Lecture 4a

$$H = -t \sum_{\langle ij \rangle, \sigma} \hat{c}^\dagger_{i\sigma} c_{j,\sigma}$$ ← hopping on 1D chain

$$+ U \sum_i n_{i\uparrow} n_{i\downarrow}$$ ← on-site Coulomb

$n_{i\uparrow} = c^\dagger_{i\uparrow} c_{i\uparrow}$

$$+ V \sum_{\substack{\langle ij \rangle \\ \sigma, \sigma'}} n_{i\sigma} n_{j\sigma'}$$ ← n.n. Coulomb (direct)

$$+ V' \sum_{\substack{\langle ij \rangle \\ \sigma, \sigma'}} \left(-\tfrac{1}{2} \underline{n_{i\sigma} n_{j\sigma'}} - 2\, \underline{\vec{S}_i \cdot \vec{S}_j} \right)$$ ← n.n. Coulomb (exchange)

$$\hat{H} = -t \sum_{\langle ij \rangle, \sigma} \hat{c}^\dagger_{i,\sigma} \hat{c}_{j,\sigma}$$

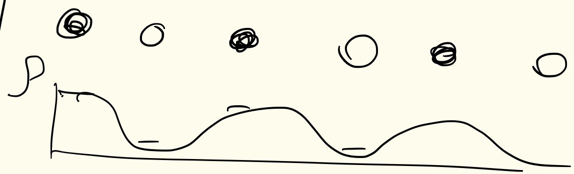
$$+ U \sum_{i} \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$$

$$\cancel{+ V \sum_{\substack{\langle ij \rangle \\ \sigma,\sigma'}} \hat{n}_{i,\sigma} \hat{n}_{j,\sigma'}}$$

$$+ V' \sum_{\substack{\langle ij \rangle \\ \sigma,\sigma'}} \left(-\tfrac{1}{2} \cancel{\hat{n}_{i\sigma} \hat{n}_{j\sigma'}} - 2 \hat{\vec{S}}_i \cdot \hat{\vec{S}}_j \right)$$

$\boxed{1 e^- / \text{atom}}$

$V \gg 1$



"Charge density wave"

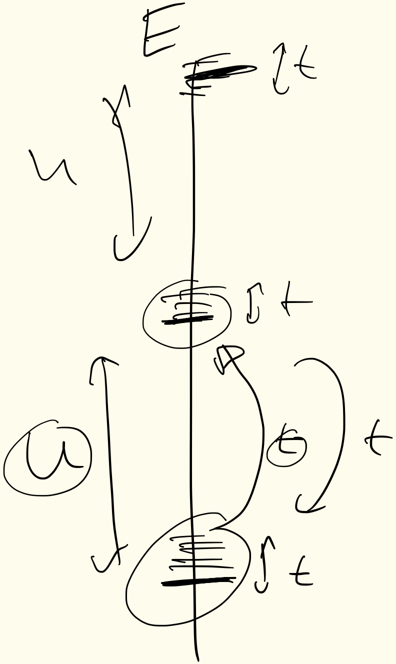
interactions

$\Rightarrow$ order.

$U \neq \infty$ $\quad t \neq 0$

$t/U \ll 1$

$$\Delta E^{(2)} = -\sum_n \frac{\langle gs|H'|n\rangle\langle n|H'|gs\rangle}{E_n - E_0}$$



Z

"Hubbard Sektors"

1 doubly occ. site

$$-\,t^2/U = \Delta E^{(2)}$$

no doubly occ. sites.

$$\Delta E^{(2)} = -\sum_n \frac{\langle gs | H' | n \rangle \langle n | H' | gs \rangle}{E_n - E_0}$$

$$H_0 = U \sum_i n_{i\uparrow} n_{i\downarrow}$$

$$H' = -t \sum_{\langle ij \rangle} c_i^\dagger c_j$$

$\langle gs | H' | n \rangle \sim t$

$E_n - E_0 \sim U$

$$\Delta E^{(2)} = -\frac{t^2}{U}$$

$t/U \ll 1$ $\equiv J$

$$\Delta E^{(2)} = + \frac{t^2}{U} \sum_{\langle ij \rangle} \left(\vec{S}_i \cdot \vec{S}_j - 1/4 \right)$$

$$V' \sum_{\langle ij \rangle} - \vec{S}_i \cdot \vec{S}_j$$

(RKKY)

$$V' \gg J$$

Heisenberg model

$$H = \sum_{\langle ij \rangle} -V' \vec{S}_i \vec{S}_j$$

$$= -V' \sum_{\langle ij \rangle} \left(S_i^z S_j^z + \frac{1}{2} S_i^+ S_j^- + \frac{1}{2} S_i^- S_j^+ \right)$$

