Ground states of quantum antiferromagnets in two dimensions

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Mott insulator: square lattice antiferromagnet

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

Ground state has long-range magnetic Néel order, or “collinear magnetic (CM) order”

\[
H = \sum_{<ij>} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j
\]

Néel order parameter: \( \mathbf{n}_i = (-1)^{i_x + i_y} \mathbf{S}_i \)

\( \langle \mathbf{n} \rangle \neq 0 \)
Decompose the magnetic order parameter as

\[ n = z_\alpha^* \vec{\sigma}_{\alpha \beta} z_\beta \]

where \( \vec{\sigma} \) are the Pauli matrices, and \( z_\alpha \) are complex spinors (\( \alpha = \uparrow, \downarrow \)) which carry spin \( S = 1/2 \).

**Key question:** Can the \( z_\alpha \) become the elementary “spinon” excitations of a fractionalized phase?

Physics must be invariant under the U(1) gauge transformation

\[ z_\alpha \rightarrow e^{i\theta} z_\alpha \]
Possible theory for fractionalization and topological order

**Naive expectation:** Low energy theory of fractionalized phase of spinons
is a U(1) gauge theory of the $S = 1/2$ $z_\alpha$ complex scalars

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

where $v < 0$ for easy plane case, and $v = 0$ for SU(2) symmetry.

This expectation is too naive, and ignores the crucial confinement properties of compact U(1) gauge theory and the influence of “Berry phases”.

**Z₂ gauge theory for fractionalization and topological order**

Break U(1) gauge symmetry down to Z₂ by condensing a charge 2 Higgs scalar Φ (E. Fradkin and S. Shenker, Phys. Rev. D 19, 3682 (1979)). Under a gauge transformation:

\[ \Phi \rightarrow e^{2i\theta} \Phi \]

Simplest gauge-invariant and spin-rotation invariant coupling between Φ and \( z_\alpha \):

\[ \Phi^* \epsilon_{\alpha\beta} z_\alpha \partial_r z_\beta. \]

‘Higgs’ phase with \( \langle \Phi \rangle \neq 0 \) has the properties:

- Description in terms of an effective \( Z_2 \) gauge theory. The spinons \( z_\alpha \) are deconfined and carry a \( Z_2 \) gauge charge.
- Vison (vortex) excitation which carries \( Z_2 \) gauge flux
- Four-fold degeneracy on a torus.
- Coplanar spin correlations generated by coupling between Φ and \( z_\alpha \).

Collinear magnetic order with $\langle \Phi \rangle = 0$.

A spin density wave:

$$\langle \vec{S}_i \rangle \propto (\cos(K \cdot r_i), \sin(K \cdot r_i), 0)$$

$$K = (\pi, \pi).$$
Coplanar magnetic order with $\langle \Phi \rangle \neq 0$.

A spin density wave:

$$\langle \vec{S}_i \rangle \propto (\cos(\mathbf{K} \cdot \mathbf{r}_i), \sin(\mathbf{K} \cdot \mathbf{r}_i), 0)$$

with

$$\mathbf{K} = (\pi + \langle \Phi \rangle, \pi + \langle \Phi \rangle).$$

Experimental realization: $CsCuCl_3$
Topologically ordered phase described by $Z_2$ gauge theory
Central questions:

Vary $J_{ij}$ smoothly until CM order is lost and a paramagnetic phase with $\langle n \rangle = 0$ is reached.

• What is the nature of this paramagnet?

• What is the critical theory of (possible) second-order quantum phase transition(s) between the CM phase and the paramagnet?
Berry Phases

\[ e^{iS\mathcal{A}} \]

\[ \mathcal{A} = 2 \sum A_\tau \pmod{4\pi} \]

\[ A_\tau \rightarrow \frac{1}{2} \times \left( \text{Area of triangle formed by } n(\tau), n(\tau + \Delta \tau), \text{ and an arbitrary reference } n_o \right) \]
Berry Phases

