Topological order in Mott insulators and dimer models

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http://ipht.cea.fr/Images/Pisp/gmisguich

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Outline

□ The Lieb-Shultz-Mattis (D=1, 1961)-Hastings (D>1, 2004) theorem:

Mott insulators with a gap should be either

- conventionally ordered,
- or topologically ordered

Heisenberg (« RVB ») spin liquids and Kitaev's toric code

Quantum dimer models as toy models for (Z2) topological order: Entanglement and vortex excitations





Part I The Lieb-Schultz-Mattis-Hastings theorem

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 Electrons hopping on a lattice
 + odd number of electrons per unit cell.
 (would be a metal according to non-interacting band theory)
 Consider a *half-filled* system for simplicity.

$$H = \sum_{\substack{i < j \\ \sigma = \uparrow \downarrow}} t_{ij} \left(c_{i\sigma}^+ c_{j\sigma} + H.c. \right)$$

Strong on-site electron-electron repulsion (=Hubbard model)

 \rightarrow insulator (charge excitations are gapped)

$$+U\sum_{i}C_{i\uparrow}^{+}C_{i\uparrow}C_{i\downarrow}^{+}C_{i\downarrow}$$

In the limit of infinite repulsion

 \rightarrow spin-1/2 Heisenberg model with an **odd** number of sites/cell

$$H = \sum_{i < j} J_{ij} \vec{S}_i \cdot \vec{S}_j$$
, $J_{ij} = 4 rac{{t_{ij}}^2}{U}$

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The Lieb-Shutlz-Mattis theorem

D=1 Lieb-Schultz-Mattis (D=1: 1961)

D>1 Hastings [PRB 69, 104431 (2004)] (see also Affleck 1988; Bonesteel 1989; Oshikawa 2000, GM *et al.* 2002) Nachtergaele & Sims, Com. Math. Phys. 276, 437 (2007).

"A system with a half-odd-integer spin in the unit cell

(+ periodic boundary conditions, $[S_{tot}^z, H]=0$ & dimensions $L_1 \times L_2 \times ... \times L_D$ with $L_2 \times ... \times L_d = odd$) cannot have simultaneously a gap and a unique ground-state (in the thermodynamic limit). "



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Oshikawa's argument (I)



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Oshikawa's argument (II)

 \Box H_a is translation invariant \Rightarrow k is well defined and indep. of θ $U = \prod \exp\left(2i\pi \frac{x_i}{L_x}S_i^z\right)$ U does generally not commute with translations : $TU = UT \exp\left(2i\pi \frac{S_{\rm tot}^z}{L_r}\right) \exp\left(2i\pi CS\right)$ **-**2π x-translation Magnetization per site Momentum shift : $k_0 = k_{2\pi} + 2\pi C(S + \vec{m}^z)$ \mathbf{k}_0 θ 2π Consider $m^z=0$, S=1/2 and C=odd (=n L_v in 2D): $k_0 = k_{2\pi} + \pi$ □ If (we assume that) the gap to excited states do not close during the adiabatic process, $k_0 + \pi$ θ The ground state is (at least) two-fold degenerate k₀ 0 2π G. Misguich 7

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Part II short-range resonating valencebond (RVB) spin liquids & (Z₂) topological order

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Some examples of topologically ordered spin model

Kitaev's "toric code" (but no conserved particle number/magnetization)



Balents, Fisher & Girvin, Phys. Rev. B **65**, 224412 (2002) Sheng & Balents, Phys. Rev. Lett. **94**, 146805 (2005)

$$H = J_{z} \sum_{h \text{ hexagon}} \left(\left(S_{h1}^{z} + \dots + S_{h6}^{z} \right)^{2} + J_{\perp} \sum_{h \text{ hexagon}} \left(\left(S_{h1}^{x} + \dots + S_{h6}^{x} \right)^{2} + \left(S_{h1}^{y} + \dots + S_{h6}^{y} \right)^{2} \right)$$



 $J_{\perp} \ll J_{z}$

h hexagon

SU(2) symmetric (=Heisenberg-like) spin models

Raman-Moessner-Sondhi, Phys. Rev. B **72**, 064413 (2005) Ring exchange on the triangular lattice ? (GM *et al.*, PRB 1999)

Experiments. Candidates to be "spin liquids", apparently all gapless...why ?