Spin $- S$

$$\hat{H} \, |\uparrow\uparrow\uparrow\uparrow\uparrow\rangle = \underline{-V' N S^2} \, |\uparrow\uparrow\uparrow\uparrow\uparrow\rangle$$

$$|\downarrow\downarrow\downarrow\rangle \qquad |\rightarrow\rightarrow\rightarrow\rightarrow\rangle$$

$|\uparrow\uparrow\uparrow\uparrow\rangle$

$$S_i^- |gs\rangle \equiv |i\rangle$$

$$\hat{H}|i\rangle = -V' \sum_{\langle ij \rangle} \left(S_i^z S_j^z + \frac{1}{2} S_i^+ S_j^- + \frac{1}{2} S_i^- S_j^+ \right) |i\rangle$$

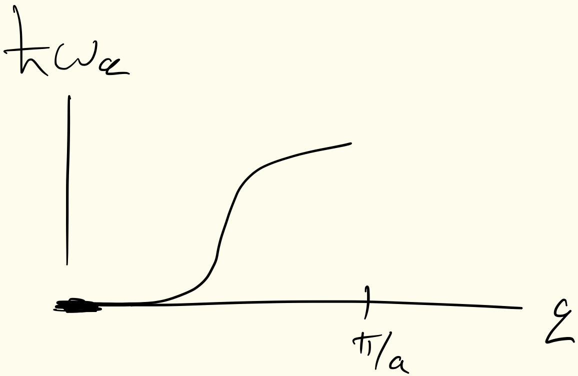
$$= \left(-N V' S^2 + 2 V' S^2 \right) |i\rangle \qquad \left((-N+2) V' S^2 \right)$$

$$- V' S \left(|i+1\rangle + |i-1\rangle \right)$$

$$|q\rangle = \frac{1}{\sqrt{N}} \sum_j e^{iq(ja)} |j\rangle$$

$$\hat{H} |q\rangle = \Big(\underbrace{-NV'S^2}_{\uparrow} + \underbrace{4V'S \sin^2\left(\tfrac{qa}{2}\right)}_{\uparrow} \Big) |q\rangle$$

$$E_0 \quad + \quad \hbar\omega_q$$



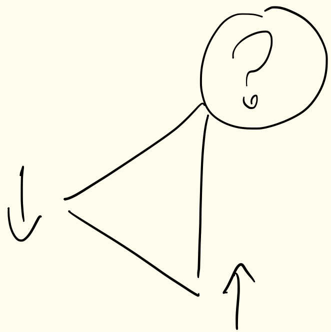
Magnons

$$q \simeq 0 \Rightarrow \hbar\omega_q \sim \frac{q^2}{2m}$$

Lecture 4b

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

$\uparrow \downarrow \uparrow \downarrow \uparrow$



geometric frustration.

bipartite

A B A B

B A B A

A B A B

$A = \uparrow$

$B = \downarrow$

Néel

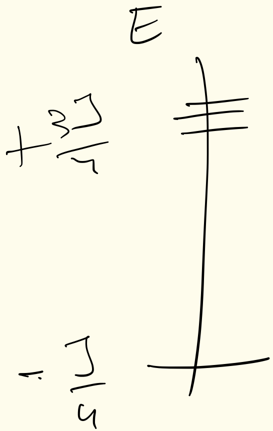
$\hat{H} \quad |\uparrow\downarrow\uparrow\downarrow\uparrow\rangle$

$$J \sum_{\langle ij \rangle} S_i^z S_j^z + \frac{1}{2}\left(S_i^+ S_j^- + S_i^- S_j^+\right)$$

$$\hat{H}\,|\text{néel}\rangle = \dots |\text{néel}\rangle$$

$$+ \dots |\text{Spin flips}\rangle$$

$$J\,\vec{S}_1\cdot\vec{S}_2 = \frac{J}{2}\Big(\underbrace{(S_1+S_2)^2}_{S^2} - S_1^2 - S_2^2\Big)$$



$$\begin{cases} |\uparrow\uparrow\rangle \\ \sqrt{\tfrac{1}{2}}\left(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle\right) \longleftarrow \sqrt{\tfrac{1}{2}}\left(|\rightarrow\rightarrow\rangle + |\leftarrow\leftarrow\rangle\right) \\ |\downarrow\downarrow\rangle \end{cases}$$

$$\sqrt{\tfrac{1}{2}}\left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right)$$

