Stability of time-reversal symmetry breaking spin liquid states in high-spin fermionic systems

Edina Szirmai

International School and Workshop on Anyon Physics of Ultracold Atomic Gases
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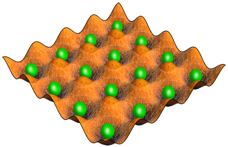
Quantum simulations with ultracold atoms



- Quantum simulation of fundamental models (properties, phenomena).
- Novel behavior, completely new phases are expected due to the high spin.

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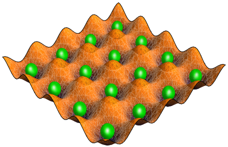

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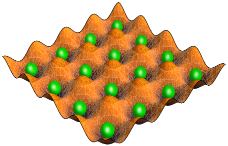
A possible explanation for the mechanism of high-T_c superconductivity and their strange behavior in the non-superconducting phase based on the strong magnetic fluctuation in dopped Mott insulators. These fluctuation can be treated within the spin liquid concept.

- High-T_c superconductors

Quantum simulations with ultracold atoms



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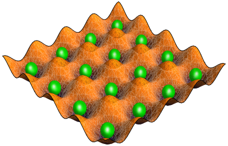
In topological phases of spin liquids the quasiparticles have fractional statistics. They are nonlocal and resist well against local perturbations. Promising qbit candidates.

- High-T_c superconductors
- Quantum information

Quantum simulations with ultracold atoms



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Low energy excitations above spin liquids can be described by effective gauge theories. Aim: to study various gauge theories with ultracold atoms.

- High-T_c superconductors
- Quantum information
- Simulation of gauge theories

Atoms loaded into an optical lattice

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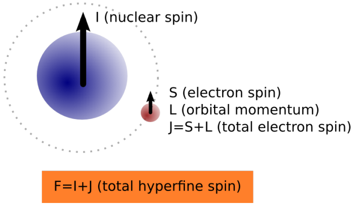

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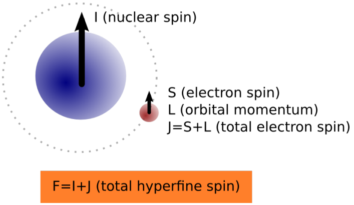

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Easy to control the model parameters:

- Interaction strength: Feshbach resonance
- Localization: laser intensity
- Lattice geometry

Outline

- Part I
  - Fundamentals of high spin systems
  - Spin wave description
  - Valence bond picture
- Part II
  - Competing spin liquid states of spin-3/2 fermions in a square lattice
  - Competing spin liquid states of spin-5/2 fermions in a honeycomb lattice
    - Properties of chiral spin liquid state
    - Stability of the spin liquid states beyond the mean-field approximation
    - Finite temperature behavior
    - Experimentally measurable quantities

In collaboration with:

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PRA 84 011611 (2011)

EPL 93, 66005 (2011)

Fundamental properties of high-spin systems

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The Hubbard Hamiltonian with n.n hopping and on-site interaction:

$$H = -t \sum_{<i,j>} c^{\dagger}_{i,\alpha} c_{j,\alpha} + \sum_{i} U^{\alpha,\beta}_{\gamma,\delta} c^{\dagger}_{i,\alpha} c^{\dagger}_{i,\beta} c_{i,\delta} c_{i,\gamma}.$$

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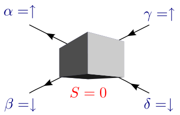
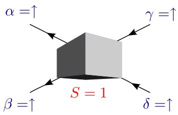
$$S = |F_1 - F_2|, \ldots |F_1 + F_2|$$
$$S_z = -S, \ldots S$$

F: individual atoms, S: total spin of 2 scattering atoms

2 components: $\uparrow$, and $\downarrow$





$F_1 = F_2 = \frac{1}{2}$,
$S = 0$: $S_z = 0$,
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4 components: $\pm\frac{3}{2}$, and $\pm\frac{1}{2}$

