Deconfined quantum criticality

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

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Lorenz Bartosch (Harvard)
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Talk online at http://sachdev.physics.harvard.edu

Outline

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

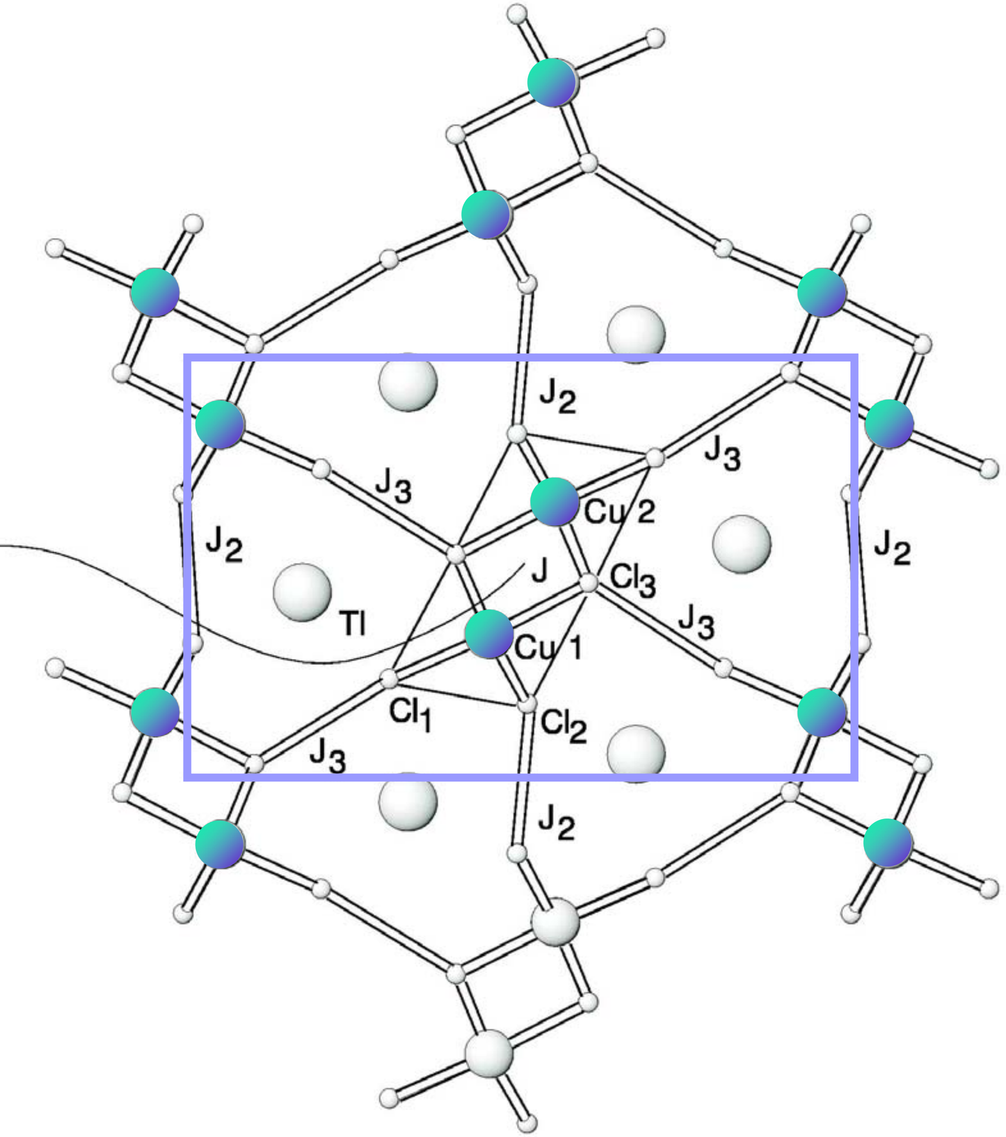
II. Magnetic quantum phase transitions of Mott insulators on the square lattice
A. Breakdown of LGW theory
B. Berry phases
C. Spinor formulation and deconfined criticality

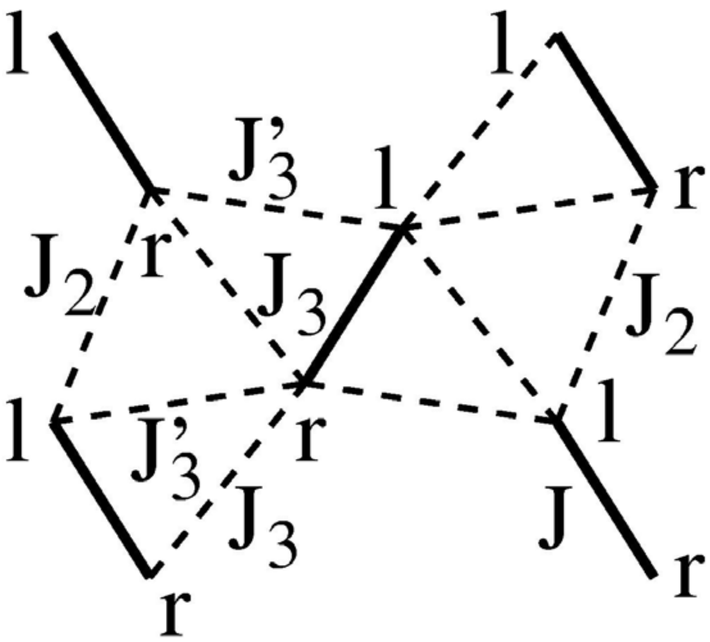
I. Magnetic quantum phase transitions in "dimerized" Mott insulators:

Landau-Ginzburg-Wilson (LGW) theory:

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

$TlCuCl_3$



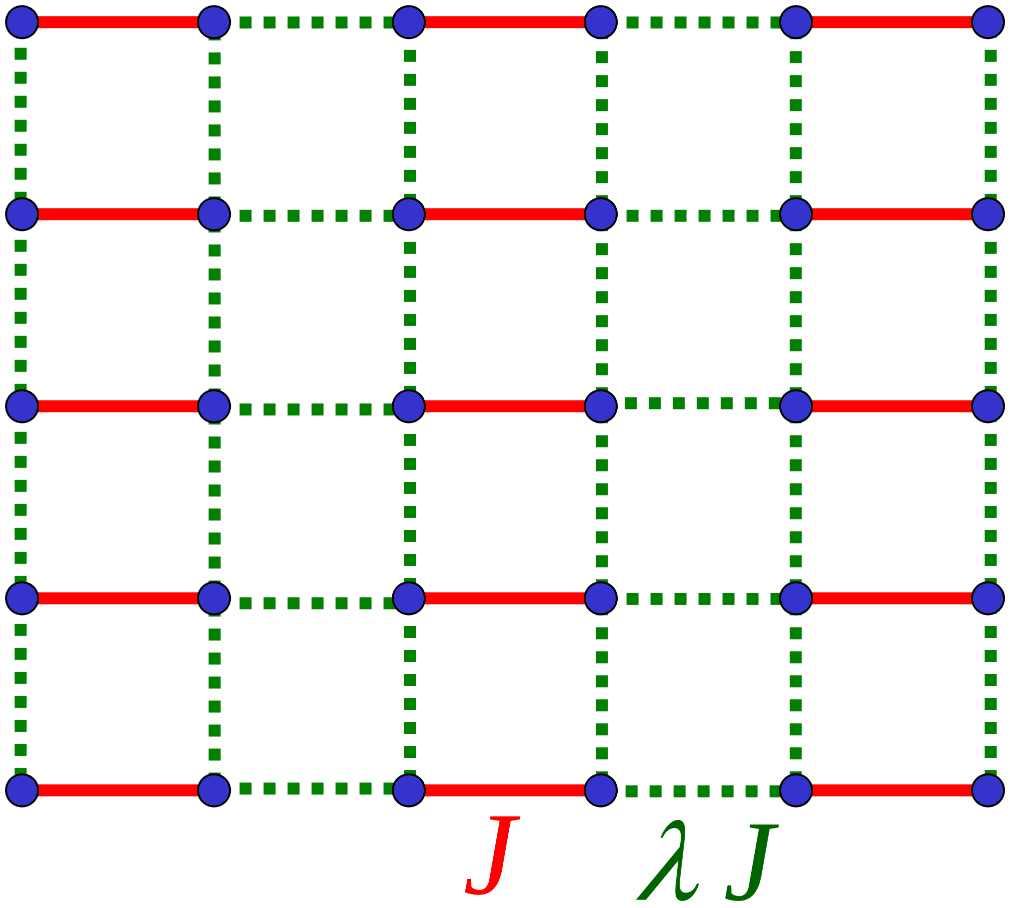


M. Matsumoto, B. Normand, T.M. Rice, and M. Sigrist, cond-mat/0309440.

Coupled Dimer Antiferromagnet

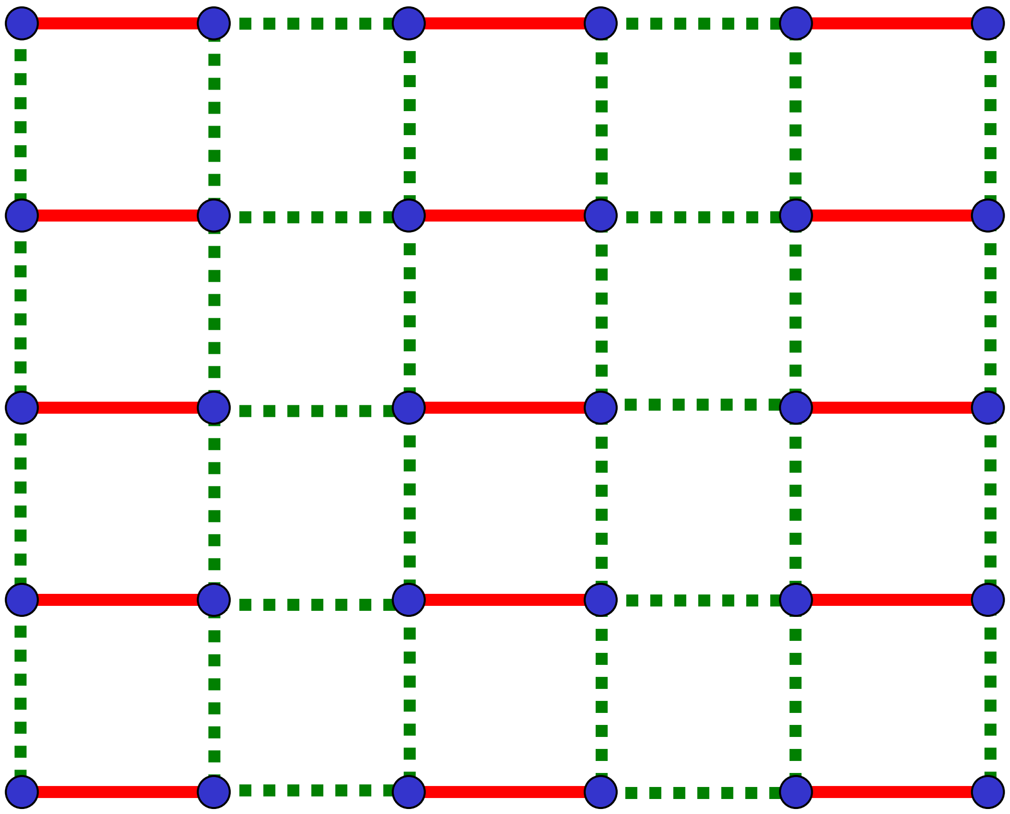
M. P. Gelfand, R. R. P. Singh, and D. A. Huse, *Phys. Rev. B* **40**, 10801-10809 (1989).
N. Katoh and M. Imada, *J. Phys. Soc. Jpn.* **63**, 4529 (1994).
J. Tworzydlo, O. Y. Osman, C. N. A. van Duin, J. Zaanen, *Phys. Rev.* B **59**, 115 (1999).
M. Matsumoto, C. Yasuda, S. Todo, and H. Takayama, *Phys. Rev.* B **65**, 014407 (2002).

S=1/2 spins on coupled dimers



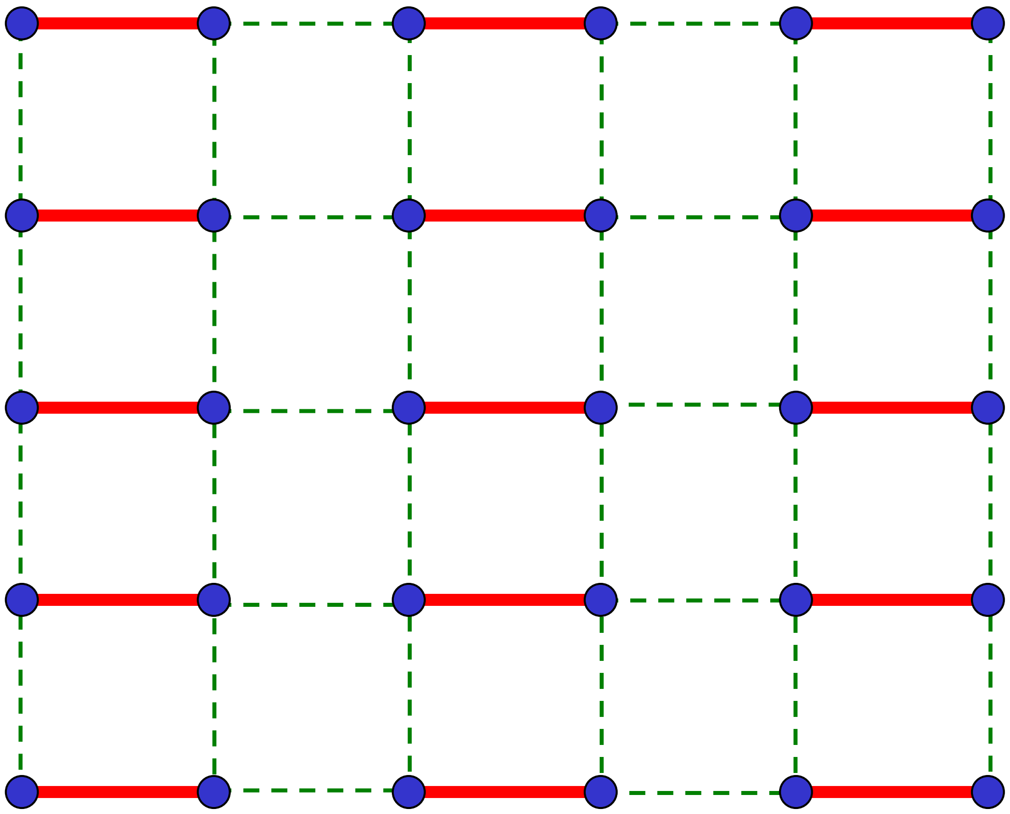
$$H = \sum_{<ij>} J_{ij} \vec{S}_i \cdot \vec{S}_j$$

$$0 \le \lambda \le 1$$



$\boxed{\lambda \text{ close to } 0}$

Weakly coupled dimers



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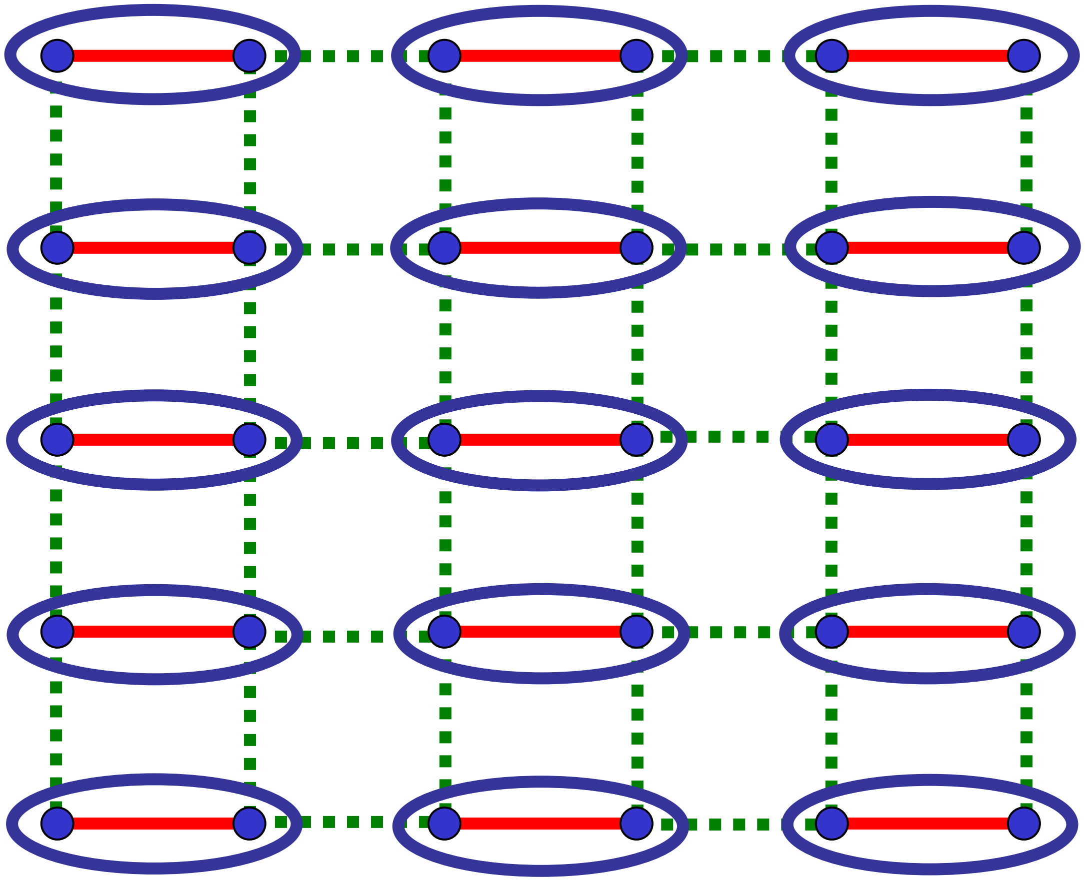
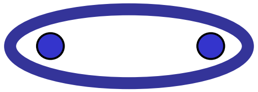
Weakly coupled dimers