Spontaneous Symmetry Breaking

$$J\sum_{\langle ij\rangle}\vec{S}_i\cdot\vec{S}_j$$

$S_{tot} = 0$

$$\alpha|\uparrow\downarrow\uparrow\downarrow\rangle + \beta|\downarrow\uparrow\downarrow\uparrow\rangle + \gamma|\rightarrow\leftarrow\rightarrow\leftarrow\rangle + \delta|\leftarrow\rightarrow\rangle \ldots$$

- Goldstone modes
- Mermin-Wagner thm
- rigidity of the order parameter

$$\langle SB | \underline{\sum_{i \in A} S_i^2 - \sum_{j \in B} S_j^2} | SB \rangle \sim N S$$

$|\text{Néel}\rangle$ $= |\uparrow\downarrow\uparrow\downarrow\rangle$

Spin flips

$$\hat{S}^- |S, M_s = S\rangle = \ldots |S, M_s - 1\rangle$$

$$\hat{a}^+ |n\rangle = \ldots |n+1\rangle$$

$$\hat{S}_i^z = S - \hat{a}_i^\dagger \hat{a}_i$$

$|S\, m_s\rangle$ | $|n\rangle$

$|S, S\rangle \equiv |n=0\rangle$

$\boxed{\langle \hat{a}_i^\dagger \hat{a}_i \rangle \ll S}$ assume

$$\hat{S}_i^z = S - \hat{a}_i^\dagger a_i$$

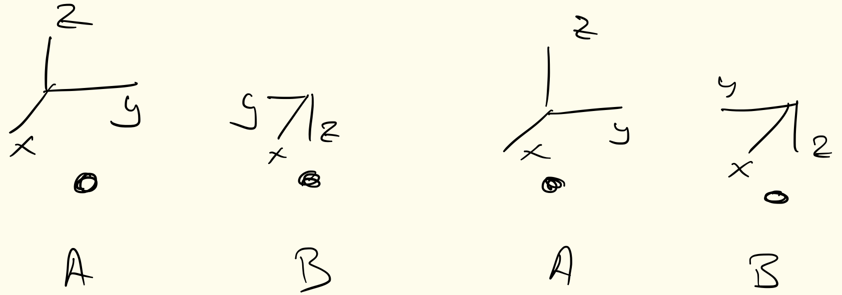
Holstein-Primakoff

comm. rel.

$$\Rightarrow \quad \hat{S}_i^+ = \sqrt{2S - \hat{a}_i^\dagger \hat{a}_i}\, \hat{a}_i \approx \sqrt{2S}\, \hat{a}_i$$

$$\hat{S}_i^- = \hat{a}_i^\dagger \sqrt{2S - \hat{a}_i^\dagger \hat{a}_i} \approx \hat{a}_i^\dagger \sqrt{2S}$$

$$\langle a_i^\dagger a_i \rangle \ll S \qquad O\left(\frac{\langle a^\dagger a \rangle}{S}\right)$$



$$\Longleftarrow \tilde{S}$$

$$\tilde{S}^{x,y,z}_{i\in A} = S^{x,y,z}_{i\in A}$$

$$\tilde{S}^{x}_{j\in B} = S^{x}_{j\in B}$$

$$\tilde{S}^{y}_{j\in B} = -S^{y}_{j\in B}$$

$$\tilde{S}^{z}_{j\in B} = -S^{z}_{j\in B}$$

$$\mathcal{H} = -J \sum_{\langle ij \rangle} \left(\tilde{S}_i^z \tilde{S}_j^z - \frac{1}{2} \left(\tilde{S}_i^+ \tilde{S}_j^+ + \tilde{S}_i^- \tilde{S}_j^- \right) \right)$$

$$= -NJS^2 + JS \sum_i \left(a_i^\dagger a_i + a_{i+1}^\dagger a_{i+1} + a_i a_{i+1} + a_i^\dagger a_{i+1}^\dagger \right)$$

$$+ O(S^0)$$

$$H = -NJS^2 + JS \sum_k \left(2 a_k^\dagger a_k + \cos(ka) \left(a_k^\dagger a_{-k}^\dagger + a_k a_{-k} \right) \right)$$

?

