Title: Quantum Spin Simulations (PHYS 7380) - Lecture 2

Date: Apr 06, 2010 11:00 AM

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Abstract:

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Quantum Spin Simulations

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lations

PERIMETER SCHOLARS INTERNATIONAL

Course on "Quantum Spin Simulations", April 5-23, 2010.

Instructor: Anders Sandvik Tutor Denis Dalidovich

This course introduces quantum spin systems and several computational methods for studying their ground-state and finite-temperature properties. Exact diagonalization and quantum Monte Carlo algorithms and their computer implementations are discussed in detail (including the use of lattice symmetries in complete and Lanczos diagonalization studies, and quantum Monte Carlo methods based on the stochastic series expansion as well as ground-state projection in the valence-bond basis). Applications of the methods are illustrated by results for some of the most essential models in quantum magnetism, such as the S=1/2 Heisenberg antiferromagnet in one and two dimensions, as well as extended models useful for studying quantum phase transitions between antiferromagnetic and magnetically disordered states in two dimensions.

PART 1: Introduction to quantum spin systems and quantum magnetism
[April 05] Classical and quantum spin systems and their significance; origin of quantum antiferromagnetism

PART 2: Exact diagonalization methods

PART 3: Quantum Monte Carlo methods

)rigin of antiferromagnetic interactions

nsights from a simple system: the 2-site Hubbard model

$$H_{12} = -t(c^\dagger_{2\uparrow}c_{1\uparrow} + c^\dagger_{1\uparrow}c_{2\uparrow} + c^\dagger_{2\downarrow}c_{1\downarrow} + c^\dagger_{1\downarrow}c_{2\downarrow}) + U(n_{1\uparrow}n_{1\downarrow} + n_{2\uparrow}n_{2\downarrow})$$

-particle subspace (half-filled band)

6 states in the Hilbert space: $|\uparrow\downarrow\rangle, \quad |\downarrow\uparrow\rangle, \quad |\uparrow\uparrow\rangle, \quad |\downarrow\downarrow\rangle, \quad |02\rangle, \quad |20\rangle$

details of the solution in tutorial

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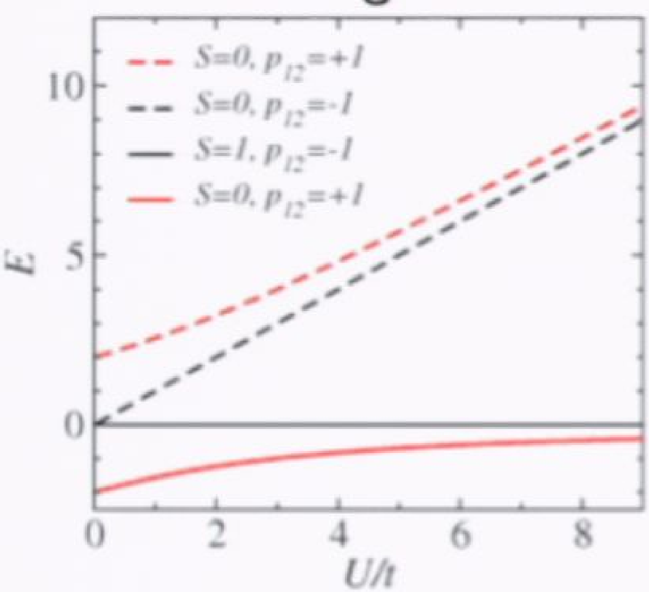
J large, 2 lowest states

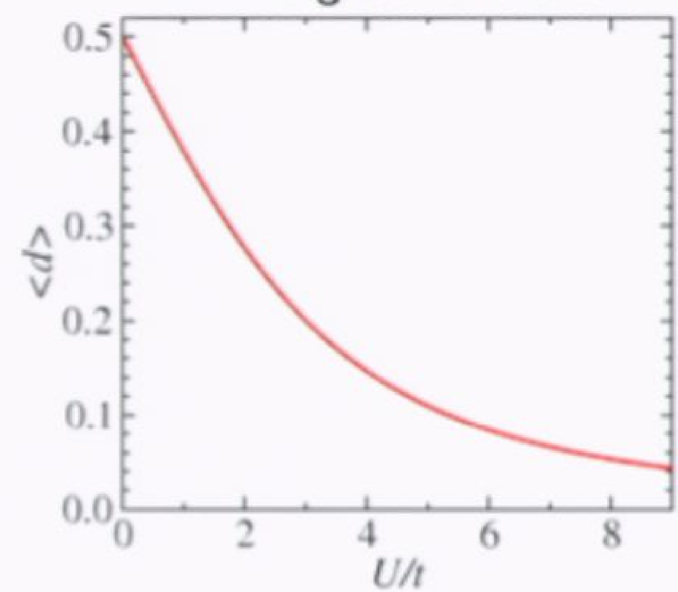
- total-spin singlet (S=0)
- small gap to S=1 states
- one-to-one with states of 2-site Heisenberg

$$\Delta = J \rightarrow \frac{4t^2}{U}$$

energies



double-occupation in the ground state



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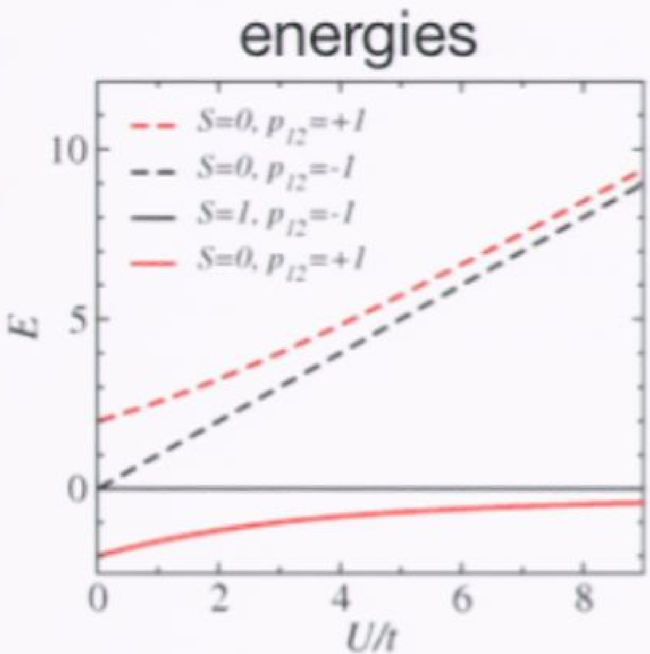

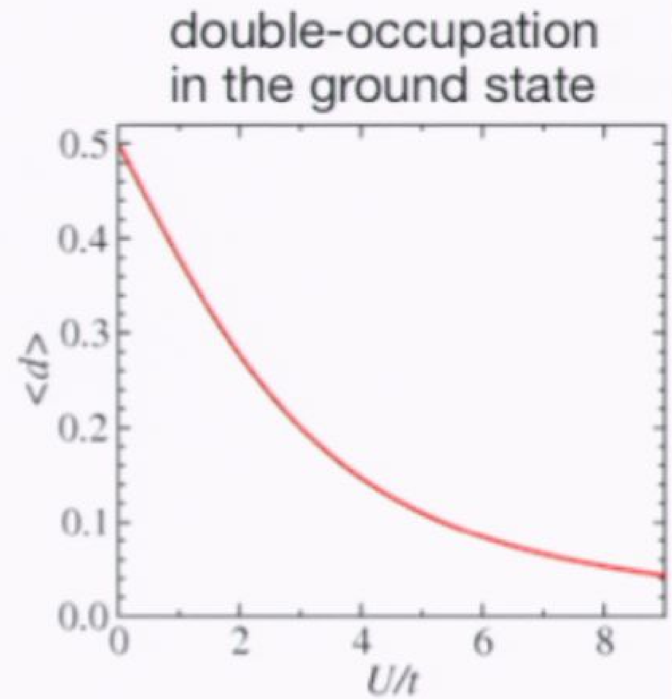

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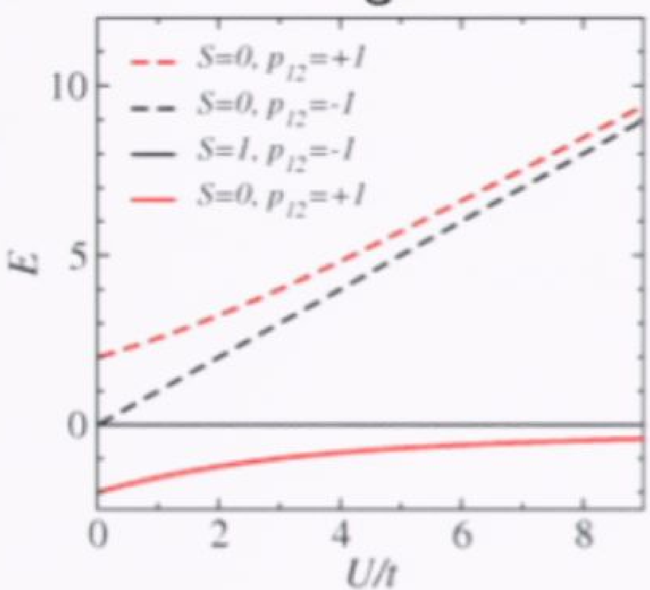

