Bogoliubov transformations

$$H = E_0 + \left| J \right| Sz \sum_k c_k^+ c_k^- + d_k^+ d_k^- + \gamma_k (c_k d_{-k}^- + c_{-k}^+ d_k^+)$$
Independants sub-lattices

Coupling between sub-lattices

diagonalization: Bogoliubov transform (see BCS theory)

$$c_k = u_k \alpha_k + v_k \beta_{-k}^+$$
 New bosonic operators with u_k , v_k real and: $\left[\alpha, \alpha^+\right] = \left[\beta, \beta^+\right] = 1$
$$\left[\alpha, \beta\right] = 0$$

Conditions on u_k v_k

(1)
$$\left[c_{k}, c_{k}^{+}\right] = 1 \iff \left[u_{k}\alpha_{k} + v_{k}\beta_{-k}^{+}, u_{k}\alpha_{k}^{+} + v_{k}\beta_{-k}\right] = u_{k}^{2}\left[\alpha_{k}, \alpha_{k}^{+}\right] + v_{k}^{2}\left[\beta_{-k}^{+}, \beta_{-k}\right] = 1$$

Bogoliubov transformations

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Conditions on uk Vk

(2) Eliminate cross terms like ($\alpha\beta$) to diagonalize H:

Ex: terms in
$$\alpha_k^+ \beta_{-k}^+ \implies u_k v_k + \gamma_k v_k^2$$

 $\alpha_{-k}^+ \beta_k^+ \implies u_k v_k + \gamma_k u_k^2$
 $\Rightarrow 2u_k v_k + \gamma_k (u_k^2 + v_k^2) = 0$

same condition for hermitic conjugates $\alpha_{\scriptscriptstyle k}eta_{\scriptscriptstyle -k}$

Bogoliubov transformations

$$H = E_0 + \left| J \right| Sz \sum_{k} c_k^+ c_k + d_k^+ d_k + \gamma_k (c_k d_{-k} + c_{-k}^+ d_k^+)$$
Indépendants sub-lattices

Coupling between sub-lattices

diagonalization: Bogoliubov transform (see BCS)

$$c_k = u_k \alpha_k + v_k \beta_{-k}^+$$
 (1) $|u_k^2 - v_k^2 = 1|$

$$(1) \quad |u_k^2 - v_k^2 = 1$$

$$d_k = u_k \beta_k + v_k \alpha_{-k}^+$$

(2)
$$2u_k v_k + \gamma_k (u_k^2 + v_k^2) = 0$$

Off diagonal terms are zero with these 2 conditions

Diagonal terms in H:

$$\alpha_k^+ \alpha_k \implies u_k^2 + \gamma_k u_k v_k$$

$$\alpha_k \alpha_k^+ \implies v_k^2 + \gamma_k u_k v_k$$

$$\alpha_k \alpha_k^+ \implies v_k^2 + \gamma_k u_k v_k$$

$$\downarrow u_k^2 - 1 + v_k^2$$

$$\downarrow u_k^2 - 1 + v_k^2 + 2\gamma_k u_k v_k + 2\gamma_k u_k v_k$$

$$= (1 + \alpha_k^+ \alpha_k + \beta_k^+ \beta_k)(u_k^2 + v_k^2 + 2\gamma_k u_k v_k) - 1$$

Diagonalized AF Hamiltonian

$$H = E_0 - \frac{N|J|Sz}{2} + \sum_k \omega_k (1 + \alpha_k^+ \alpha_k^- + \beta_k^+ \beta_k^-) \quad \text{E}_0: \text{ energy of classical N\'e\'el}$$

$$\omega_k = |J|Sz(u_k^2 + v_k^2 + 2\gamma_k u_k v_k^-) = |J|Sz(\cosh(2\theta_k^-) + \gamma_k \sinh(2\theta_k^-))$$

$$u_k^2 - v_k^2 = 1 \qquad \qquad 2u_k v_k^- + \gamma_k (u_k^2 + v_k^2^-) = 0$$

Expression of magnons energy as a function of γ_k

we set:
$$u_k = \cosh(\theta_k)$$
 $\implies \sinh(2\theta_k) + \gamma_k \cosh(2\theta_k) = 0$

$$v_k = \sinh(\theta_k) \qquad \sinh(2\theta_k) + \gamma_k \sqrt{1 - \sinh^2(2\theta_k)} = 0$$

$$\implies \sinh(2\theta_k) = -\frac{\gamma_k}{\sqrt{1 - \gamma_k^2}}$$

$$\cosh(2\theta_k) = \frac{1}{\sqrt{1 - \gamma_k^2}}$$

$$\cosh(2\theta_k) = \frac{1}{\sqrt{1 - \gamma_k^2}}$$

Dispersion relation of AF magnons

AF magnons: 2 degenerate modes

$$\omega_k = JSz\sqrt{1 - \gamma_k^2}$$

in 1D: 2 neighbors

$$\gamma_k = \frac{1}{z} \sum_{\delta} e^{i\vec{k}.\vec{\delta}} = \frac{1}{2} \left[\cos(ka) + \cos(-ka) \right] = \cos(ka)$$

