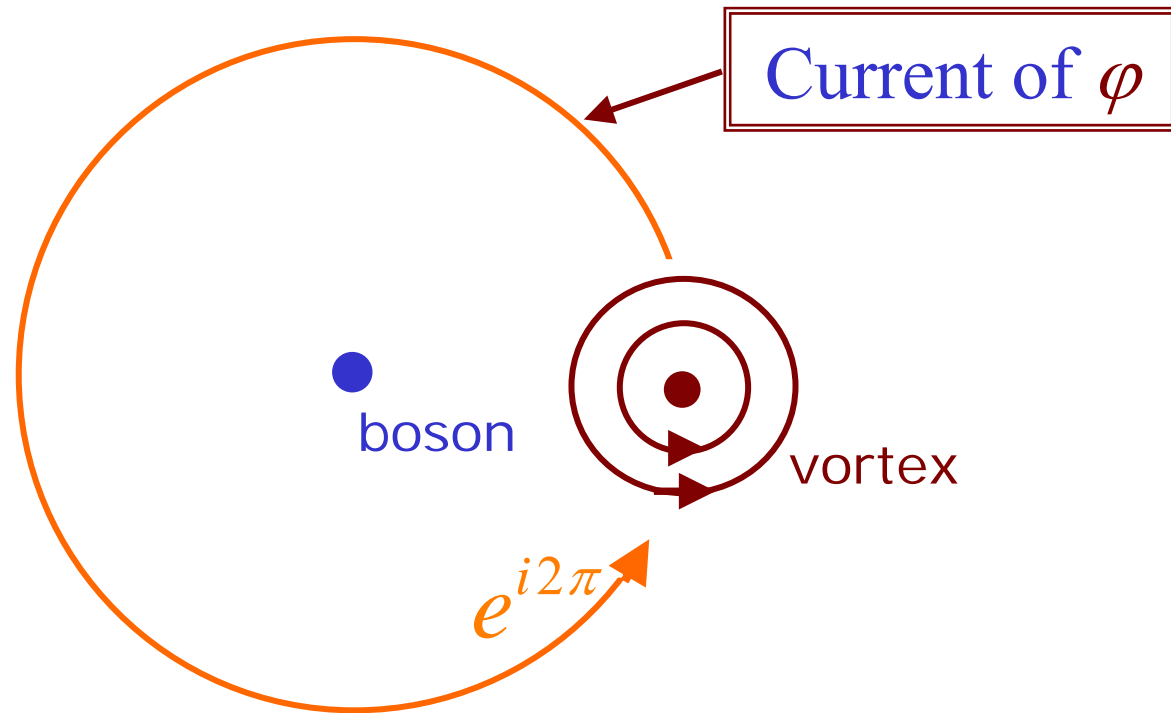
## *A vortex in the vortex field is the original boson*

A vortex in  $\varphi$  carries  $2\pi$  flux in the ‘magnetic field’

$B = \epsilon_{\tau\mu\nu}\partial_\mu A_\nu$ . But this is just the original boson number operator. Consequently, in the path integral viewpoint, the world line of the vortex in  $\varphi$  is just the world line of the original boson.

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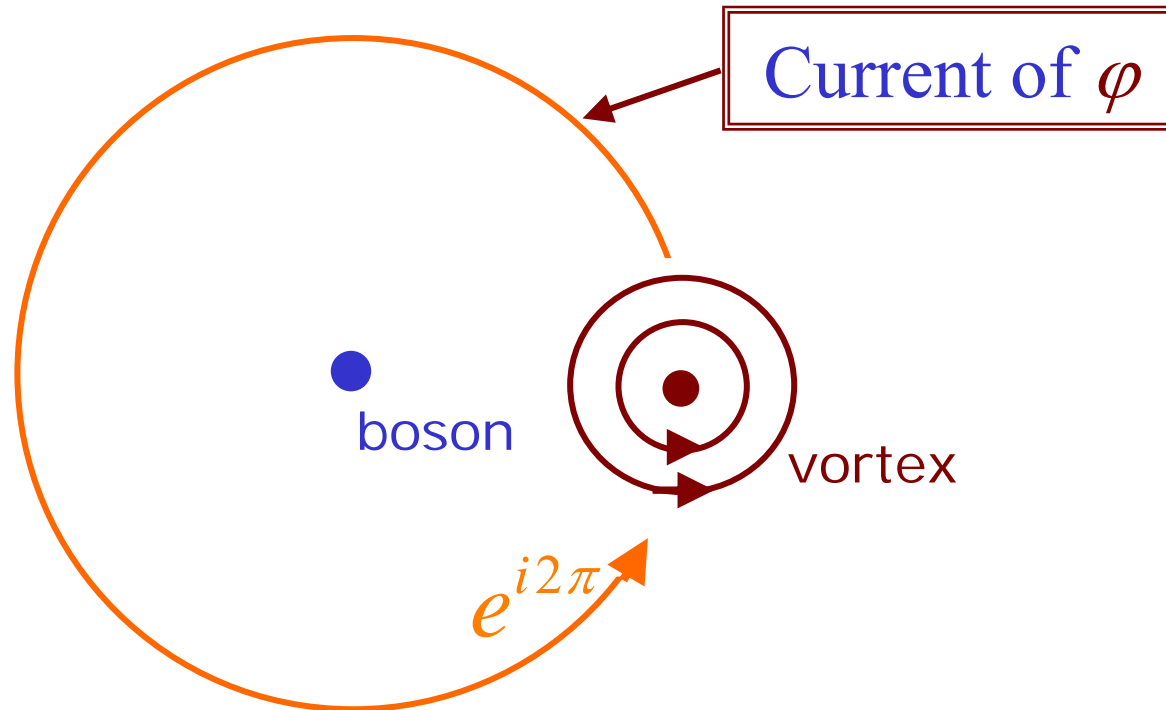
The wavefunction of a vortex acquires a phase of  $2\pi$  each time the vortex encircles a boson