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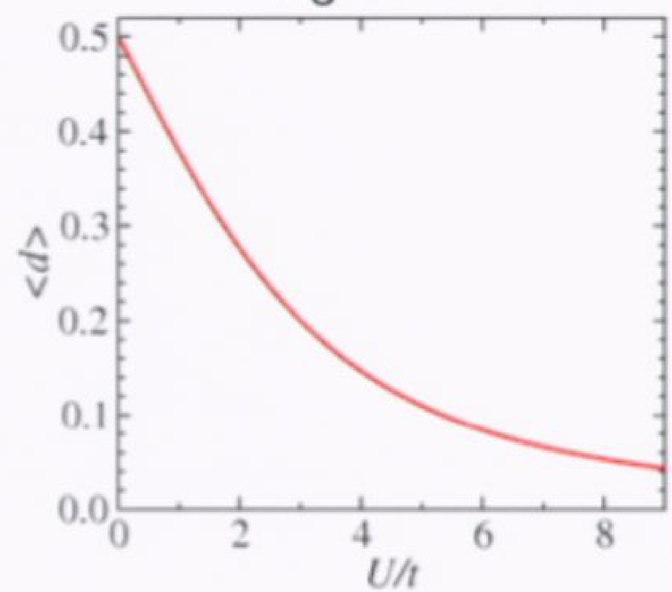

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Origin of antiferromagnetic interactions

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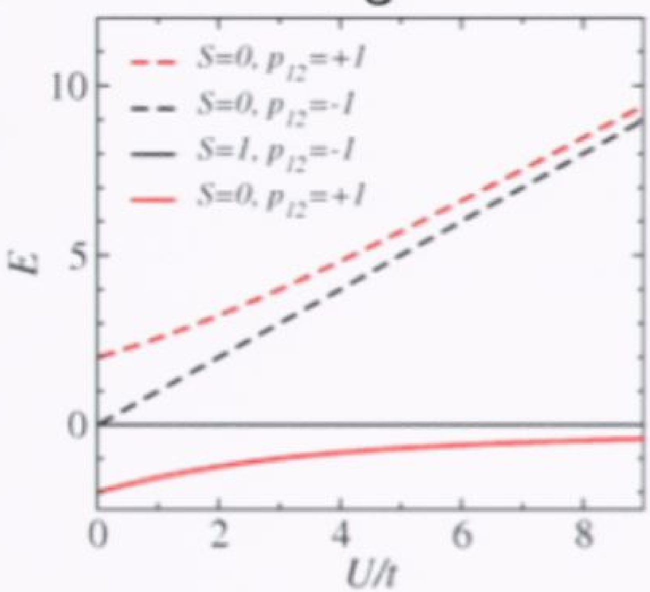

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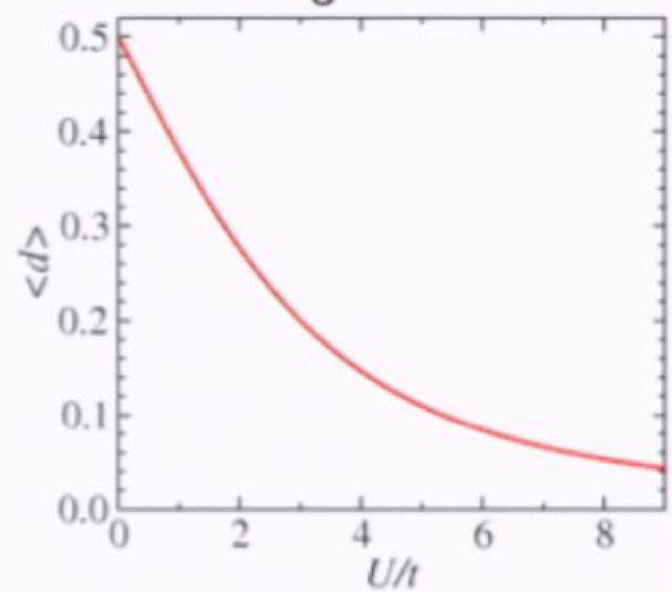

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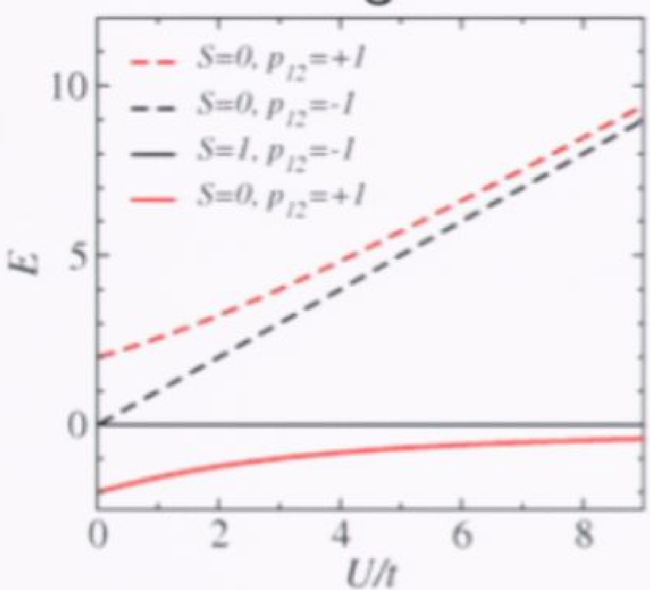

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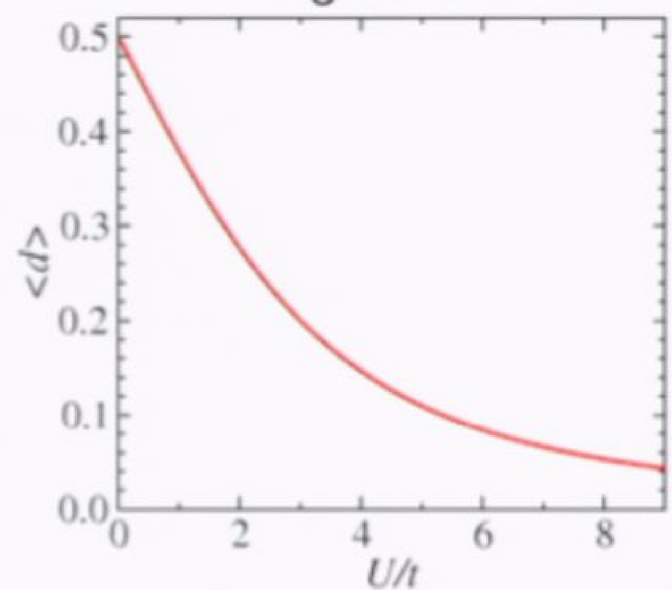

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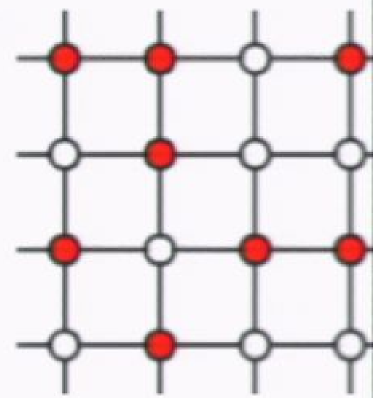

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U>>t : use degenerate perturbation theory (e.g., Schiff)

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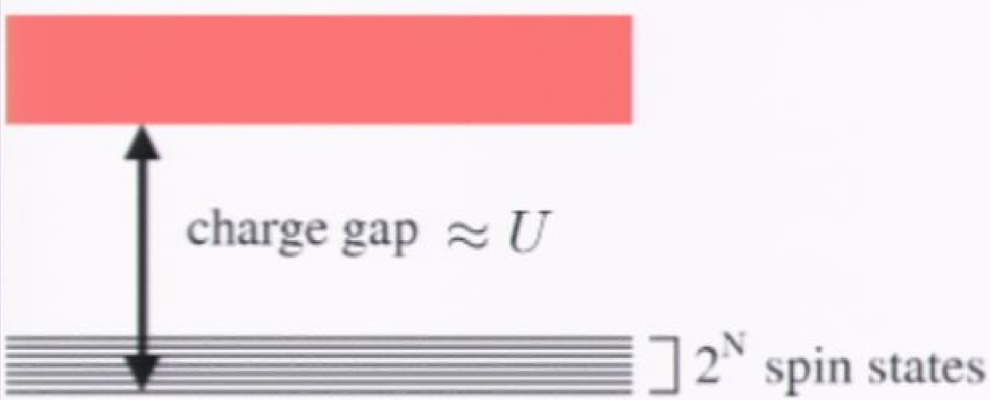

