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

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

Leon Balents (UCSB)
Matthew Fisher (UCSB)
T. Senthil (MIT)
Ashvin Vishwanath (MIT)
Parent compound of the high temperature superconductors: \( \text{La}_2\text{CuO}_4 \)

**A Mott insulator**

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

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

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

spin density wave order parameter:

\[
\bar{\phi} = \eta_i \frac{\vec{S}_i}{S} \quad ; \quad \eta_i = \pm 1 \text{ on two sublattices}
\]

\[\langle \bar{\phi} \rangle \neq 0\]
Parent compound of the high temperature superconductors: \( \text{La}_2\text{CuO}_4 \)

**A Mott insulator**

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

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

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

spin density wave order parameter:

\[
\bar{\phi} = \eta_i \frac{\vec{S}_i}{S} \quad ; \quad \eta_i = \pm 1 \text{ on two sublattices}
\]

\[
\langle \bar{\phi} \rangle \neq 0
\]
Parent compound of the high temperature superconductors: \( \text{La}_2\text{CuO}_4 \)

**A Mott insulator**

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

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

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

spin density wave order parameter:

\[
\bar{\phi} = \eta_i \frac{\vec{S}_i}{S} \quad ; \quad \eta_i = \pm 1 \text{ on two sublattices}
\]

\[ \langle \bar{\phi} \rangle \neq 0 \]
Doped state is a paramagnet with $\langle \tilde{\phi} \rangle = 0$
and also a high temperature superconductor with
the BCS pairing order parameter $\langle \Psi_{\text{BCS}} \rangle \neq 0$.
$
\Rightarrow \text{With increasing } \delta, \text{ there must be one or more}
\text{quantum phase transitions involving}
(i) \text{onset of a non-zero } \langle \Psi_{\text{BCS}} \rangle
(ii) \text{restoration of spin rotation invariance by a transition}
\text{from } \langle \tilde{\phi} \rangle \neq 0 \text{ to } \langle \tilde{\phi} \rangle = 0
$
First study magnetic transition in Mott insulators..........
Outline

A. Magnetic quantum phase transitions in “dimerized” Mott insulators
   \textit{Landau-Ginzburg-Wilson (LGW) theory}

B. Mott insulators with spin $S=1/2$ per unit cell
   \textit{Berry phases, bond order, and the breakdown of the LGW paradigm}

C. Technical details
   \textit{Duality and dangerously irrelevant operators}
A. Magnetic quantum phase transitions in “dimerized” Mott insulators:

Landau-Ginzburg-Wilson (LGW) theory:
Second-order phase transitions described by fluctuations of an order parameter associated with a broken symmetry
TlCuCl$_3$

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


$S=1/2$ spins on coupled dimers

\[ H = \sum_{\langle ij \rangle} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j \]

0 \leq \lambda \leq 1
\( \lambda \) close to 0

Weakly coupled dimers
$\lambda$ close to 0

Weakly coupled dimers

\[ \langle \vec{S}_i \rangle = 0, \langle \vec{\phi} \rangle = 0 \]
$\lambda$ close to 0

Weakly coupled dimers

$\begin{align*}
\uparrow \downarrow - \downarrow \uparrow &= \frac{1}{2} \left( |\uparrow \downarrow\rangle - |\downarrow \uparrow\rangle \right) \\
\text{Excitation: } S=1 \text{ triplon}
\end{align*}$
\( \lambda \) close to 0

Weakly coupled dimers

\[ \text{Excitation: } S=1 \text{ triplon} \]

\[ \text{=} \frac{1}{\sqrt{2}} (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle) \]
Weakly coupled dimers

\[ \lambda \text{ close to } 0 \]

Excitation: \( S=1 \) *triplon*

\[ = \frac{1}{\sqrt{2}} \left( |\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle \right) \]
$\lambda$ close to 0