The area of the triangle formed by $n(\tau)$, $n(\tau + \Delta \tau)$, and an arbitrary reference $n_0$ is given by:

$$A_\tau \rightarrow \frac{1}{2} \times \text{Area of triangle formed by } n(\tau), n(\tau + \Delta \tau), \text{ and } n_0$$

The total area $\mathcal{A}$ is then:

$$\mathcal{A} = 2 \sum A_\tau \pmod{4\pi}$$
Theory for quantum fluctuations of Neel state

Discretize spacetime to a cubic lattice of sites $a$, include spin Berry phases, and account for gauge invariance and invariance under $A_\tau \rightarrow A_\tau + 2\pi$

$$Z = \prod_a \int d z_{a\alpha} d A_{a\mu} \delta (|z_{a\alpha}|^2 - 1) \exp \left( \frac{1}{g} \sum_{a,\mu} z_{a\alpha}^* e^{i A_{a\mu}} z_{a+\mu,\alpha} + \text{c.c.} \right)$$

$$+ i 2 S \sum_a \eta_a A_{a\tau}$$

$$+ \frac{1}{e^2} \sum_{\Box} \cos (\Delta_\mu A_{av} - \Delta_\nu A_{a\mu})$$

Here $\eta_a = \pm 1$ on the 2 square sublattices, and $z_{a\alpha}, \alpha = 1 \ldots N$, is a $N$-component complex scalar.

\[ Z = \prod_{a} \int d\bar{z}_{a\alpha} dA_{a\mu} \delta(|z_{a\alpha}|^2 - 1) \]
\[ \exp \left( \frac{1}{g} \sum_{a,\mu} \bar{z}_{a\alpha}^* \ e^{iA_{a\mu}} z_{a+\mu,\alpha} + \text{c.c.} + i2S \sum_{a} \eta_{a} A_{a\tau} + \frac{1}{e^2} \sum \cos (\Delta_{\mu} A_{a\nu} - \Delta_{\nu} A_{a\mu}) \right) \]
At large $g$, we can integrate $z_\alpha$ out, and work with effective action for the $A_{a\mu}$

$$Z = \prod_{a,\mu} \int dA_{a\mu} \exp \left( \frac{1}{e^2} \sum \cos (\Delta_\mu A_{av} - \Delta_\nu A_{a\mu}) + i2S \sum \eta_a A_{a\tau} \right)$$

This is compact QED in 2+1 dimensions with static charges $\pm 2S$ 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

\[ Z_{\text{dual}} = \sum_{\{m_j\}} \exp \left( -\frac{\pi}{2e^2} \sum_{j,j'} \frac{m_j m_{j'}}{|r_j - r_{j'}|} + 4\pi i S \sum_j m_j \chi'_j \right) \]

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

\[ Z_{\text{dual}} = \sum_{\{h_j\}} \exp \left( -\frac{e^2}{2} \sum_j (\Delta_\mu h_j - 2S\Delta_\mu x_j)^2 \right) \]

with the \( h_j \) integer heights.
The Berry phases now lead to height ‘offsets’ \( x_j = 0, 1/4, 1/2, 3/4 \) on the four dual sublattices.
For $S=1/2$ and large $e^2$, low energy height configurations are in exact one-to-one correspondence with dimer coverings of the square lattice.


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

$\Rightarrow$ There is a definite average height of the interface

$\Rightarrow$ **Ground state has bond order.**

Two possible bond-ordered paramagnets for $S=1/2$

There is a broken lattice symmetry, and the ground state is at least four-fold degenerate.

Topologically ordered phase described by $Z_2$ gauge theory
\[ Z = \prod_a \int d\bar{z}_{a\alpha} dA_{a\mu} \delta (|z_{a\alpha}|^2 - 1) \]

\[ \exp \left( \frac{1}{g} \sum_{a,\mu} z_{a\alpha}^* e^{iA_{a\mu}} z_{a+\mu,\alpha} + \text{c.c.} + i \sum_a \eta_a A_{a\tau} + \frac{1}{e^2} \sum \cos (\Delta_\mu A_{a\nu} - \Delta_\nu A_{a\mu}) \right) \]
Bond order in a frustrated $S=1/2$ XY magnet