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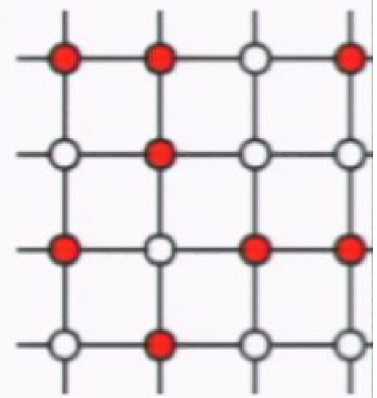

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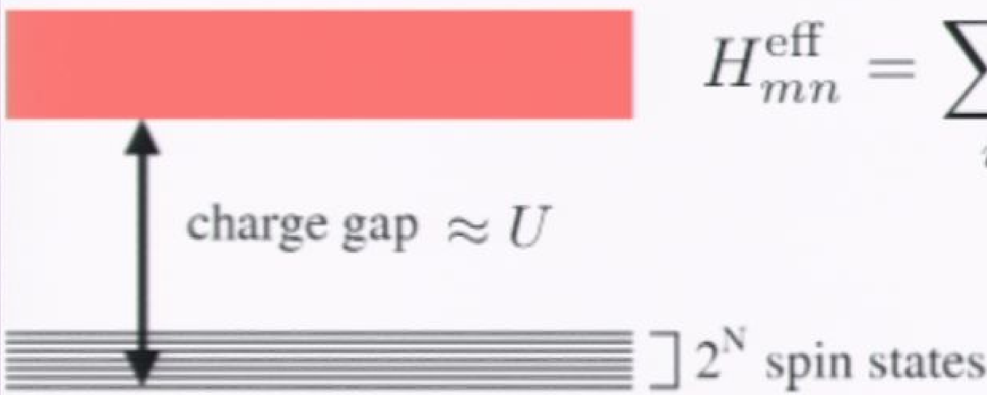

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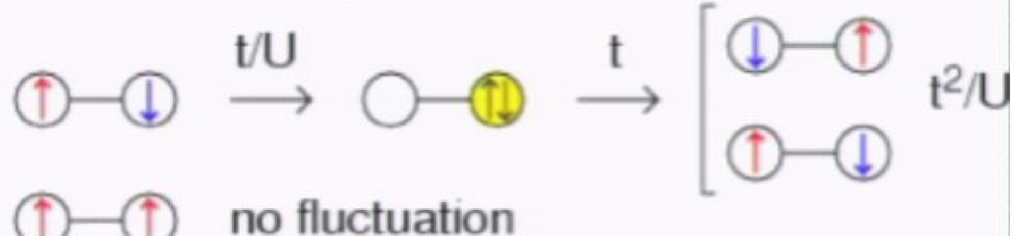

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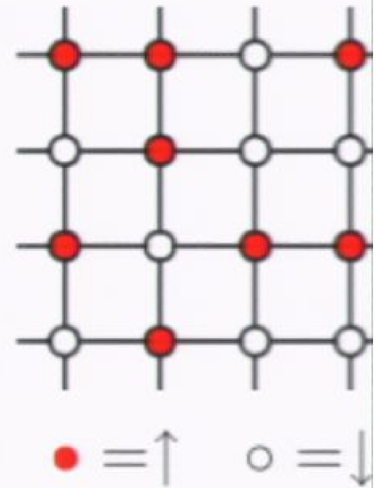

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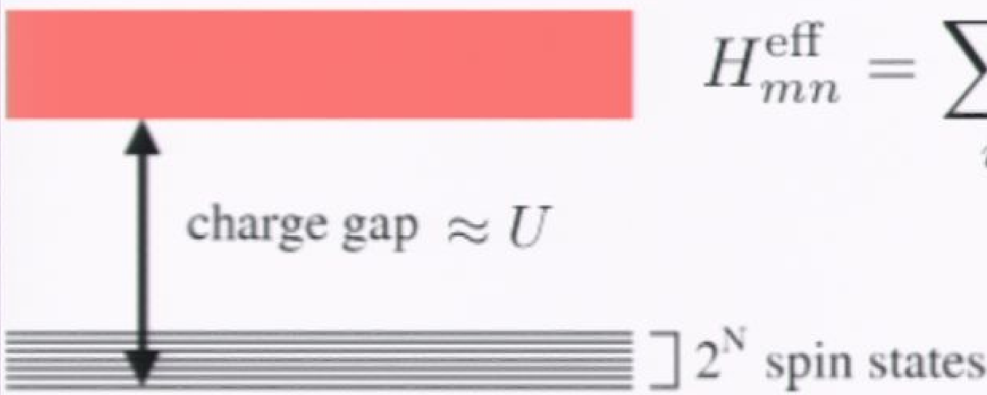

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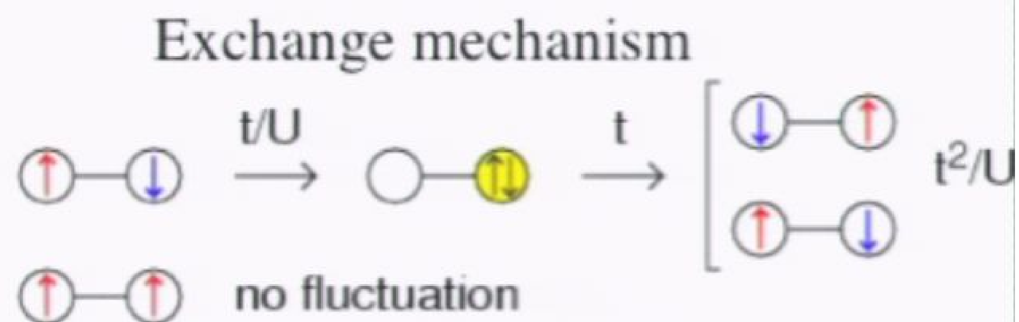

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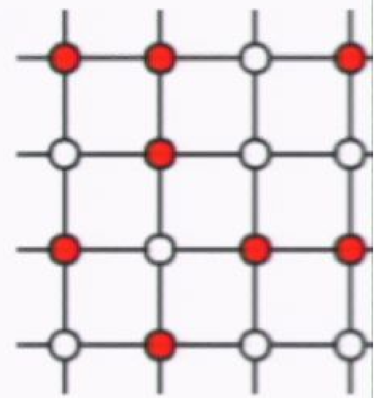

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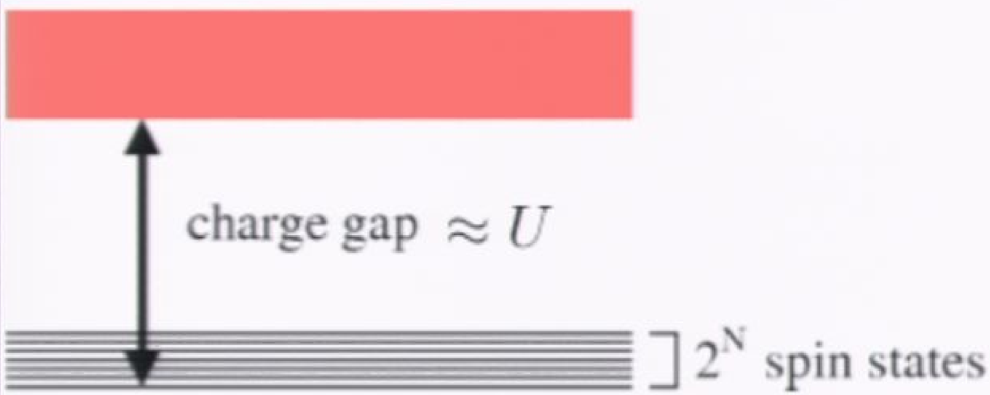

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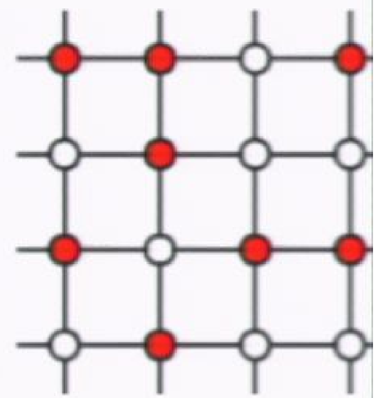

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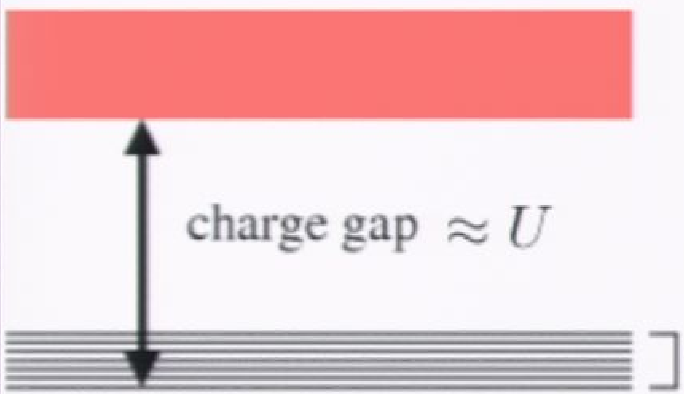