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$$S_z = -S, \dots S$$

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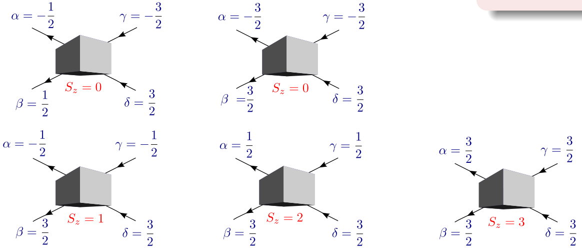

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$S = 0$: $S_z = 0$,

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$S = 2$: $S_z = -2, \dots, 2$

$S = 3$: $S_z = -3, \dots, 3$

Fundamental properties of high-spin systems

The Hamiltonian:

$$H = H_{kin} + H_{int}$$

where H_{int} contains many types of scattering processes.

on-site interaction

$\Longrightarrow$

Pauli's principle

The only nonzero terms are completly antisymmetric for the exchange of the spin of the two scattering particles.

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spin-1/2 fermions

Only singlet scatterings are allowed:

- $S_{tot} = 0$

$\Longrightarrow$

$H = -t\sum_{\langle i,j\rangle}(c^{\dagger}_{i,\sigma}c_{j,\sigma} + H.c.) + \sum_i U_0 \mathscr{P}^{(i)}_0$, and $\mathscr{P}^{(i)}_0 = c^{\dagger}_{i,\uparrow}c^{\dagger}_{i,\downarrow}c_{i,\downarrow}c_{i,\uparrow} = n_{i\uparrow}n_{i\downarrow}$ projects to the singlet subspace $S_{tot} = 0$.

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spin-3/2 fermions

Classification of the allowed scattering processes:

- $S_{tot} = 0$
- $S_{tot} = 2$

$\Longrightarrow$

$$H = -t\sum_{\langle i,j \rangle}(c^{\dagger}_{i,\sigma} c_{j,\sigma} + H.c.) + \sum_i \left[U_0 \mathscr{P}^{(i)}_0 + U_2 \mathscr{P}^{(i)}_2 \right],$$

and $\mathscr{P}^{(i)}_S = c^{\dagger}_{i,\sigma_1} c^{\dagger}_{i,\sigma_2} c_{i,\sigma_3} c_{i,\sigma_4} \hat{P}_S$, where $\hat{P}_S$ projects to the subspace $S_{tot} = S$.

T. L. Ho PRL (1998)

T. Ohmi and K. Machida JPSJ (1998)

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spin-5/2 fermions

Classification of the allowed scattering processes:

- $S_{tot} = 0$
- $S_{tot} = 2$
- $S_{tot} = 4$

$\Longrightarrow$

$$H = -t\sum_{\langle i,j\rangle}(c^\dagger_{i,\sigma}c_{j,\sigma} + H.c.) + \sum_i \left[U_0\mathscr{P}^{(i)}_0 + U_2\mathscr{P}^{(i)}_2 + U_4\mathscr{P}^{(i)}_4\right],$$

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Effective spin models in the strong coupling limit

The Hubbard Hamiltonian with n.n hopping and on-site interaction:

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spin independent interaction $\rightarrow$ SU(N) symmetry

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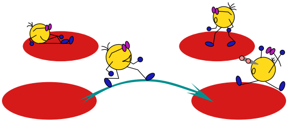
Strongly repulsive limit: $U/t \rightarrow \infty$

repulsive interaction, $f = 1/(2F+1)$ filling ($\#$ of particles $= \#$ of sites)

Perturbation theory up to leading order with respect to t.

