Berry phases and magnetic quantum critical points of Mott insulators in two dimensions

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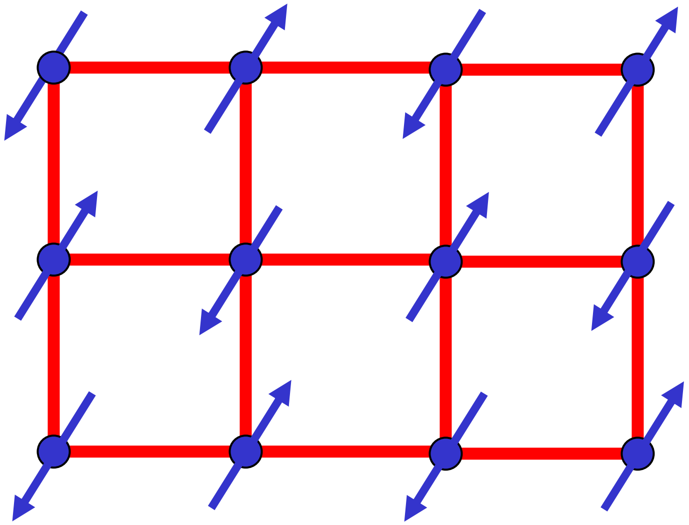
Parent compound of the high temperature superconductors: La_2CuO_4

Mott insulator: square lattice antiferromagnet



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

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

Néel order parameter: $\boldsymbol{n}_i = (-1)^{i_x + i_y}\, \vec{S}_i$

$$\langle \boldsymbol{n} \rangle \neq 0$$

Central questions:

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

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I. Effective lattice model: compact U(1) gauge theory, Berry phases, and monopoles.

Bond order in the paramagnet.

II. The CP^{N-1} representation (physical case: $N=2$)

III. "Solvable" limits and duality:

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 $N=2$

Berry phases make monopoles irrelevant at critical point

IV. Theory of quantum critical point

V. Conclusions: emergent "fractionalized" degrees of freedom at the quantum critical point, distinct from order parameters of both confining phases.

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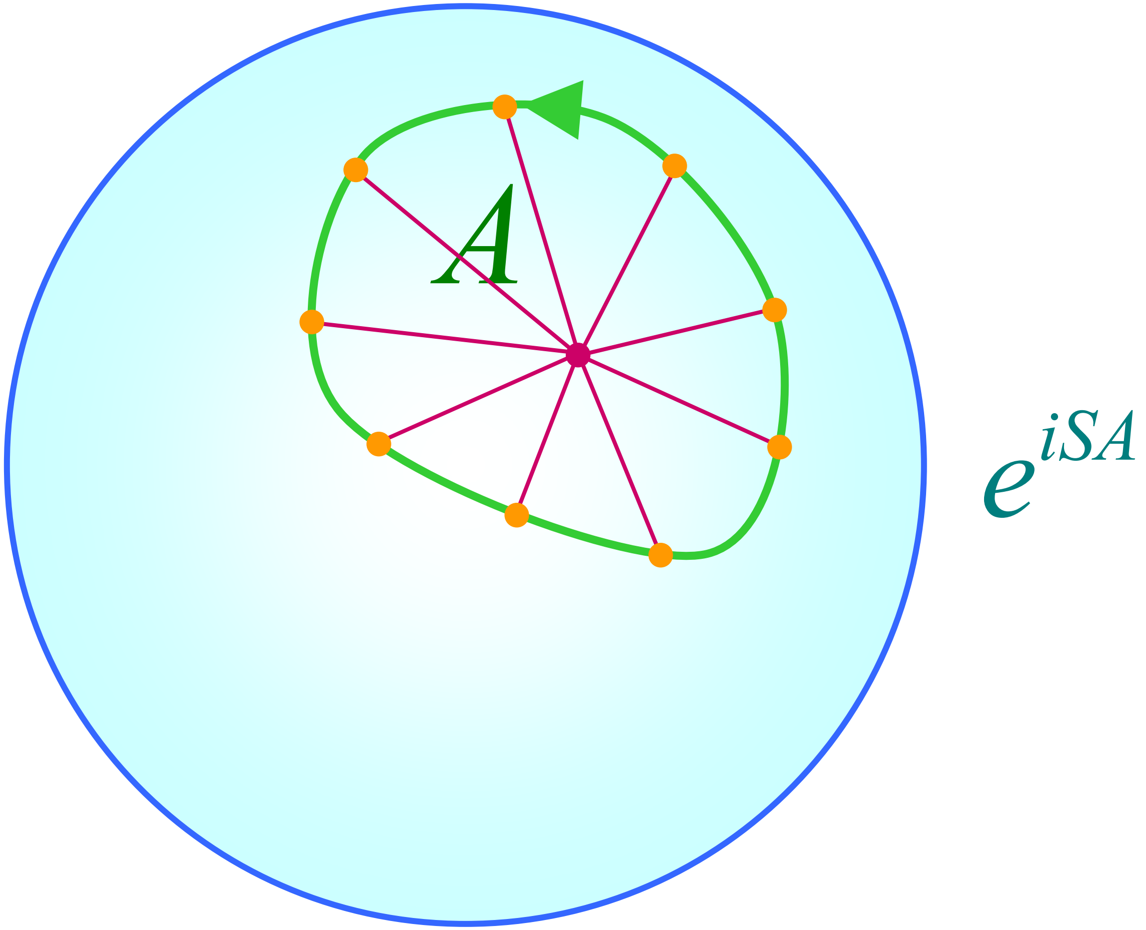
I. Effective lattice model: compact U(1) gauge theory, Berry phases, and monopoles