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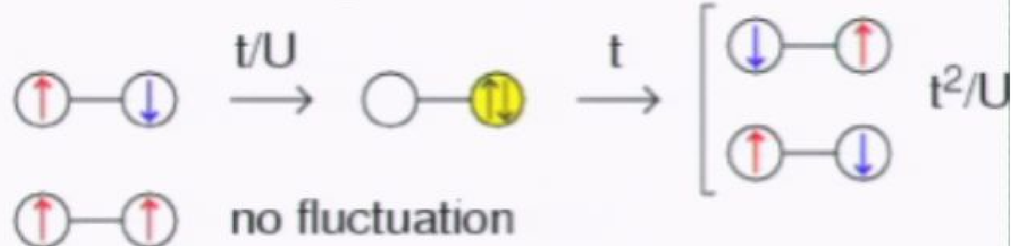

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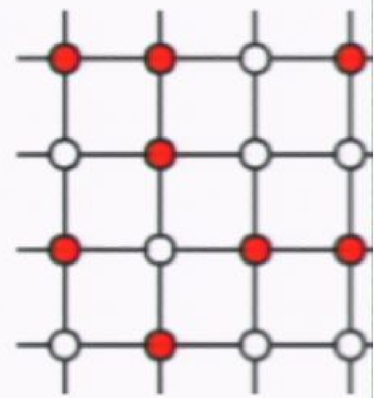

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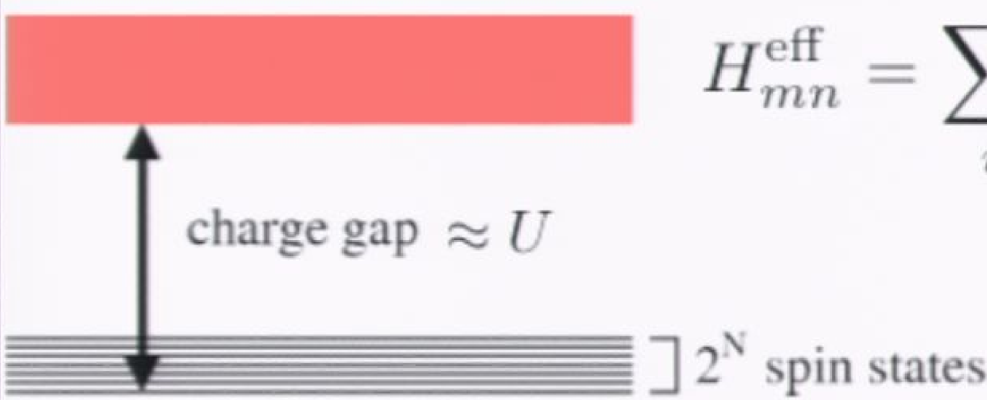

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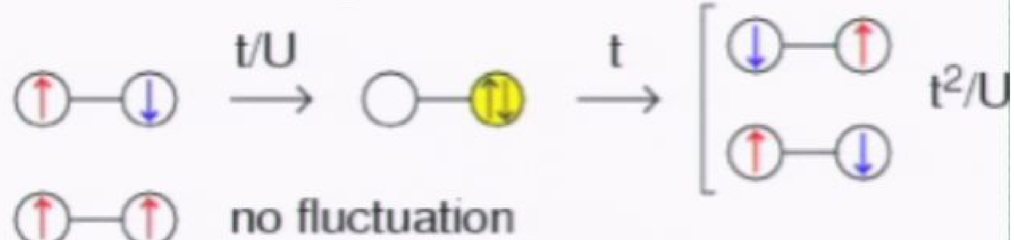

Spin band overlaps with other states for finite U when N→∞

The antiferromagnetic (Néel) state and quantum fluctuations

The ground state of the Heisenberg model (bipartite 2D or 3D lattice)

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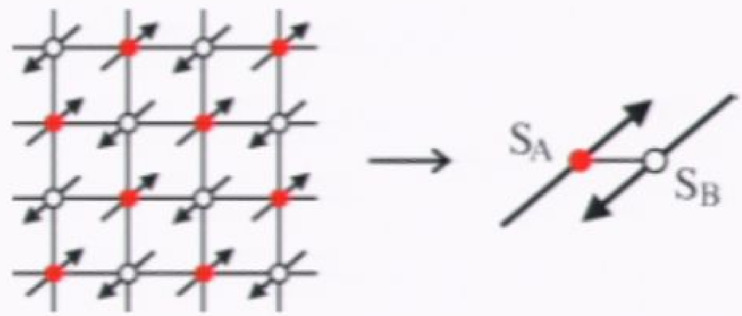

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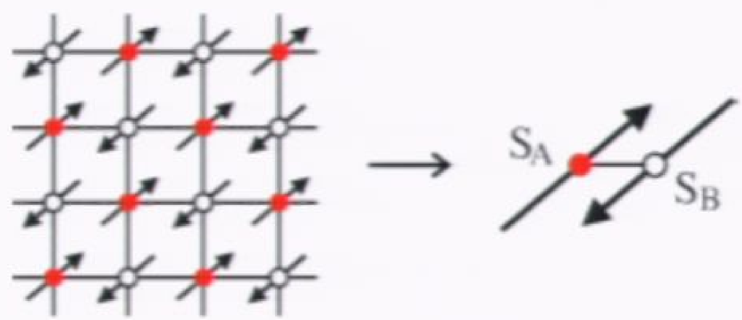

If there is order ($m_s>0$), the direction of the vector is fixed ($N=\infty$)

- conventionally this is taken as the z direction

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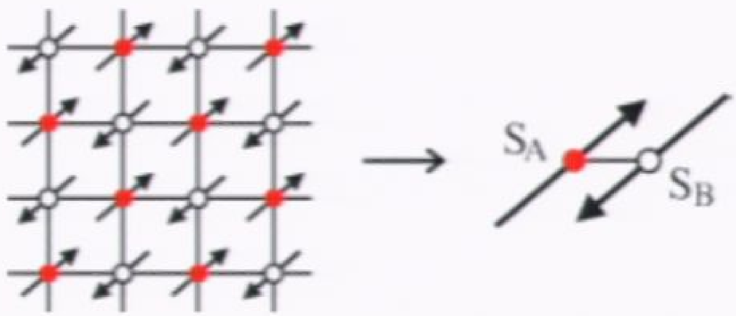

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PERIMETER SCHOLARS INTERNATIONAL
April 5-23, 2010, Course on

Quantum spin simulations

Anders W. Sandvik, Boston University

Part 1: Introduction to quantum spin systems

- what they are, where they come from, why study them
- some simple analytical calculations (details in tutorials)
- related classical physics (phase transitions)

Part 2: Exact diagonalization studies (small systems)

- use of symmetries
- full diagonalization (all states), the Lanczos method (low-energy states)
- Physics of spin chains

Quantum spins

Spin magnitude S; basis states $|S^z{}_1, S^z{}_2, \ldots, S^z{}_N\rangle$, $S^z{}_i = -S, \ldots, S-1, S$

Commutation relations:

$$[S_i^x, S_i^y] = i\hbar S_i^z \quad (\text{we set } \hbar = 1)$$

$$[S_i^x, S_j^y] = [S_i^x, S_j^z] = \ldots = [S_i^z, S_j^z] = 0 \quad (i \neq j)$$

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Ladder (raising and lowering) operators:

$$S_i^+ = S_i^x + iS_i^y, \qquad S_i^- = S_i^x - iS_i^y$$

$$S_i^+|S_i^z\rangle = \sqrt{S(S+1) - S_i^z(S_i^z+1)}|S_i^z+1\rangle,$$

$$S_i^-|S_i^z\rangle = \sqrt{S(S+1) - S_i^z(S_i^z-1)}|S_i^z-1\rangle,$$

Spin (individual) squared operator: $S_i^2|S_i^z\rangle = S(S+1)|S_i^z\rangle$

Why study quantum spin systems?