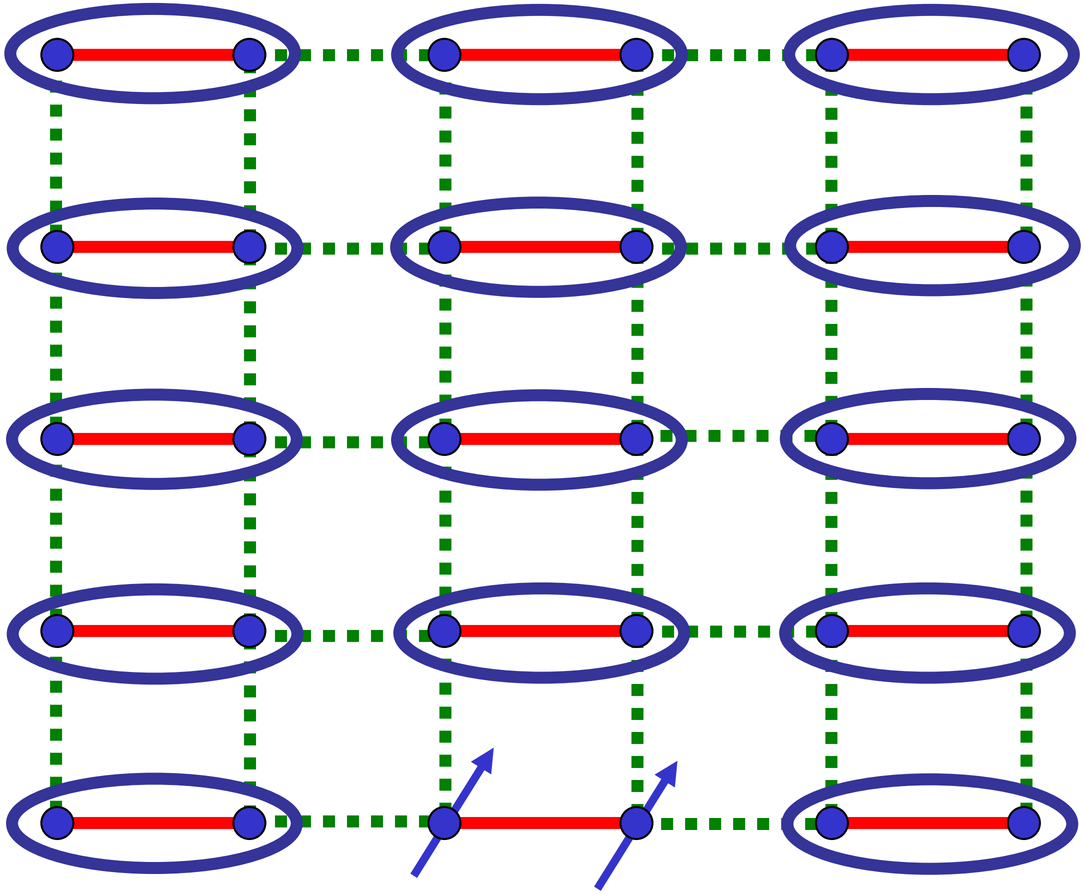
Paramagnetic ground state

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

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

$\boxed{\lambda \text{ close to } 0}$

Weakly coupled dimers

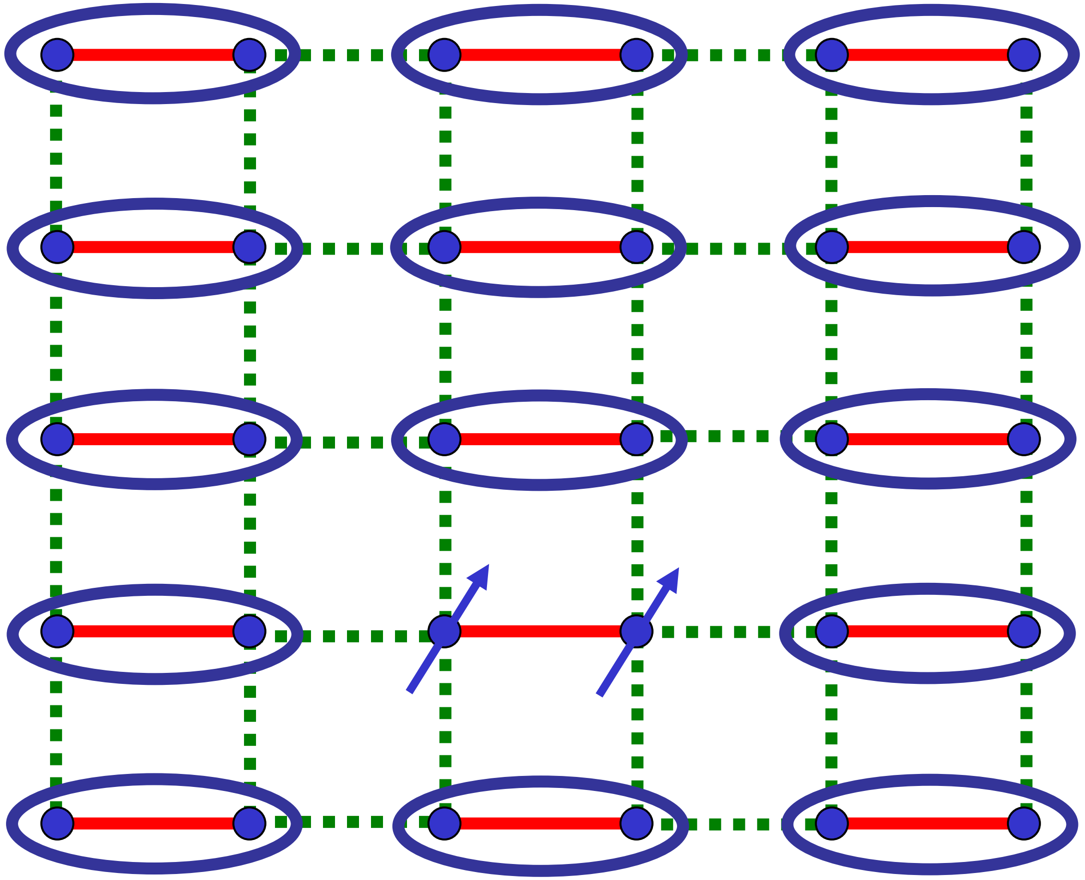


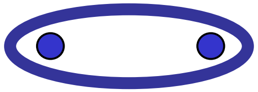
$$= \frac{1}{\sqrt{2}}\left(\left|\uparrow\downarrow\right\rangle - \left|\downarrow\uparrow\right\rangle\right)$$

Excitation:
S=1 quasipartcle

λ close to 0

Weakly coupled dimers



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

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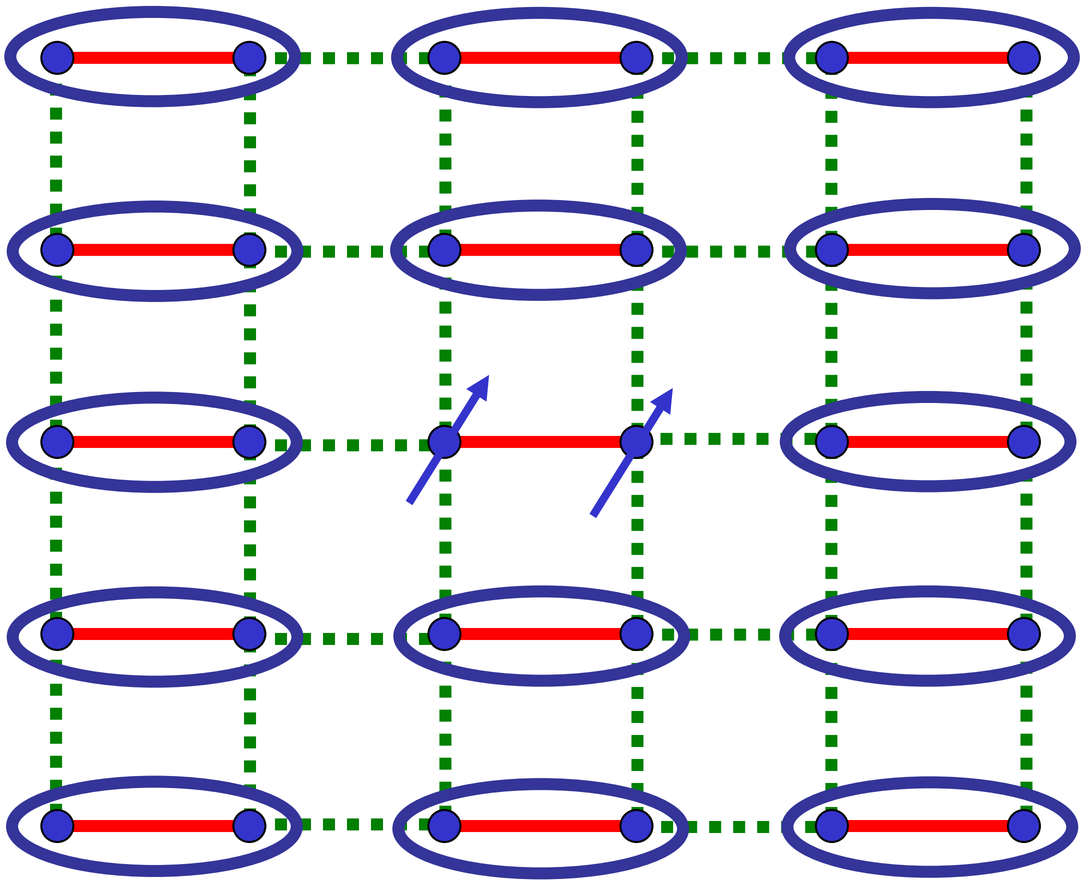

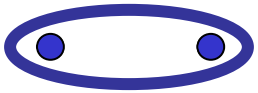 $= \frac{1}{\sqrt{2}}\left(\left|\uparrow\downarrow\right\rangle - \left|\downarrow\uparrow\right\rangle\right)$

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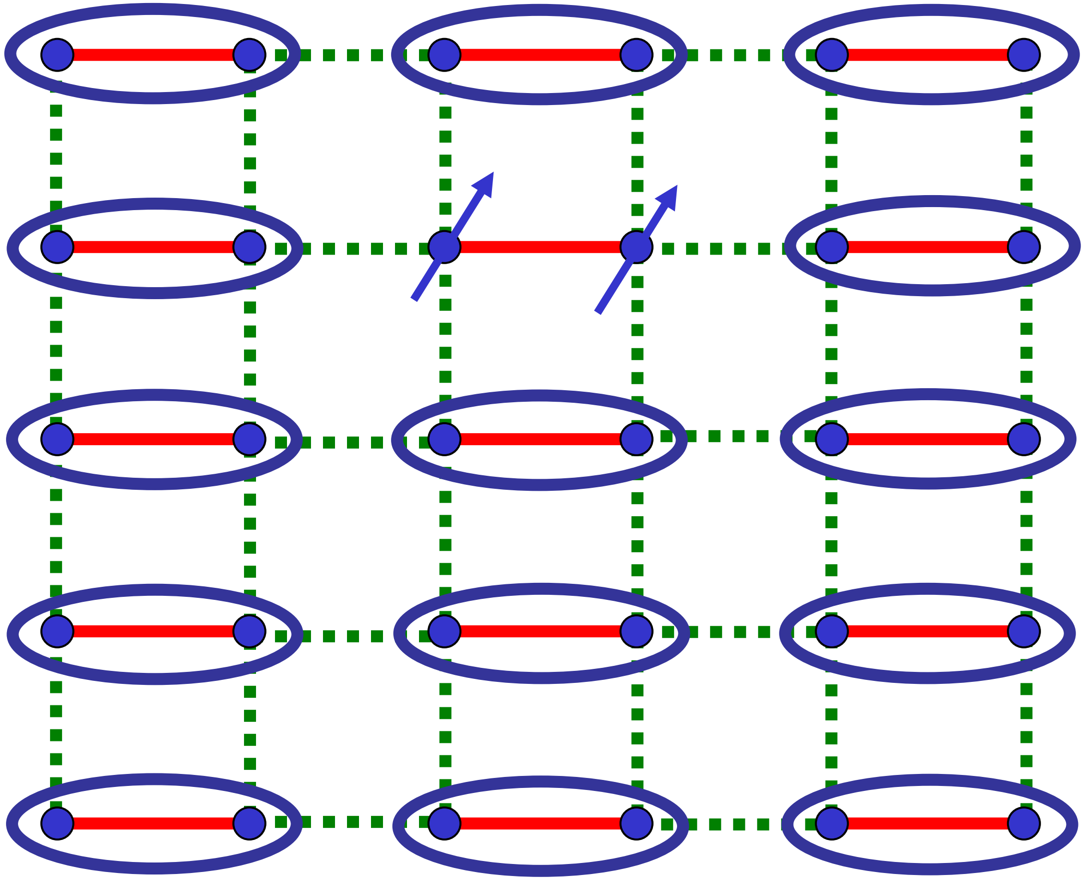

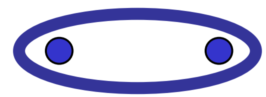 $= \frac{1}{\sqrt{2}}\left(\left|\uparrow\downarrow\right\rangle - \left|\downarrow\uparrow\right\rangle\right)$

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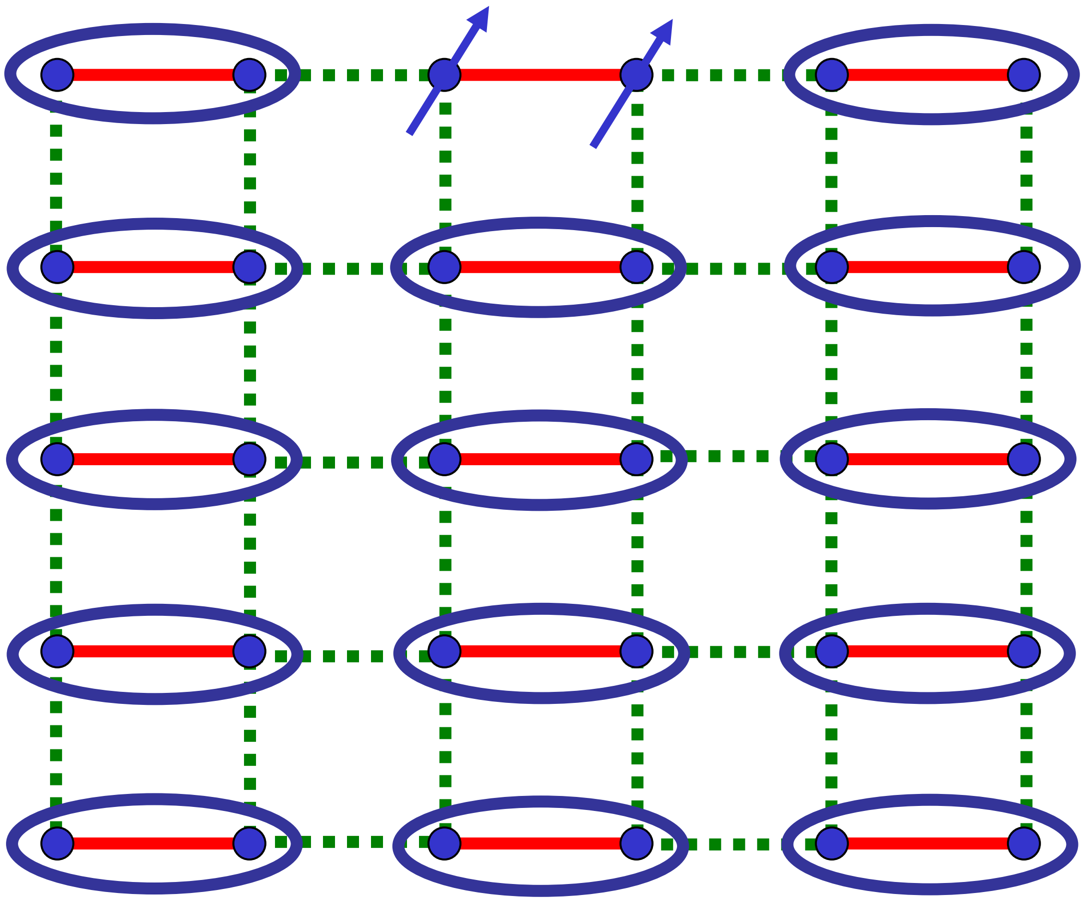

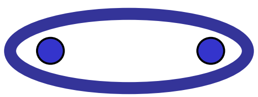 $= \frac{1}{\sqrt{2}}\left(\left|\uparrow\downarrow\right\rangle - \left|\downarrow\uparrow\right\rangle\right)$

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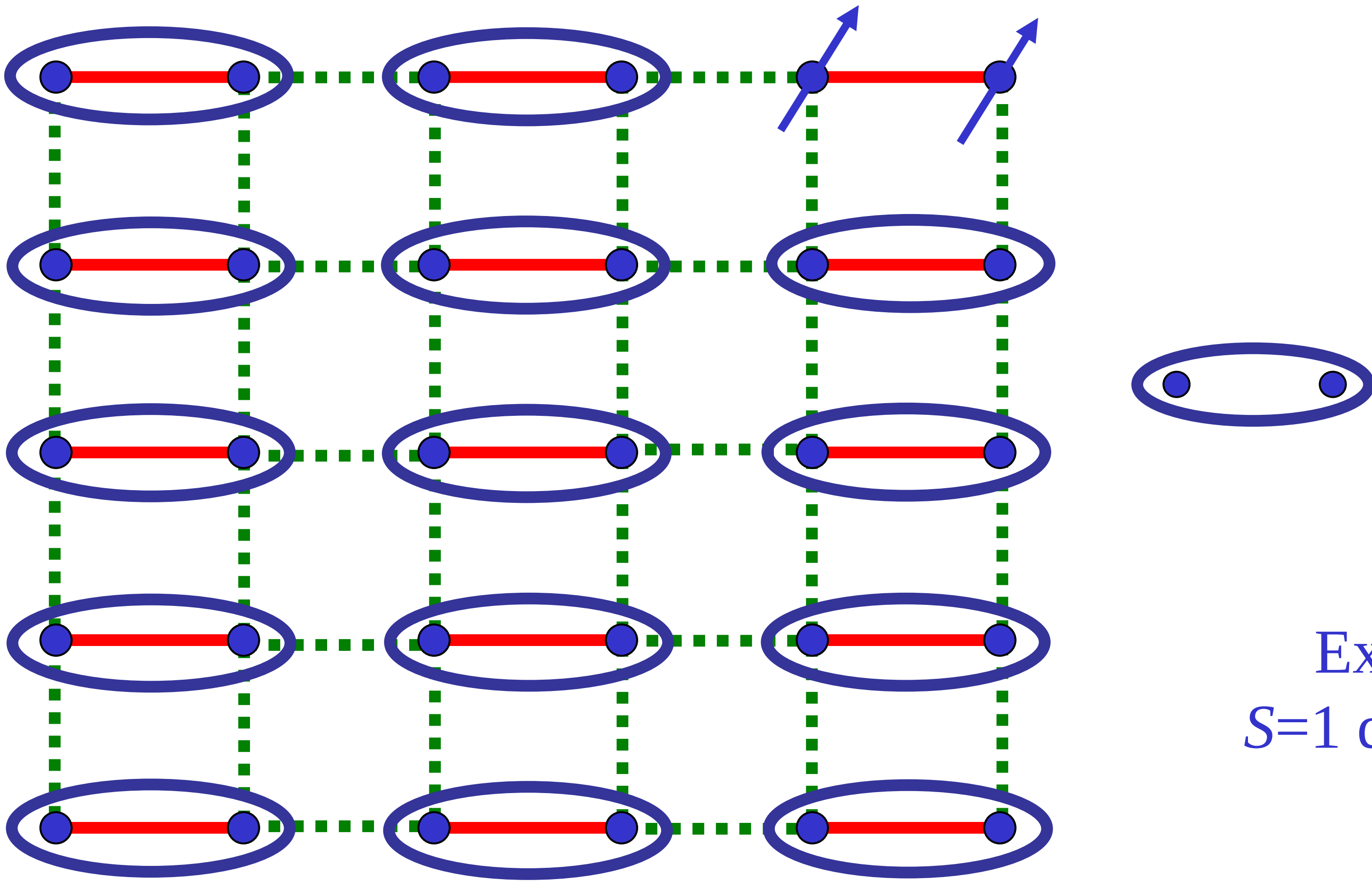

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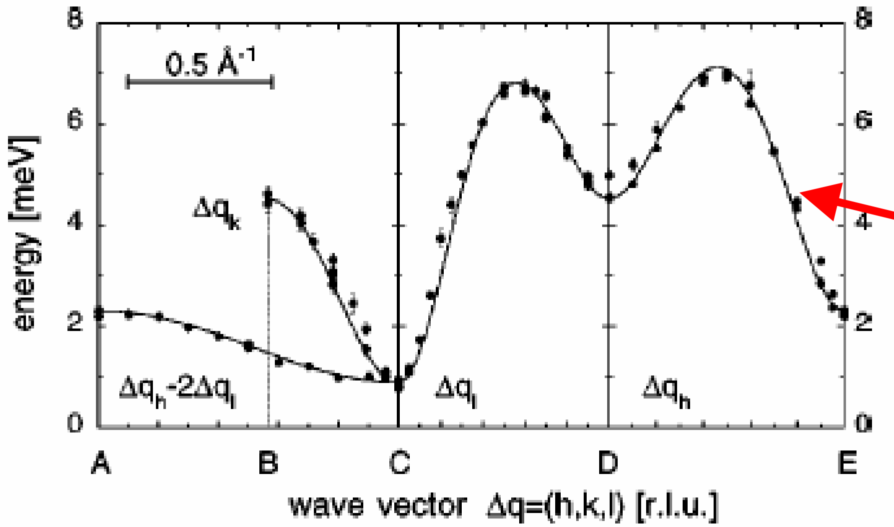
S=1 quasipartcle