## D. Boson-vortex duality

### *2. Bosons in a lattice at fractional filling $f$*

L. Balents, L. Bartosch, A. Burkov, S. Sachdev, K. Sengupta,  
*Physical Review B* **71**, 144508 and 144509 (2005),  
cond-mat/0502002, and cond-mat/0504692.

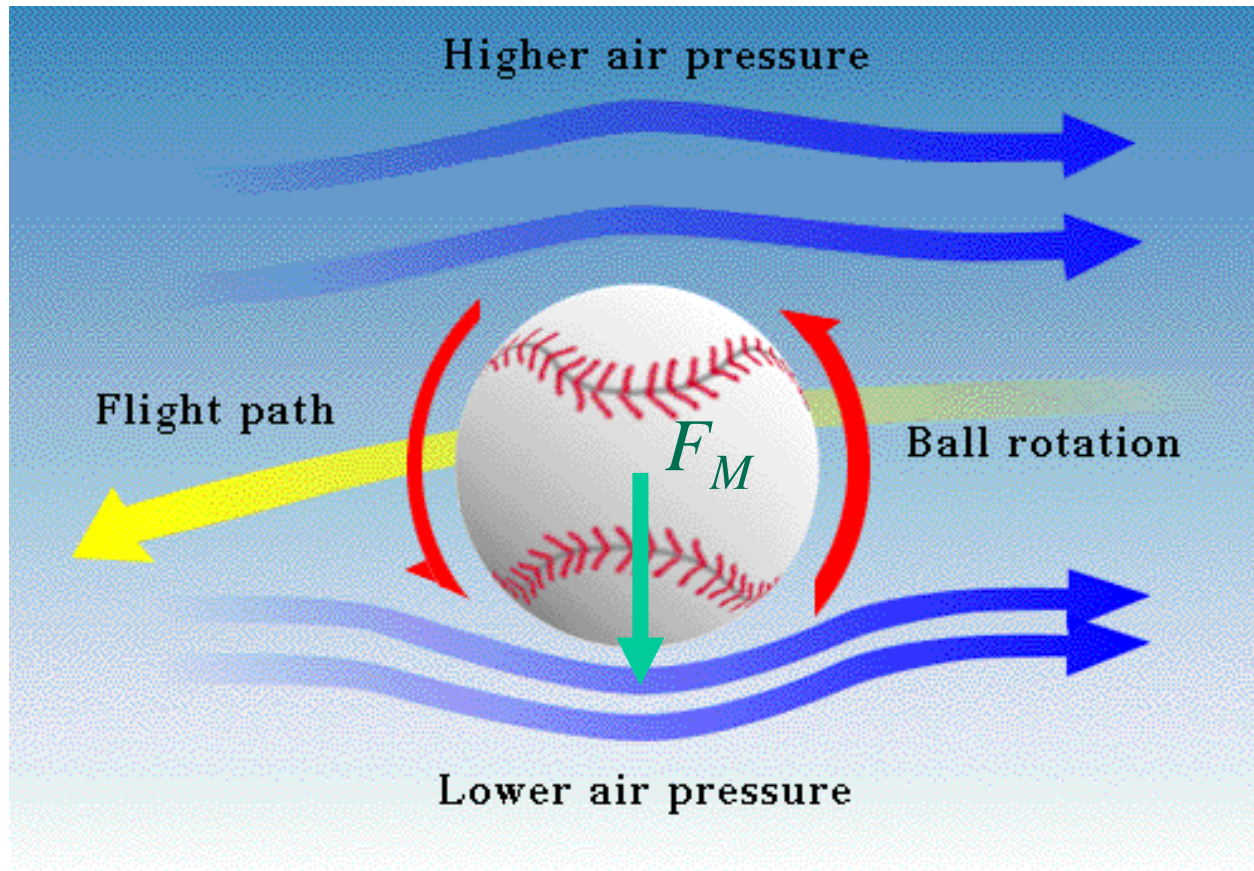
# Boson-vortex duality



The wavefunction of a vortex acquires a phase of  $2\pi$  each time the vortex encircles a boson

Strength of “magnetic” field on vortex field  $\varphi$   
= density of bosons =  $f$  flux quanta per plaquette

In ordinary fluids, vortices experience the Magnus Force



$$F_M = (\text{mass density of air}) \cdot (\text{velocity of ball}) \cdot (\text{circulation})$$