Weakly coupled dimers

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

Excitation: $S=1$ *triplon*
\( \lambda \) close to 0

Weakly coupled dimers

![Diagram with dimers and arrows indicating excitations]

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

Excitation: \( S=1 \) triplon
\( \lambda \) close to 0

Weakly coupled dimers

\[ \begin{array}{c}
\uparrow \downarrow - \downarrow \uparrow = 2
\end{array} \]

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

Energy dispersion away from antiferromagnetic wavevector

\[ \epsilon_p = \Delta + \frac{c_x^2 p_x^2 + c_y^2 p_y^2}{2\Delta} \]

\( \Delta \rightarrow \) spin gap
TlCuCl₃


For quasi-one-dimensional systems, the triplon linewidth takes the exact universal value \( 1.20 k_B T e^{-\Delta/k_B T} \) at low T


Coupled Dimer Antiferromagnet
\( \lambda \) close to 1

Weakly dimerized square lattice
$\lambda$ close to 1

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

spin density wave order parameter: $\phi = \eta_i \frac{\vec{S}_i}{S}$ ; $\eta_i = \pm 1$ 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$_3$. 
\[ \lambda_c = 0.52337(3) \]
M. Matsumoto, C. Yasuda, S. Todo, and H. Takayama,

LGW theory for quantum criticality

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

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


For $\lambda < \lambda_c$ oscillations of $\bar{\phi}$ about $\bar{\phi} = 0$ lead to the following structure in the dynamic structure factor $S(p, \omega)$

$$\varepsilon(p) = \Delta + \frac{c^2 p^2}{2\Delta} ; \quad \Delta = \sqrt{\lambda_c - \lambda}/c$$

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

*Berry phases, bond order, and the breakdown of the LGW paradigm*
Mott insulator with two $S=1/2$ spins per unit cell
Mott insulator with one $S=1/2$ spin per unit cell
Mott insulator with one $S=1/2$ spin per unit cell

Ground state has Neel order with $\vec{\phi} \neq 0$
Mott insulator with one $S=1/2$ spin per unit cell

Destroy Neel order by perturbations which preserve full square lattice symmetry e.g. second-neighbor or ring exchange. The strength of this perturbation is measured by a coupling $g$.

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

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

Large $g \Rightarrow$ paramagnetic ground state with $\langle \tilde{\phi} \rangle = 0$
Mott insulator with one $S=1/2$ spin per unit cell

Possible large $g$ paramagnetic ground state (Class A) with $\langle \tilde{\phi} \rangle = 0$
Mott insulator with one $S=1/2$ spin per unit cell

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

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

$$\Psi_{\text{bond}}(i) = \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j e^{i\arctan(r_j - r_i)}$$
Mott insulator with one $S=1/2$ spin per unit cell

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

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

$$
\Psi_{\text{bond}} (i) = \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j e^{i \arctan(r_j - r_i)}
$$
Mott insulator with one $S=1/2$ spin per unit cell

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

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

$$\Psi_{\text{bond}} (i) = \sum_{\langle ij \rangle} \tilde{S}_i \cdot \tilde{S}_j e^{i \arctan(r_j - r_i)}$$
Mott insulator with one $S=1/2$ spin per unit cell

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

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

$$\Psi_{\text{bond}} (i) = \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j e^{i \arctan(r_j - r_i)}$$
Mott insulator with one $S=1/2$ spin per unit cell

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

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

$$\Psi_{\text{bond}}(i) = \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j e^{i\arctan(r_j-r_i)}$$
Mott insulator with one $S=1/2$ spin per unit cell

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

$$\Psi_{\text{bond}}(i) = \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j e^{i \arctan(r_j - r_i)}$$
Mott insulator with one $S=1/2$ spin per unit cell

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

$$\Psi_{\text{bond}} (i) = \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j e^{i \arctan(r_j - r_i)}$$
Mott insulator with one $S=1/2$ spin per unit cell

