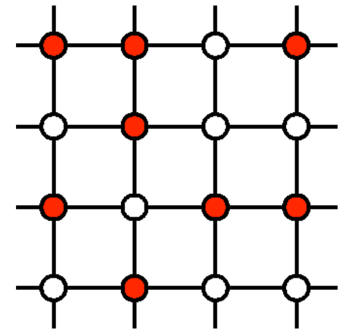
N-site Hubbard model (e.g, square lattice); half-filling

- cannot be solved exactly for N>2 (can in 1D), numerically up to N≈20
- one can identify “spin excitations” and “charge excitations”
- low-energy effective spin model (Heisenberg) can be derived



$\bullet = \uparrow \quad \circ = \downarrow$

$$H = -t \sum_{\langle i,j \rangle} \sum_{\sigma=\uparrow,\downarrow} c^{+}_{i,\sigma} c_{j,\sigma} + U \sum_i n_{i,\uparrow} n_{i,\downarrow} = H_t + H_U$$

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

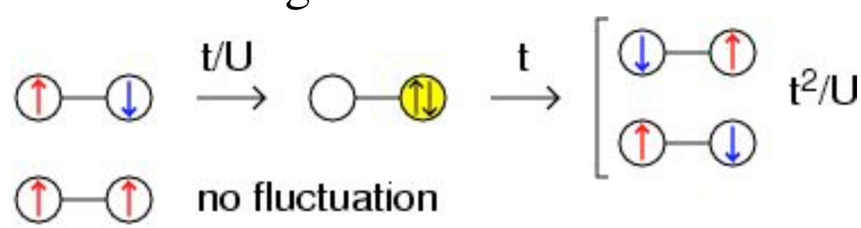
- **U=∞**, one particle on every site; 2^N degenerate spin states
- degeneracy lifted in order t^2/U (1 doubly-occupied site, d=1)
- leads to the Heisenberg model

$$H^{\text{eff}}_{mn} = \sum_i \frac{\langle n|H_t|i\rangle\langle i|H_t|m\rangle}{E_0 - E_i}$$

$|i\rangle : \; d=1$

$|m\rangle, |n\rangle : \; d=0$

Exchange mechanism



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

- only low-energy states of the Heisenberg model (up to E<<U) are relevant

The antiferromagnetic (Néel) state and quantum fluctuations

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

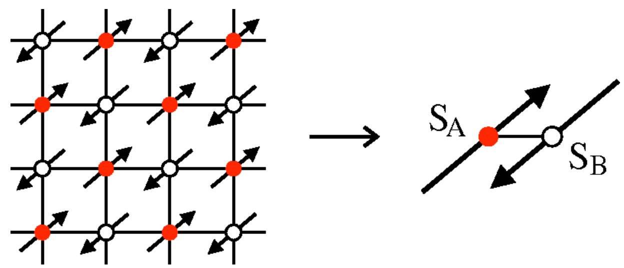
$$H = J\sum_{\langle ij\rangle}\vec{S}_i\cdot\vec{S}_j = J\sum_{\langle ij\rangle}[S_i^z S_j^z + \tfrac{1}{2}(S_i^+ S_j^- + S_i^- S_j^+)]$$

Does the long-range "staggered" order survive quantum fluctuations?

- order parameter: staggered (sublattice) magnetization

$$\vec{m}_s = \frac{1}{N}\sum_{i=1}^{N}\phi_i\vec{S}_i, \qquad \phi_i = (-1)^{x_i+y_i} \quad \text{(2D square lattice)}$$

$$\vec{m}_s = \frac{1}{N}\left(\vec{S}_A - \vec{S}_B\right)$$



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

- conventionally this is taken as the z direction

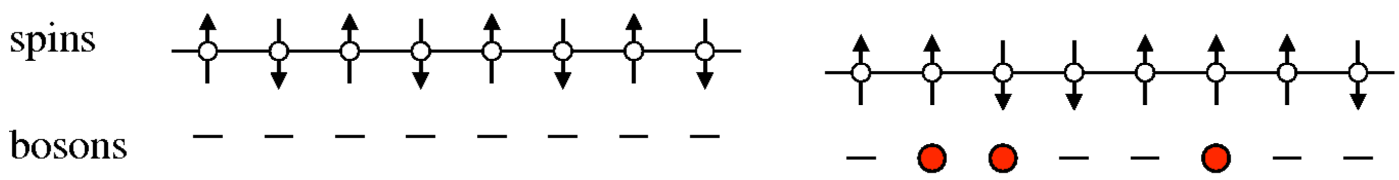
$$\langle m_s\rangle = \frac{1}{N}\sum_{i=1}^{N}\phi_i\langle S_i^z\rangle = |\langle S_i^z\rangle|$$

- For S→∞ (classical limit) <m_s>→S
- what happens for small S (especially S=1/2)?