Lecture 4c

$$H = -NJS^2 + JS\sum_k \left(2a_k^\dagger a_k + \cos(ka)\left(a_k^\dagger a_{-k}^\dagger + a_k a_{-k}\right)\right)$$

$$= -NJS(S+1) + JS\sum_k \left(\hat{a}_k^\dagger \;\; \hat{a}_{-k}\right)\begin{pmatrix} 1 & \gamma_k \\ \gamma_k & 1 \end{pmatrix}\begin{pmatrix} \hat{a}_k \\ \hat{a}_{-k}^\dagger \end{pmatrix}$$

$\gamma_k = \cos(ka)$

$$\hat{\alpha}_k^\dagger = A_k \hat{a}_k^\dagger + B_k \hat{a}_{-k}$$

Bogoliubov

$$H = E_0 + JS\sum_k \left(\alpha_k^\dagger \;\; \alpha_{-k}\right)\begin{pmatrix} \varepsilon_k & 0 \\ 0 & \varepsilon_k \end{pmatrix}\begin{pmatrix} \alpha_k \\ \alpha_{-k}^\dagger \end{pmatrix}$$

$$[\alpha_u, \alpha^+_{u'}] = \delta_{u,u'}$$

$$= \left(|A_u|^2 - |B_u|^2\right)\delta_{u,u'}$$

$$A_u = \cosh(\theta_u) \qquad (\theta_u = \theta_{-u}) \qquad \left(\cosh^2 + \sinh^2 = \cosh(2\theta)\right)$$

$$B_u = \sinh(\theta_u)$$

$$H = -NJS(S+1) + JS\sum_u \left(\hat{\alpha}^+_u \hat{\alpha}_{-u}\right)\begin{pmatrix} \cosh(2\theta_u) - \gamma_k \sinh(2\theta_u) & \gamma c - s \\ \gamma c - s & c - \gamma s \end{pmatrix}\begin{pmatrix} \alpha_u \\ \alpha^+_{-u} \end{pmatrix}$$

$$\boxed{\gamma_u \cosh(2\theta_u) - \sinh(2\theta_u) = 0} \Rightarrow \boxed{\theta_u = \frac{1}{2}\,\mathrm{atanh}(\gamma_u)}$$

$$\gamma_k = \tanh(2\theta_k)$$

$$1-\gamma^2 = 1-\tanh^2 = \frac{\cosh^2 - \sinh^2}{\cosh^2}$$

$$= 1/\cosh^2$$

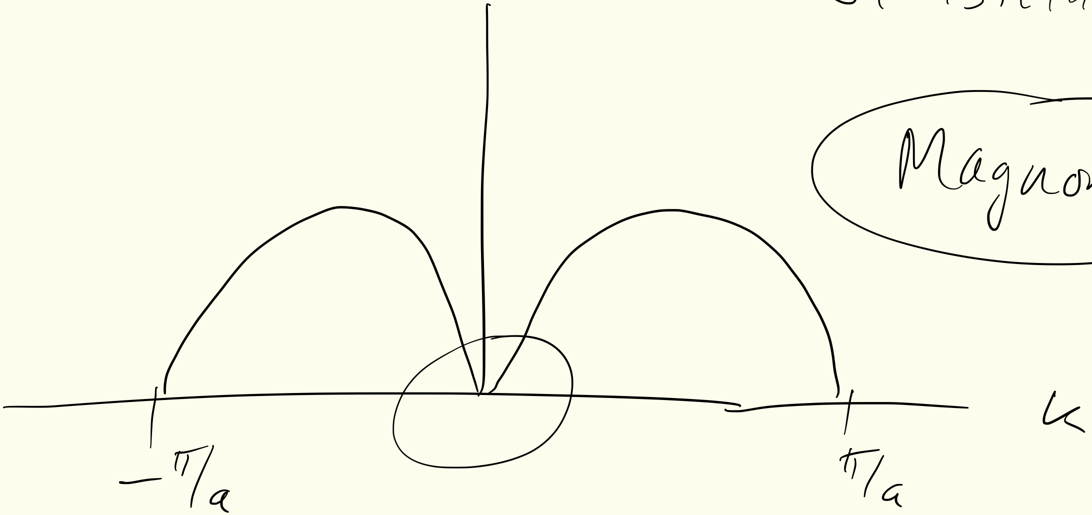
$$\varepsilon_k = \cosh(2\theta_k) - \gamma_k \sinh(2\theta_k)$$