- t preserves S and S_z
- nearest-neighbor hopping



Effective spin models in the strong coupling limit

Effective Hamiltonian (spin-F fermions in the $U/t \to \infty$ limit)

$$H = J \sum_{\langle i,j \rangle} c^\dagger_{i,\alpha} c^\dagger_{j,\beta} c_{j,\alpha} c_{i,\beta}$$

- nearest-neighbor interaction
- the same spin dependence that has the original model

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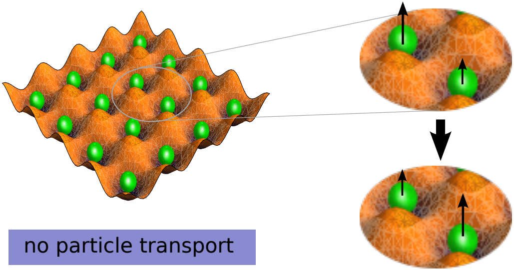

no particle transport

Mott state

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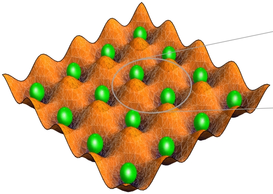

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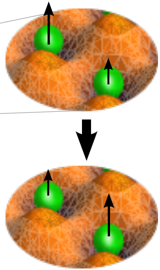

Mott state

Without long range spin order/preserved spin rotational invariance:
spin liquid state

Effective spin models in the strong coupling limit

($n_i = c^\dagger_{i,\sigma} c_{i,\sigma}$, and $\mathbf{S}_i = c^\dagger_{i,\sigma} \mathbf{F}_{\sigma,\sigma'} c_{i,\sigma'}$)

Spin exchange appears explicitly in the Hamiltonian:

- $F = \frac{1}{2}$: AFM Heisenberg model

$$H_{eff} = J \sum_{\langle i,j \rangle} \left(\mathbf{S}_i \mathbf{S}_j - \frac{1}{4} n_i n_j \right)$$

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$$H^{F=3/2}_{eff} = \sum_{\langle i,j \rangle} \left[a_0\, n_i n_j + a_1 \mathbf{S}_i \mathbf{S}_j + a_2 (\mathbf{S}_i \mathbf{S}_j)^2 + a_3 (\mathbf{S}_i \mathbf{S}_j)^3 \right]$$

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- $F = \frac{5}{2}$:

$$H^{F=5/2}_{eff} = \sum_{\langle i,j \rangle} \left[a_0\, n_i n_j + a_1 \mathbf{S}_i \mathbf{S}_j + a_2 (\mathbf{S}_i \mathbf{S}_j)^2 + a_3 (\mathbf{S}_i \mathbf{S}_j)^3 + a_4 (\mathbf{S}_i \mathbf{S}_j)^4 + a_5 (\mathbf{S}_i \mathbf{S}_j)^5 \right]$$

Let us consider a two-site problem:

$$\mathscr{H}_{i,j} = J\mathbf{S}_i\mathbf{S}_j$$

- Site-by-site picture:
  $\left|S_i^z = F, S_j^z = -F\right\rangle$: $E_{i,j} = -JF^2$.
  BUT this is not an eigenstate of $\mathscr{H}_{i,j} = JS_i^z S_j^z + \frac{J}{2}(S_i^+ S_j^- + S_i^- S_j^+)$.
  Let S^z fluctuate to gain energy

$\Rightarrow$ theory of AFM spin waves

Antiferromagnetic Heisenberg model: $H_{eff} = J\sum_{\langle i,j\rangle}\left(\mathbf{S}_i\mathbf{S}_j - \frac{1}{4}n_i n_j\right)$

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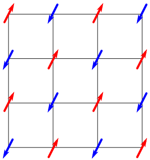
Fluctuation above the classical Néel state:



- Sublattice magnetization:
  $\langle S_A^z\rangle = -\langle S_B^z\rangle = F - \Delta F$.
- Description: magnon picture.