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

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

$$\Psi_{\text{bond}} (i) = \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j e^{i \arctan(r_j-r_i)}$$
Mott insulator with one $S=1/2$ spin per unit cell

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

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

$$\Psi_{\text{bond}} (i) = \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j e^{i \arctan (r_j - r_i)}$$
Mott insulator with one $S=1/2$ spin per unit cell

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

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

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


Resonance in benzene leads to a symmetric configuration of valence bonds

*(F. Kekulé, L. Pauling)*

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

Excitations of the paramagnet with non-zero spin

\[ \langle \Psi_{\text{bond}} \rangle \neq 0; \text{Class A} \]
Excitations of the paramagnet with non-zero spin

\[ \langle \Psi_{\text{bond}} \rangle \neq 0; \text{ Class A} \]
Excitations of the paramagnet with non-zero spin

$\langle \Psi_{\text{bond}} \rangle \neq 0$; Class A
Excitations of the paramagnet with non-zero spin

$\langle \Psi_{\text{bond}} \rangle \neq 0; \text{Class A}$
Excitations of the paramagnet with non-zero spin

$\langle \Psi_{\text{bond}} \rangle \neq 0$; Class A
Excitations of the paramagnet with non-zero spin

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

\( S=1/2 \) spinons, \( z_\alpha \), are confined into a \( S=1 \) triplon, \( \tilde{\varphi} \)

\[ \tilde{\varphi} \sim z_\alpha^* \tilde{\sigma}_{\alpha\beta} z_\beta \]
Excitations of the paramagnet with non-zero spin

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

\[ \langle \Psi_{\text{bond}} \rangle = 0; \text{Class B} \]

\( S=1/2 \) spinons, \( z_\alpha \), are confined into a \( S=1 \) triplon, \( \tilde{\varphi} \)

\[ \tilde{\varphi} \sim z_\alpha \tilde{\sigma}_{\alpha \beta} z_\beta \]
Excitations of the paramagnet with non-zero spin

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

\[ \langle \Psi_{\text{bond}} \rangle = 0; \text{Class B} \]

\( S=1/2 \) spinons, \( z_\alpha \), are confined into a \( S=1 \) triplon, \( \tilde{\phi} \)

\[ \tilde{\phi} \sim z_\alpha^* \tilde{\sigma}_{\alpha\beta} z_\beta \]
Excitations of the paramagnet with non-zero spin

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

\[ \langle \Psi_{\text{bond}} \rangle = 0; \text{Class B} \]

\( S=1/2 \) spinons, \( Z_\alpha \), are confined into a \( S=1 \) triplon, \( \vec{\varphi} \)

\[ \vec{\varphi} \sim Z_\alpha \vec{\sigma}_{\alpha\beta} Z_\beta \]
Excitations of the paramagnet with non-zero spin

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

\[ \langle \Psi_{\text{bond}} \rangle = 0; \text{Class B} \]

\( S=1/2 \) spinons, \( z_\alpha \), are confined into a \( S=1 \) triplon, \( \phi \)

\[ \phi \sim z^{*}_\alpha \sigma_{\alpha\beta} z_\beta \]

\( S=1/2 \) spinons can propagate independently across the lattice
Quantum theory for destruction of Neel order

**Ingredient missing from LGW theory:**
**Spin Berry Phases**

$e^{iSA}$
Quantum theory for destruction of Neel order

Ingredient missing from LGW theory:
Spin Berry Phases

\[ e^{iSA} \]
Quantum theory for destruction of Neel order
Quantum theory for destruction of Neel order

Discretize imaginary time: path integral is over fields on the sites of a cubic lattice of points $a$
Quantum theory for destruction of Neel order