For a vortex in a superfluid, this is

$$\begin{aligned}\mathbf{F}_M &= (m\rho) \left( \left( \mathbf{v}_s - \frac{d\mathbf{r}_v}{dt} \right) \times \hat{\mathbf{z}} \right) \left( \oint \mathbf{v}_s \cdot d\mathbf{r} \right) \\ &= nh\rho \left( \mathbf{v}_s - \frac{d\mathbf{r}_v}{dt} \right) \times \hat{\mathbf{z}}\end{aligned}$$

where  $\rho$  = number density of bosons

$\mathbf{v}_s$  = local velocity of superfluid

$\mathbf{r}_v$  = position of vortex

For a vortex in a superfluid, this is

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where  $\mathbf{E} = \rho\mathbf{v}_s \times \hat{\mathbf{z}}$  and  $\mathbf{B} = -h\rho\hat{\mathbf{z}}$

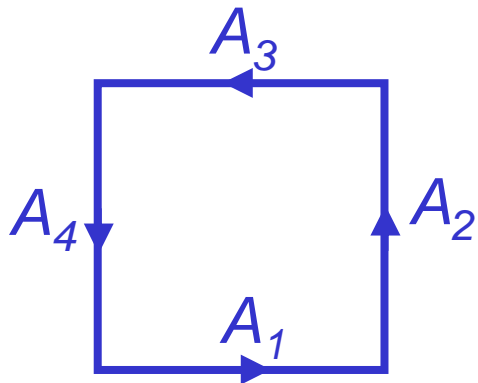
### Dual picture:

The vortex is a quantum particle with dual “electric” charge  $n$ , moving in a dual “magnetic” field of strength =  $h \times$  (number density of Bose particles)

- The vortices are quantum particles moving in a periodic potential with the symmetry of the square lattice, and in the presence of a dual “magnetic” field of strength  $= h\rho$ , where  $\rho$  is the number density of bosons per unit cell.
- The vortex motion can be described by the effective Hofstadter Hamiltonian:

$$\mathcal{H}_v = -t \sum_{\langle ij \rangle} (e^{iA_{ij}} \varphi_i^* \varphi_j + \text{c.c.})$$

where  $\varphi_i$  is an operator which annihilates a vortex particle at site  $i$  of a square lattice.



$$A_1 + A_2 + A_3 + A_4 = 2\pi f$$

where  $f$  is the boson filling fraction.

## Bosons at filling fraction $f = 1$

- At  $f=1$ , the “magnetic” flux per unit cell is  $2\pi$ , and the vortex does not pick up any phase from the boson density.
- The effective dual “magnetic” field acting on the vortex is zero, and the corresponding component of the Magnus force vanishes.

## Bosons at rational filling fraction $f=p/q$

Quantum mechanics of the vortex “particle” in a periodic potential with  $f$  flux quanta per unit cell

Space group symmetries of Hofstadter Hamiltonian:

$T_x, T_y$  : Translations by a lattice spacing in the  $x, y$  directions

$R$  : Rotation by 90 degrees.

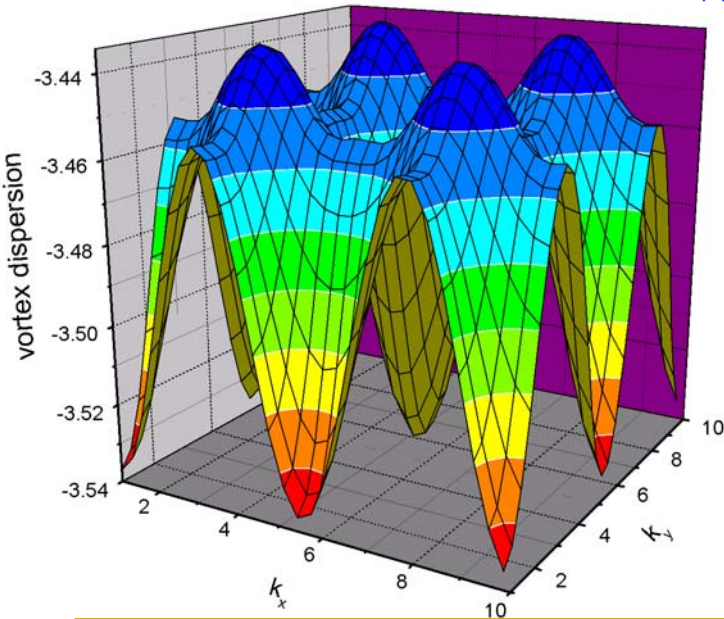
Magnetic space group:

$$T_x T_y = e^{2\pi i f} T_y T_x \ ;$$

$$R^{-1} T_y R = T_x \ ; \ R^{-1} T_x R = T_y^{-1} \ ; \ R^4 = 1$$

The low energy vortex states must form a representation of this algebra

# Vortices in a superfluid near a Mott insulator at filling $f=p/q$ Hofstadter spectrum of the quantum vortex “particle” with field operator $\varphi$



At filling  $f=p/q$ , there are  $q$  species of vortices,  $\varphi_\ell$  (with  $\ell=1\dots q$ ), associated with  $q$  degenerate minima in the vortex spectrum. These vortices realize the smallest,  $q$ -dimensional, representation of the magnetic algebra.