Solid-state physics

- localized electronic spins in Mott insulators (e.g., high-Tc cuprates)
- large variety of lattices, interactions, physical properties
- search for "exotic" quantum states in such systems (e.g., spin liquid)

Ultracold atoms (in optical lattices)

- spin hamiltonians can (?) be engineered
- some bosonic systems very similar to spins (e.g., "hard-core" bosons)

Quantum information theory / quantum computing

- possible physical realizations of quantum computers using interacting spins
- many concepts developed using spins (e.g., entanglement)

Lecture contents and goals

Quantum spin systems discussed from a computational perspective

- Thorough introduction before details of computational methods
  - including some analytical calculations and related classical physics

Models

- S=1/2 Heisenberg model and its extensions, 1D, 2D lattices

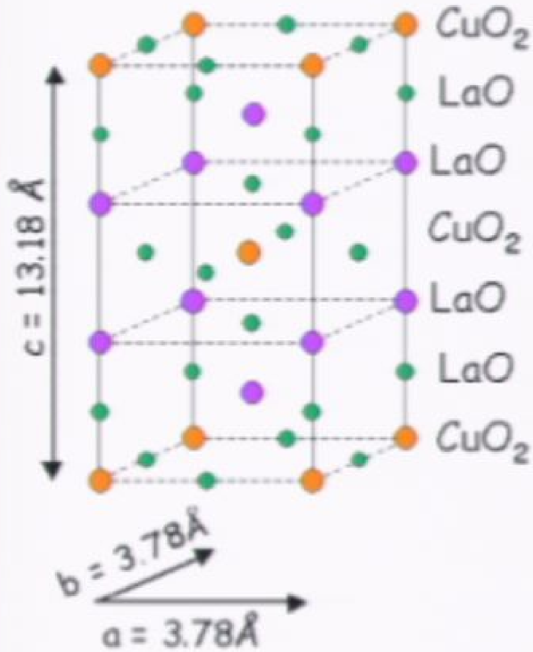
Methods

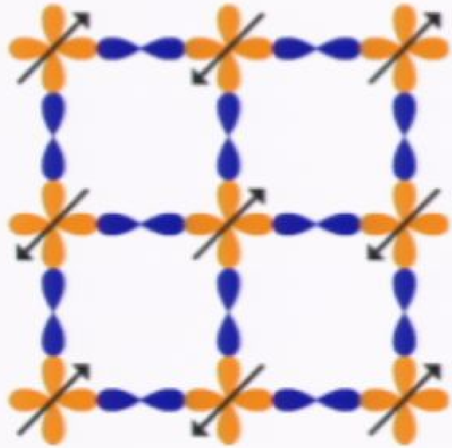
- finite-lattice methods; exact diagonalization, quantum Monte Carlo
- primarily focusing on “unbiased” (numerically exact) methods
- some discussion of variational methods
- algorithms and implementations in detail

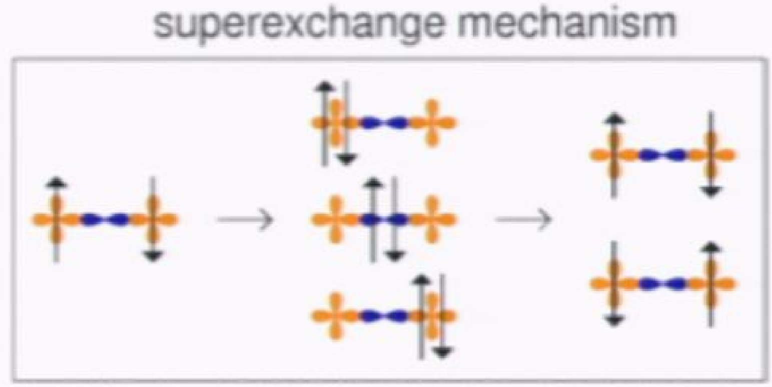
Physics

- illustrative results for key models and phenomena
- various types of ordered and disordered ground states
- quantum phase transitions

Prototypical Mott insulator; high-Tc cuprates (antiferromagnets)



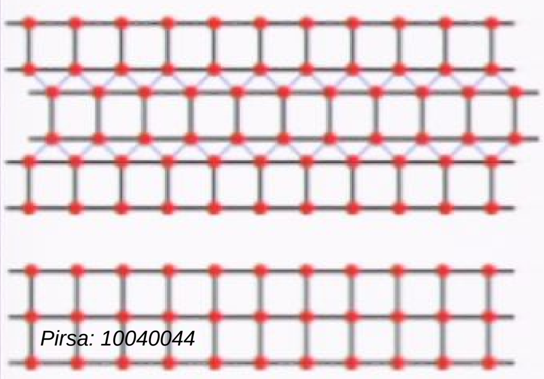


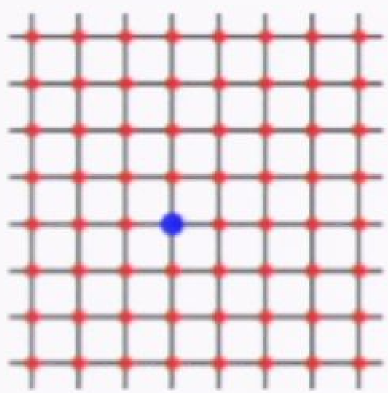


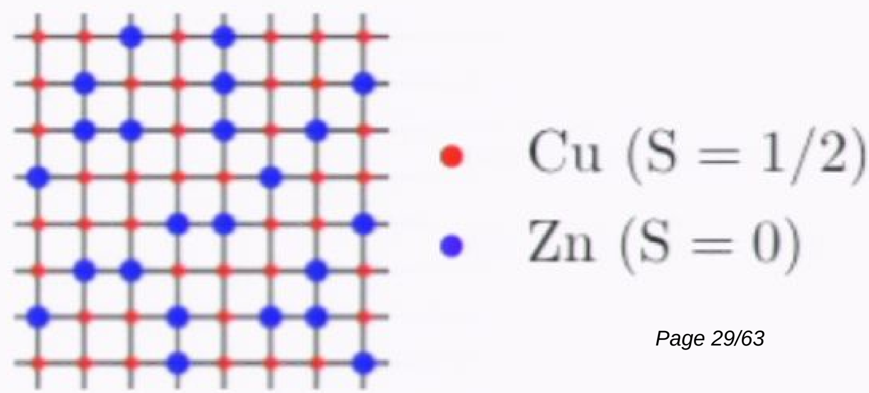
CuO_2 planes, localized spins on Cu sites
- Lowest-order spin model: S=1/2 Heisenberg
- Super-exchange coupling, J≈1500K

$$H = J \sum_{\langle i,j \rangle} \vec{S}_i \cdot \vec{S}_j$$

Many other quasi-1D and quasi-2D cuprates
- chains, ladders, impurities and dilution, frustrated interactions, ...







rigin of antiferromagnetic interactions

nsights from a simple system: the 2-site Hubbard model

$$H_{12} = -t(c^\dagger_{2\uparrow}c_{1\uparrow} + c^\dagger_{1\uparrow}c_{2\uparrow} + c^\dagger_{2\downarrow}c_{1\downarrow} + c^\dagger_{1\downarrow}c_{2\downarrow}) + U(n_{1\uparrow}n_{1\downarrow} + n_{2\uparrow}n_{2\downarrow})$$

-particle subspace (half-filled band)

6 states in the Hilbert space: $|\uparrow\downarrow\rangle,\quad |\downarrow\uparrow\rangle,\quad |\uparrow\uparrow\rangle,\quad |\downarrow\downarrow\rangle,\quad |02\rangle,\quad |20\rangle$

details of the solution in tutorial

large, 2 lowest states

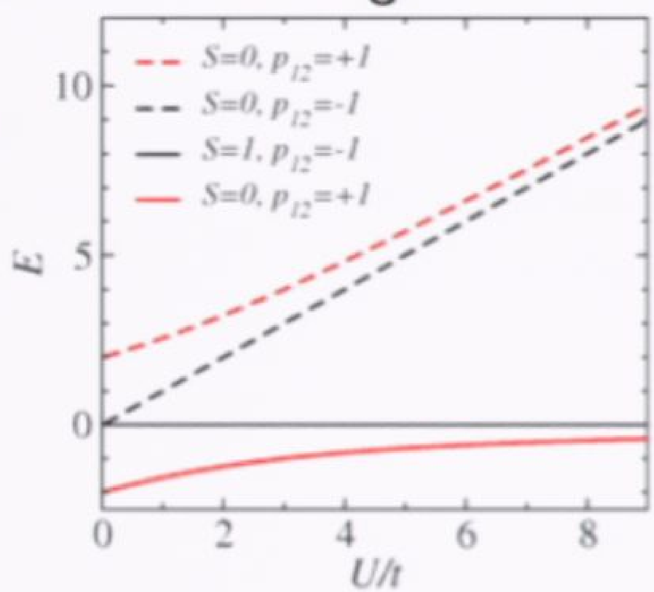
total-spin singlet (S=0)

small gap to S=1 states

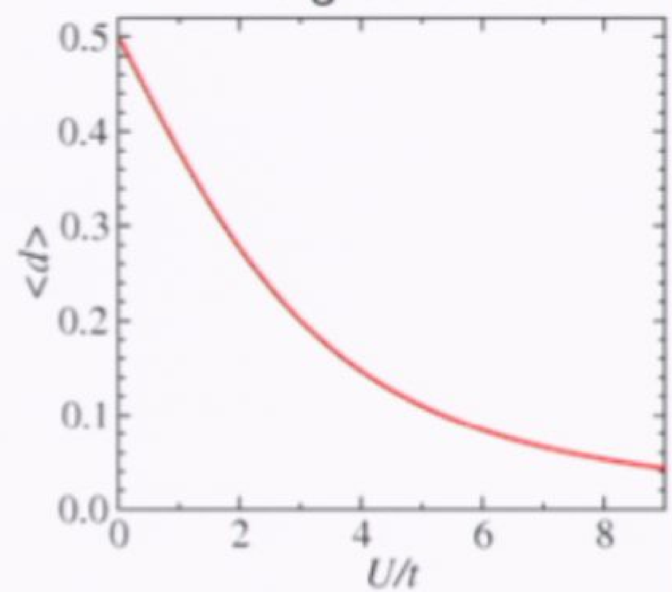
one-to-one with states of 2-site Heisenberg

$$\Delta = J \to \frac{4t^2}{U}$$

energies



double-occupation in the ground state



$$|\psi_0\rangle = \frac{1}{\sqrt{2+8t^2/U^2}}\left[|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle + \frac{2t}{U}(|20\rangle + |02\rangle)\right] \longrightarrow \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$$