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

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

$\eta_a \rightarrow \pm 1$ on two square sublattices;

\[ (\mu = x, y, \tau) \]
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 \( \vec{\phi}_a = 2\eta_a \vec{S}_a \rightarrow \vec{\phi}_a = (0,0,1) \) in classical Neel state;

\[ \eta_a \rightarrow \pm 1 \] on two square sublattices;

\[ A_{a\mu} \rightarrow \text{half oriented area of spherical triangle} \]

formed by \( \vec{\phi}_a, \vec{\phi}_{a+\mu} \), and an arbitrary reference point \( \vec{\phi}_0 \).
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 $\bar{\phi}_a = 2\eta_a \bar{S}_a \rightarrow \bar{\phi}_a = (0,0,1)$ in classical Neel state;

$\eta_a \rightarrow \pm 1$ on two square sublattices;

$A_{a\mu} \rightarrow half$ oriented area of spherical triangle formed by $\bar{\phi}_a, \bar{\phi}_{a+\mu}$, and an arbitrary reference point $\bar{\phi}_0$
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 $\vec{\phi}_a = 2\eta_a \vec{S}_a \rightarrow \vec{\phi}_a = (0,0,1)$ in classical Neel state;

$\eta_a \rightarrow \pm 1$ on two square sublattices;

$A_{a\mu} \rightarrow \text{half}$ oriented area of spherical triangle formed by $\vec{\phi}_a$, $\vec{\phi}_a+\mu$, and an arbitrary reference point $\vec{\phi}_0$
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 $\vec{\phi}_a = 2\eta_a \vec{S}_a \rightarrow \vec{\phi}_a = (0,0,1)$ in classical Neel state;

$\eta_a \rightarrow \pm 1$ on two square sublattices;

$A_{a\mu} \rightarrow \text{half}$ oriented area of spherical triangle formed by $\vec{\phi}_a$, $\vec{\phi}_{a+\mu}$, and an arbitrary reference point $\vec{\phi}_0$. 

\[ \vec{\gamma}_a, \vec{\gamma}_{a+\mu} \]
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 $\vec{\phi}_a = 2\eta_a \vec{S}_a \rightarrow \vec{\phi}_a = (0,0,1)$ in classical Neel state;

$\eta_a \rightarrow \pm 1$ on two square sublattices;

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

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

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

Change in choice of $\vec{\phi}_0$ is like a “gauge transformation”
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 \( \vec{\phi}_a = 2\eta_a \vec{S}_a \rightarrow \vec{\phi}_a = (0,0,1) \) in classical Neel state;
\( \eta_a \rightarrow \pm 1 \) on two square sublattices;
\( A_{a\mu} \rightarrow \text{half oriented area of spherical triangle} \)
formed by \( \vec{\phi}_a, \vec{\phi}_{a+\mu}, \) and an arbitrary reference point \( \vec{\phi}_0 \)

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

Change in choice of \( \vec{\phi}_0 \) is like a “gauge transformation”

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 ±1 on sublattices
Quantum theory for destruction of Neel order

Partition function on cubic lattice

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

Modulus of weights in partition function: those of a classical ferromagnet at a “temperature” \( g \)

Small \( g \) \( \Rightarrow \) ground state has Neel order with \( \langle \bar{\phi} \rangle \neq 0 \)

Large \( g \) \( \Rightarrow \) paramagnetic ground state with \( \langle \bar{\phi} \rangle = 0 \)

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 $A_{a\mu}$

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

with $e^2 \sim g^2$

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

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

\[ Z_{\text{dual}} = \sum_{\{m_j\}} \exp \left( -\frac{\pi}{2e^2} \sum_{j,j'} \frac{m_j m_{j'}}{|r_j - r_{j'}|} + 2\pi i \sum_{j} m_j \chi_j \right) \]

with the \( m_j \) integer monopole charges. Each monopole carries a Berry phase (F.D.M. Haldane, *Phys. Rev. Lett.* 61, 1029 (1988)) determined by the fixed \( \chi_j = 0, 1/4, 1/2, 3/4 \) on the four dual sublattices.
Alternative representation is in terms of a “height” model

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

with the $h_{\bar{j}}$ integer heights.
The Berry phases now lead to height ‘offsets’ $\chi_{\bar{j}} = 0, 1/4, 1/2, 3/4$ on the four dual sublattices.
For large $e^2$, low energy height configurations are in exact one-to-one correspondence with nearest-neighbor valence bond pairings of the sites square lattice.