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

$$H = 2J \sum_{\langle ij \rangle} \left( S_i^x S_j^x + S_i^y S_j^y \right) - K \sum_{\langle i j k l \rangle} \left( S_i^+ S_j^- S_k^- S_l^- + S_i^- S_j^+ S_k^+ S_l^+ \right)$$
Nature of quantum critical point

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

\[ \exp \left( \frac{1}{g} \sum_{a,\mu} \bar{z}_{a\alpha}^* e^{iA_{a\mu}} z_{a+\mu,\alpha} + \text{c.c.} + i2S \sum_a \eta_\alpha A_{a\tau} + \frac{1}{\epsilon^2} \sum \cos (\Delta_\mu A_{a\nu} - \Delta_\nu A_{a\mu}) \right) \]

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

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

\[ \exp \left( \frac{1}{g} \sum_{a,\mu} z_{a\alpha}^* e^{iA_{a\mu}} z_{a+\mu,\alpha} + \text{c.c.} + i2S \sum_a \eta_a A_a \tau + \frac{1}{e^2} \sum \cos (\Delta_\mu A_a - \Delta_\nu A_a) \right) \]

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

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

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

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

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

\[ \exp \left( \frac{1}{g} \sum_{a,\mu} \tilde{z}_{a\alpha}^* e^{iA_{a\mu}} \tilde{z}_{a+\mu,\alpha} + \text{c.c.} + i2S \sum_a \eta_\alpha A_{a\tau} + \frac{1}{\epsilon^2} \sum \cos (\Delta_\mu A_{a\nu} - \Delta_\nu A_{a\mu}) \right) \]

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

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

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

The Dasgupta-Halperin mapping now yields the dual theory

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

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

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

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

\[ \exp \left( \frac{1}{g} \sum_{a,\mu} \bar{z}_{a\alpha} e^{iA_{a\mu}} z_{a+\mu,\alpha} + \text{c.c.} + i2\sqrt{2} \sum_a \eta_a A_{a\tau} + \frac{1}{e^2} \sum_{\square} \cos (\Delta_{\mu} A_{a\nu} - \Delta_{\nu} A_{a\mu}) \right) \]

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

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

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

Upon including Berry phases, the previous theory becomes

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

$$
+ \frac{1}{g} \sum_{a,\mu} \cos (\Delta_\mu \theta_a - A_{a\mu}) + i2S \sum_a \eta_a A_{a\tau} \left. \right)
$$

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

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

where $q$ is the smallest integer such that

$$e^{i\pi Sq} = 1$$

i.e. $q = 4$ for $S$ half-odd-integer, $q = 2$ for $S$ odd integer, and $q = 1$ for $S$ even integer.

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

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

For \( S = 1/2 \), this is an \textbf{inverted XY model with a four-fold anisotropy}, \textit{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 \textbf{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 \textit{bond-ordered} paramagnet.

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

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

**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

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

\[ \exp \left( \frac{1}{g} \sum_{a,\mu} \bar{z}_{a\alpha} e^{iA_{a\mu}} z_{a+\mu,\alpha} + \text{c.c.} + i2S \sum_a \eta_a A_{a\tau} + \frac{1}{e^2} \sum \cos (\Delta_{\mu} A_{a\nu} - \Delta_{\nu} A_{a\mu}) \right) \]

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Identical critical theories for \(S=1/2\)!
Nature of quantum critical point

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

\[ \exp \left( \frac{1}{g} \sum_{a,\mu} \bar{z}^*_{a\alpha} e^{iA_{a\mu}} z_{a+\mu,\alpha} + \text{c.c.} + i2S \sum_a \eta_a A_{a\tau} + \frac{1}{e^2} \sum \cos (\Delta_\mu A_{a\nu} - \Delta_\nu A_{a\mu}) \right) \]

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Identical critical theories for \(S=1/2\)!
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

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

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

Evaluation of functional determinant for $S = 1/2$ shows

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

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

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

E. Easy plane case for $N=2$

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

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

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

Critical theory is not expressed in terms of order parameter of either phase.