$$= \cosh(2\theta_k)\left(1-\gamma_k^2\right)$$

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

$$\Rightarrow \boxed{\hat{H} = -NJS(S+1) + 2JS\sum_k |\sin(ka)|\left(\hat{\alpha}_k^\dagger \hat{\alpha}_k + \frac{1}{2}\right)}$$

$$\hbar\omega_k = 2JS'|\sin(ka)|$$



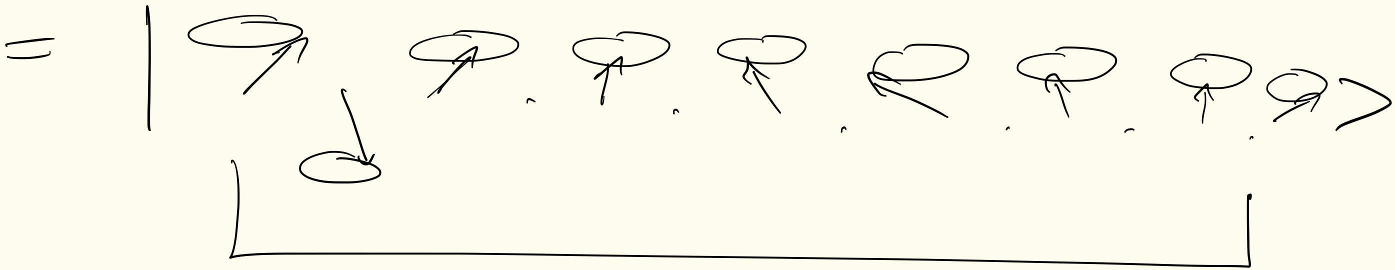
Magnons

$k \to 0$

$$\boxed{\hbar\omega_k = c\,k}$$

Goldstone modes.

$$\alpha_k^\dagger \,|\uparrow\;\downarrow\;\uparrow\;\downarrow\;\uparrow\;\downarrow\rangle$$



$$\lambda = 2\pi/k$$

$$|\nearrow\;\swarrow\;\nearrow\;\swarrow\;\nearrow\;\swarrow\;\nearrow\;\swarrow\rangle$$

$$\alpha_u^\dagger \alpha_u^\dagger \alpha_u \alpha_u$$

$$\underline{\alpha^\dagger \alpha} \qquad \underline{\alpha^\dagger \alpha}$$

$$H = \sum_k \frac{\hbar^2 k^2}{2m} \hat{a}_k^\dagger \hat{a}_k + \frac{1}{2V} \sum_{kk'q} V_q \, \hat{a}_{k+q}^\dagger \hat{a}_{k'-q}^\dagger \hat{a}_{k'} \hat{a}_k$$

N bosons

f.e. ^4He

$$a_0^\dagger a_0 |gs\rangle \approx N |gs\rangle$$

$\hat{H} |gs\rangle$

"mean field theory"

"RPA"

$$H = \frac{V_0}{2V} \boxed{a_0^\dagger a_0^\dagger a_0 a_0}$$

$$\boxed{V_q = V_0}$$

$$+ \sum_k \frac{\hbar^2 k^2}{2m} a_k^\dagger a_k$$

$$+ \frac{V_0}{2V} \sum_{k \neq 0} \Big(4\, a_0^\dagger a_k^\dagger a_0 a_k + a_k^\dagger a_{-k}^\dagger a_0 a_0$$

$$+ a_0^\dagger a_0^\dagger a_k a_{-k} \Big)$$

$$\boxed{a_0^\dagger a_0 \to N}$$

$$\boxed{a_0^\dagger a_0 + \sum_{k\neq 0} a_k^\dagger a_k = N}$$

Bogoliubov approx.

$$V_0 \equiv g\left(1 + \frac{g}{V}\sum_{k\neq 0} \frac{m}{k^2}\right)$$

$$\hat{H} = g\frac{N^2}{2V} + \sum_k \frac{k^2}{2m} a_k^\dagger a_k + \frac{gmN}{2V}\sum_{k\neq 0}\Big(2a_k^\dagger a_k + a_k^\dagger a_{-k}^\dagger$$

$$+ a_k a_{-k} + \frac{mgN}{2V}\Big)$$

$$= E_0 + \sum_k \sqrt{\frac{gN}{mV}k^2 + \left(\frac{k^2}{2m}\right)^2}\ \hat{b}_k^\dagger \hat{b}_k$$

$$\hbar\omega_k \propto k.$$