The  $q$  vortices form a *projective* representation of the space group

$$T_x : \varphi_\ell \rightarrow \varphi_{\ell+1} \quad ; \quad T_y : \varphi_\ell \rightarrow e^{2\pi i \ell f} \varphi_\ell$$

$$R : \varphi_\ell \rightarrow \frac{1}{\sqrt{q}} \sum_{m=1}^q \varphi_m e^{2\pi i \ell m f}$$

## Boson-vortex duality

The  $q \varphi_\ell$  vortices characterize *both* superconducting and density wave orders

Superconductor/insulator :  $\langle \varphi_\ell \rangle = 0 / \langle \varphi_\ell \rangle \neq 0$

# Boson-vortex duality

The  $q$   $\varphi_\ell$  vortices characterize *both* superconducting and density wave orders

Density wave order:

Status of space group symmetry determined by

density operators  $\rho_{\mathbf{Q}}$  at wavevectors  $\mathbf{Q}_{mn} = \frac{2\pi p}{q}(m, n)$

$$\rho_{mn} = e^{i\pi mnf} \sum_{\ell=1}^q \varphi_\ell^* \varphi_{\ell+n} e^{2\pi i \ell m f}$$

$$T_x : \rho_{\mathbf{Q}} \rightarrow \rho_{\mathbf{Q}} e^{i\mathbf{Q} \cdot \hat{x}} \quad ; \quad T_y : \rho_{\mathbf{Q}} \rightarrow \rho_{\mathbf{Q}} e^{i\mathbf{Q} \cdot \hat{y}}$$

$$R : \rho(\mathbf{Q}) \rightarrow \rho(R\mathbf{Q})$$

# Field theory with projective symmetry

Degrees of freedom:

$q$  complex  $\varphi_\ell$  vortex fields

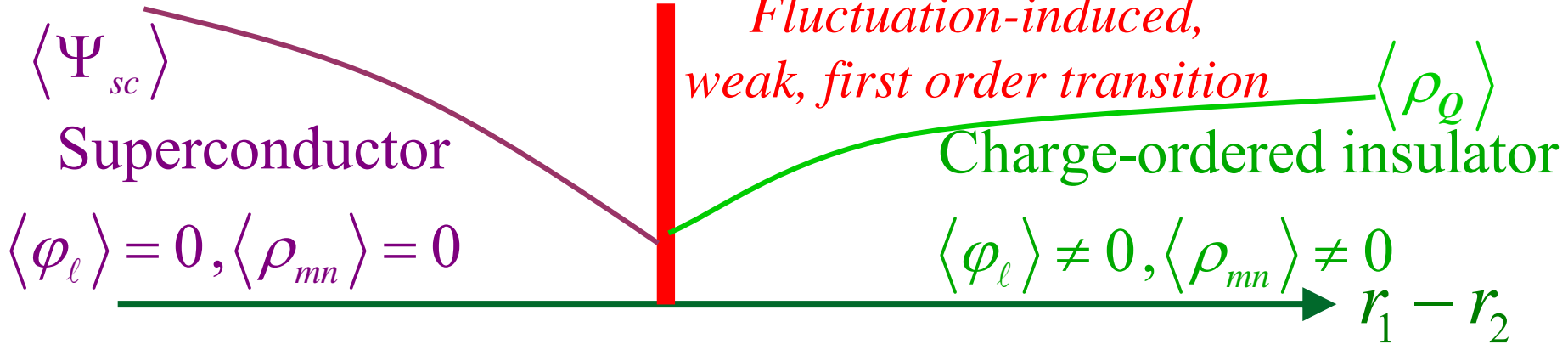
1 non-compact U(1) gauge field  $A_\mu$

$$\mathcal{S} = \int d^2x d\tau \left[ \sum_\ell \{ |(\partial_\mu - iA_\mu)\varphi_\ell|^2 + s|\varphi_\ell|^2 \} + \frac{1}{2e^2} (\epsilon_{\mu\nu\lambda} \partial_\nu A_\lambda)^2 + \sum_{lmn} \gamma_{lmn} \varphi_\ell^* \varphi_{\ell+m}^* \varphi_{\ell+n} \varphi_{\ell+m-n} \right]$$