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

⇒ There is a definite average height of the interface

⇒ **Ground state has bond order.**

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

Neel order
\[ \langle \bar{\phi} \rangle \neq 0 \]

Bond order
\[ \langle \Psi_{\text{bond}} \rangle \neq 0 \]
Not present in LGW theory of \( \bar{\phi} \) order
Naïve approach: add bond order parameter to LGW theory “by hand”

Neel order
\[ \langle \phi \rangle \neq 0, \langle \Psi_{\text{bond}} \rangle = 0 \]

First order transition

Bond order
\[ \langle \phi \rangle = 0, \langle \Psi_{\text{bond}} \rangle \neq 0 \]

Neel order
\[ \langle \phi \rangle \neq 0, \langle \Psi_{\text{bond}} \rangle = 0 \]

Coexistence
\[ \langle \phi \rangle \neq 0, \langle \Psi_{\text{bond}} \rangle \neq 0 \]

Bond order
\[ \langle \phi \rangle = 0, \langle \Psi_{\text{bond}} \rangle \neq 0 \]

"disordered"
\[ \langle \phi \rangle = 0, \langle \Psi_{\text{bond}} \rangle = 0 \]

Bond order
\[ \langle \phi \rangle = 0, \langle \Psi_{\text{bond}} \rangle \neq 0 \]
Bond order in a frustrated $S=1/2$ XY magnet


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

\[ H = 2J \sum_{\langle ij \rangle} (S_i^x S_j^x + S_i^y S_j^y) - K \sum_{\langle ijk \rangle} \left( S_i^+ S_j^- S_k^+ S_l^- + S_i^- S_j^+ S_k^- S_l^+ \right) \]
\[ Z = \prod_a \int d\bar{\phi}_a \delta(\bar{\phi}_a^2 - 1) \exp \left( \frac{1}{g} \sum_{a,\mu} \bar{\phi}_a \cdot \bar{\phi}_{a+\mu} + i \sum_a \eta_a A_{a\tau} \right) \]

Neel order
\[ \langle \bar{\phi} \rangle \neq 0 \]

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

Not present in LGW theory of \( \bar{\phi} \) order
Alternative formulation to describe transition:
Express theory in terms of a complex spinor \( z_{a\alpha}, \alpha = \uparrow, \downarrow \), with

\[
\mathbf{n}_a = z_{a\alpha}^* \sigma_{\alpha\beta} z_{a\beta}
\]

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

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

**Theory of a second-order quantum phase transition between Neel and bond-ordered phases**

At the quantum critical point:

- \( A_\mu \rightarrow A_\mu + 2\pi \) periodicity can be ignored
  (Monopoles interfere destructively and are dangerously irrelevant).
- \( S=1/2 \) spinons \( z_\alpha \), with \( \bar{\phi} \sim z_\alpha^* \tilde{\sigma}_{\alpha\beta} z_\beta \), are globally propagating degrees of freedom.

---

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

---


Phase diagram of S=1/2 square lattice antiferromagnet

Neel order
\[ \langle \vec{\phi} \rangle \sim \langle z^*_\alpha \tilde{\sigma}_{\alpha\beta} z_\beta \rangle \neq 0 \]

Bond order \[ \langle \Psi_{\text{bond}} \rangle \neq 0 \]
(associated with condensation of monopoles in \( A_\mu \)),
\[ S = 1/2 \] spinons \( z_\alpha \) confined,
\[ S = 1 \] triplon excitations