Write down path integral for quantum spin fluctuations

Key ingredient: Spin Berry Phases



$$e^{iSA}$$

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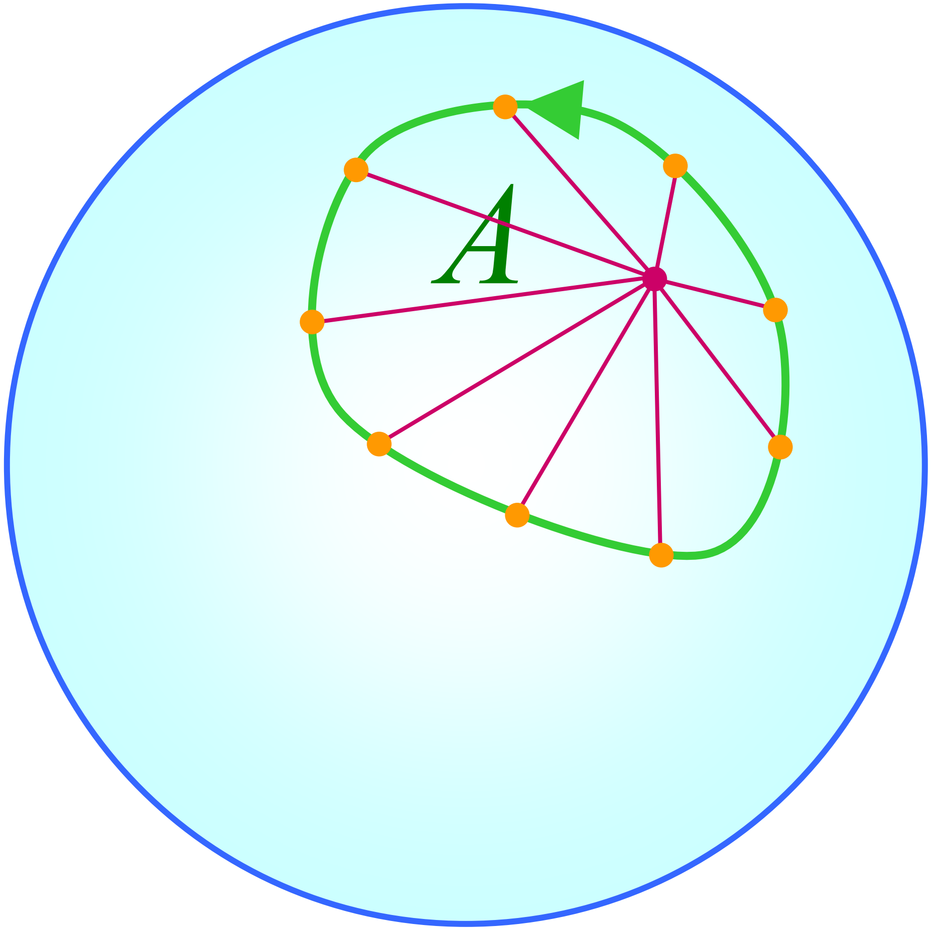

$$e^{iSA}$$

I. Effective lattice model: compact U(1) gauge theory, Berry phases, and monopoles

Path integral for quantum spin fluctuations on spacetime discretized on a cubic lattice:

- Action depends upon relative orientation of Neel order at nearby points in spacetime

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

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

$\boldsymbol{n}_a \sim \eta_a \vec{S}_a \rightarrow$ Neel order parameter;

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Path integral for quantum spin fluctuations on spacetime discretized on a cubic lattice:

- Action depends upon relative orientation of Neel order at nearby points in spacetime

- Complex Berry phase term on every temporal link.

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

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

$\boldsymbol{n}_a \sim \eta_a \vec{S}_a \rightarrow$ Neel order parameter;

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

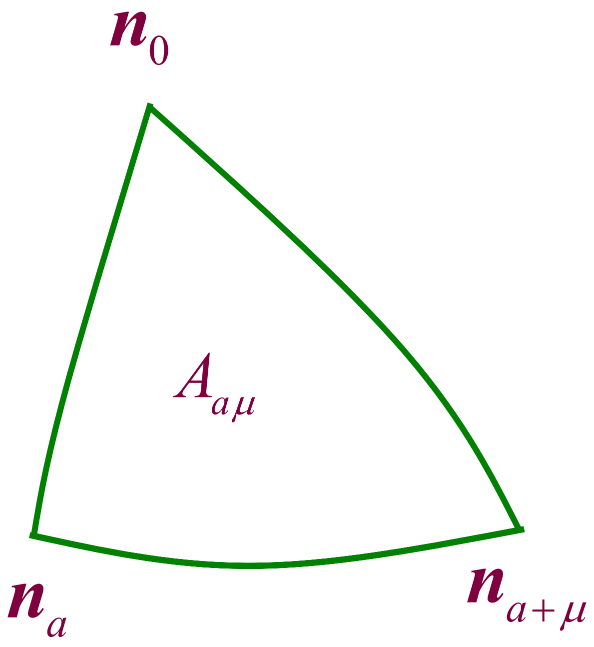
formed by $\boldsymbol{n}_a$, $\boldsymbol{n}_{a+\mu}$, and an arbitrary reference point $\boldsymbol{n}_0$

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

Small g → Spin-wave theory about Neel state receives minor modifications from Berry phases.

Large g → Berry phases are crucial in determining structure of paramagnetic phase with $\langle \boldsymbol{n}_a \rangle = 0$

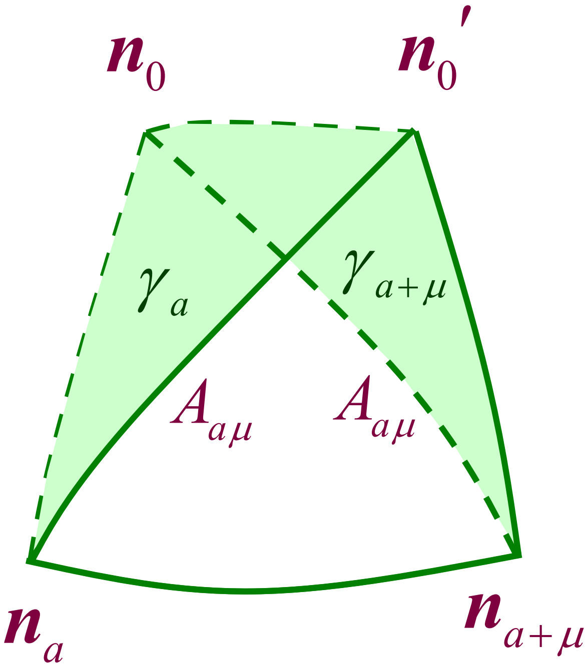
Integrate out $\boldsymbol{n}_a$ ***to obtain effective action for*** $A_{a\mu}$


$\boldsymbol{n}_0$
$A_{a\mu}$
$\boldsymbol{n}_a$
$\boldsymbol{n}_{a+\mu}$

Change in choice of $\boldsymbol{n}_0$ is like a "gauge transformation"

$$A_{a\mu} \to A_{a\mu} - \gamma_{a+\mu} + \gamma_a$$

(γ_a is the oriented area of the spherical triangle formed by $\boldsymbol{n}_a$ and the two choices for $\boldsymbol{n}_0$).