 \Box CS₂CUCl₄ [Anisotropic S=1/2 triangular lattice, Coldea *et al.* 2003]

 \Box K-(BEDT-TTF)₂Cu₂(CN)₃ [Shimizu *et al.* 2003]

□ ZnCu₃(OH)₆Cl₂ [Helton *et al.* 2007, Mendels *et al.* 2007, Ofer *et al.* 2007, Imai *et al.* 2007]

□ Na₄Ir₃O₈ [3D lattice of corner sharing triangles, "hyper kagome", Okamoto *et al.* 2007]

□ He³ films [Nuclear magnetism on a triangular lattice, Masutomi *et al.* 2004]



Short-range RVB picture

P. W. Anderson's idea (1973) : (short-ranged) resonating valence-bond (RVB)

Linear superposition of many (exponential) low-energy short-range valence-bond configurations



Spatially *uniform* state (P.W. Anderson, 1973)

 $\Box \text{ Spin-}\frac{1}{2} \text{ excitations } ?$

Crystal of singlets \rightarrow linear potential between spinons Liquid of singlets \rightarrow we *may* expect deconfined spinons







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Topological degeneracy & spinon fractionalization

fractional spin-¹/₂ magnetic excitation (spinon)





adiabatic process \rightarrow New ground-state

Topological degeneracy (X.-G. Wen 1991) ↔ fractionalization See also Oshikawa & Senthil PRL 96, 060601 (2006) 2-fold degeneracy \Rightarrow Satisfies LSMH

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Schwinger bosons

Schwinger boson representation of the SU(2) spin algebra

$$S^{z} = \frac{1}{2} \begin{pmatrix} b^{+}_{\uparrow} b_{\uparrow} - b^{+}_{\downarrow} b_{\downarrow} \end{pmatrix}$$
$$S^{+} = b^{+}_{\uparrow} b_{\downarrow} \qquad S^{-} = b^{+}_{\downarrow} b_{\uparrow}$$
$$b^{+}_{\uparrow} + b^{+}_{\downarrow} b_{\downarrow} = 2S \text{ at each site}$$

$$\vec{S}_{r} \cdot \vec{S}_{r'} = S^{2} - \frac{1}{2} A_{rr'}^{+} A_{rr'} \quad \text{Heisenberg interaction}$$

$$\vec{A}_{rr'}^{+} = \left(b_{\uparrow r}^{+} b_{\downarrow r'}^{+} - b_{\downarrow r}^{+} b_{\uparrow r'}^{+} \right) \text{Bond operator - spin singlet}$$

Path integral formulation

$$Z = \operatorname{Tr}[\exp(-\beta H)]$$

$$= \int D[b_{r\uparrow}(\tau), b_{r\downarrow}(\tau), \lambda_{r}(\tau)] \exp(-S_{eff})$$

$$S_{eff}' = \int d\tau \sum_{r} \left(b_{r\uparrow}^{+} \partial_{\tau} b_{r\uparrow} + b_{r\downarrow}^{+} \partial_{\tau} b_{r\downarrow} \right) + i \int d\tau \sum_{r} \lambda_{r} \left(b_{r\uparrow}^{+} b_{r\uparrow} + b_{r\downarrow}^{+} b_{r\downarrow} - 2S \right)$$

$$- \int d\tau \sum_{rr'} \left\{ \frac{\int_{rr'}}{2} \frac{(b_{\uparrow r} b_{\downarrow r'} - b_{\downarrow r} b_{\uparrow r'})^{+} (b_{\uparrow r} b_{\downarrow r'} - b_{\downarrow r} b_{\uparrow r'})}{A_{rr'}} \right\}$$
Hubbard-Stratonovich \rightarrow spinons interacting with bond fields $Q_{rr'}$

$$Z = \int D[b_{r\uparrow}, b_{r\downarrow}, Q_{rr'}, \lambda_{r}] \exp(-S_{eff}')$$

$$S_{eff}' = \int d\tau \sum_{rr'} \left\{ 2 \frac{|Q_{rr'}|^{2}}{J_{rr'}} - Q_{rr'}^{+} \frac{(b_{\uparrow r} b_{\downarrow r'} - b_{\downarrow r} b_{\uparrow r'})}{A_{rr'}} - Q_{rr'}(b_{\uparrow r} b_{\downarrow r'} - b_{\downarrow r} b_{\uparrow r'}) - Q_{rr'}(b_{\uparrow r}^{+} b_{\downarrow r'}^{+} - b_{\downarrow r}^{+} b_{\uparrow r'}^{+})$$

$$+ \cdots \qquad (exact so far)$$

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Saddle point approximation

Saddle point approximation - equivalent to a self-consistent mean field approx.