Energy dispersion away from antiferromagnetic wavevector

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

$\Delta \to$ spin gap

$TlCuCl_3$



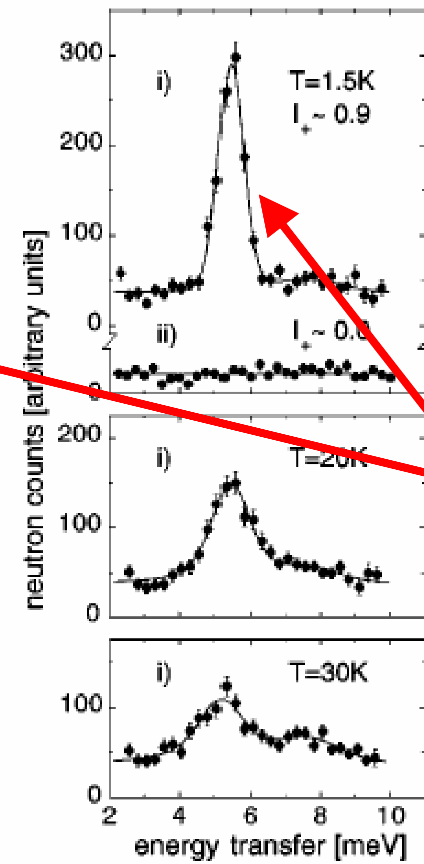
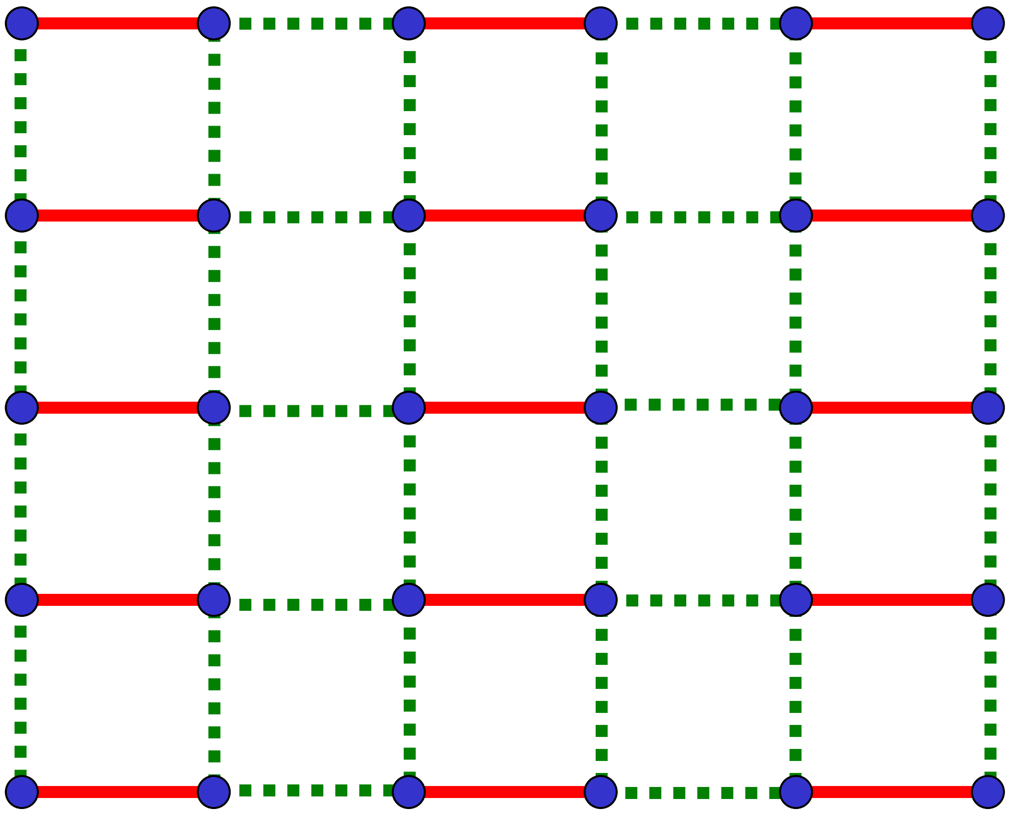


FIG. 1. Measured neutron profiles in the a^*c^* plane of $TlCuCl_3$ for $i=(1.35,0,0)$, $ii=(0,0,3.15)$ [r.l.u]. The spectrum at $T=1.5$ K

S=1 quasi-particle

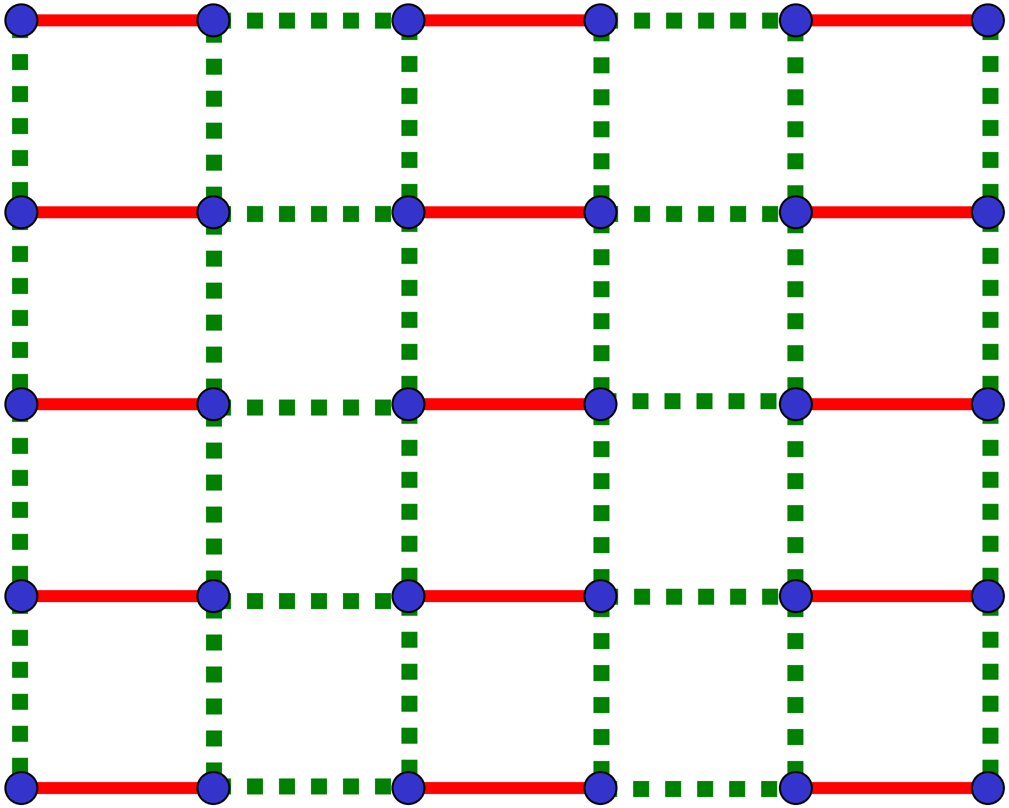
N. Cavadini, G. Heigold, W. Henggeler, A. Furrer, H.-U. Güdel, K. Krämer and H. Mutka, *Phys. Rev.* B 63 172414 (2001).

Coupled Dimer Antiferromagnet



λ close to 1

Weakly dimerized square lattice



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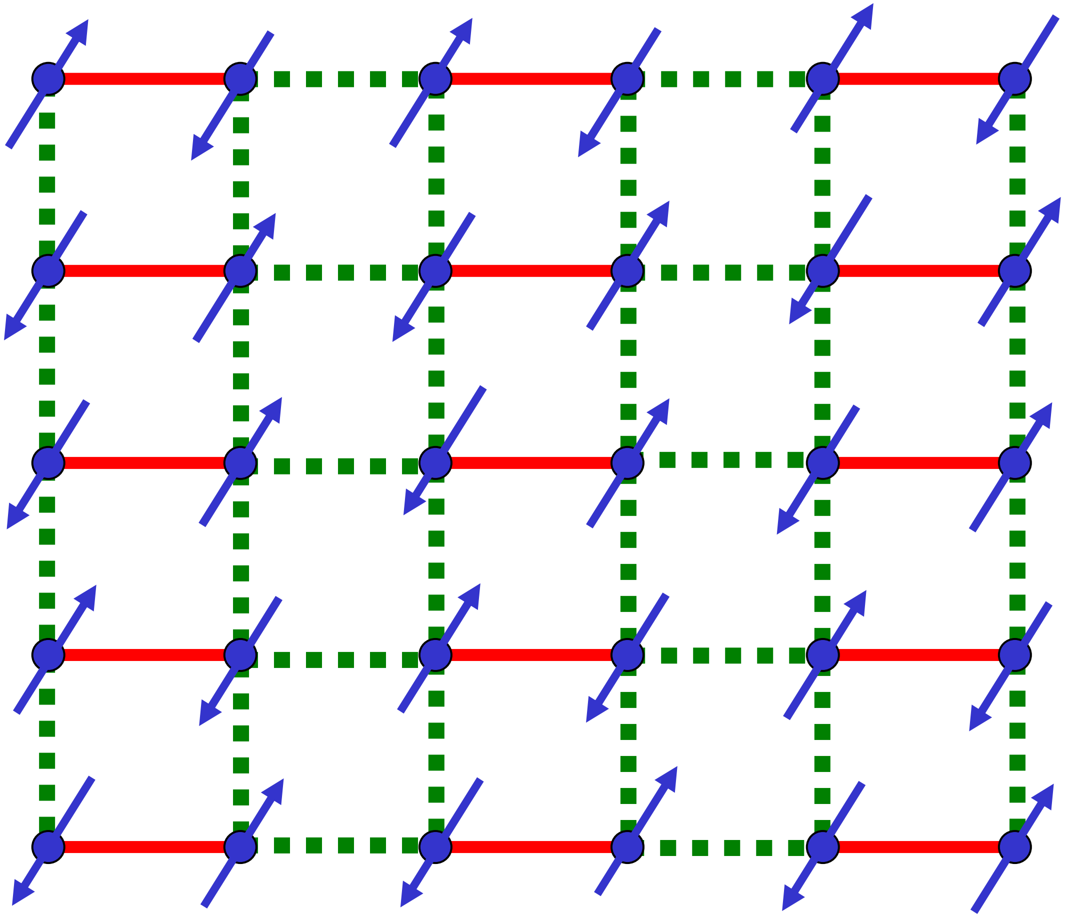


Excitations:
2 spin waves (***magnons***)

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

Ground state has long-range spin density wave (Néel) order at wavevector ***K***= (π,π)

$$\boxed{\left\langle \vec{\varphi} \right\rangle \neq 0}$$

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

$TlCuCl_3$

Neutron Diffraction Study of the Pressure-Induced Magnetic Ordering in the Spin Gap System $TlCuCl_3$

Akira OOSAWA*, Masashi FUJISAWA[1], Toyotaka OSAKABE, Kazuhisa KAKURAI and Hidekazu TANAKA[2]

Advanced Science Research Center, Japan Atomic Energy Research Institute, Tokai, Ibaraki 319-1195
[1]*Department of Physics, Tokyo Institute of Technology, Oh-okayama, Meguro-ku, Tokyo 152-8551*
[2]*Research Center for Low Temperature Physics, Tokyo Institute of Technology, Oh-okayama, Meguro-ku, Tokyo 152-8551*

(Received February 3, 2003)

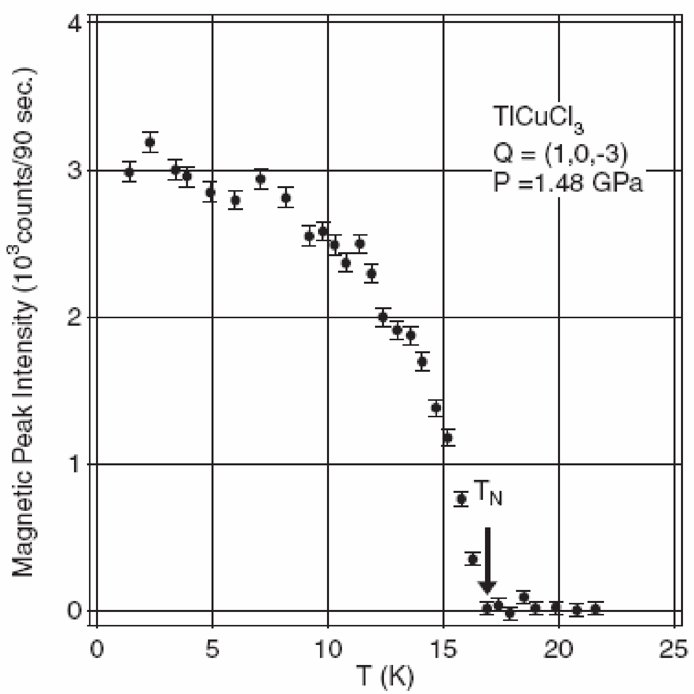


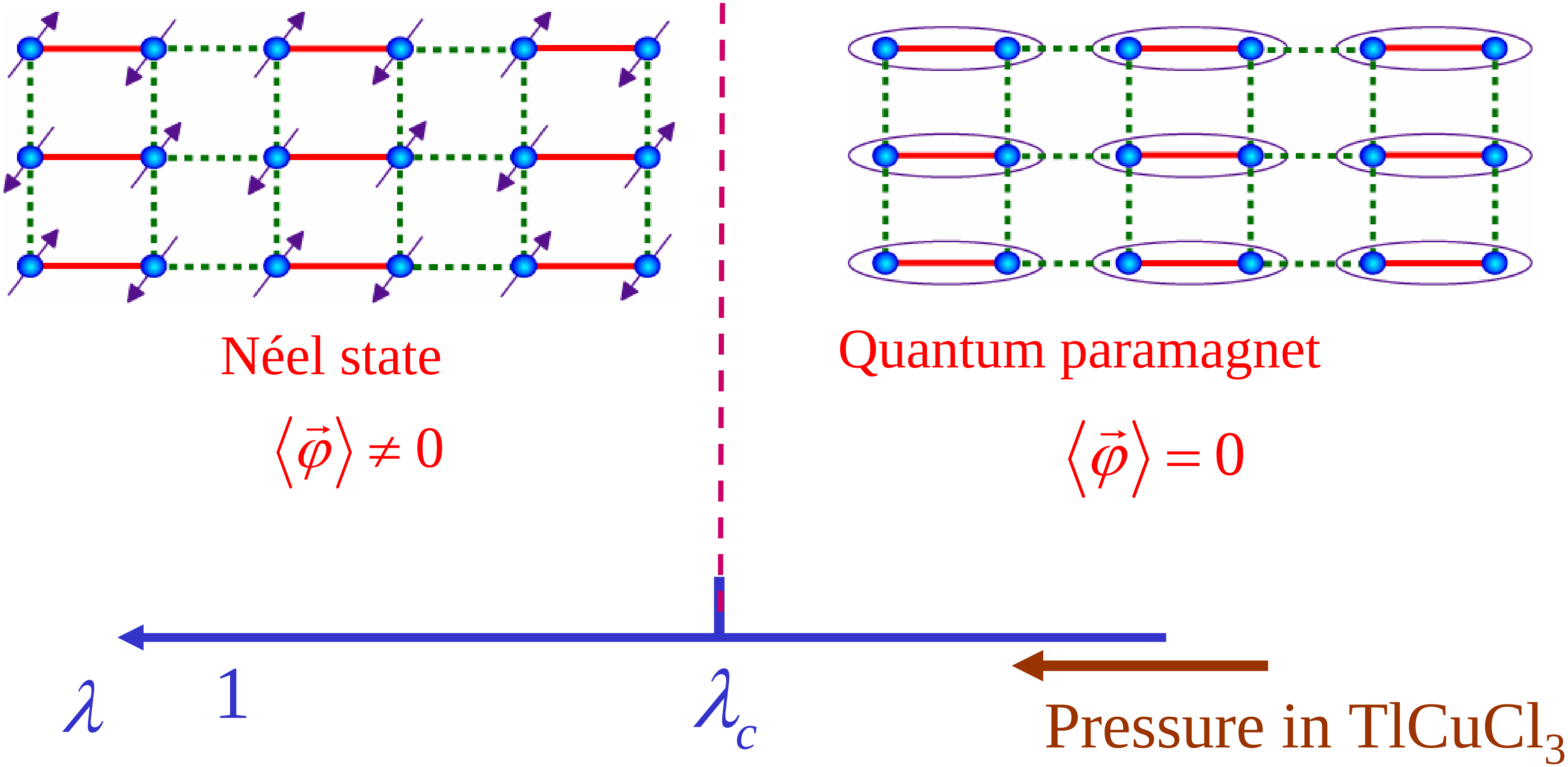
Fig. 3. Temperature dependence of the magnetic Bragg peak intensity for $Q = (1, 0, -3)$ reflection measured at $P = 1.48$ GPa in $TlCuCl_3$.