The area of the triangle is uncertain modulo 4π, and the action is invariant under

$$A_{a\mu} \to A_{a\mu} + 4\pi$$

These principles strongly constrain the effective action for $A_{a\mu}$ which provides description of the large g phase

Simplest large g effective action for the $A_{a\mu}$

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

with $e^2 \sim g^2$

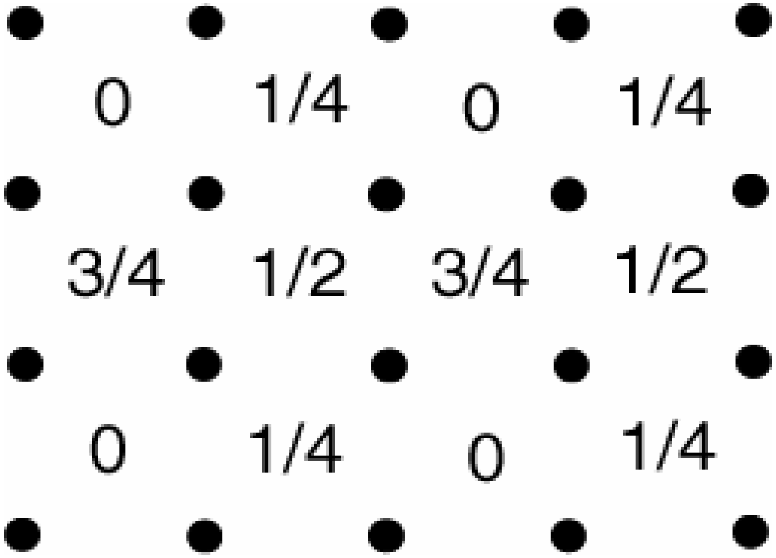
This is compact QED in 2+1 dimensions with static charges ± 1 on two sublattices.

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).

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

$$Z_{\text{dual}} = \sum_{\{m_{\bar{\jmath}}\}} \exp\left(-\frac{\pi}{2e^2} \sum_{\bar{\jmath},\bar{\jmath}'} \frac{m_{\bar{\jmath}} m_{\bar{\jmath}'}}{|r_{\bar{\jmath}} - r_{\bar{\jmath}'}|} + 2\pi i \sum_{\bar{\jmath}} m_{\bar{\jmath}} \mathcal{X}_{\bar{\jmath}} \right)$$

with the $m_{\bar{\jmath}}$ integer monopole charges. Each monopole carries a Berry phase (F.D.M. Haldane, *Phys. Rev. Lett.* **61**, 1029 (1988)) determined by the fixed $\mathcal{X}_{\bar{\jmath}} = 0, 1/4, 1/2, 3/4$ on the four dual sublattices.



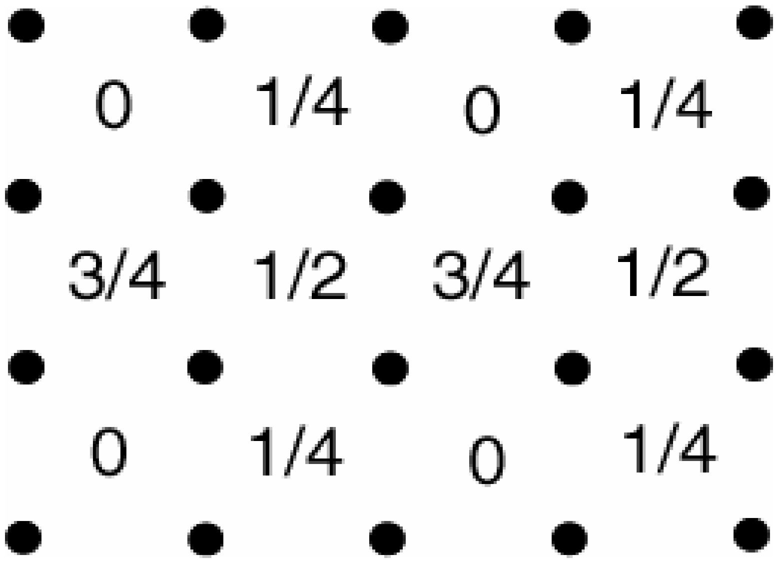
N. Read and S. Sachdev, *Phys. Rev. Lett*. **62**, 1694 (1989).