$$\begin{split} \vec{S}_{r} \cdot \vec{S}_{r'} &= S^{2} - \frac{1}{2} A_{rr'}^{+} A_{rr'} \\ \left\langle A_{rr'}^{+} A_{rr'} \right\rangle &\approx A_{rr'}^{+} \left\langle A_{rr'} \right\rangle + \left\langle A_{rr'}^{+} \right\rangle A_{rr'} - \left\langle A_{rr'}^{+} \right\rangle \left\langle A_{rr'} \right\rangle \\ 2Q_{rr'}^{0} &= J_{rr'} \left\langle A_{rr'} \right\rangle \\ \left\langle b_{r\uparrow}^{+} b_{r\uparrow} + b_{r\downarrow}^{+} b_{r\downarrow} \right\rangle &= 2S \end{split}$$

Note:

Can be motivated as a large-N limit With *N*: number of boson flavors (Read & Sachdev)

■ Mean-field Hamiltonian :
$$H_{MF} = -\sum_{\langle rr' \rangle} Q_{rr'}^{0+} \underbrace{\left(b_{\uparrow r} b_{\downarrow r'} - b_{\downarrow r} b_{\uparrow r'}\right)}_{A_{rr'}} + H.c$$

$$-\sum_{r} \lambda_r^0 \left(b_{\uparrow r}^+ b_{\uparrow r} + b_{\downarrow r}^+ b_{\downarrow r} - 2S\right)$$

□ Bogoliubov transformation → mean-field RVB spin liquid with free (gapped) spinons, (we assume no Bose condensation (i.e. magnetic/Néel LRO) ok for small enough S)

□ Is such an approximation reliable ? Effect of the (neglected) fluctuations ?

Fluctuations about the saddle point: Z₂ gauge field

❑ Most important fluctuation modes for the long-distance properties of the system ? ⇒ Gauge modes

Parametrize the sign fluctuations the bond field Q

Mean field value

$$Q_{ij}(\tau) = Q_{ij}^{0} \sigma_{ij}^{z}(\tau)$$

$$\sigma_{ij}^{z}(\tau) = \pm 1$$

$$Z_{2} \text{ gauge invariance} \qquad \eta_{i} = \pm 1$$

$$b_{\uparrow i} \rightarrow \eta_{i} b_{\uparrow i}$$

$$b_{\downarrow i} \rightarrow \eta_{i} b_{\downarrow i}$$

$$\sigma_{ij}^{z} \rightarrow \eta_{i} \eta_{j} \sigma_{ij}^{z}$$

$$Quantization \rightarrow Gauss Law$$

$$G_{i} = \exp\left[i\pi(b_{i\uparrow}^{+}b_{i\uparrow} + b_{i\downarrow}^{+}b_{i\downarrow})\right]\prod_{j} \sigma_{ij}^{x} \qquad \sigma^{x}\sigma^{z} = -\sigma^{z}\sigma^{x}$$

$$\forall i \quad G_{j}|phys\rangle = G_{j}|phys\rangle$$

$$= \text{local constraint of physical states}$$

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A toy model describing the fluctuations





A toy model describing the fluctuations: toric code limit

"Toric code" limit

$$\begin{array}{c} t = 0 \\ \Gamma = 0 \\ V = \infty \end{array} \right\} \rightarrow H = \Delta \sum_{i} \left(b_{i\uparrow}^{+} b_{i\uparrow} + b_{i\downarrow}^{+} b_{i\downarrow} \right) - K \sum_{ijkl} \sigma_{ji}^{z} \sigma_{jk}^{z} \sigma_{kl}^{z} \sigma_{ji}^{z} \\ b_{i\uparrow}^{+} b_{i\uparrow} + b_{i\downarrow}^{+} b_{i\downarrow} = 0 \text{ or } 1 \\ \underbrace{(-1)^{b_{i\uparrow}^{+} b_{i\uparrow} + b_{i\downarrow}^{+} b_{i\downarrow}}_{\text{Gauss law}} \right] \rightarrow 2 \left(b_{i\uparrow}^{+} b_{i\uparrow} + b_{i\downarrow}^{+} b_{i\downarrow} \right) = 1 - \prod_{j} \sigma_{ij}^{z} \\ H = -\frac{\Delta}{2} \sum_{i} \left(\prod_{j} \sigma_{ij}^{z} \right) - K \sum_{ijkl} \sigma_{ij}^{z} \sigma_{jk}^{z} \sigma_{kl}^{z} \sigma_{li}^{z} \\ = \text{Kitaev's toric code} \\ (= \text{solvable toy model for a topologically ordered ground state} \right)$$