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

T=0

$\lambda_c = 0.52337(3)$

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



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 $TlCuCl_3$ across the quantum phase transition (M. Matsumoto, B. Normand, T.M. Rice, and M. Sigrist, *Phys. Rev. Lett.* **89**, 077203 (2002))

LGW theory for quantum criticality

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

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

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

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

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

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

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   A. Breakdown of LGW theory
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   C. Spinor formulation and deconfined criticality

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

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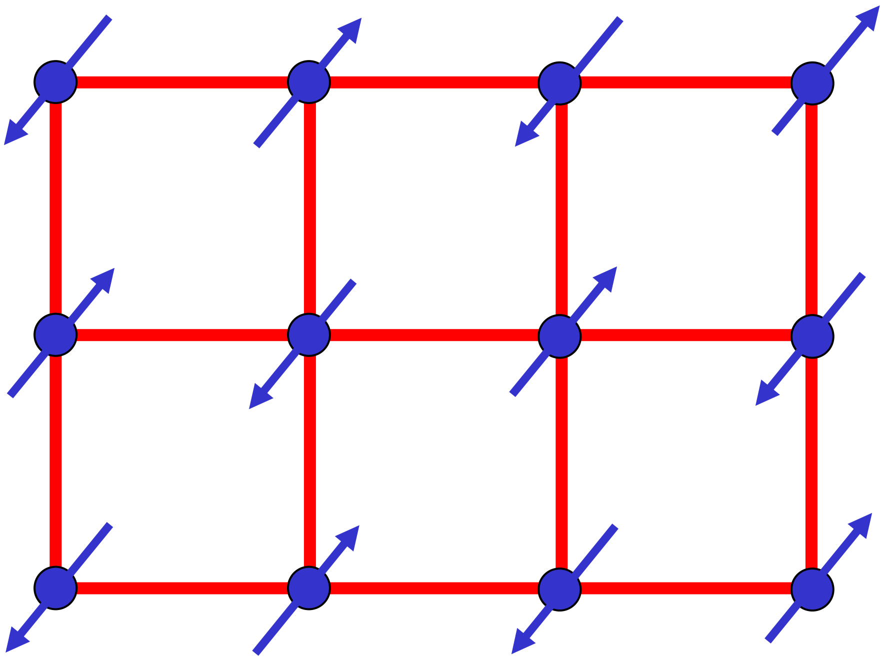
Square lattice antiferromagnet

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



Ground state has long-range Néel order

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

$\eta_i = \pm 1$ on two sublattices

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

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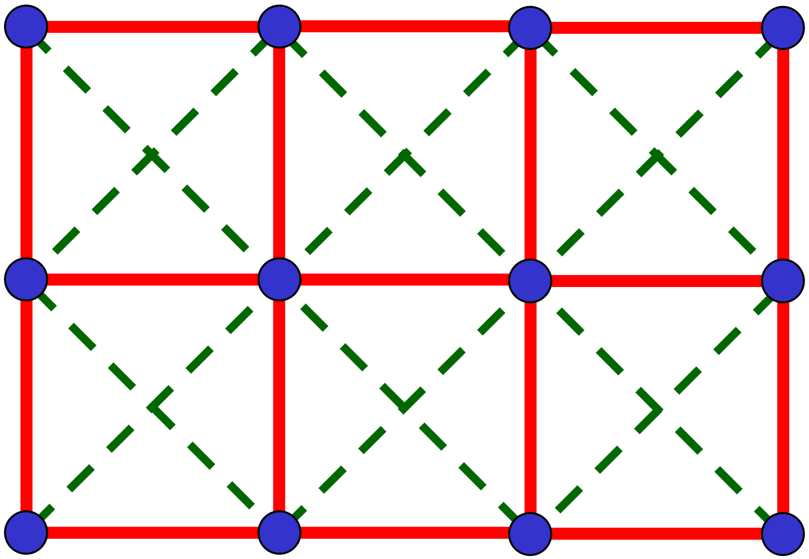

Destroy Neel order by perturbations which preserve full square lattice symmetry *e.g.* second-neighbor or ring exchange.

$$\boxed{\text{What is the state with } \langle \vec{\varphi} \rangle = 0 \text{ ?}}$$

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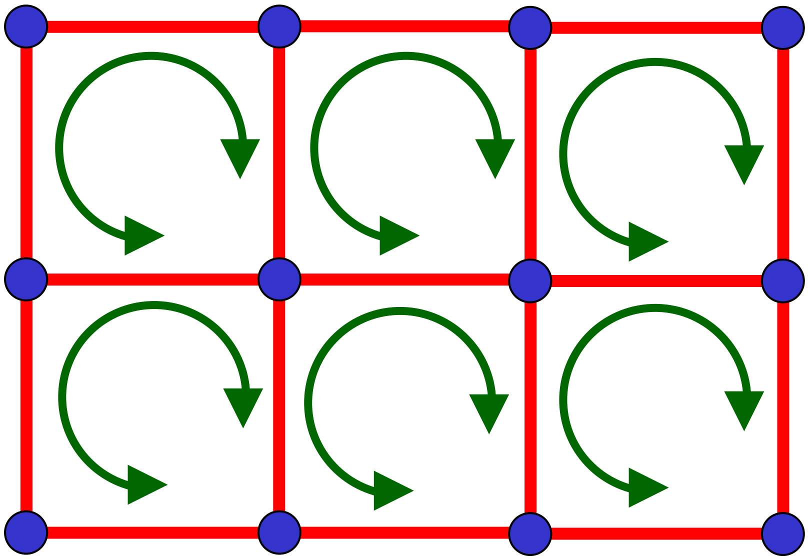

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$$S_\varphi = \int d^2x d\tau \left[\frac{1}{2} \left(\left(\nabla_x \vec{\varphi} \right)^2 + c^2 \left(\partial_\tau \vec{\varphi} \right)^2 + r \vec{\varphi}^2 \right) + \frac{u}{4!} \left(\vec{\varphi}^2 \right)^2 \right]$$

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

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

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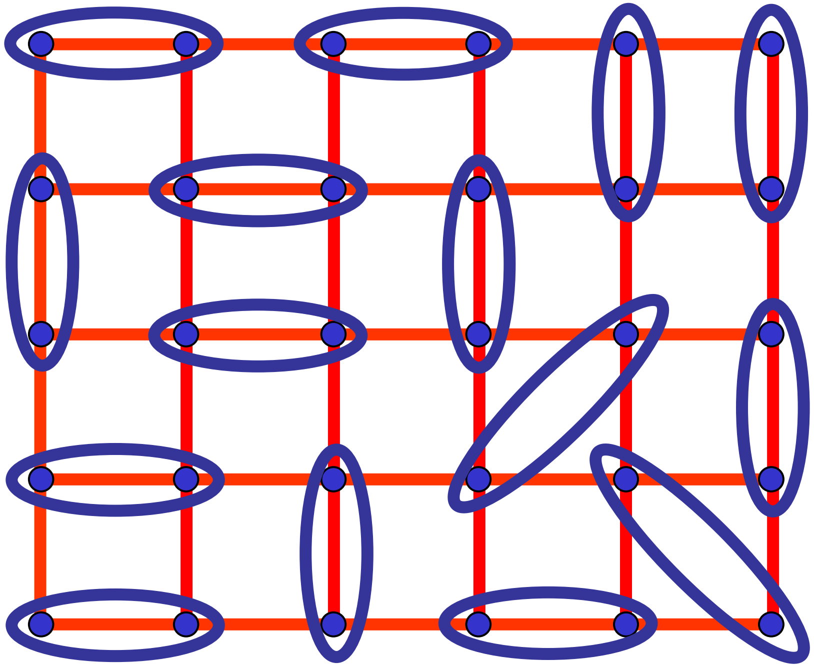

"Liquid" of valence bonds has fractionalized *S=1/2* excitations

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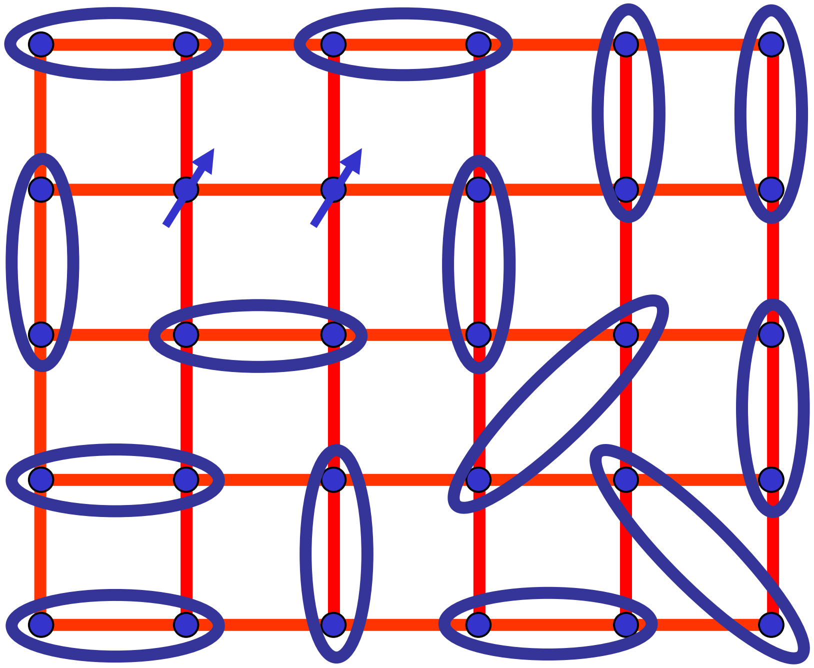

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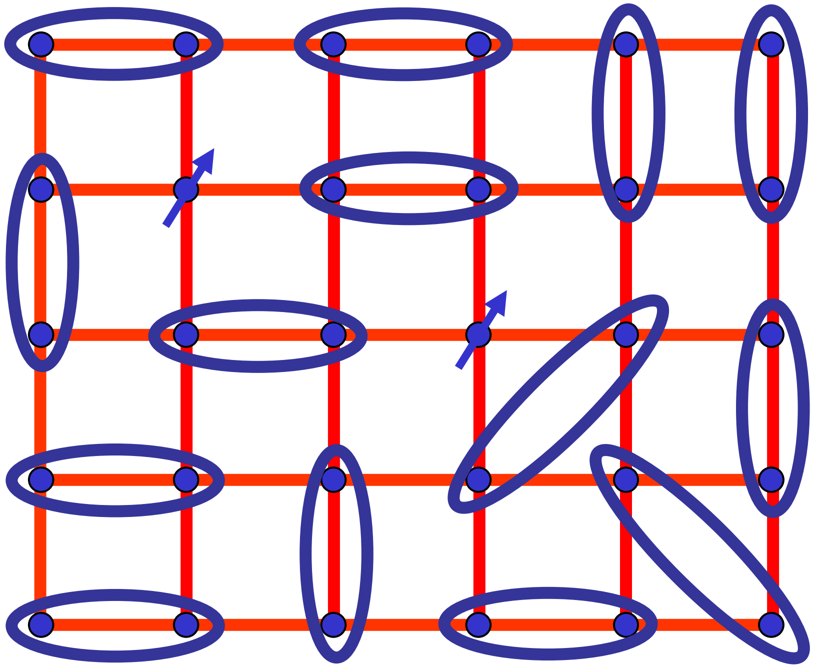

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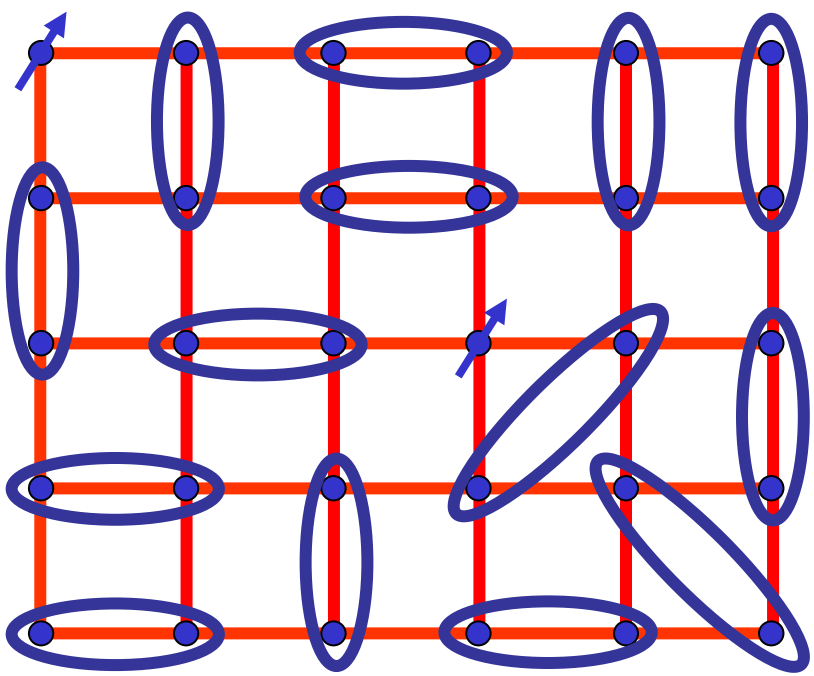

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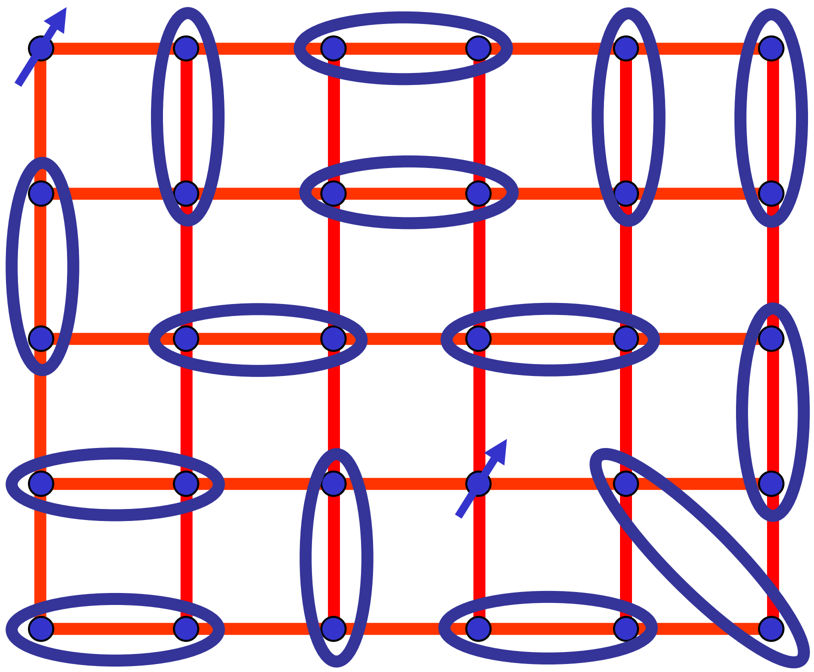

"Liquid" of valence bonds has fractionalized $S=1/2$ excitations

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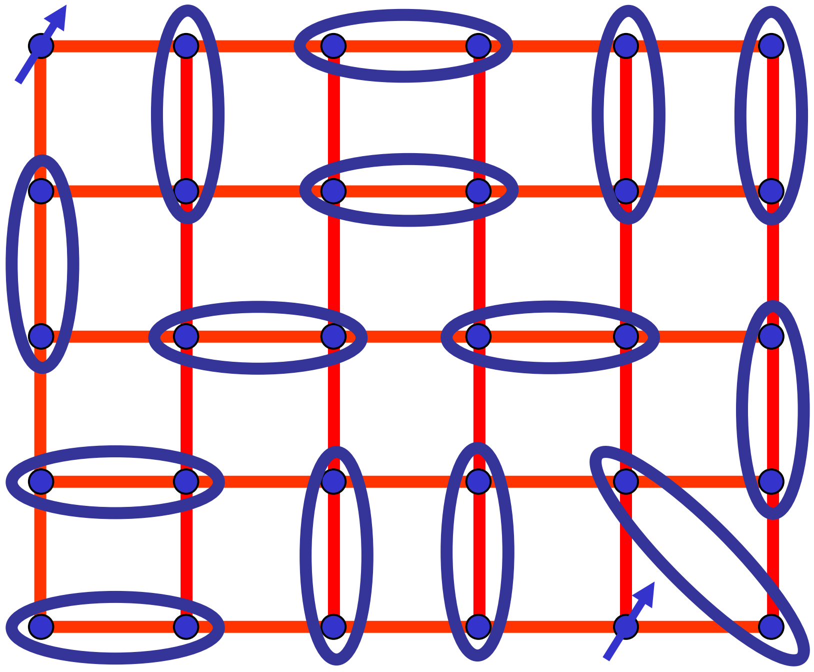
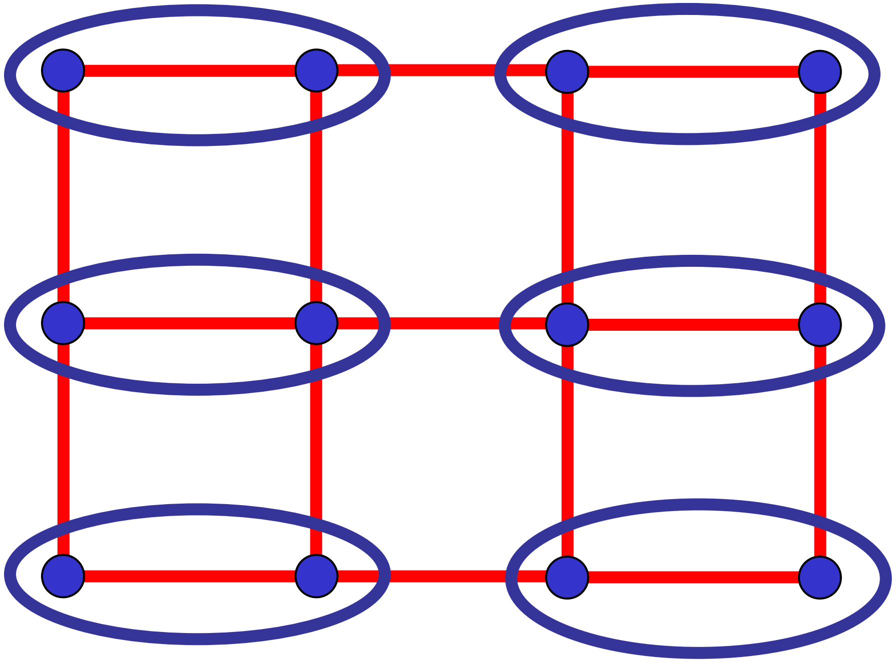


"Liquid" of valence bonds has fractionalized *S=1/2* excitations

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



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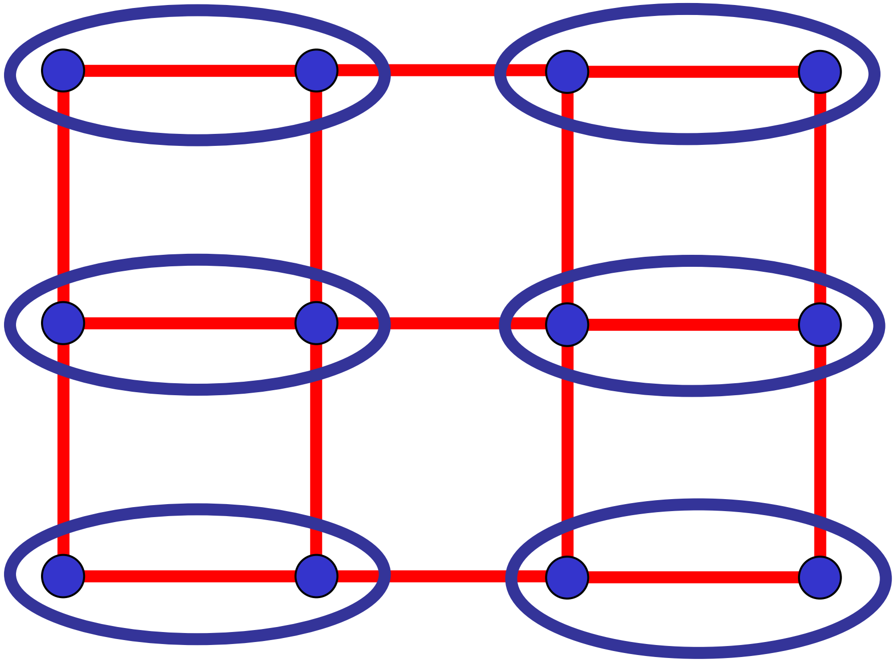

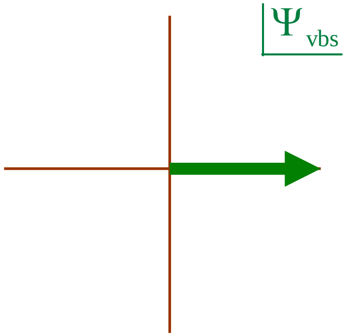

Such a state breaks the symmetry of rotations by $n\pi/2$ about lattice sites, and has $\langle \Psi_{\text{vbs}} \rangle \neq 0$, where Ψ_{vbs} is the ***VBS order parameter***

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

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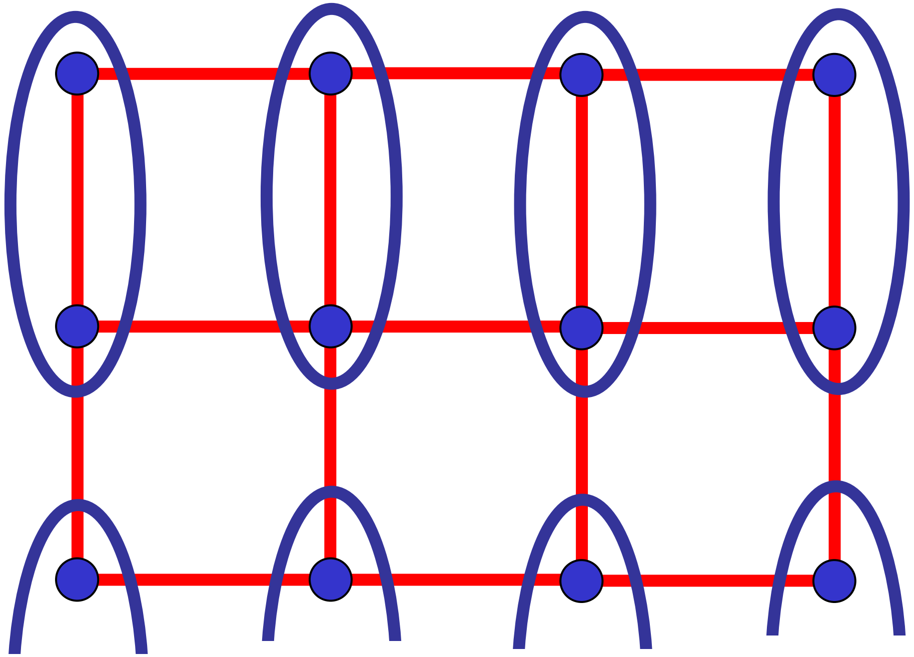