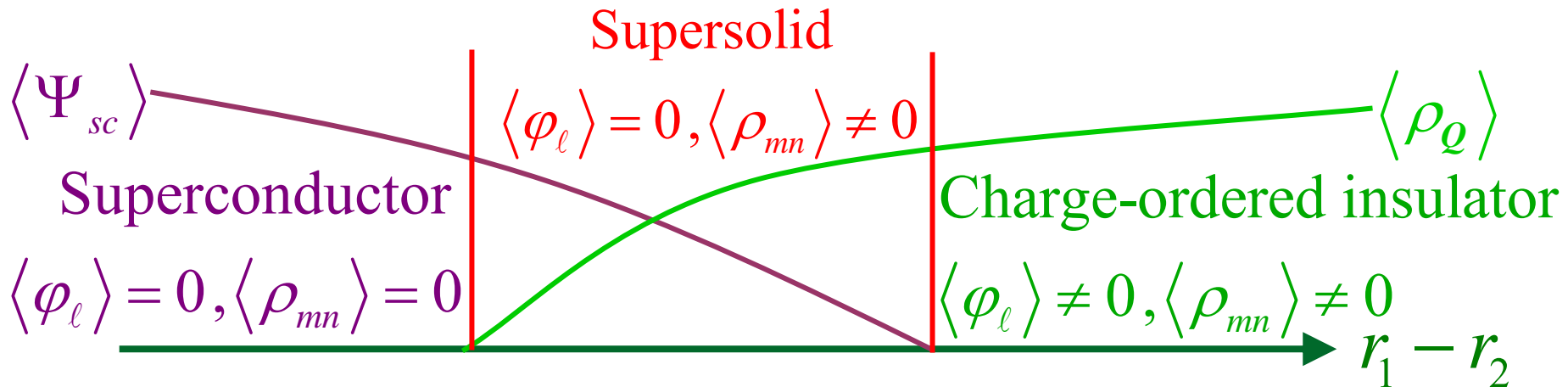
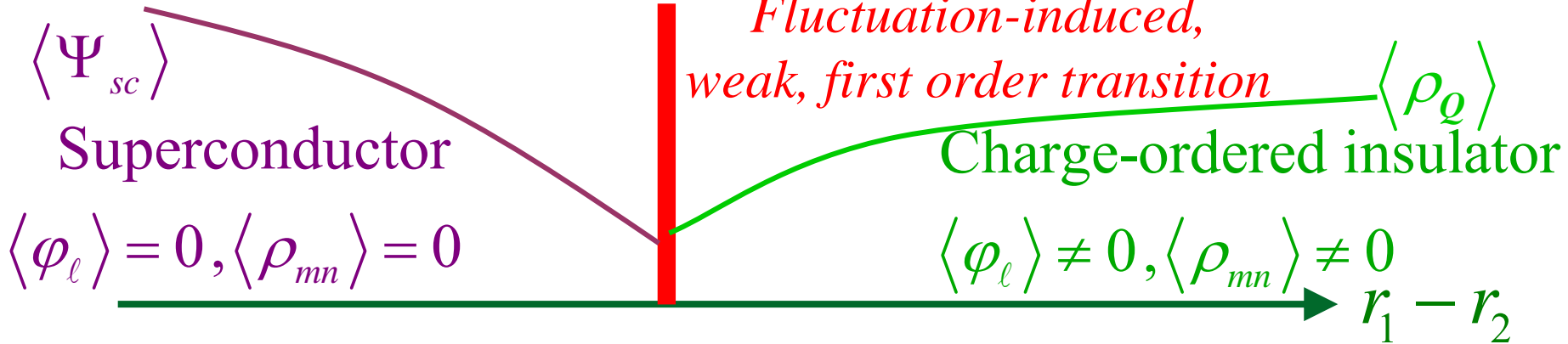
The projective symmetries constrain the couplings  $\gamma_{mn}$  to obey

$$\begin{aligned} \gamma_{mn} &= \gamma_{-m,-n} \quad ; \quad \gamma_{mn} = \gamma_{m,m-n} \quad ; \quad \gamma_{mn} = \gamma_{m-2n,-n} \\ \gamma_{\bar{m}\bar{n}} &= \frac{1}{q} \sum_{mn} \gamma_{mn} e^{-2\pi i f [n(\bar{m}-\bar{n}) + \bar{n}(m-n)]} \end{aligned}$$