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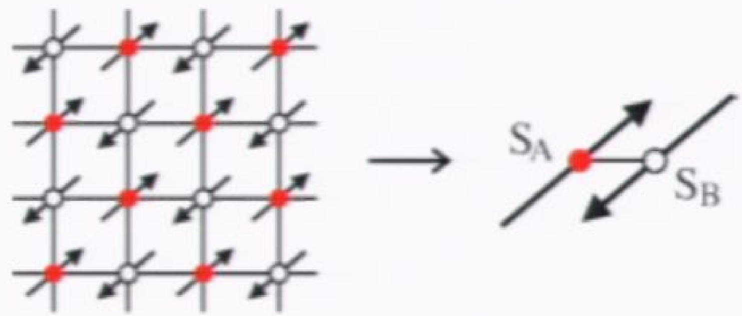

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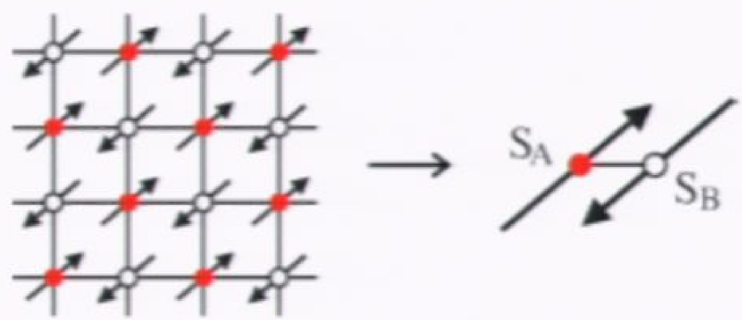

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Spin-wave theory

Perturbation around the exact $S \to \infty$ (classical) Néel state

- spins have complicated commutation relations
- map spins→bosons; simpler commutation rules, but complicated form of H
- simple lowest-order form in an 1/S expansion (linear spin-wave theory)

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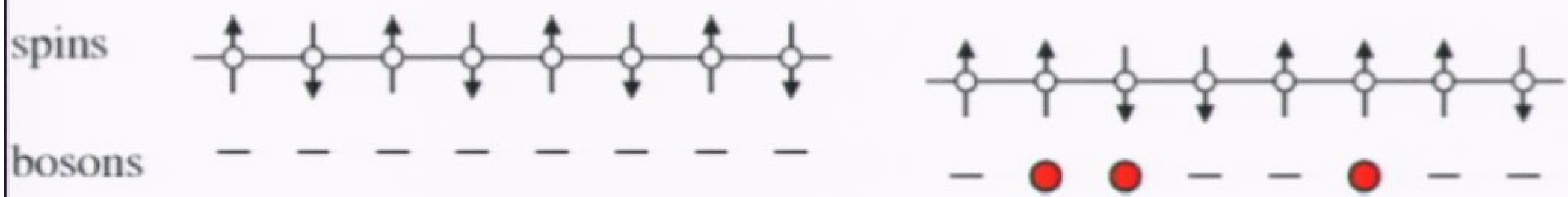

$(S = 1/2)$

physical subspace : $n_i = a_i^+ a_i \in \{0, 1, \ldots, 2S\}$

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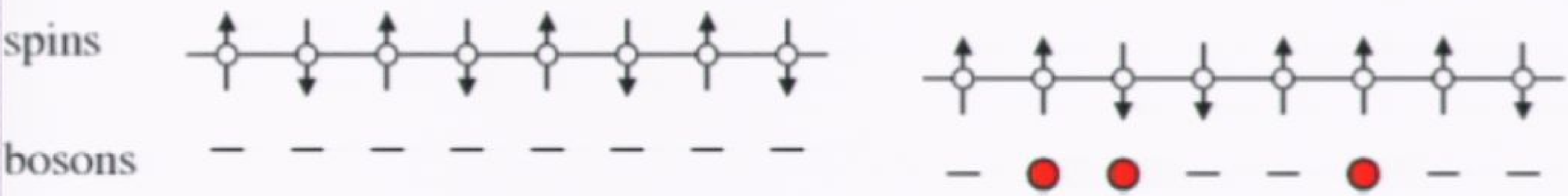

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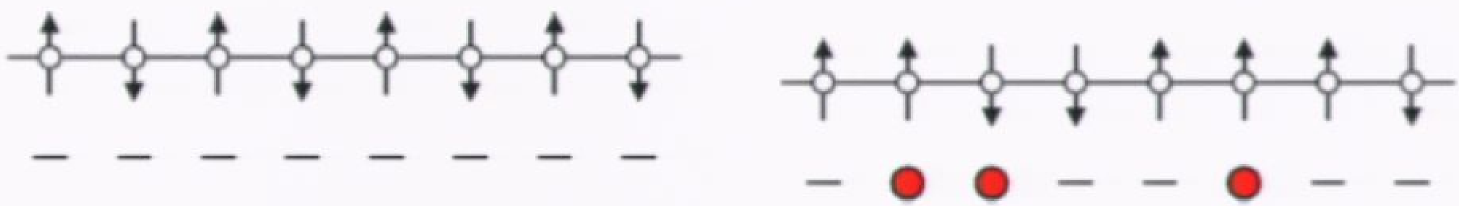

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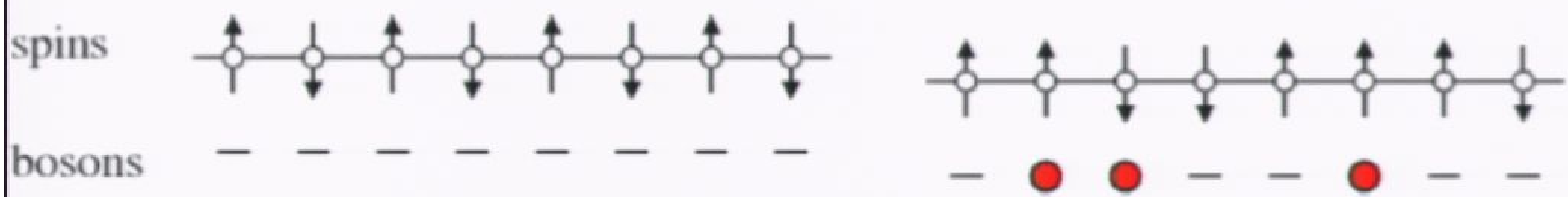

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We can diagonalize this model (write it in terms of boson number operators)

- details in tutorial (and related homework)

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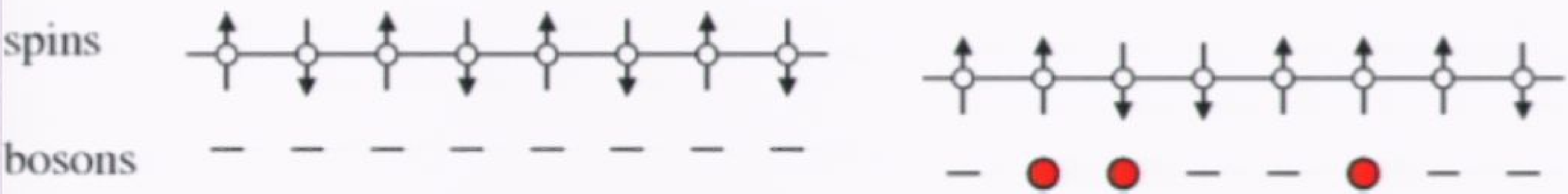