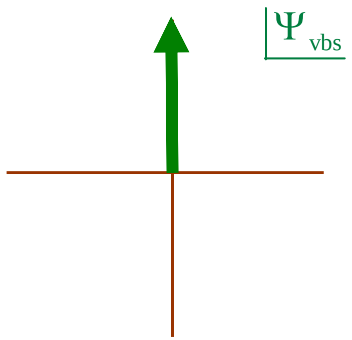

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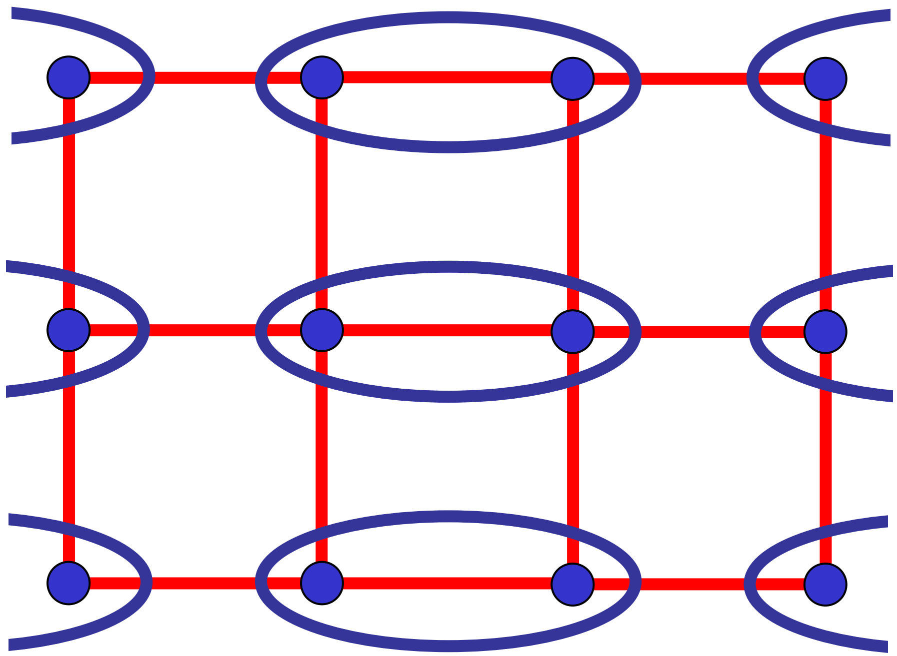

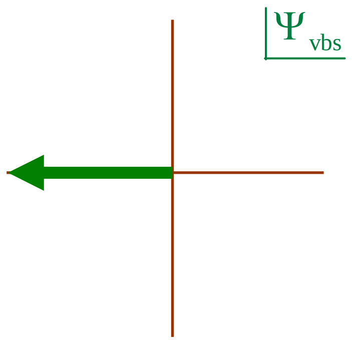

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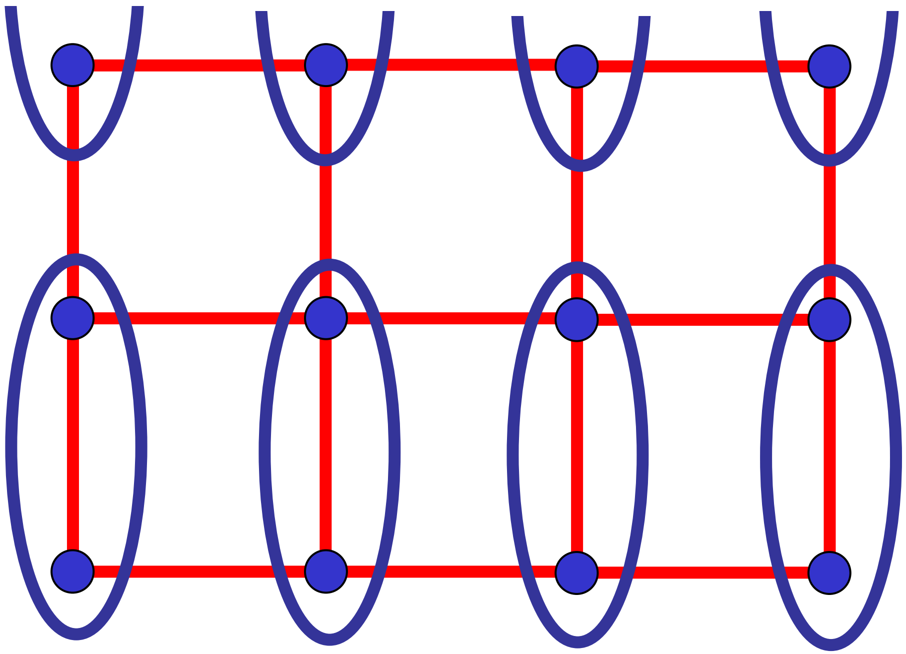

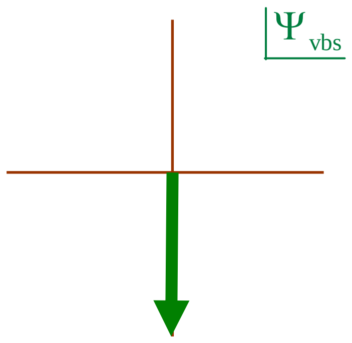

Such a state breaks the symmetry of rotations by $n\pi/2$ about lattice sites, and has $\langle \Psi_{\text{vbs}} \rangle \neq 0$, where Ψ_{vbs} is the ***VBS order parameter***

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

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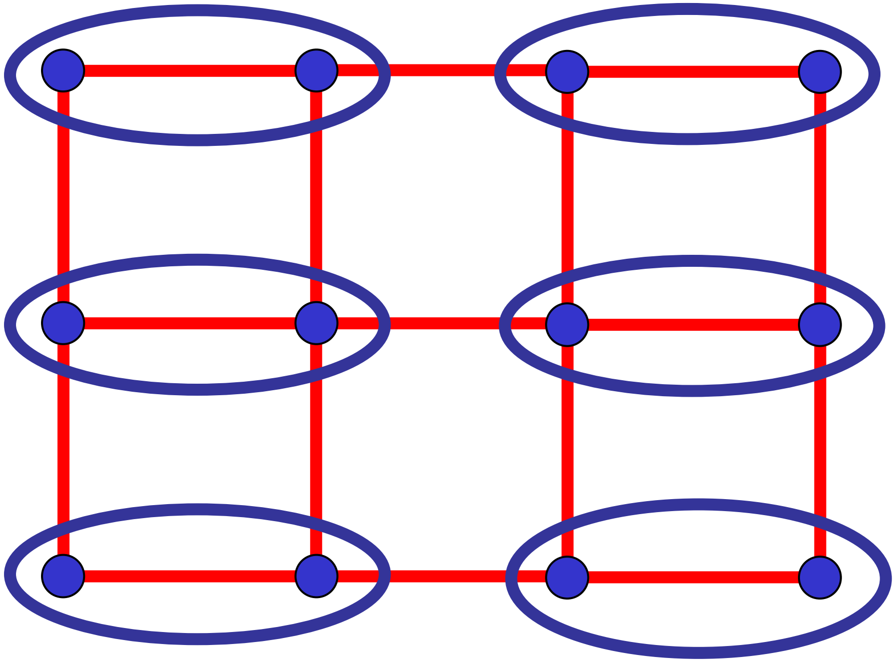

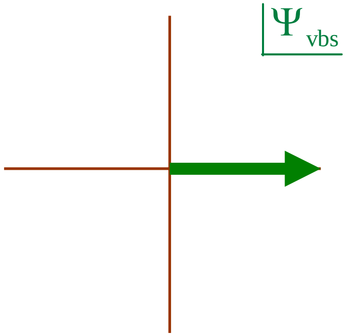

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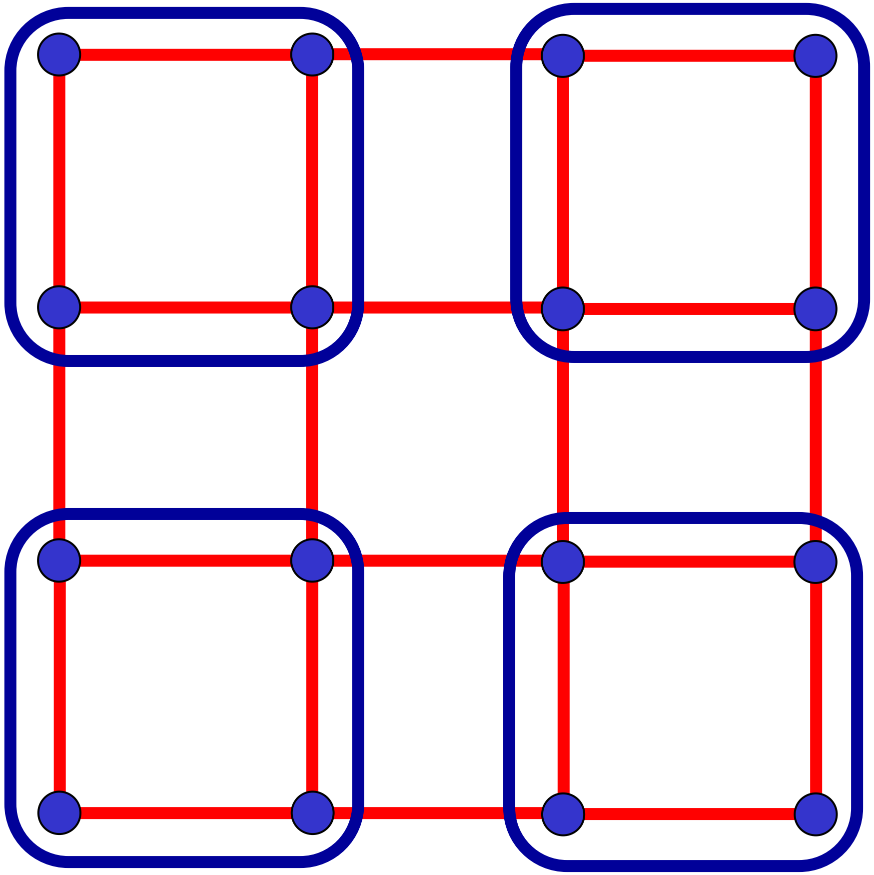

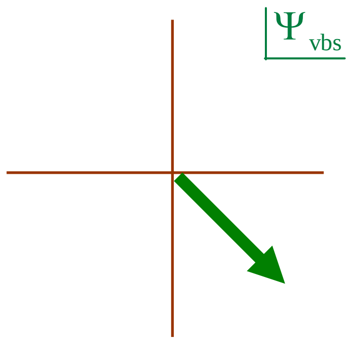

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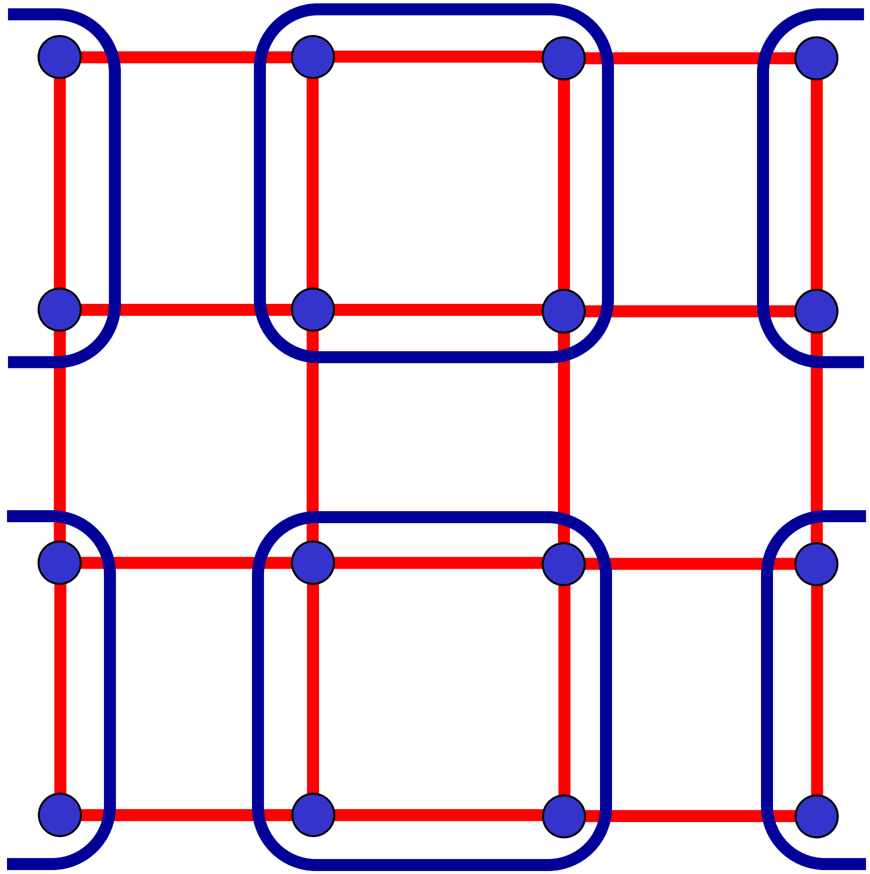

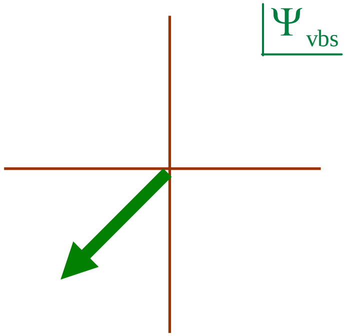

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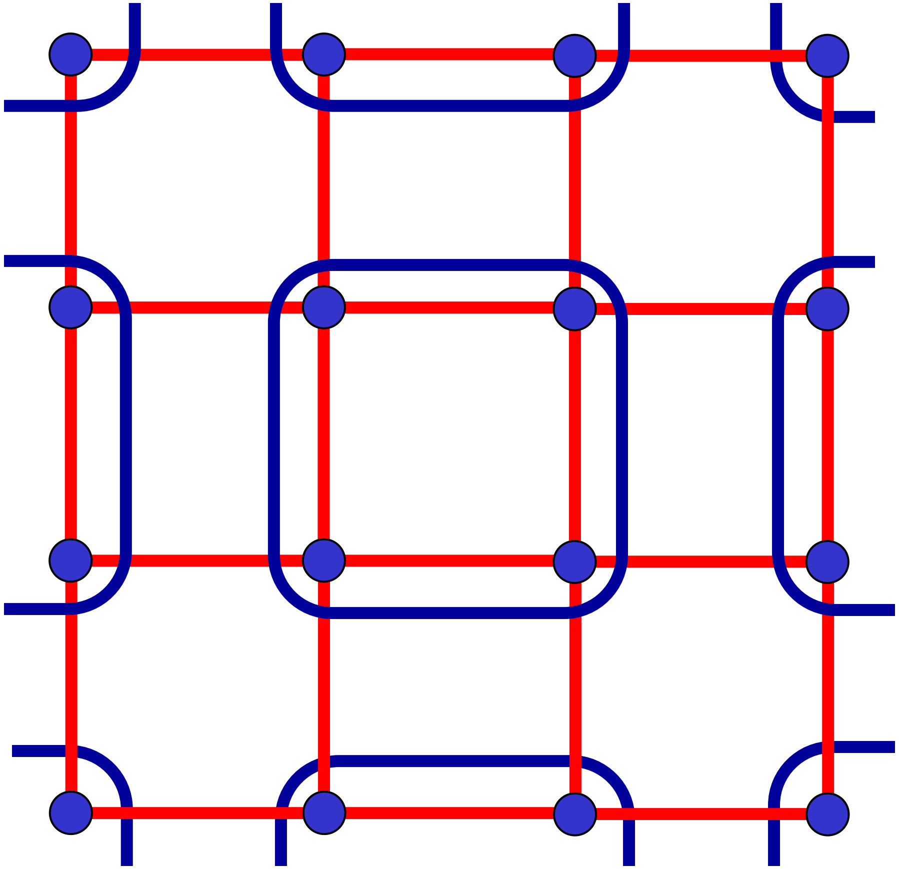

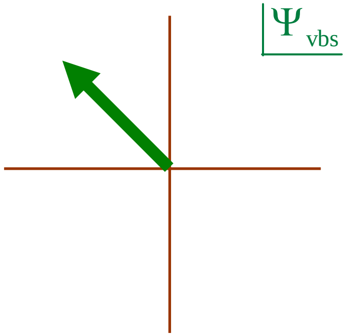

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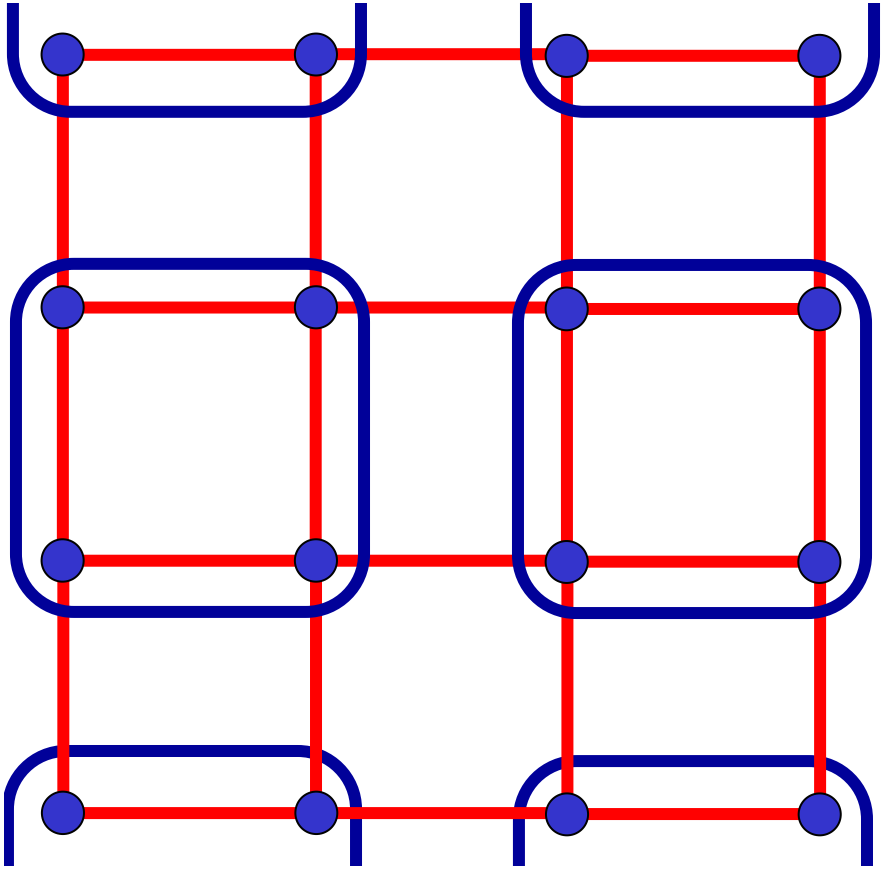