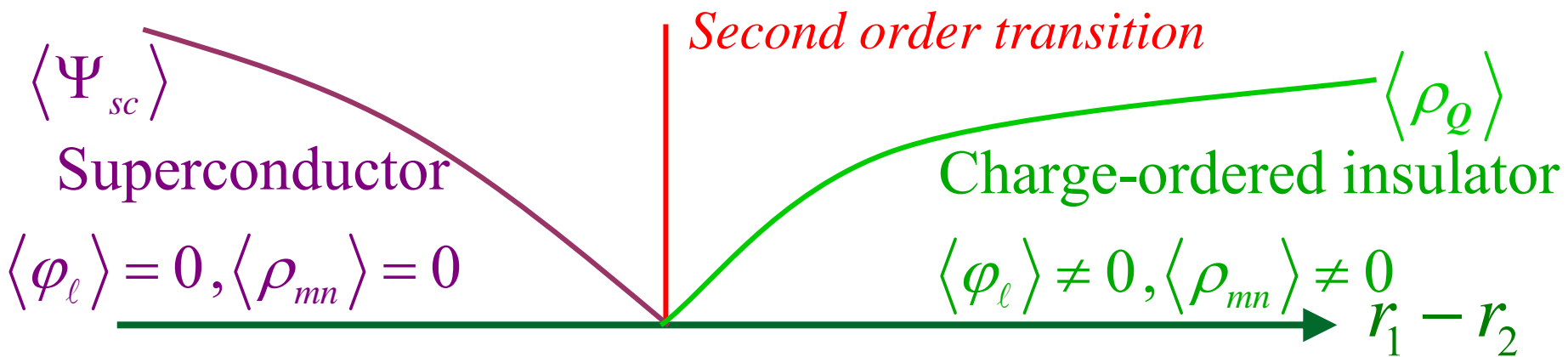
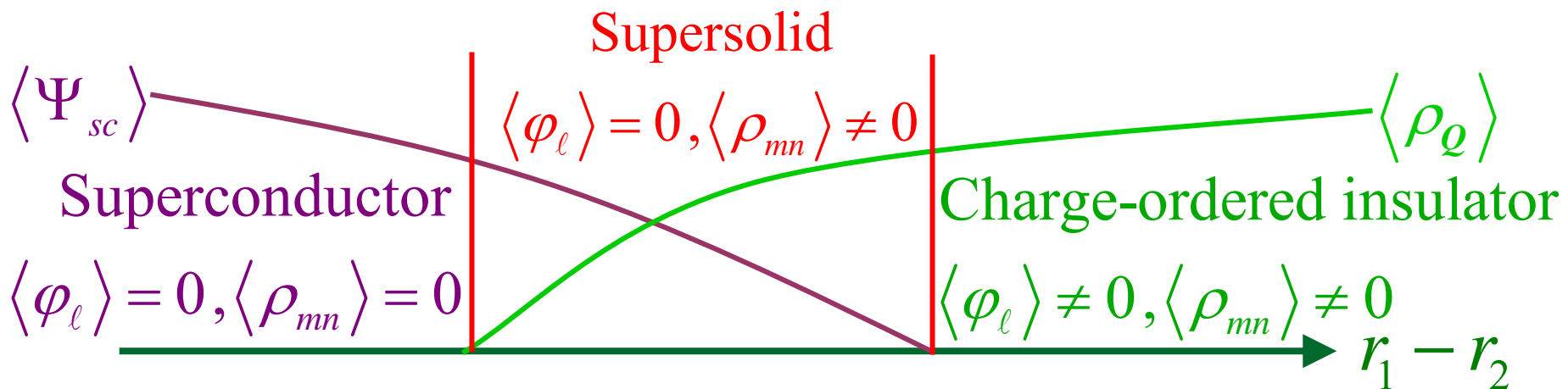
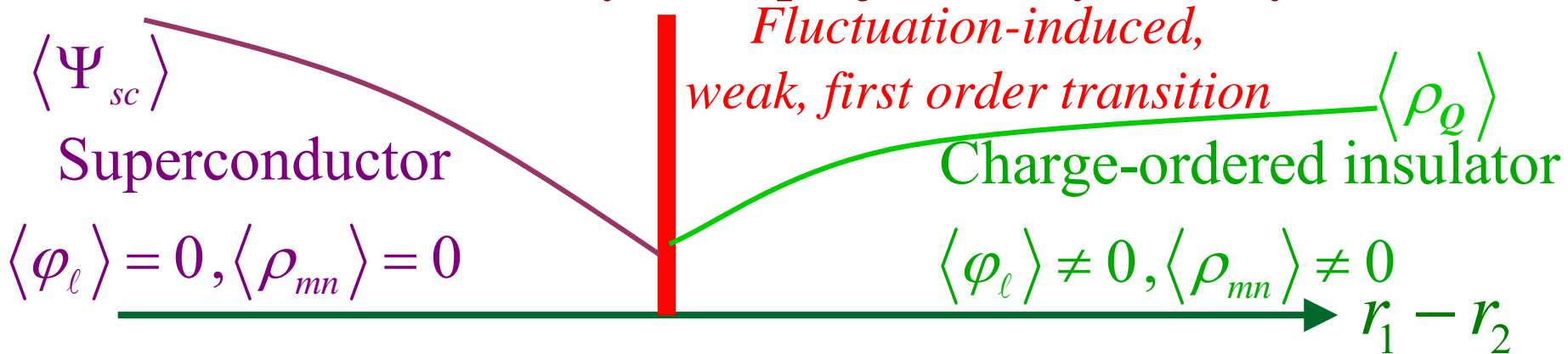
# Field theory with projective symmetry