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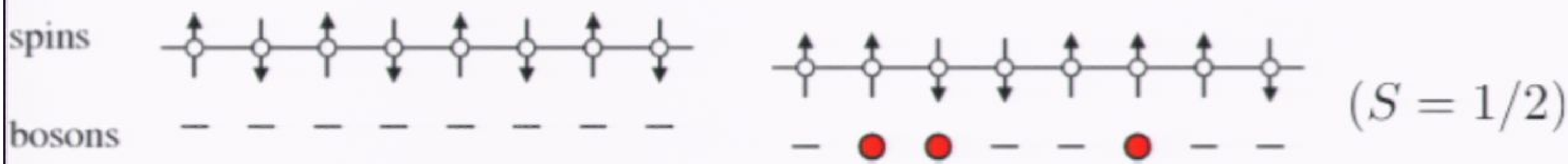

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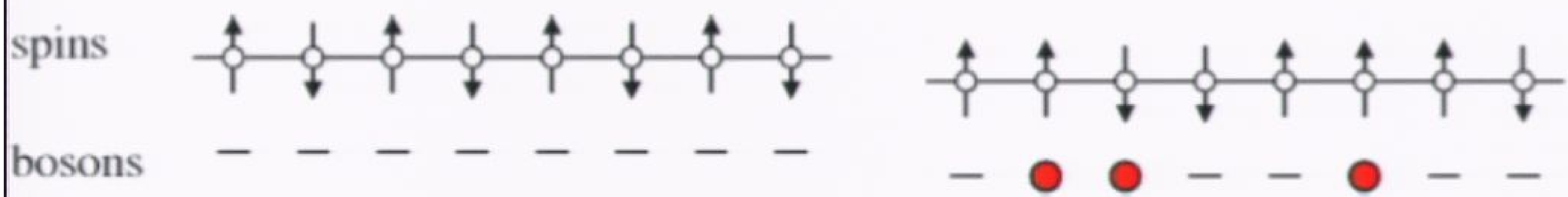

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Now eliminate *aa* and a^+a^+ operators

- accomplished with **Bogolubov transformation:**

$$\begin{aligned} \alpha_{\mathbf{k}} &= \cosh(\Theta_{\mathbf{k}})a_{\mathbf{k}} + \sinh(\Theta_{\mathbf{k}})a_{-\mathbf{k}}^+ \\ a_{\mathbf{k}} &= \cosh(\Theta_{\mathbf{k}})\alpha_{\mathbf{k}} - \sinh(\Theta_{\mathbf{k}})\alpha_{-\mathbf{k}}^+ \end{aligned}$$

These operators satisfy standard boson commutation relations

- we can choose the angles Θ_k to suit our needs (to diagonalize) →

After some manipulations we can cast the hamiltonian in the form

$$H = E_0 + \sum_{\mathbf{k}} \omega(\mathbf{k}) \alpha^{+}_{\mathbf{k}} \alpha_{\mathbf{k}},$$

with zero-point energy

$$E_0 = -2SJ \sum_{\mathbf{k}} \frac{\gamma^2_{\mathbf{k}}}{1 + \sqrt{1 - \gamma^2_{\mathbf{k}}}} - 2NS^2 J,$$

The sum can be evaluated, e.g., by converting to an integral (N→∞)

- evaluate numerically, e.g., using Mathematica (or Matlab, Maple...)

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Substitute (Fourier transform) in the hamiltonian →

$$H = -2NS^2J + 4SJ\sum_{\mathbf{k}} n_{\mathbf{k}} + 2SJ\sum_{\langle ij\rangle} \gamma_{\mathbf{k}}(a_{\mathbf{k}}a_{-\mathbf{k}} + a_{\mathbf{k}}^+ a_{-\mathbf{k}}^+),$$

$$\gamma_{\mathbf{k}} = [\cos(k_x) + \cos(k_y)]$$

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$$2\cosh(\Theta_{\mathbf{k}})\sinh(\Theta_{\mathbf{k}})$$

After some manipulations we can cast the hamiltonian in the form

$$H = E_0 + \sum_{\mathbf{k}} \omega(\mathbf{k}) \alpha_{\mathbf{k}}^{+} \alpha_{\mathbf{k}},$$

with zero-point energy

$$E_0 = -2SJ \sum_{\mathbf{k}} \frac{\gamma_{\mathbf{k}}^2}{1 + \sqrt{1 - \gamma_{\mathbf{k}}^2}} - 2NS^2 J,$$

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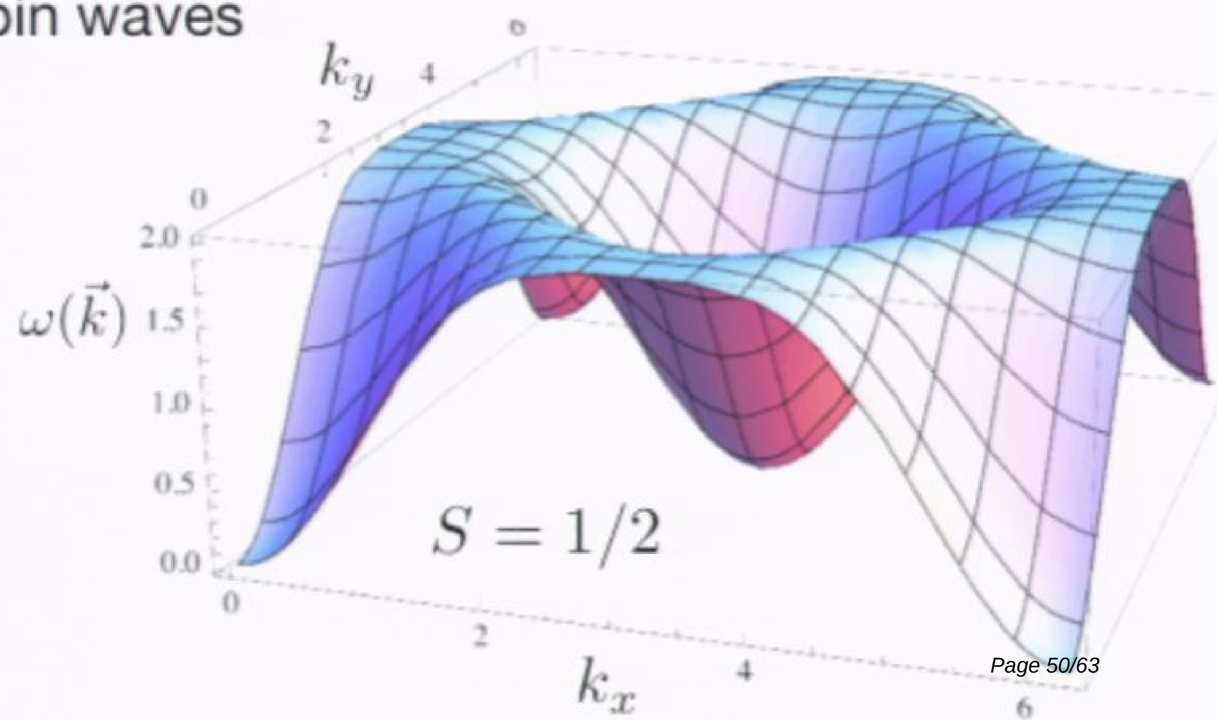

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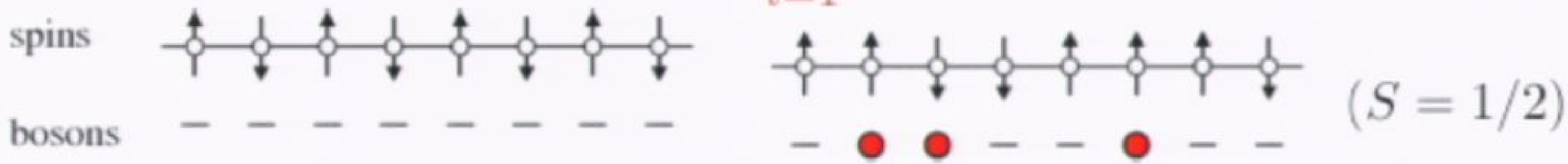

Spin-wave theory

Perturbation around the exact S→∞ (classical) Néel state

- spins have complicated commutation relations
- map spins→bosons; simpler commutation rules, but complicated form of H
- simple lowest-order form in an 1/S expansion (linear spin-wave theory)

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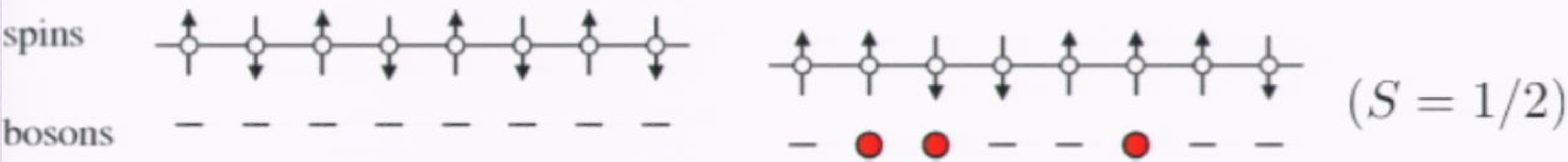

physical subspace : $n_i = a_i^+ a_i \in \{0, 1, \ldots, 2S\}$

Lowest-order mapping (also exact for S=1/2 in physical subspace)**:**

$$i \in \uparrow \text{sublattice}: \quad S_i^z = S - n_i, \qquad S_i^+ = \sqrt{2S}a_i, \qquad S_i^- = \sqrt{2S}a_i^+$$

$$i \in \downarrow \text{sublattice}: \quad S_i^z = n_i - S, \qquad S_i^+ = \sqrt{2S}a_i^+, \qquad S_i^- = \sqrt{2S}a_i.$$