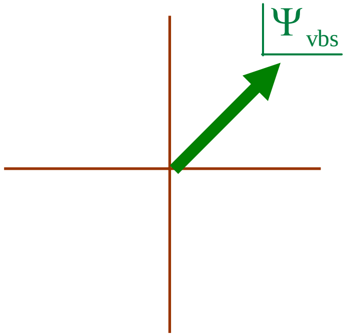

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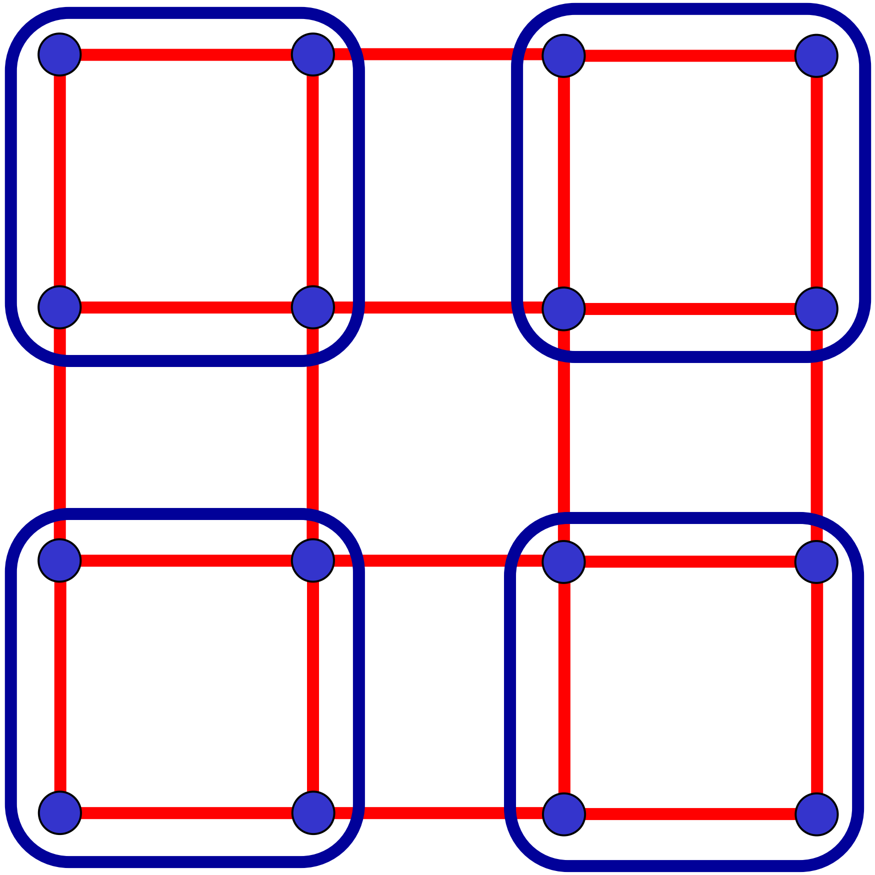

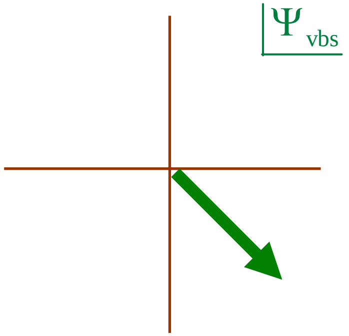

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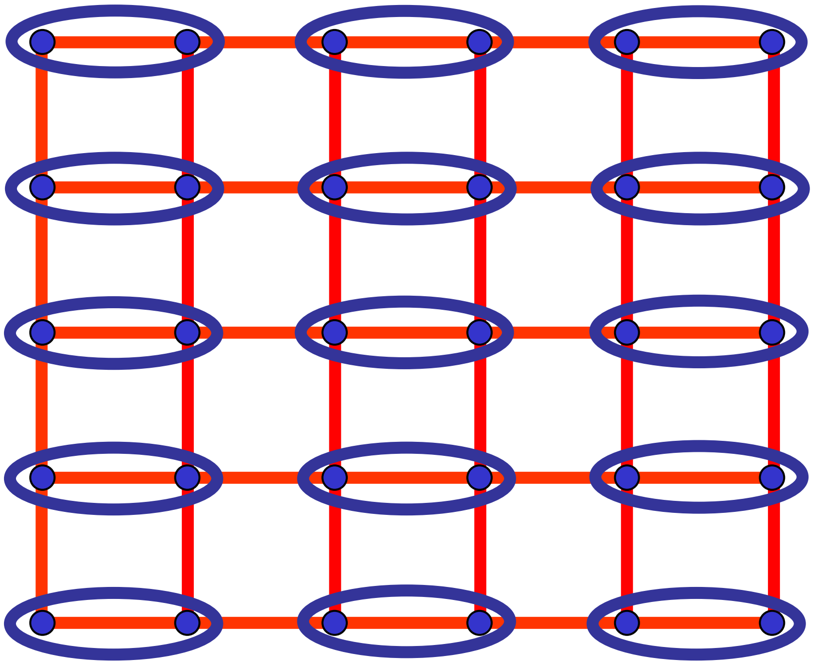

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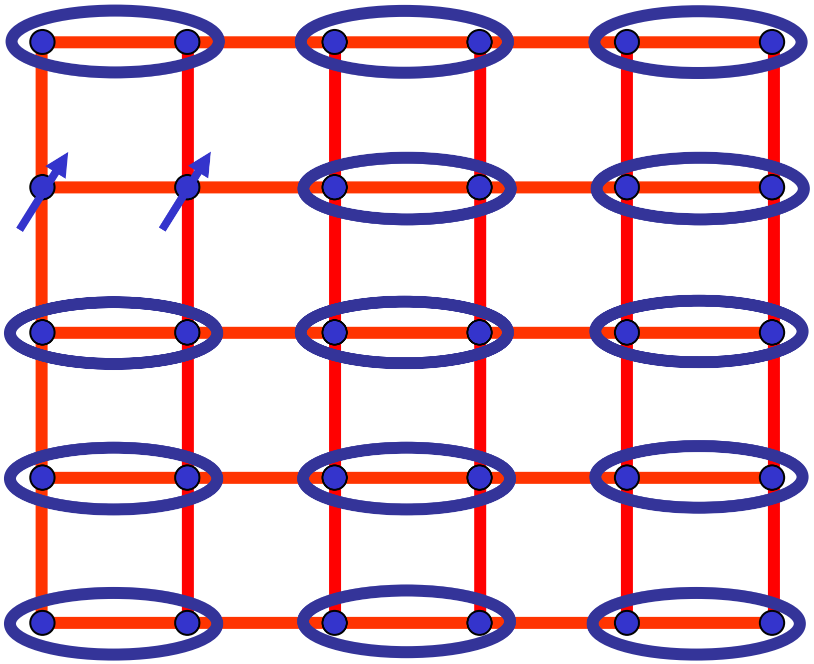

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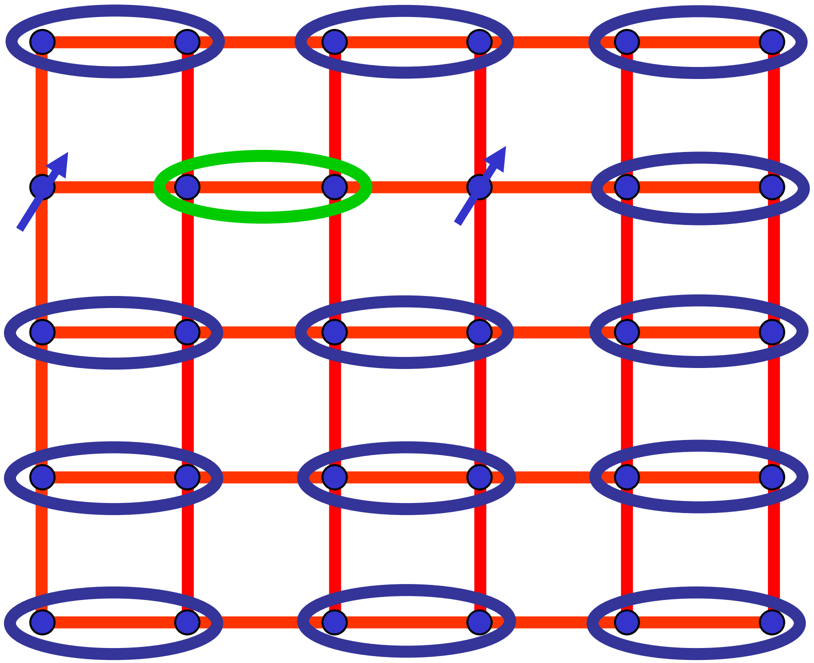

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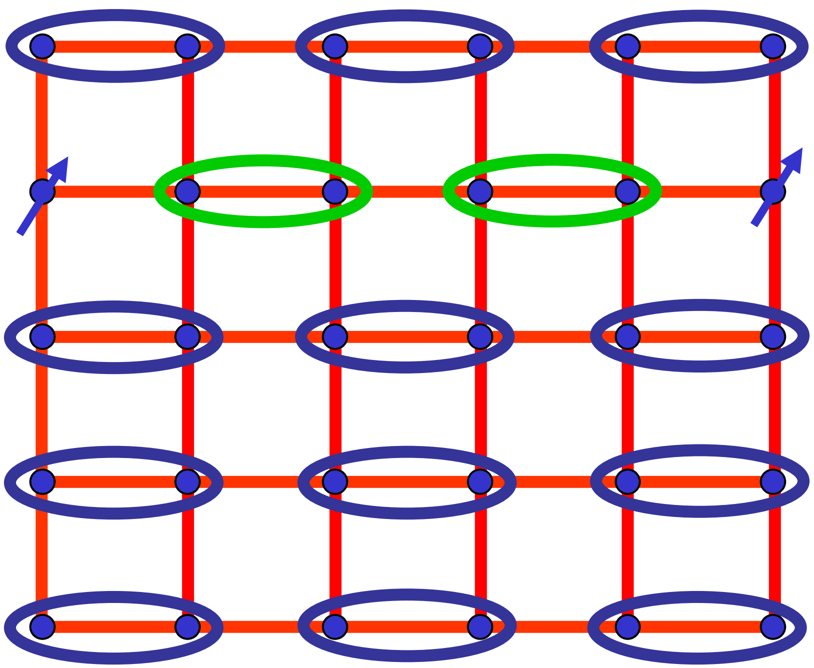

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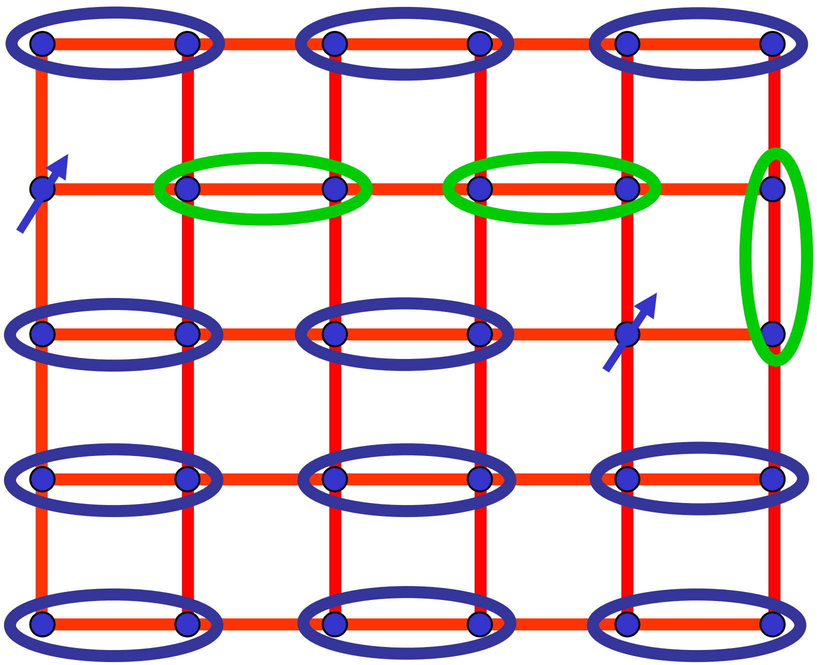

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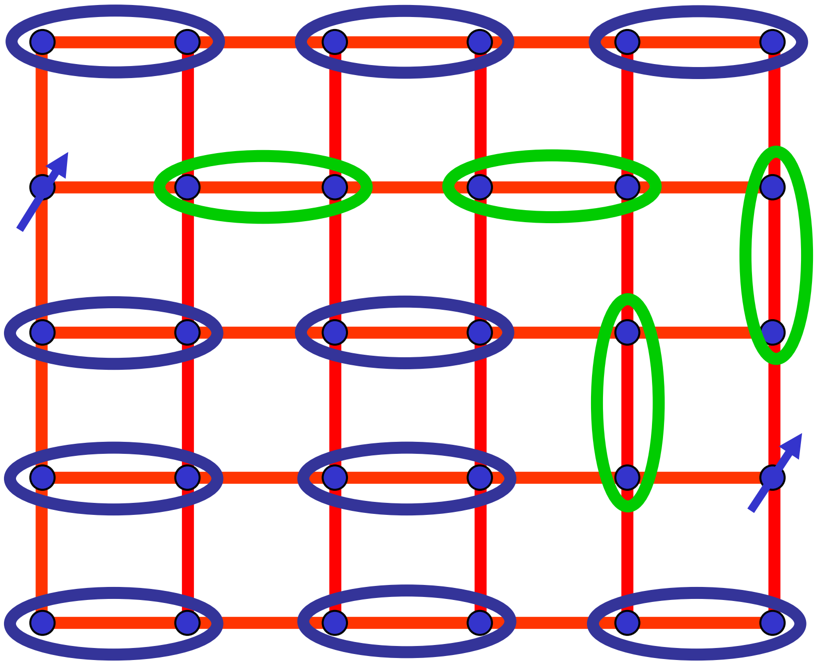


LGW theory of multiple order parameters

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

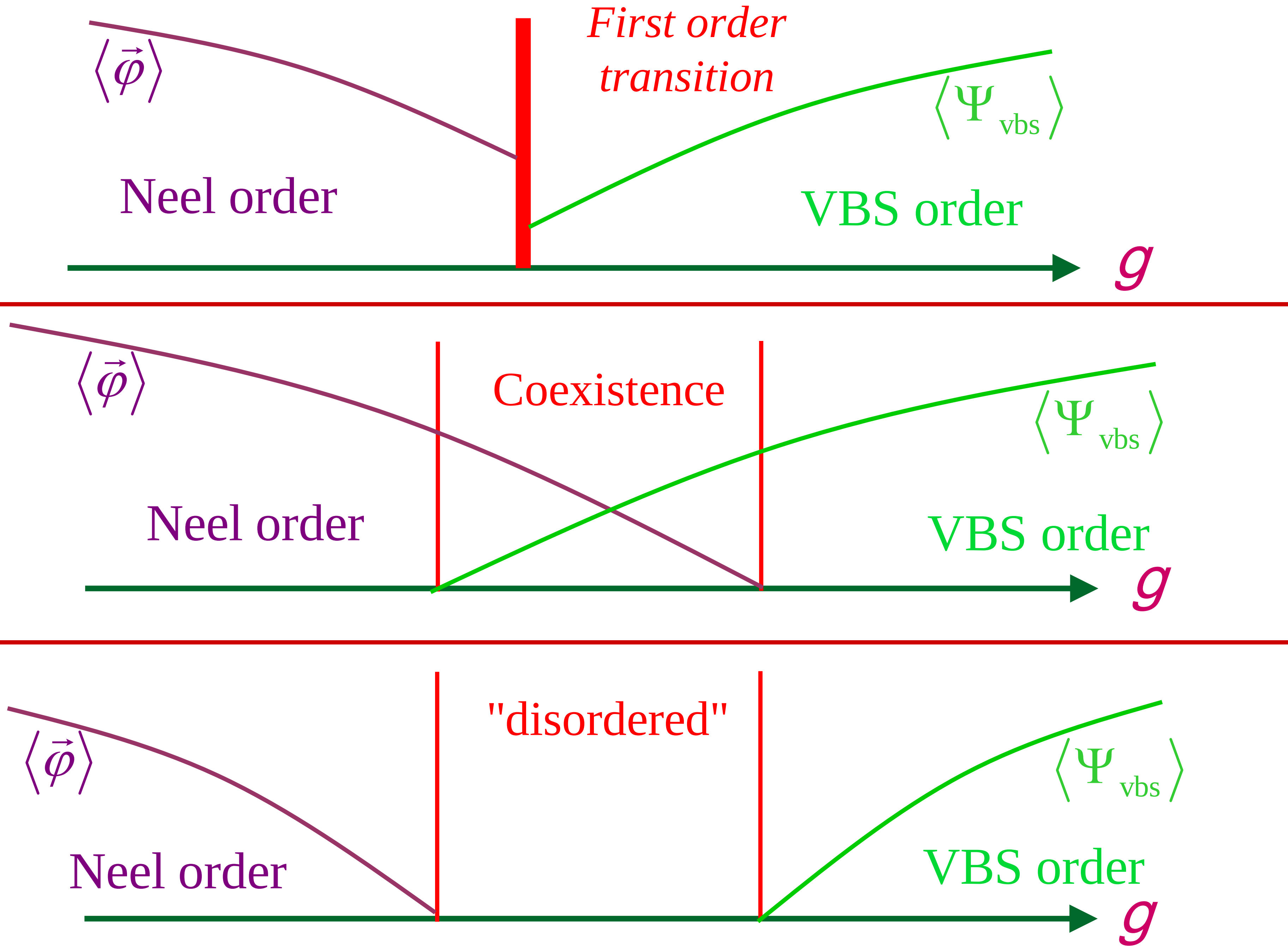
$$F_{\text{vbs}}\left[\Psi_{\text{vbs}}\right] = r_1 \left|\Psi_{\text{vbs}}\right|^2 + u_1 \left|\Psi_{\text{vbs}}\right|^4 + \cdots$$

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

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

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

<u>LGW theory of multiple order parameters</u>



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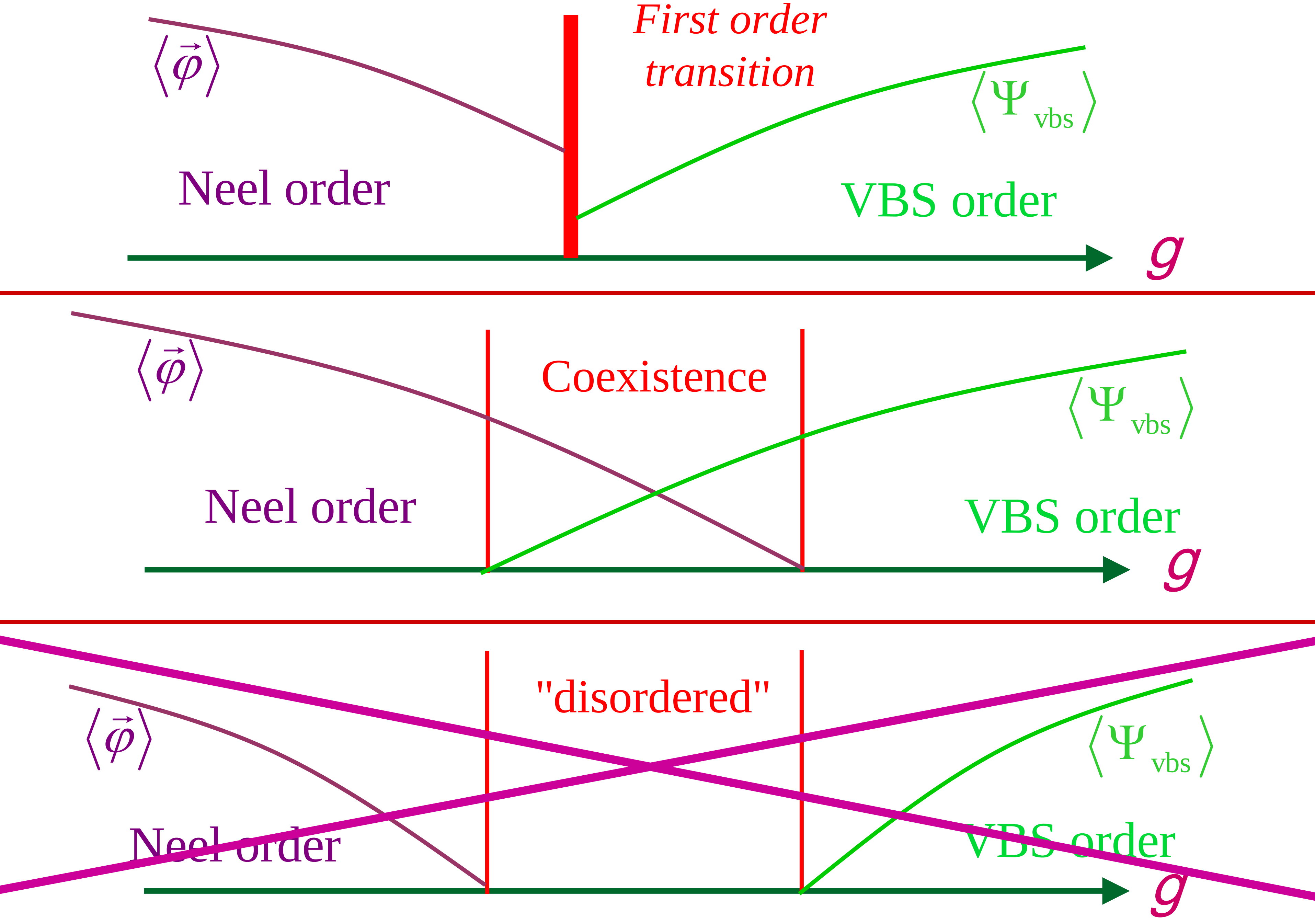