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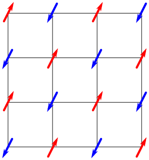

- Sublattice magnetization:
  $\langle S_A^z\rangle = -\langle S_B^z\rangle = F - \Delta F$.
- Description: magnon picture.
- Large $\Delta F \rightarrow$ "quantum melting" $\rightarrow$

Spin liquid

Basic concepts of AFM SWT and magnon picture:

- Description of the spin wave excitations $\rightarrow$ boson operators.
- Holstein-Primakoff transformation (and similar for sublattice B):

$$S^+_{A,j} = \left(2F - a^\dagger_j a_j\right)^{1/2} a_j \qquad S^-_{A,j} = a^\dagger_j \left(2F - a^\dagger_j a_j\right)^{1/2}$$

$$S^z_{A,j} = 2 - a^\dagger_j a_j$$

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- The ground state energy/bond (LSWT): $E_{i,j} = -JF(F+\zeta)$, with $0 < \zeta < 1$ and geometry-dependent.

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- If ΔF large from the LSWT:
  - Beyond LSWT.
  - Change concept.

Effective spin models in the strong coupling limit

- Even in case of the simplest $F = \frac{1}{2}$ case there exist lattices that have ground state without breaking of spin rotational invariance (no Néel order) in the thermodynamic limit.
- Various disordered spin sates occur in e.g.
  - finite systems,
  - frustrated systems,
  - systems described by Hamiltonian with higher power of $\mathbf{S}_i\mathbf{S}_j$.
- To describe these disordered states a powerful possibility:

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valence bond picture.

Valence bond picture

$F = 1/2$ AFM Heisenberg model

Fazekas, *Electron Correlation and Magnetism* (1999)

Affleck, Kennedy, Lieb, Tasaki, *Valence Bond Ground States in Isotropic Quantum Antiferromagnets* (1988)

Valence bond picture

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- Bond-by-bond picture:
  $\mathcal{H}_{i,j} = -JF(F+1) + \frac{J}{2}(\mathbf{S}_i + \mathbf{S}_j)^2 \quad \Rightarrow \quad |\mathbf{S}_i + \mathbf{S}_j| = 0$ (singlet)
  $E_{i,j} = -JF(F+1)$

  $\Rightarrow$ theory of valence bonds

Valence bond picture

Let us consider now larger lattice:

$$\mathscr{H} = \sum_{\langle i,j \rangle} \mathscr{H}_{i,j} = J \sum_{\langle i,j \rangle} \mathbf{S}_i \mathbf{S}_j$$

$$[ij] = \frac{1}{\sqrt{2}}[\alpha(i)\beta(j) - \beta(i)\alpha(j)] =$$ 

singlet bond

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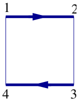
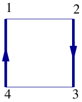
singlet bond

Singlet state on a lattice: letting all spins participate in pair bonds.

- The singlet basis for $L = 4$:

$[12][34] =$ 

and
$[23][41] =$ 

Valence bond picture

Let us consider now larger lattice:

$$\mathcal{H} = \sum_{\langle i,j \rangle} \mathcal{H}_{i,j} = J \sum_{\langle i,j \rangle} \mathbf{S}_i \mathbf{S}_j$$

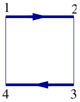
$$[ij] = \frac{1}{\sqrt{2}} [\alpha(i)\beta(j) - \beta(i)\alpha(j)] =$$

singlet bond

Singlet state on a lattice: letting all spins participate in pair bonds.

- The singlet basis for $L = 4$:

$[12][34] =$



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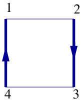
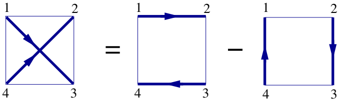


- One spin – one bond.
- Only non-crossing bonds:



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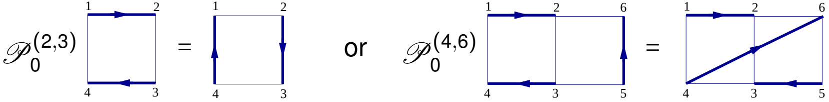
singlet bond

$$F = \frac{1}{2}$$

$\mathbf{S}_i\mathbf{S}_j = -\frac{1}{2}\mathscr{P}_0^{(i,j)} + \frac{1}{4}$, and $\mathscr{P}_0^{(i,j)}$ projects to the singlet subspace



Resonate between different configurations of the valence (singlet) bonds.