Linear spin-wave hamiltonian (2D square lattice)

$$H = -2NS^2J + 4SJ\sum_{i=1}^{N} n_i + SJ\sum_{\langle ij\rangle}(a_i a_j + a_i^+ a_j^+).$$

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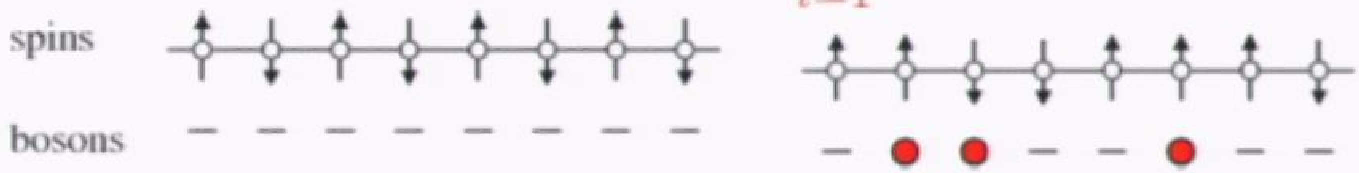

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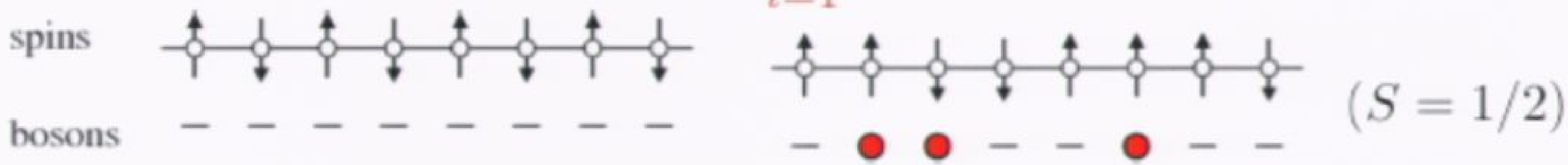

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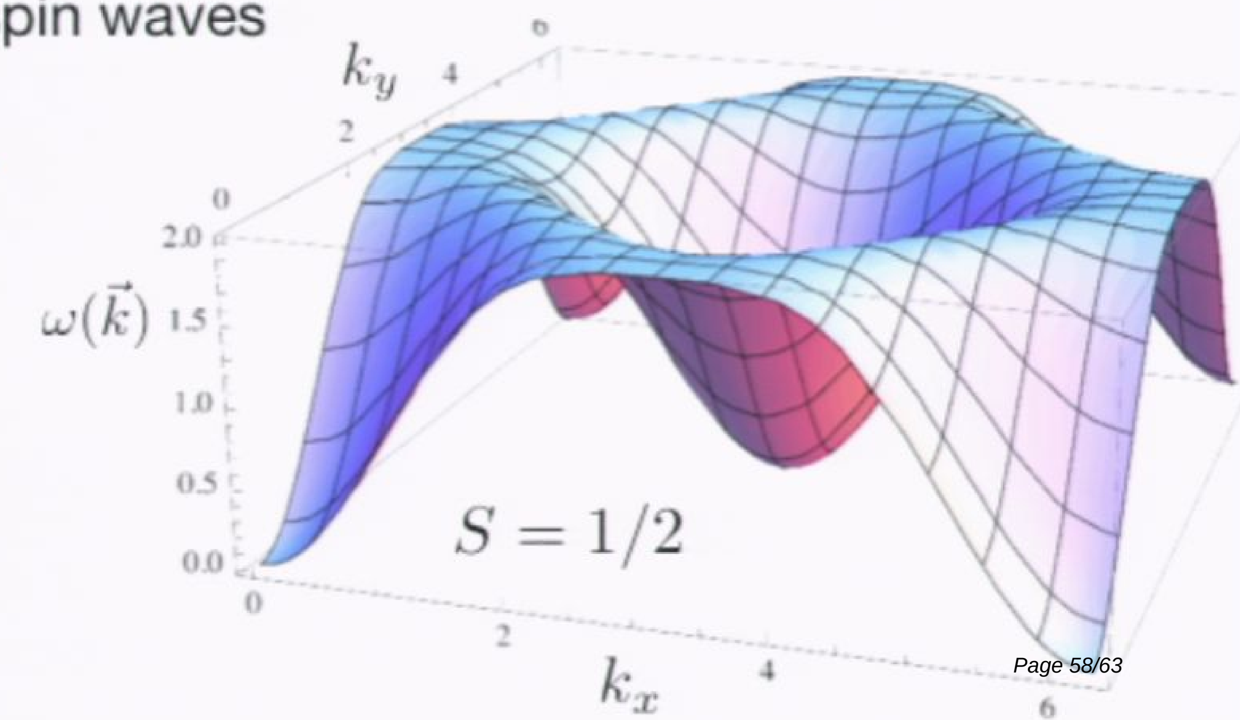

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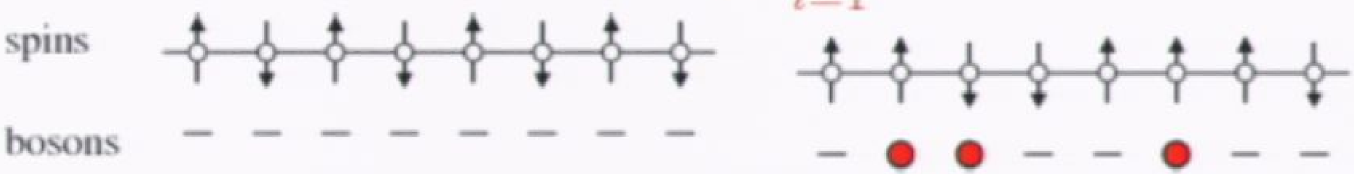

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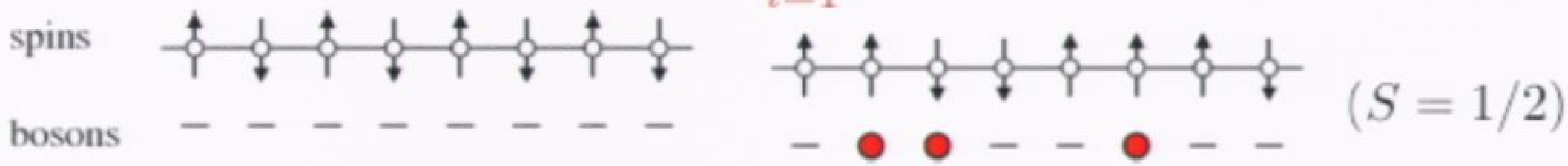

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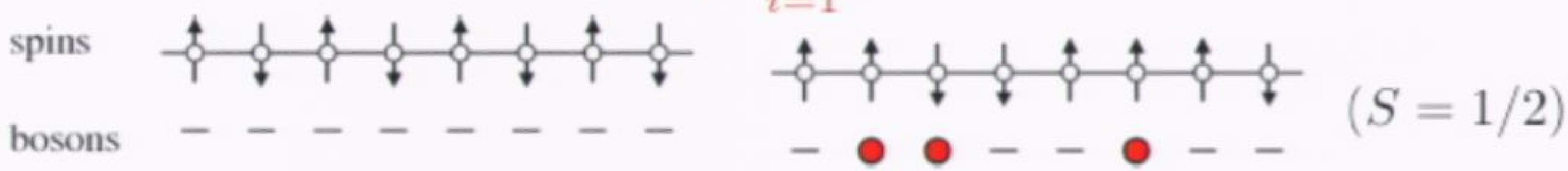

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Numerical evaluation gives **$<m_s>=0.3034$ for S=1/2**

Conclusion: Linear spin-wave theory predicts an ordered ground state

- the quantum fluctuations reduce the order by 40% from the classical value
- this turns out to be very close to the true value (obtained with QMC)

Non-magnetic states

Two spins, i and j, in isolation, $H_{ij} = J_{ij}\vec{S}_i \cdot \vec{S}_j = J_{ij}[S_i^z S_j^z + \frac{1}{2}(S_i^+ S_j^- + S_i^- S_j^+$

For $J_{ij}>0$ the ground state is the singlet;

$$|\phi_{ij}^s\rangle = \frac{|\uparrow_i\downarrow_j\rangle - |\downarrow_i\uparrow_j\rangle}{\sqrt{2}}, \qquad E_{ij} = -3J_{ij}/4$$

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