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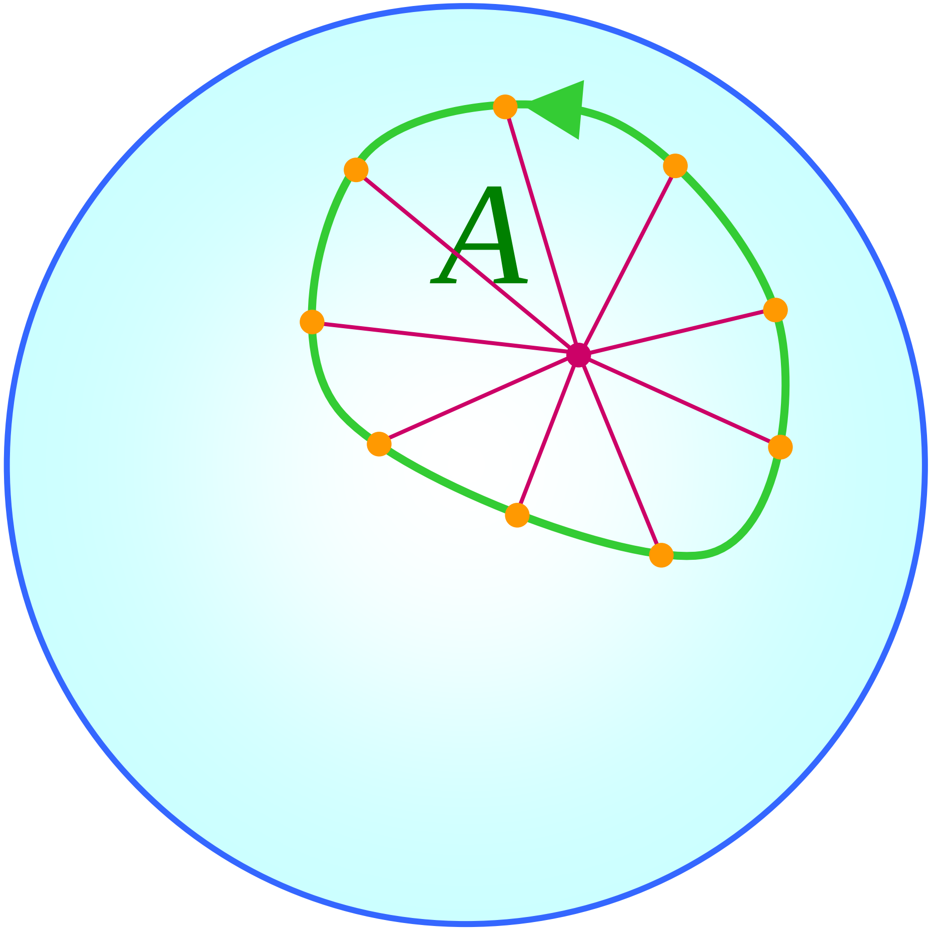
II. Magnetic quantum phase transitions of Mott insulators on the square lattice:

B. Berry phases

Quantum theory for destruction of Neel order

Ingredient missing from LGW theory: Spin Berry Phases



$$e^{iSA}$$

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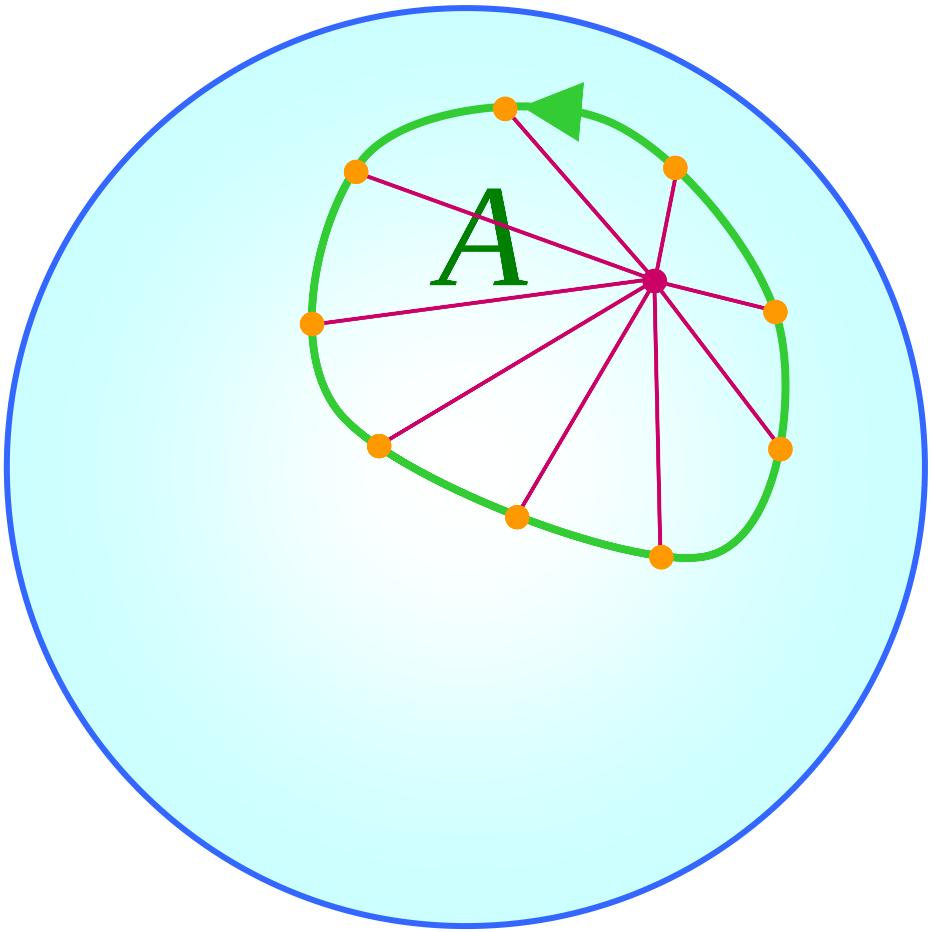

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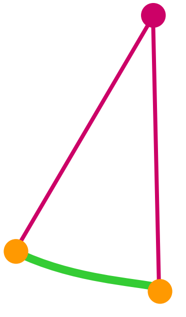
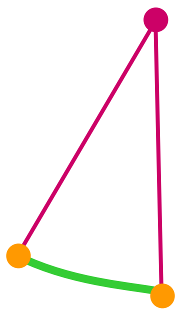


Quantum theory for destruction of Neel order

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

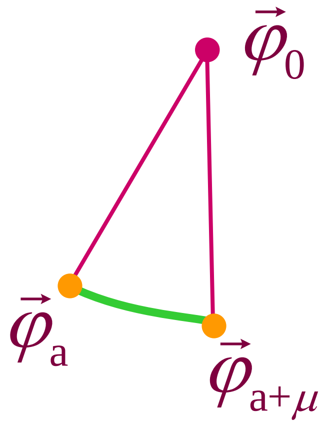


Quantum theory for destruction of Neel order

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

Recall $\vec{\varphi}_{\mathrm{a}} = 2\eta_a \vec{S}_a \rightarrow \vec{\varphi}_{\mathrm{a}} = (0,0,1)$ in classical Neel state;

$\eta_{\mathrm{a}} \rightarrow \pm 1$ on two square sublattices ;



$(\mu = x, y, \tau)$

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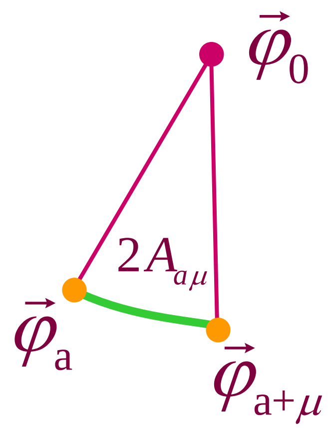
$A_{a\mu} \rightarrow$ *half* oriented area of spherical triangle

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



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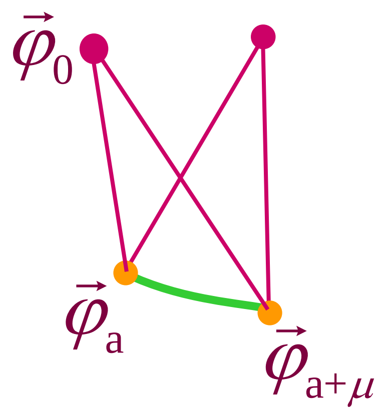

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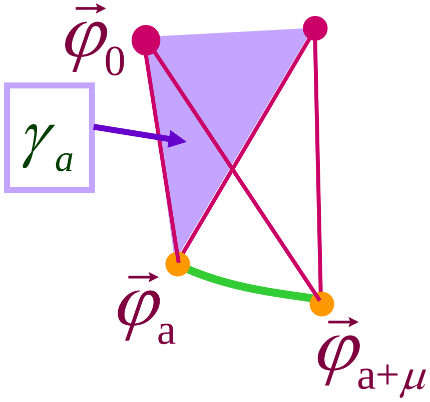

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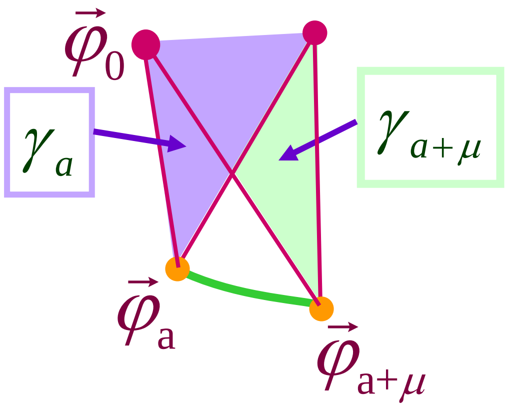

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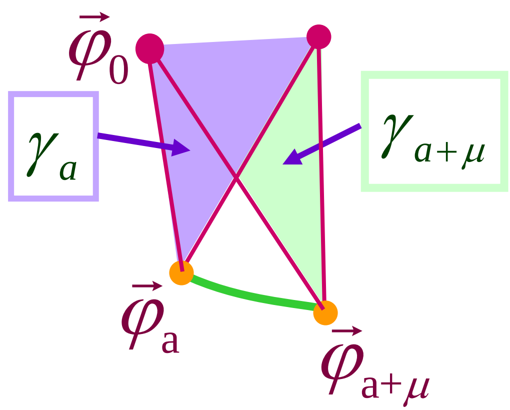
$$2A_{a\mu} \rightarrow 2A_{a\mu} - \gamma_{a+\mu} + \gamma_a$$

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



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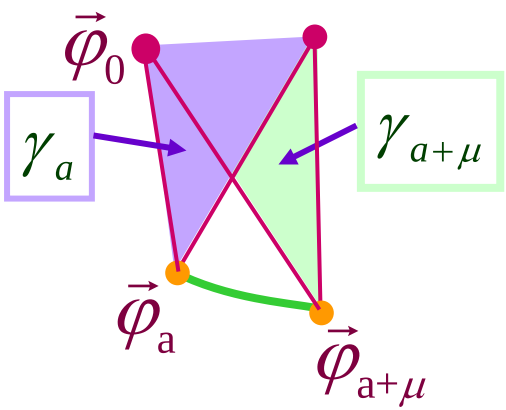
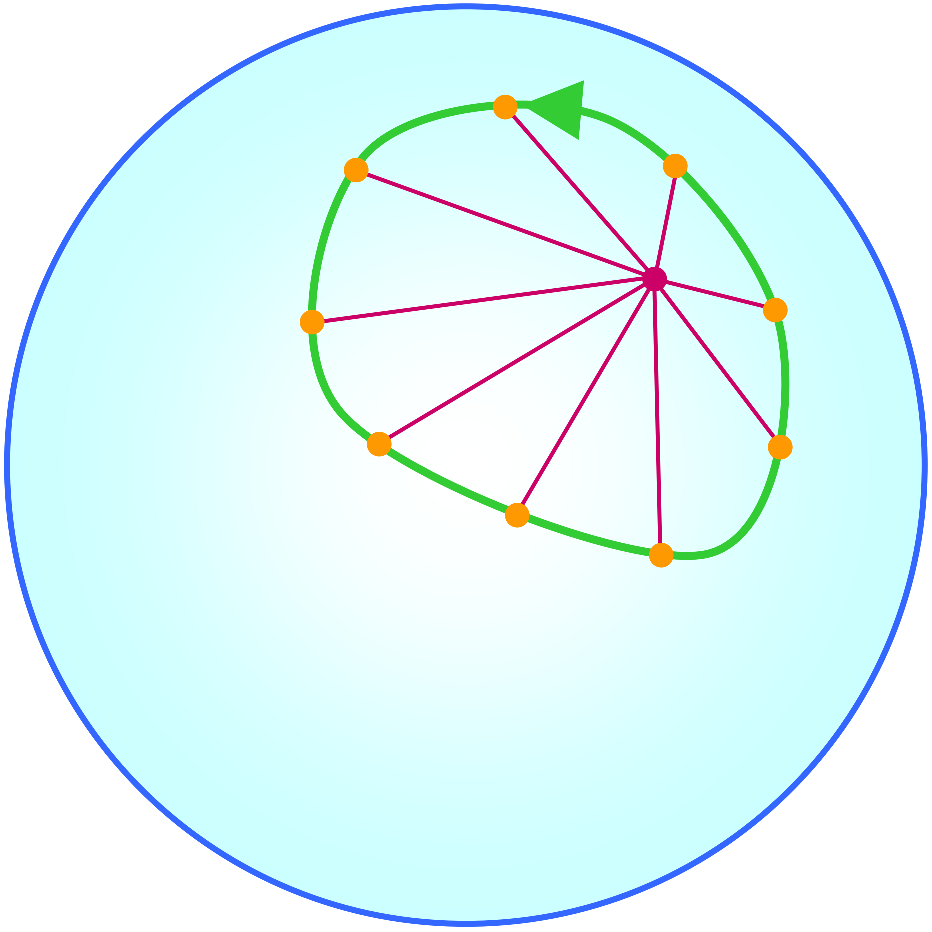


The area of the triangle is uncertain modulo 4π, and the action has to be invariant under $A_{a\mu} \rightarrow A_{a\mu} + 2\pi$

Quantum theory for destruction of Neel order

Ingredient missing from LGW theory: Spin Berry Phases



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

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

Quantum theory for destruction of Neel order

Partition function on cubic lattice

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

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

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

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

Quantum theory for destruction of Neel order

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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

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

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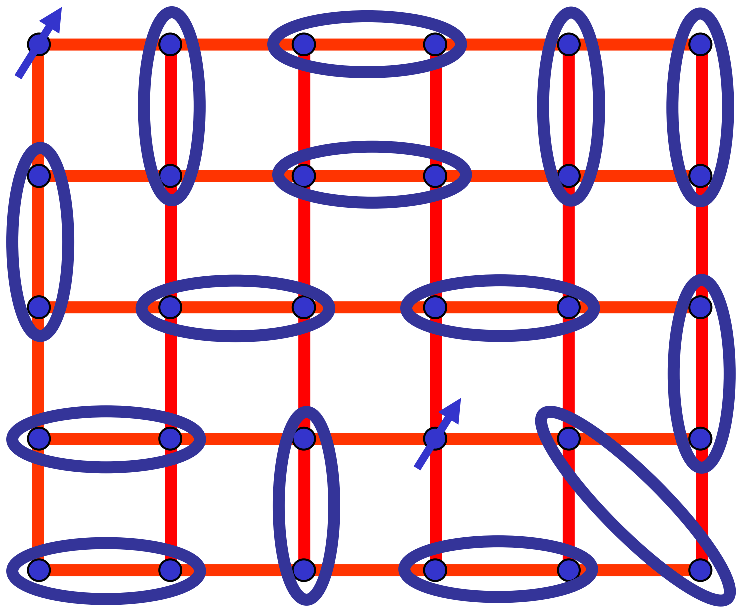
Rewrite partition function in terms of spinors $z_{a\alpha}$, with $\alpha = \uparrow, \downarrow$ and

$$\vec{\varphi}_a = z_{a\alpha}^* \vec{\sigma}_{\alpha\beta} z_{a\beta}$$



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Remarkable identity from spherical trigonometry

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

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

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

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

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

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

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

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

with $e^2 \sim g^2$

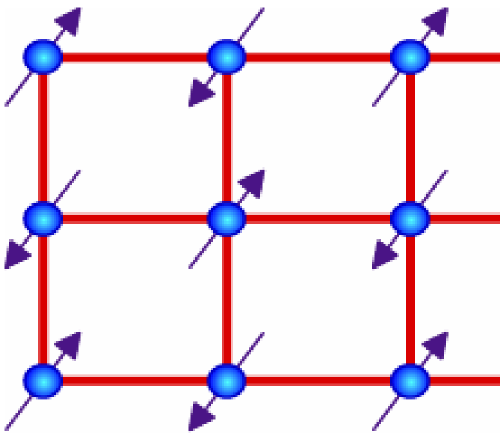
This is compact QED in 3 spacetime dimensions with static charges ± 1 on two sublattices.

This theory can be reliably analyzed by a duality mapping.

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

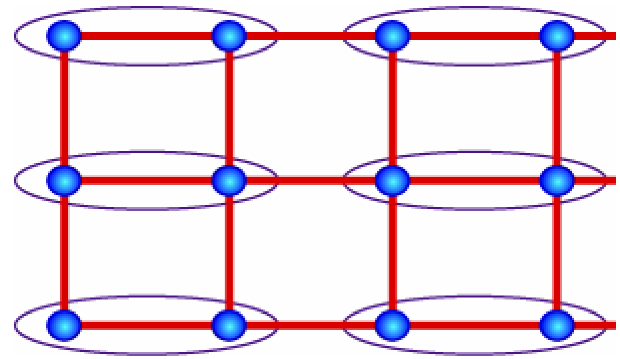
N. Read and S. Sachdev, *Phys. Rev. Lett*. **62**, 1694 (1989).
S. Sachdev and R. Jalabert, *Mod. Phys. Lett*. B **4**, 1043 (1990).
K. Park and S. Sachdev, *Phys. Rev*. B **65**, 220405 (2002).