Second-order critical point described by
\[
S_{\text{critical}} = \int d^2 x d\tau \left[ \left| (\partial_\mu - i A_\mu) z_\alpha \right|^2 + r |z_\alpha|^2 + \frac{u}{2} \left( |z_\alpha|^2 \right)^2 + \frac{1}{4e^2} \left( \partial_\mu A_\nu - \partial_\nu A_\mu \right)^2 \right]
\]
at its critical point \( r = r_c \), where \( A_\mu \) is non-compact

S. Sachdev cond-mat/0401041.
The line $\lambda_4 = 0$ is described by

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

where $A_\mu$ is non-compact.
B. Mott insulators with spin $S=1/2$ per unit cell:

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

*Order parameters/broken symmetry*

*Emergent gauge excitations, fractionalization.*
C. Technical details

*Duality and dangerously irrelevant operators*
Nature of quantum critical point

\[ Z = \prod_a \int d\mathbf{z}_{a\alpha} dA_{a\mu} \delta (|\mathbf{z}_{a\alpha}|^2 - 1) \]

\[ \exp \left( -\frac{1}{g} \sum_{a,\mu} \mathbf{z}_{a\alpha}^* e^{iA_{a\mu}} \mathbf{z}_{a+\mu,\alpha} + \text{c.c.} + i \sum_a \eta_a A_{a\tau} + \frac{1}{e^2} \sum \cos (\Delta_\mu A_{a\nu} - \Delta_\nu A_{a\mu}) \right) \]

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

A. Non-compact QED with scalar matter
B. Compact QED with scalar matter
C. \( N=1 \): Compact QED with scalar matter and Berry phases
D. \( N \to \infty \) theory
E. Easy plane case for \( N=2 \)
Nature of quantum critical point

\[ Z = \prod_a \int d z_{a\alpha} A_{a\mu} \delta (|z_{a\alpha}|^2 - 1) \]

\[ \exp \left( \frac{1}{g} \sum_{a,\mu} z_{a\alpha}^* e^{i A_{a\mu}} z_{a+\mu,\alpha} + c.c. + i \sum_a \eta_a A_{a\tau} + \frac{1}{e^2} \sum_a \cos (\Delta_{\mu} A_{a\nu} - \Delta_{\nu} A_{a\mu}) \right) \]

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

A. Non-compact QED with scalar matter
B. Compact QED with scalar matter
C. \( N=1 \): Compact QED with scalar matter and Berry phases
D. \( N \to \infty \) theory
E. Easy plane case for \( N=2 \)
A. $N=1$, non-compact U(1), no Berry phases

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

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

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

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

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

Nature of quantum critical point

\[ Z = \prod_a \int d\bar{z}_{a\alpha} dA_{a\mu} \delta (|z_{a\alpha}|^2 - 1) \]

\[ \exp \left( \frac{1}{g} \sum_{a,\mu} \bar{z}_{a\alpha} e^{iA_{a\mu}} z_{a+\mu,\alpha} + \text{c.c.} + i \sum_a \eta A_{a\tau} + \frac{1}{e^2} \sum \cos (\Delta_{\mu} A_{a\nu} - \Delta_{\nu} A_{a\mu}) \right) \]

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

A. Non-compact QED with scalar matter
B. Compact QED with scalar matter
C. \( N=1 \): Compact QED with scalar matter and Berry phases
D. \( N \rightarrow \infty \) theory
E. Easy plane case for \( N=2 \)
Nature of quantum critical point

\[ Z = \prod_z \int dz_{\alpha} dA_{\alpha \mu} \delta (|z_{\alpha}|^2 - 1) \]

\[ \exp \left( \frac{1}{g} \sum_{a, \mu} z_{a \alpha}^* \sum_{\alpha} e^{iA_{a \mu}} z_{a+\mu, \alpha} + \text{c.c.} + i \sum_{a} \eta_{a} A_{a \tau} + \frac{1}{e^2} \sum \cos (\Delta_{\mu} A_{a \nu} - \Delta_{\nu} A_{a \mu}) \right) \]