$$\rightarrow \omega_k = JSz\sqrt{1-\gamma_k^2} = JSz|\sin(ka)|$$

 $\omega_k \approx JSz|ka|$ $\frac{\pi}{\pi} \text{ ka}$

Periodicity $k_{BZ} = \pi/a$

Magnetic Brillouin zone ≠ cristal Brillouin zone

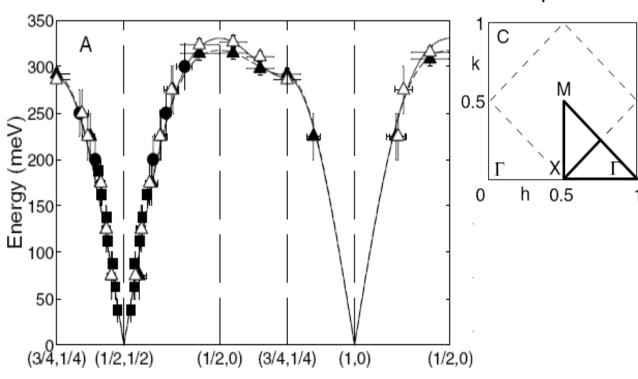
Linear dispersion at low energy / wave-vector (ferro: quadratic)

Dispersion relation of AF magnons

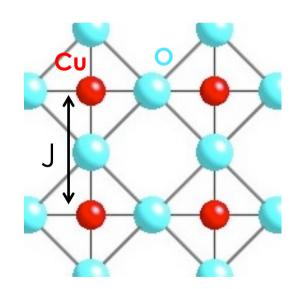
La₂ × Sr_x CuO₄: high Tc superconductor

$$La_2CuO_4$$
 2D square (z=4)

$$\omega_k = 4JS\sqrt{1 - \frac{1}{4}\left[\cos(k_x a) + \cos(k_y a)\right]^2}$$



First nearest neighbors only!



 CuO_2 plane (Cu^{2+} : S=1/2)

AF ground state in the harmonic approximation

$$H = E_0 - \frac{NJSz}{2} + JSz \sum_{k} \sqrt{1 - \gamma_k^2} (1 + \alpha_k^+ \alpha_k^- + \beta_k^+ \beta_k^-)$$

Ground state $\langle \alpha_k^+ \alpha_k \rangle = \langle \beta_k^+ \beta_k \rangle = 0$ Be careful: $\langle c_k^+ c_k \rangle = \langle d_k^+ d_k \rangle \neq 0$ (harmonic approx.)

the gound state is not Néél state anymore!

$$E_{AF}^{harm} = \left\langle H \right\rangle = E_0 - \frac{NJSz}{2} + JSz \sum_{k} \sqrt{1 - \gamma_k^2} = E_0 - JSz \left[\frac{N}{2} - \sum_{k} \sqrt{1 - \gamma_k^2} \right] < E_0$$

$$\gamma_k = \frac{1}{z} \sum_{s} e^{i\vec{k}.\vec{\delta}} < 1 \iff \sqrt{1 - \gamma_k^2} \le 1$$

Ground state is Néél state renormalized by fluctuations

$$E_0 = -\frac{NJS^2z}{2} \implies E_{AF}^{harm} = -\frac{NJS^2z}{2} \left[1 + \frac{2}{NS} \sum_{k} (1 - \sqrt{1 - \gamma_k^2}) \right]$$

Correction in 1/S
Recover Néél state for large S

AF ground state in the harmonic approximation

$$E_{AF}^{harm} = -\frac{NJS^2z}{2} \left[1 + \frac{2}{NS} \sum_{k} (1 - \sqrt{1 - \gamma_k^2}) \right] \qquad \gamma_k = \frac{1}{z} \sum_{\delta} e^{i\vec{k}.\vec{\delta}}$$

$$\gamma_k = \frac{1}{z} \sum_{\delta} e^{i\vec{k}.\vec{\delta}}$$

Can be computed numerically for different lattices

$$E_{AF}^{harm} = -\frac{NJS^2z}{2} \left[1 + \frac{0.363}{S} \right]$$
 for chain (1D)

$$E_{AF}^{harm} = -\frac{NJS^2z}{2} \left[1 + \frac{0.158}{S} \right]$$
 For square (2D)

$$E_{AF}^{harm} = -\frac{NJS^2z}{2} \left[1 + \frac{0.097}{S} \right]$$
 for cube (3D)