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)



$(S = 1/2)$

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

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

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

Off-diagonal and diagonal Heisenberg terms:

$$(S_i^+ S_j^- + S_i^- S_j^+) \to S(a_i a_j + a_i^+ a_j^+),$$
$$S_i^z S_j^z \to -S^2 + S(n_i + n_j) - \cancel{n_i n_j}.$$

(i,j on different sublattices)

- the boson interaction term is neglected, because lower by factor 1/S
- in linear spin-wave theory the constraints on n_i are completely neglected

Linear spin-wave hamiltonian (2D square lattice)

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

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

- details in tutorial (and related homework)

$$a_{\mathbf{k}} = N^{-1/2}\sum_{\mathbf{r}} \mathrm{e}^{i\mathbf{k}\cdot\mathbf{r}} a_{\mathbf{r}}, \qquad a_{\mathbf{r}} = N^{-1/2}\sum_{\mathbf{k}} \mathrm{e}^{-i\mathbf{k}\cdot\mathbf{r}} a_{\mathbf{k}},$$

Substitute (Fourier transform) in the hamiltonian →

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

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

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) →

$$\frac{2\cosh(\Theta_{\mathbf{k}})\sinh(\Theta_{\mathbf{k}})}{\cosh^2(\Theta_{\mathbf{k}}) + \sinh^2(\Theta_{\mathbf{k}})} = \gamma_{\mathbf{k}}.$$

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 (per spin)

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

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

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

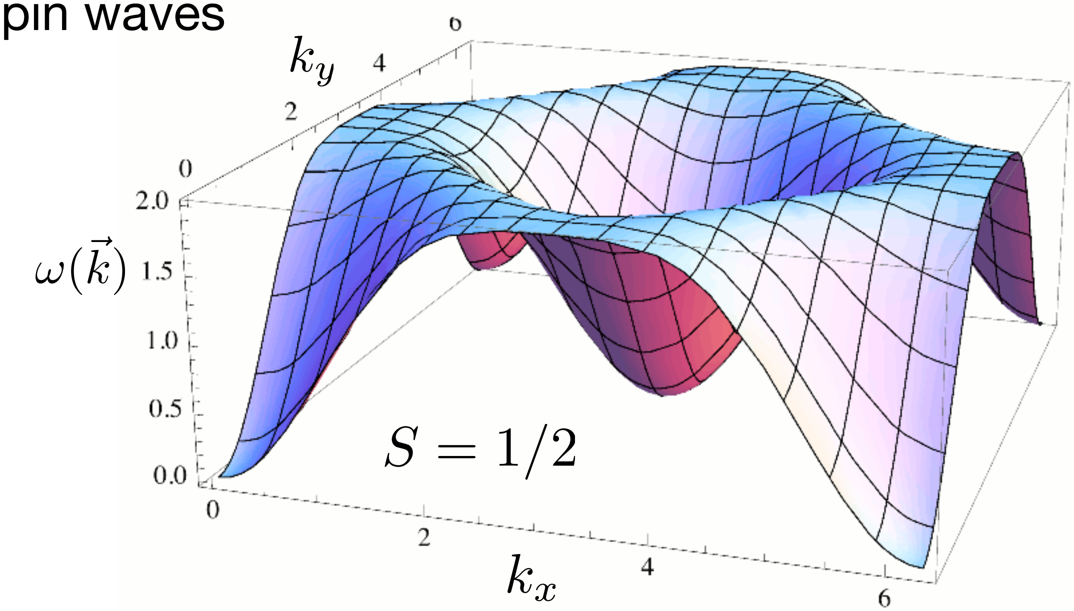
The ground state |0> has no spin waves (Bogolubov bosons)

- elementary excitatios $a^+_k|0>$

The dispersion relation is

$$\omega_{\mathbf{k}} = 4SJ\sqrt{1-\gamma^2_{\mathbf{k}}}.$$

$$\rightarrow \quad \text{velocity } c = 2\sqrt{2}S$$



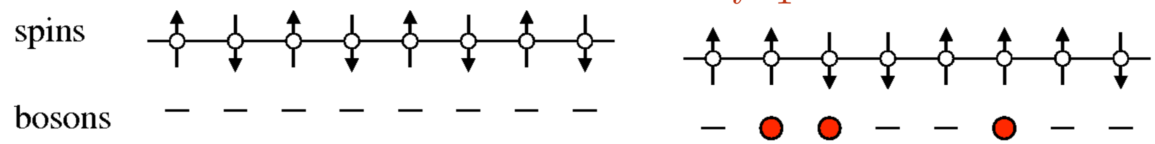
Gapless excitations at k=(0,0) and k=(π,π)

- we are using the Brillouin zone of the full lattice
- can also “fold” the zone to correspond to 2-site unit cell

The ground state has no spin waves

- but it has some density of the original a-bosons
- this density is directly related to the sublattice magnetization

$$\langle m_s \rangle = S - \langle 0|a_i^+ a_i|0\rangle = S - \frac{1}{N}\sum_{i=1}^{N}\langle 0|a_i^+ a_i|0\rangle$$



$(S = 1/2)$

Using the Bogolubov transformation gives

$$\langle m_s \rangle = S - \frac{1}{N}\sum_{\mathbf{k}} \sinh^2(\Theta_{\mathbf{k}}).$$

and one can show with some manipulations that

$$2\sinh^2(\Theta_{\mathbf{k}}) = \frac{1}{\sqrt{1-\gamma_{\mathbf{k}}^2}} - 1$$

Numerical evaluation gives **$\langle m_s \rangle$=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)
- it's not clear a priory why spin-wave theory should work, but it does here
- not always the case (reliable only when $\langle m_s \rangle$ is large)