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

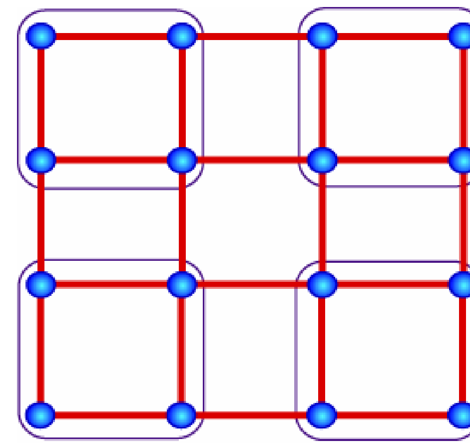


Neel order

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



or

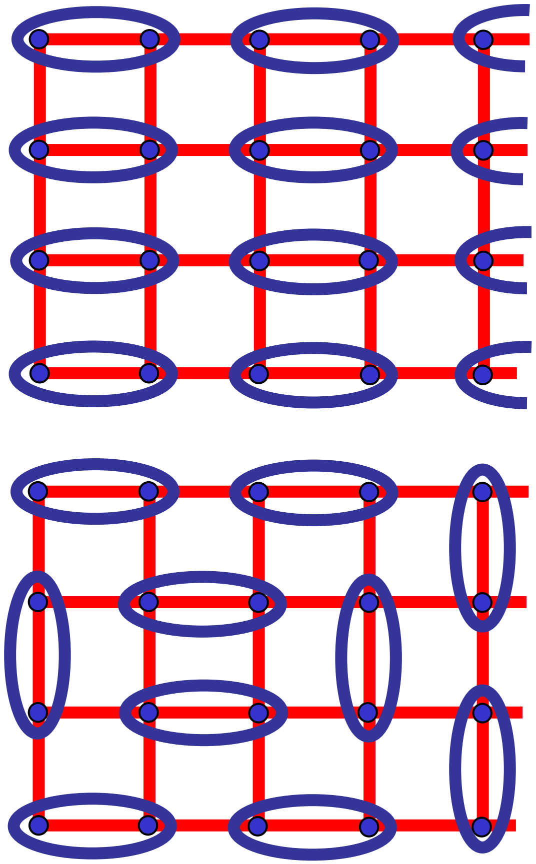


VBS order

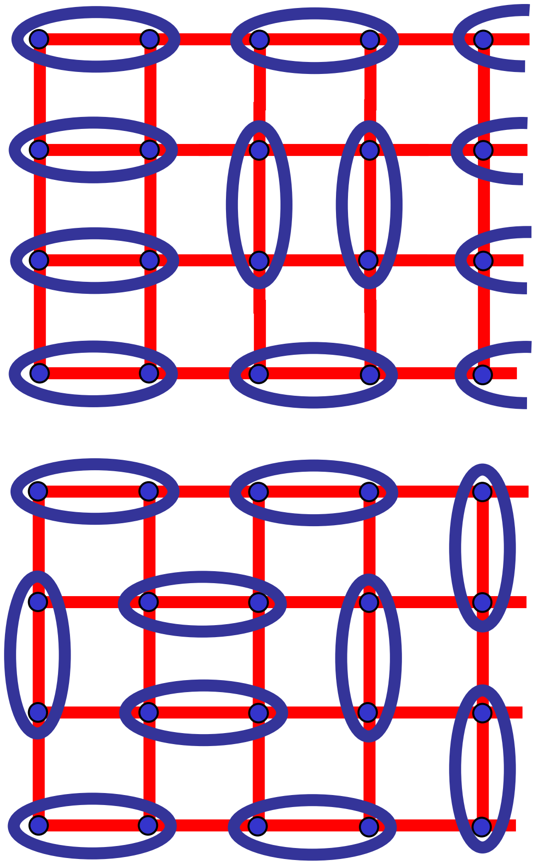
$$\left\langle \Psi_{\text{vbs}} \right\rangle \neq 0$$

Not present in LGW theory of $\vec{\varphi}$ order

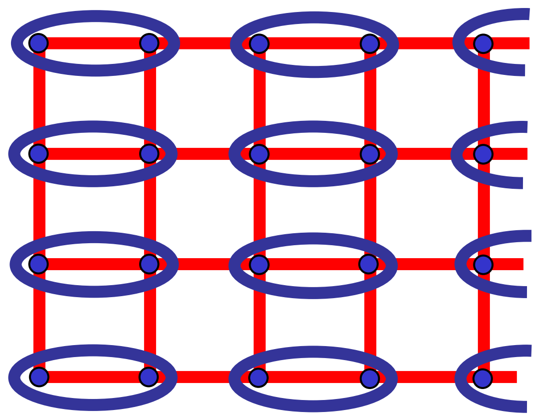
Ordering by quantum fluctuations

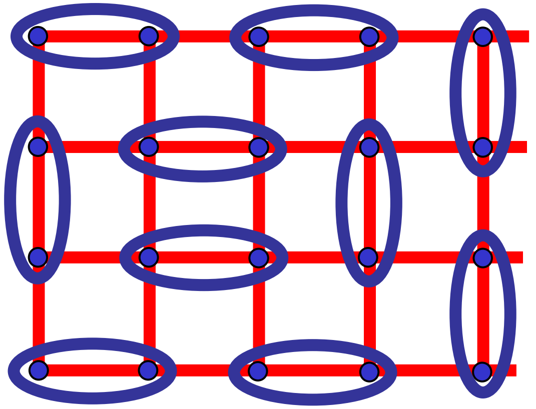


Ordering by quantum fluctuations

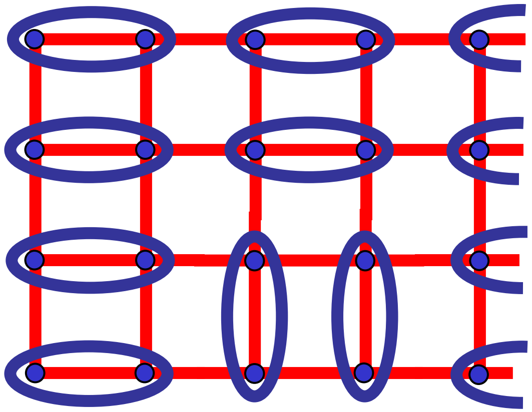


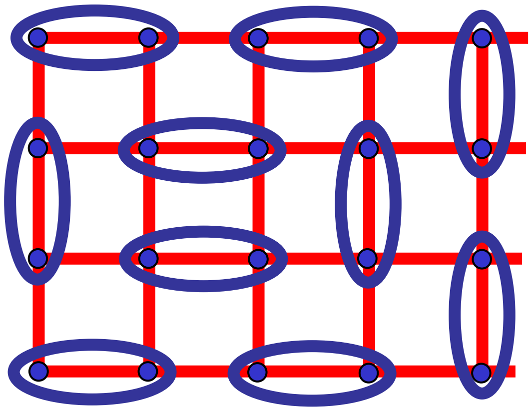
Ordering by quantum fluctuations



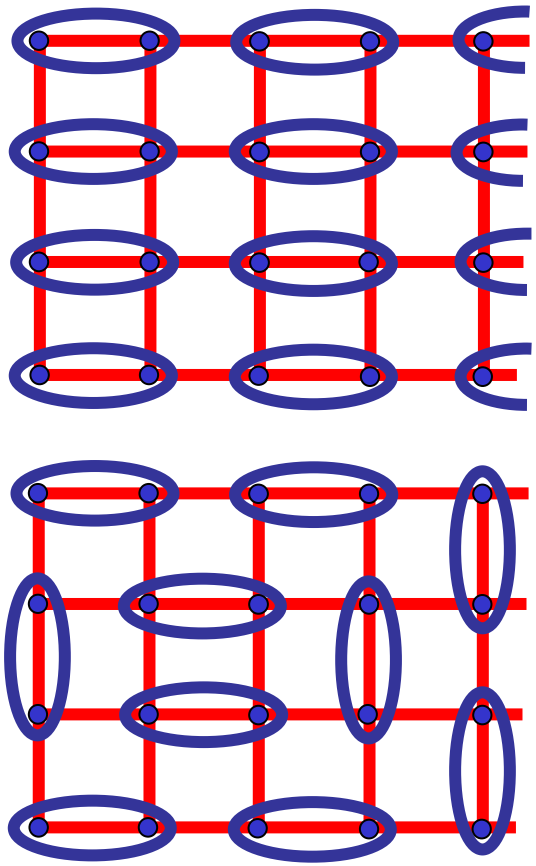


Ordering by quantum fluctuations

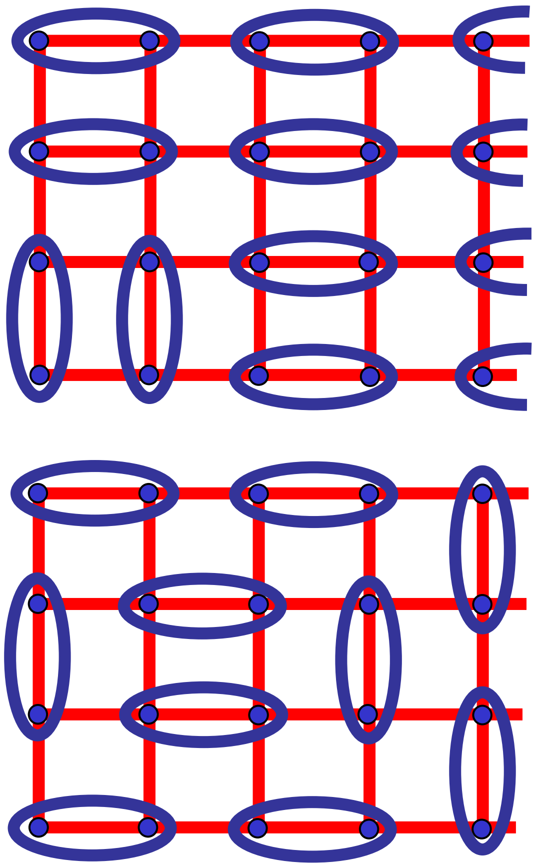




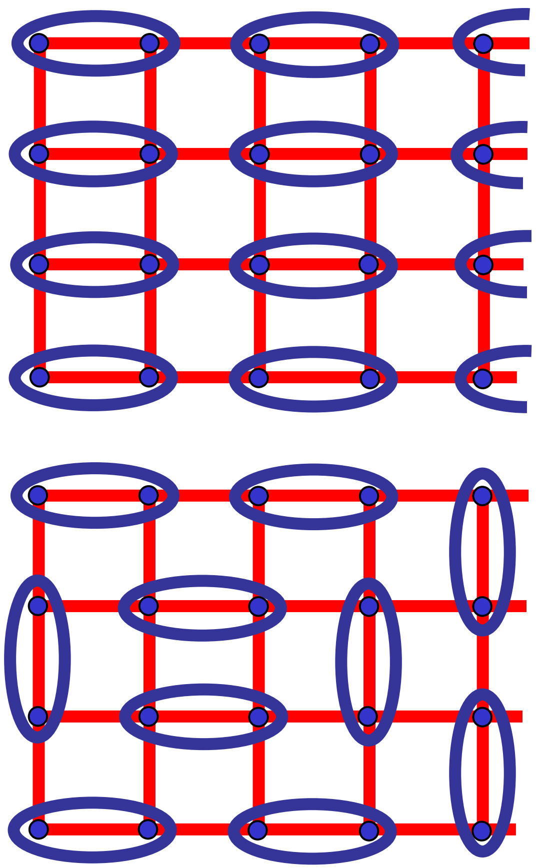
Ordering by quantum fluctuations



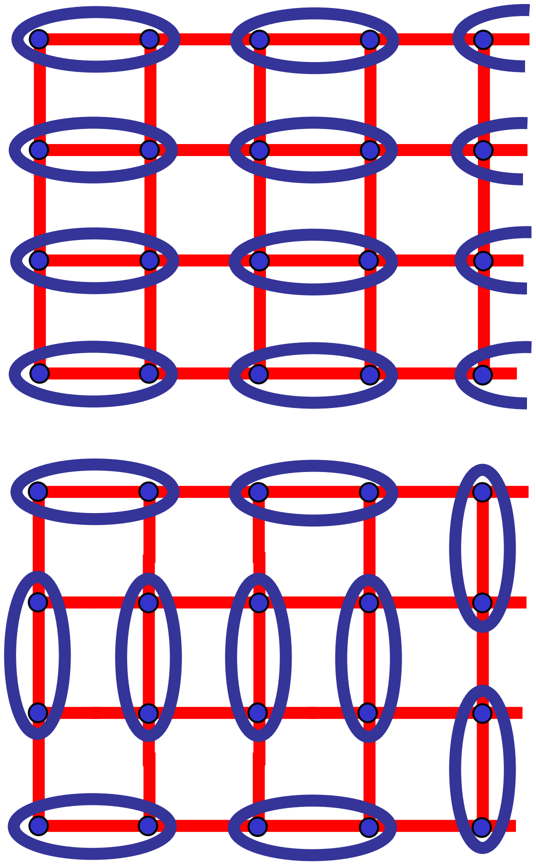
Ordering by quantum fluctuations



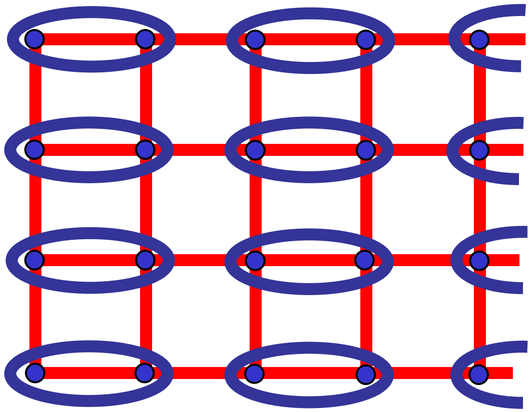
Ordering by quantum fluctuations

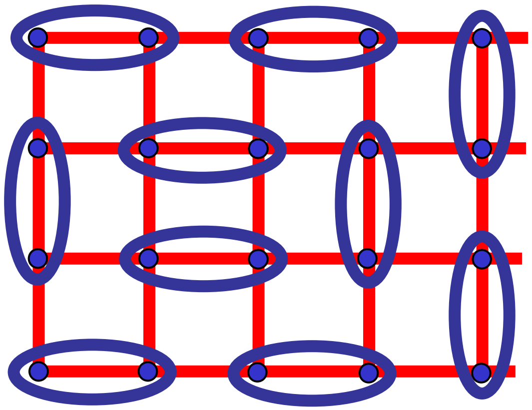


Ordering by quantum fluctuations

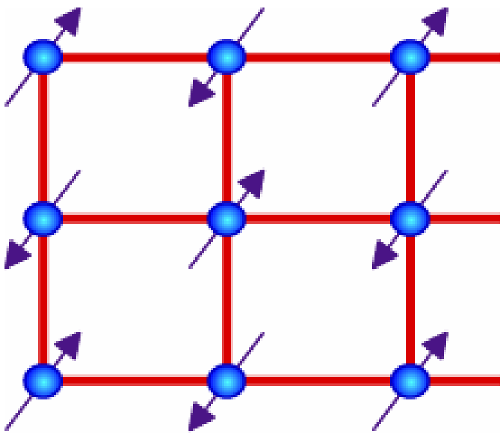


Ordering by quantum fluctuations





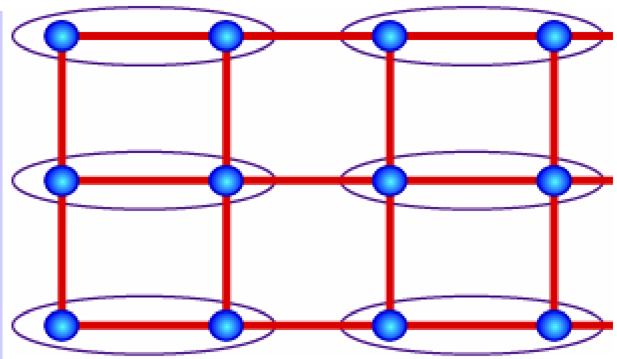
$$Z \approx \prod_a \int dz_{a\alpha} dA_{a\mu} \delta\left(\left|z_{a\alpha}\right|^2 - 1\right) \exp\left(\frac{1}{g} \sum_{a,\mu} z^*_{a\alpha} e^{iA_{a\mu}} z_{a+\mu,\alpha} + i \sum_a \eta_a A_{a\tau}\right)$$



Neel order

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

?



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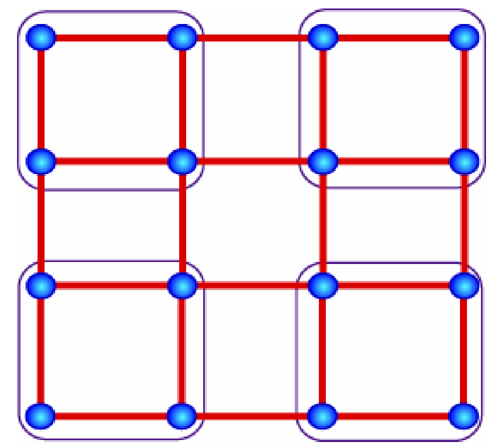


VBS order

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

Not present in LGW theory of $\vec{\varphi}$ order

0 $\rightarrow$ g

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

At the quantum critical point:

- $A_\mu \rightarrow A_\mu + 2\pi$ periodicity can be ignored

(Monopoles interfere destructively and are dangerously irrelevant).

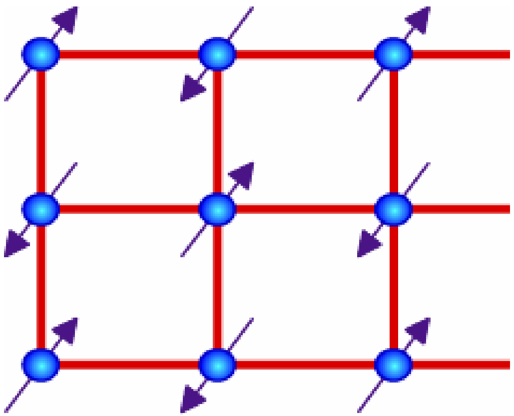
- $S=1/2$ *spinons* z_α, with $\vec{\varphi} \sim z_\alpha^* \vec{\sigma}_{\alpha\beta} z_\beta$, are globally propagating degrees of freedom.

Second-order critical point described by emergent fractionalized degrees of freedom (A_μ and z_α); Order parameters ($\vec{\varphi}$ and Ψ_{vbs}) are "composites" and of secondary importance

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

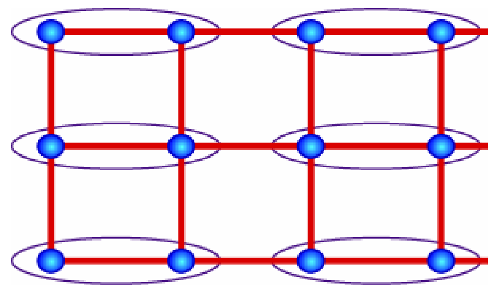
T. Senthil, A. Vishwanath, L. Balents, S. Sachdev and M.P.A. Fisher, *Science* **303**, 1490 (2004).

Phase diagram of S=1/2 square lattice antiferromagnet



Neel order

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



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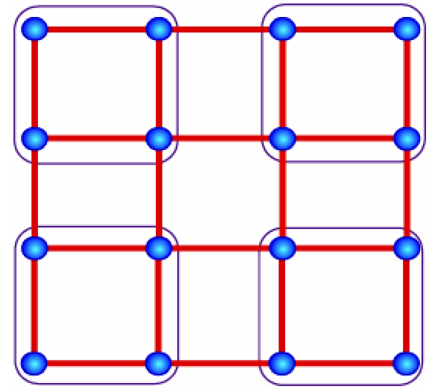

VBS order $\langle \Psi_{\text{vbs}} \rangle \neq 0$

(associated with condensation of monopoles in A_μ),

$S = 1/2$ spinons z_α confined,

$S = 1$ triplon excitations

g

Second-order critical point described by

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

at its critical point $r = r_c$, where A_μ is *non-compact*

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

Conclusions

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