Alternative representation is in terms of a “height” model

$$Z_{\mathrm{dual}} = \sum_{\{h_{\bar{\jmath}}\}} \exp\left(-\frac{e^2}{2} \sum_{\bar{\jmath}} \left(\Delta_\mu h_{\bar{\jmath}} - \Delta_\mu \mathcal{X}_{\bar{\jmath}} \right)^2 \right)$$

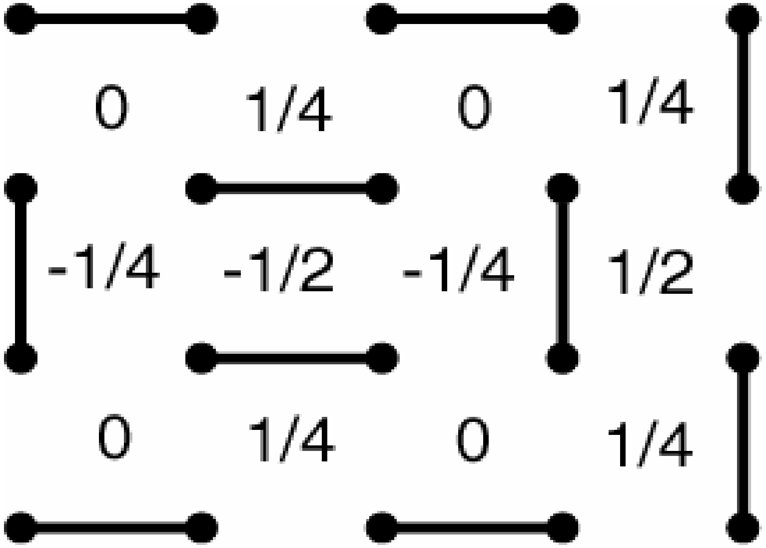
with the $h_{\bar{\jmath}}$ integer heights.

The Berry phases now lead to height ‘offsets’ $\mathcal{X}_{\bar{\jmath}} = 0, 1/4, 1/2, 3/4$ on the four dual sublattices.



For large e^2 , low energy height configurations are in exact one-to-one correspondence with dimer coverings of the square lattice

⟹ 2+1 dimensional height model is the path integral of the **Quantum Dimer Model** D. Rokhsar and S.A. Kivelson, *Phys. Rev. Lett*. **61**, 2376 (1988); E. Fradkin and S. A. Kivelson, *Mod. Phys. Lett*. B **4**, 225 (1990))



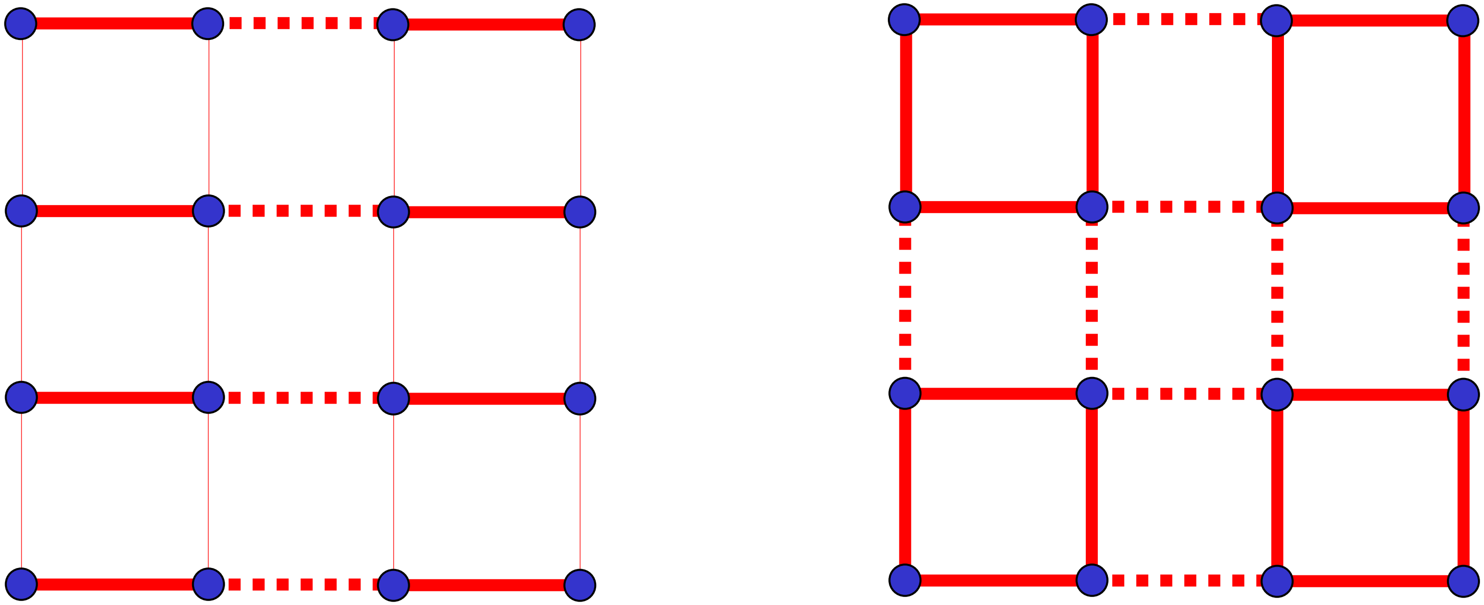
There is no roughening transition for three dimensional interfaces, which are smooth for all couplings