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

A. Non-compact QED with scalar matter
B. Compact QED with scalar matter
C. \( N=1 \): Compact QED with scalar matter and Berry phases
D. \( N \to \infty \) theory
E. Easy plane case for \( N=2 \)
B. \textit{N}=1, compact U(1), no Berry phases

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

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

The Dasgupta-Halperin mapping now yields the dual theory

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

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

This dual theory is an \textbf{inverted XY model in a “magnetic” field} and it has no phase transition. In the direct theory, the monopoles are a relevant perturbation, and they destroy the “superconducting” phase.
Nature of quantum critical point

\[ Z = \prod_a \int d\bar{z}_{a\alpha} dA_{a\mu} \delta (|z_{a\alpha}|^2 - 1) \]

\[ \exp \left( \frac{1}{g} \sum_{a,\mu} \bar{z}_{a\alpha} e^{iA_{a\mu}} z_{a+\mu,\alpha} + \text{c.c.} + i \sum_a \eta_a A_{a\tau} + \frac{1}{e^2} \sum \cos (\Delta_\mu A_{a\mu} - \Delta_\nu A_{a\mu}) \right) \]

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

A. Non-compact QED with scalar matter
B. Compact QED with scalar matter
C. \( N=1 \): Compact QED with scalar matter and Berry phases
D. \( N \to \infty \) theory
E. Easy plane case for \( N=2 \)
Nature of quantum critical point

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

\[ \exp \left( \frac{1}{g} \sum_{a,\mu} z_{a\alpha}^* e^{iA_{a\mu}} z_{a+\mu,\alpha} + \text{c.c.} + i \sum_a \eta_a A_{a\tau} + \frac{1}{e^2} \sum \cos (\Delta_{\mu} A_{a\nu} - \Delta_{\nu} A_{a\mu}) \right) \]

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

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

Upon including Berry phases, the previous theory becomes

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

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

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

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

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

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

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

\[ Z = \prod_a \int \! dz_a \alpha dA_{a\mu} \delta \left( |z_{a\alpha}|^2 - 1 \right) \]

\[ \exp \left( \frac{1}{g} \sum_{a,\mu} z_{a\alpha}^* e^{iA_{a\mu}} z_{a+\mu,\alpha} + \text{c.c.} + i \sum_a \eta_a A_{a\tau} + \frac{1}{e^2} \sum \cos (\Delta_{\mu} A_{a\nu} - \Delta_{\nu} A_{a\mu}) \right) \]

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

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

Identical critical theories!
Nature of quantum critical point

\[
Z = \prod_a \int d z_{a\alpha} d A_{a\mu} \delta (|z_{a\alpha}|^2 - 1)
\]

\[
\exp \left( \frac{1}{g} \sum_{a,\mu} z_{a\alpha}^* e^{i A_{a\mu} z_{a+\mu,\alpha} + \text{c.c.}} + i \sum_a \eta A_{a\tau} + \frac{1}{e^2} \sum \cos (\Delta_{\mu} A_{a\nu} - \Delta_{\nu} A_{a\mu}) \right)
\]

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

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

Identical critical theories!
D. $N \to \infty$, compact U(1), Berry phases

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

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

where $\frac{\delta S_{\text{monopole}}}{\delta V(r)} = 0$ and $V(r \to \infty) = 0$.

Evaluation of functional determinant for $q = 4$ shows

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

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

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

E. Easy plane case for $N=2$

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

- monopoles are relevant without Berry phases,

- monopoles are irrelevant at the critical point in the presence of Berry phases, and

- monopoles drive the appearance of bond order in the paramagnetic phase.

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

O. Motrunich and A. Vishwanath, cond-mat/0311222
Phase diagram of $S=1/2$ square lattice antiferromagnet

Neel order

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

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

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

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

$S = 1$ triplon excitations

Second-order critical point described by

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

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


S. Sachdev cond-mat/0401041.