L. Hulthén (1938)

Valence bond picture

Let us consider now larger lattice:

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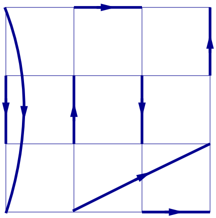
$[ij] = \frac{1}{\sqrt{2}} [\alpha(i)\beta(j) - \beta(i)\alpha(j)] =$ 

singlet bond

- Usually longer bonds appear.
- VB state: $|VB\rangle = \prod_{pairs} |[i,j]\rangle$
- RVB state: $|RVB\rangle = \sum_{conf} \prod_{pairs} \mathscr{A}(|i-j|)|[i,j]\rangle$
- Approximation: nearest-neighbor RVB



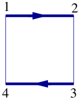
P. W. Anderson (1973)

Valence bond picture

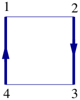
1) Simplest RVB system:

$L = 4$, isotropic HM, $F = 1/2$

$$\Psi_0 = \frac{1}{\sqrt{3}}([12][34] + [23][41]) = \frac{1}{\sqrt{3}}\Bigg(\quad + \quad \Bigg)$$



+



- $\mathscr{E}_0 = -2J$.
- $\langle \Psi_0 | S_j^z | \Psi_0 \rangle = 0$, for $\forall j$.
- $\langle \Phi_0 | S_1^z S_2^z | \Psi_0 \rangle = -1/6$, and $\langle \Phi_0 | S_1^z S_3^z | \Psi_0 \rangle = 1/12$

Valence bond picture

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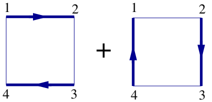

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$\Rightarrow$ No magnetic order but there is an AF correlation.

Valence bond picture

2) One-dimensional J_1-J_2 isotropic AFM HM, $F = 1/2$

$$H(J_1, J_2) = J_1 \sum_j \mathbf{S}_i \mathbf{S}_{j+1} + J_2 \sum_j \mathbf{S}_i \mathbf{S}_{j+2}$$

Valence bond picture

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- Majumdar-Ghosh model: $J_1 = 2J_2 \equiv J$.

$$H(J, J/2) = \frac{J}{4} \sum_j (\mathbf{S}_{j-1} + \mathbf{S}_j + \mathbf{S}_{j+1})^2 + const.$$

- The total spin of a "trion of site j" is either $S_{trion} = 1/2$ or 3/2
- $E = \frac{J}{4} L S_{trion} (S_{trion} + 1) + const. \quad \Rightarrow \quad S_{trion}^{(j)}(GS) = 1/2.$

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- Construct such a state.

Valence bond picture

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- Majumdar-Ghosh model: $J_1 = 2J_2 \equiv J$.

$$S^{(j)}_{trion}(GS) = 1/2$$

- 2-fold degeneracy.
- No magnetic order.
- (Discrete) translational inv. is broken!

spin liquid
$\leftrightarrow$
valence bond solid

Valence bond picture

- Dimer order parameter: $\mathscr{D}_j = A \langle \mathbf{S}_{j-1}\mathbf{S}_j - \mathbf{S}_j\mathbf{S}_{j+1} \rangle$ (with $A = -4/3J$).
- Why there is no resonance?
- Cancellations only in the MG case ($J_2/J_1 = 1/2$).

Valence bond picture

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  - Only short range AF correlations.
- RVB ground state below $J_2/J_1 \approx 0.24$.
  - Homogeneous: $\mathscr{D}_j = 0$.
  - $\langle \mathbf{S}_j^z \mathbf{S}_l^z \rangle$ decay algebraically $\rightarrow$ quasi-long range AF correlations.