# Field theory with projective symmetry

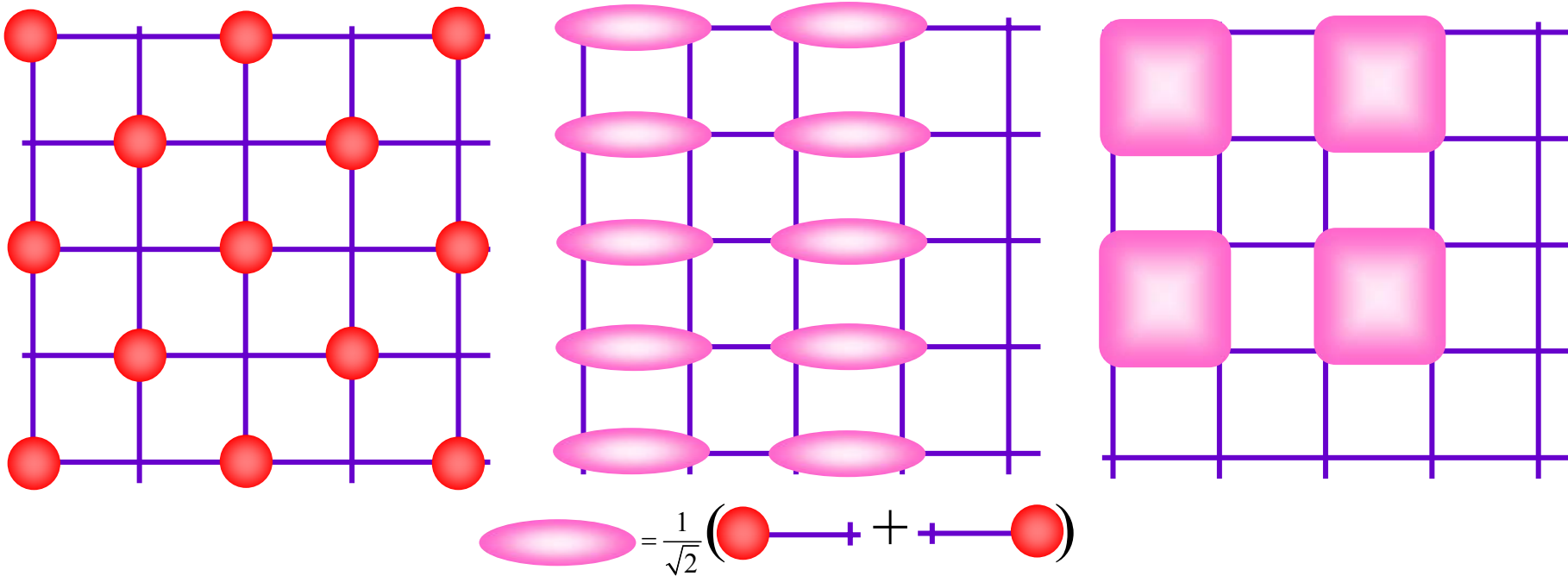


# Field theory with projective symmetry



# Field theory with projective symmetry

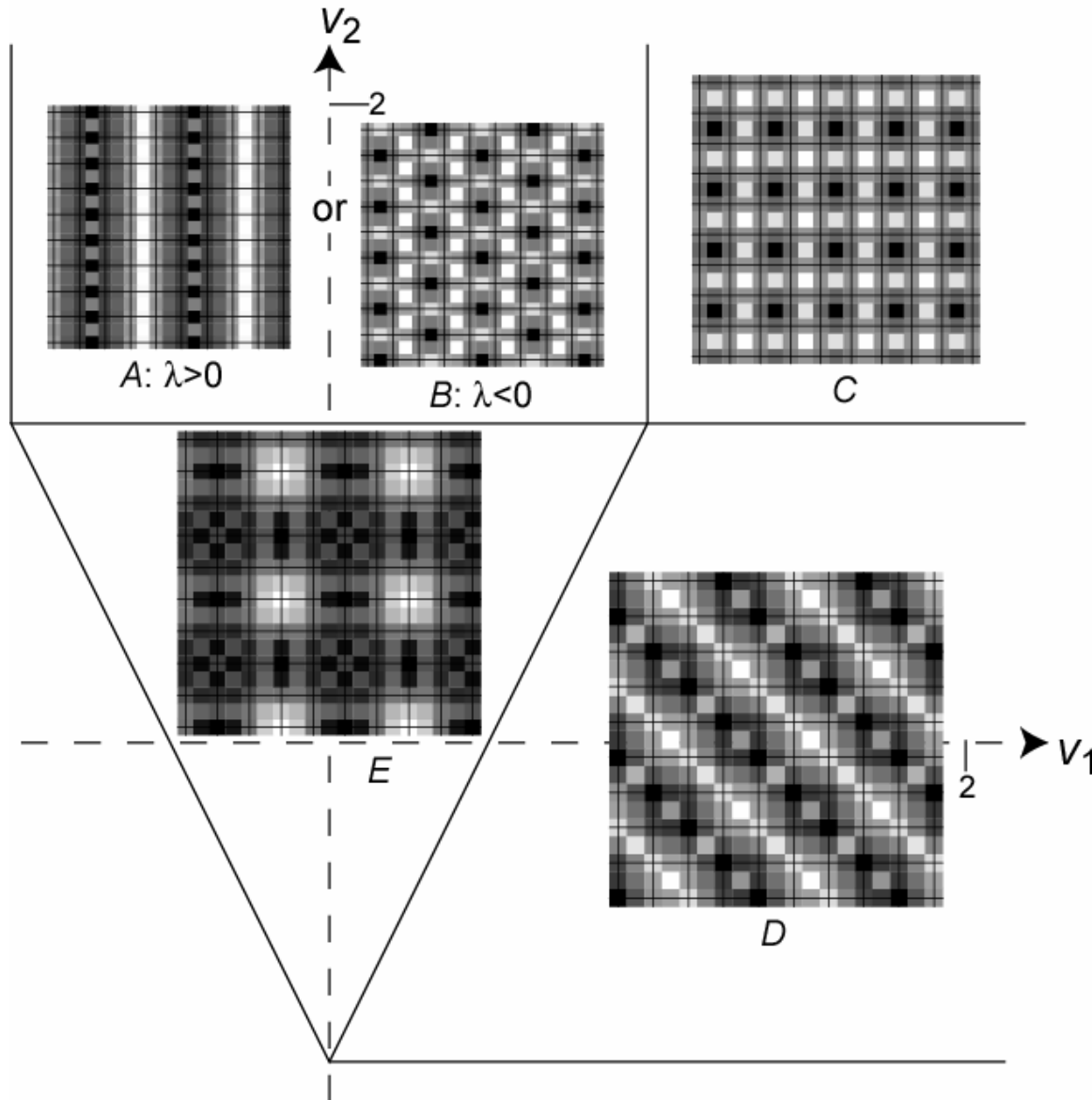
Spatial structure of insulators for  $q=2$  ( $f=1/2$ )



All insulating phases have density-wave order  $\rho(\mathbf{r}) = \sum_{\mathbf{Q}} \rho_{\mathbf{Q}} e^{i\mathbf{Q}\cdot\mathbf{r}}$  with  $\langle \rho_{\mathbf{Q}} \rangle \neq 0$

# Field theory with projective symmetry

Spatial structure of insulators for  $q=4$  ( $f=1/4$  or  $3/4$ )