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Part III Quantum dimer models

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Quantum dimer models



Dimer liquid phase in the triangular QDM

Hamiltonian [Moessner & Sondhi, 2001]



First *simple* model with a short-ranged RVB liquid. Moessner & Sondhi, Phys. Rev. Lett. (2001) Ralko *et al.*, Phys. Rev. B 74, 134301 (2006) + refs. Therein GM and Mila, Phys. Rev. B 77, 134421 (2008)

 $|g.s.\rangle = \sum_{c \in \{\text{coverings}\}} |c\rangle$

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Rokhsar-Kivelson point - triangular QDM

At J=V=1, the Hamiltonian can be written as

$$H = 2\sum_{r} |\psi_{r}\rangle \langle \psi_{r}| = \text{Sum of projectors}$$

$$|\psi_{r}\rangle = \frac{1}{\sqrt{2}} \left(|\swarrow \rangle \rangle - |\land \rangle \right)$$

$$|g.s.\rangle = \sum_{c} |c\rangle$$

$$\langle \Psi_{r}|c\rangle = \begin{cases} \frac{1}{\sqrt{2}} |c_{\backslash r \backslash}\rangle & \text{if } |c\rangle = |\cdots |\land \rangle \\ -\frac{1}{\sqrt{2}} |c_{\backslash r \backslash}\rangle & \text{if } |c\rangle = |\cdots |\land \rangle \\ 0 & \text{otherwise} \end{cases}$$

$$\langle \Psi_{r}|g.s.\rangle = 0$$

$$\Rightarrow H|g.s.\rangle = 0 \Rightarrow \text{a ground - state}$$

Excitations of the toric code



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Excitations in the dimer liquid

Magnetic Z₂ vortices (« visons ») Analogy with the toric code

Electric charge = monomer



Magnetic charge = vison



$$|g.s.\rangle = \sum_{c \in \{\text{coverings}\}} |c\rangle$$
$$|vison\rangle \approx \sum_{c \in \{\text{coverings}\}} (-1)^{N(\Omega,c)} |c\rangle$$

Contrary to the toric code, this trial state is not an exact eigenstate... See also: GM, Serban & Pasquier PRL (2002)

Variational approximation (I)



$$S_{pp'} = \langle p | p' \rangle \neq 0$$
 overlapp
 $\langle p | H | p' \rangle \neq 0$ vison hopping



Overlap and dispersion relation are computed using Pfaffians

Variational approximation (I)



Overlap and dispersion relation are computed using Pfaffians (not easy...)

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Dispersion relation of the « magnetic » vortices



Dimer crystallization – Z_2 vortex condensation



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Reduced density matrices for RK wave functions





Probing topological order with entanglement entropy

□ A. Kitaev and J. Preskill, Phys. Rev. Lett. 96, 110404(2006)





See also: M. Levin and X.-G. Wen, Phys. Rev. Lett. 96, 110405(2006)



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Reduced density matrix for RK wave functions

$$|RK\rangle = \frac{1}{Z} \sum_{c} e^{-\frac{1}{2}\beta E(c)} |c\rangle$$

GM & V. Pasquier, work in progress...

Cylinder geometry



1) Write the transfer matrix M of the classical problem

2) find the ground state $|\psi\rangle$ of M (=assume an infinitely long cylinder). In the dimer case: 1D free fermions.

3) All the probabilities of the boundary states are contained in the ground state of M (the *full* RDM spectrum) :

$$p_{b} = \left| \left\langle b \right| \psi \right\rangle \right|^{2}$$

4) Compute the entanglement entropy

$$S = -\sum_{b} \left| \left\langle b \left| \psi \right\rangle \right|^2 \log \left(\left\langle b \left| \psi \right\rangle \right|^2 \right)$$



Summary

Lieb-Shultz-Mattis-Hastings theorem:

a gapped Mott insulator is either

- topologically ordered,
- or "conventionally" ordered.



⇒ Frustrated Heisenberg magnets may provide realizations of gapped topological states ... but no experimental evidence so far.

Quantum dimer models & RK wave functions offer tractable models to study entanglement, fractionalization and topological order.



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