⟹ There is a definite average height of the interface

⟹ **Ground state has bond order.**

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

Two possible bond-ordered paramagnets



Distinct lines represent different values of $\left\langle \vec{S}_i \bullet \vec{S}_j \right\rangle$ on links

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

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

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II. The CP^{N-1} representation

Lattice model for

- the small *g* Neel phase,
- the large *g* bond-ordered paramagnet, and
- the transition(s) between them.

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

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

Here $z_{a\alpha}$, $\alpha = 1 \ldots N$, is a N-component complex scalar. We are interested in the case $N = 2$ where $\alpha = \uparrow, \downarrow$, and $\mathbf{n}_a = z_{a\alpha}^* \sigma_{\alpha\beta} z_{a\beta}$ with σ the Pauli matrices.

We will analyze a sequence of simpler models, starting with the case $N = 1$, non-compact gauge fields, and no Berry phases, and then put back these features.

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

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

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

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

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 ψ 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 ψ is a creation operator for *vortices* in the original theory of a "Ginzburg-Landau superconductor" coupled to "electromagnetism".

C. Dasgupta and B.I. Halperin, *Phys. Rev. Lett.* **47**, 1556 (1981).

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

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

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

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_{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.

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

Upon including Berry phases, the previous theory becomes

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

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

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

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.

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

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

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

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

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!*

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Identical critical theories !

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III D. $N \to \infty$, compact U(1), Berry phases

Near the critical point of the $N = \infty$ non-compact theory, integrate out z_α quanta (with gap Δ) in the presence of a Dirac monopole with $A_\mu = A_\mu^D$ with magnetic charge $q = 4$. The functional determinant yields the action of such a monopole, and the scaling dimension of the monopole insertion

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

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

Evaluation of functional determinant shows

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

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

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

G. Murthy and S. Sachdev, Nucl. Phys. B **344**, 557 (1990).

III E. Easy plane case for *N*=2

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

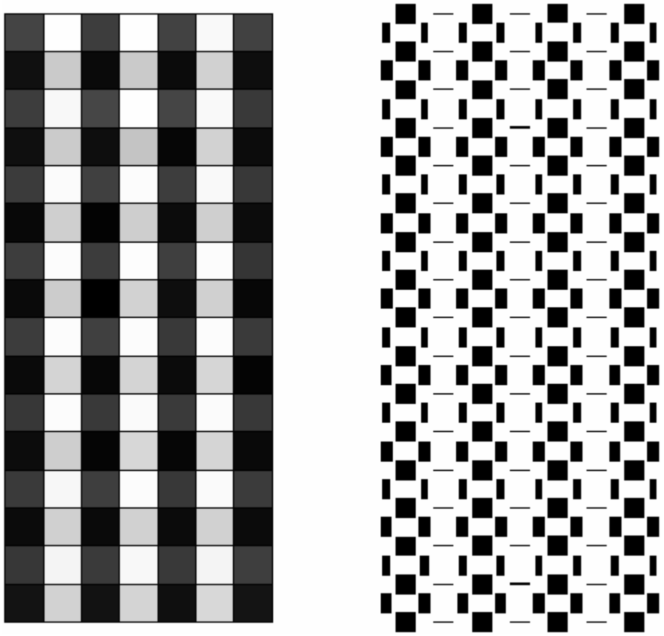
- monopoles are relevant without Berry phases,
- monopoles are irrelevant at the critical point in the presence of Berry phases, and
- monopoles drive the appearance of bond order in the paramagnetic phase.