$a \times b$  unit cells;  
 $\frac{q}{a}, \frac{q}{b}, \frac{ab}{q}$ ,  
all integers

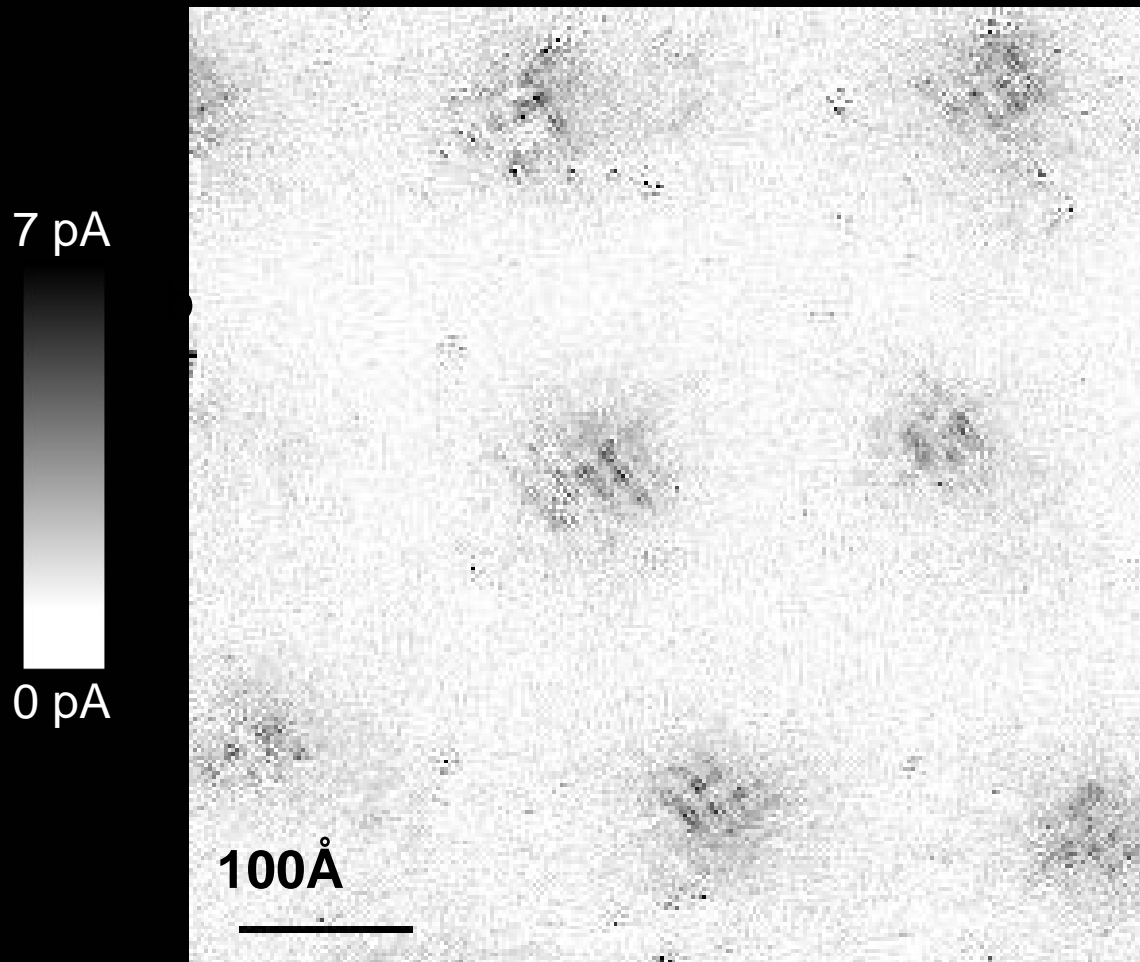
## Field theory with projective symmetry

Density operators  $\rho_Q$  at wavevectors  $Q_{mn} = \frac{2\pi p}{q}(m, n)$

$$\rho_{mn} = e^{i\pi mnf} \sum_{\ell=1}^q \varphi_{\ell}^* \varphi_{\ell+n} e^{2\pi i \ell mf}$$

Each pinned vortex in the superfluid has a halo of density wave order over a length scale  $\approx$  the zero-point quantum motion of the vortex. This scale diverges upon approaching the insulator

# Vortex-induced LDOS of $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$ integrated from 1meV to 12meV at 4K



Vortices have halos with LDOS modulations at a period  $\approx 4$  lattice spacings

J. Hoffman E. W. Hudson, K. M. Lang, V. Madhavan, S. H. Pan, H. Eisaki, S. Uchida, and J. C. Davis, *Science* 295, 466 (2002).

Prediction of VBS order near vortices: K. Park and S. Sachdev, *Phys. Rev. B* 64, 184510 (2001).

## Superfluids near Mott insulators

*The Mott insulator has average Cooper pair density,  $f = p/q$  per site, while the density of the superfluid is close (but need not be identical) to this value*

- Vortices with flux  $h/(2e)$  come in multiple (usually  $q$ ) “flavors”
- The lattice space group acts in a projective representation on the vortex flavor space.
- These flavor quantum numbers provide a distinction between superfluids: they constitute a “quantum order”
- Any pinned vortex must choose an orientation in flavor space. This necessarily leads to modulations in the local density of states over the spatial region where the vortex executes its quantum zero point motion.