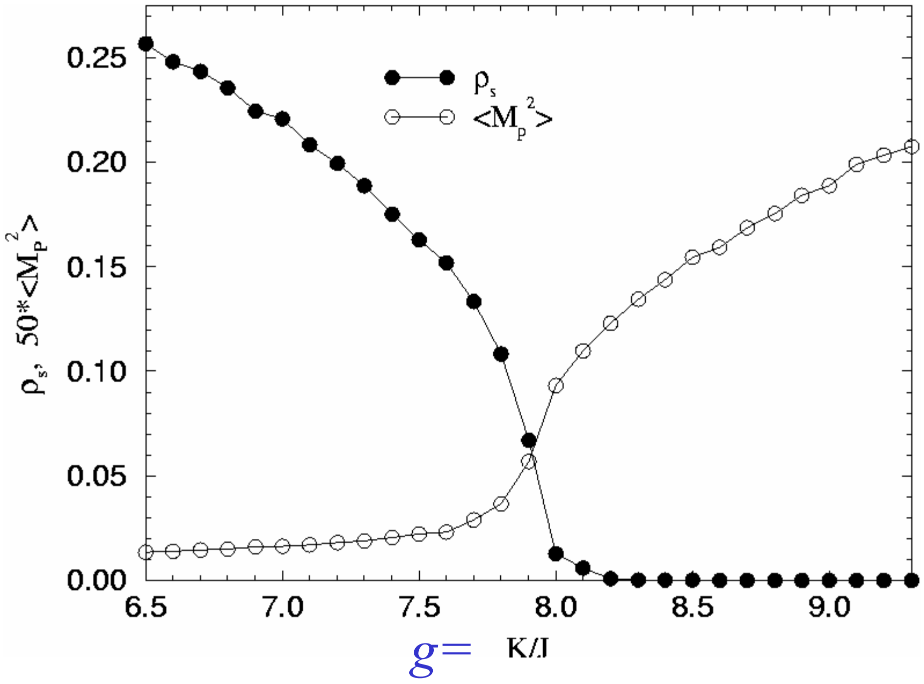
C. Lannert, M.P.A. Fisher, and T. Senthil, Phys. Rev. B **63**, 134510 (2001).
S. Sachdev and K. Park, Annals of Physics, **298**, 58 (2002).
O. Motrunich and A. Vishwanath, to appear.
T. Senthil *et al.*, to appear.

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

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

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





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

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IV. Theory for critical point

All this evidence makes it likely that Berry phases make monopoles irrelevant also at the critical point with $N = 2$ and full SU(2) symmetry.

To obtain the critical theory, take the naive continuum limit of lattice model, neglecting *both monopoles and Berry phases:*

$$\begin{aligned} \mathcal{S}_{\text{critical}} &= \int d^2x d\tau \Bigg[|(\partial_\mu - iA_\mu) z_\alpha|^2 + r\,|z_\alpha|^2 + \frac{u}{2}\left(|z_\alpha|^2\right)^2 + v|z_\uparrow|^2|z_\downarrow|^2 \\ &\qquad \frac{1}{4e^2}\left(\partial_\mu A_\nu - \partial_\nu A_\mu\right)^2 \Bigg] \end{aligned} \qquad (1)$$

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

For $r < r_c$, we have the Neel state with order parameter $\mathbf{n} = z^*_\alpha \sigma_{\alpha\beta} z_\beta$, $\langle \mathbf{n} \rangle \neq 0$.

For $r > r_c$, we have the paramagnet with bond order. The bond order is associated with modulations in the average 'electric flux' of the U(1) gauge field.

CRITICAL THEORY IS NOT EXPRESSED IN TERMS OF ORDER PARAMETER OF EITHER PHASE

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Berry phases make monopoles irrelevant at critical point

IV. Theory of quantum critical point

V. Conclusions: emergent "fractionalized" degrees of freedom at the quantum critical point, distinct from order parameters of both confining phases.