SFB 1143

Solid State Theory (SS2020)

Lecture 21: Hubbard & Heisenberg models

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§ 6.1 Hubbard & Heisenberg models

- Hubbard model:

$n_{i\sigma} = c_{i\sigma}^{+} c_{i\sigma}$

$$H = -t \sum_{\langle i,j \rangle} \sum_{\sigma=\uparrow,\downarrow} \left(c_{i\sigma}^{+} c_{j\sigma} + c_{j\sigma}^{+} c_{i\sigma} \right) + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

  - Partially filled d- and f-orbitals

very localized!

Ref: A. Auerbach, *Interacting Electrons and Quantum Magnetism* (Springer, 1994).

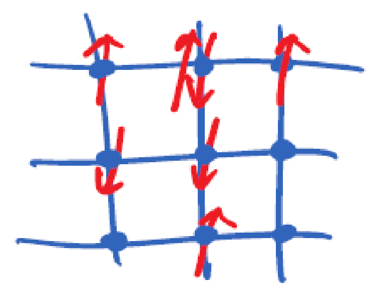
§ 6.1 Hubbard & Heisenberg models

- Hubbard model:

$n_{i\sigma} = c_{i\sigma}^{+} c_{i\sigma}$

$$H = -t \sum_{\langle i,j \rangle} \sum_{\sigma=\uparrow,\downarrow} \left(c_{i\sigma}^{+} c_{j\sigma} + c_{j\sigma}^{+} c_{i\sigma} \right) + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

half-filling : $N_e = N$



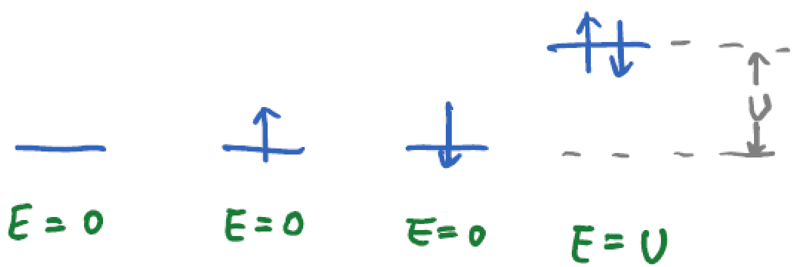
$$\varepsilon_{\vec{k}} = -2t(\cos k_x + \cos k_y)$$

metal for $U = 0$!

§ 6.1 Hubbard & Heisenberg models

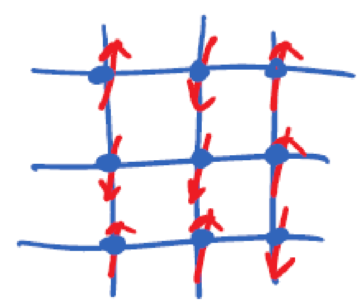
$U > 0$?

single site : $H_U = U\, n_\uparrow n_\downarrow$



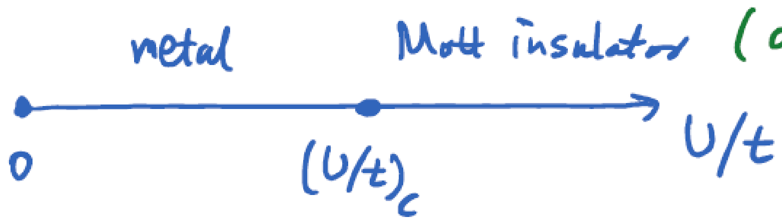
$U \to \infty$:
half-filled

single occupancy



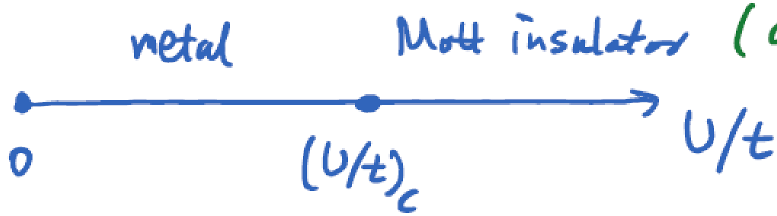
2^N configurations

§ 6.1 Hubbard & Heisenberg models



(driven by interactions, despite band half-filled)

§ 6.1 Hubbard & Heisenberg models



(driven by interactions, despite band half-filled)

$U \gg t$: second-order perturbation theory (in t/U)

$$H_{eff}^{(2)} = J \sum_{\langle i,j \rangle} \vec{S}_i \cdot \vec{S}_j$$

$S = 1/2$

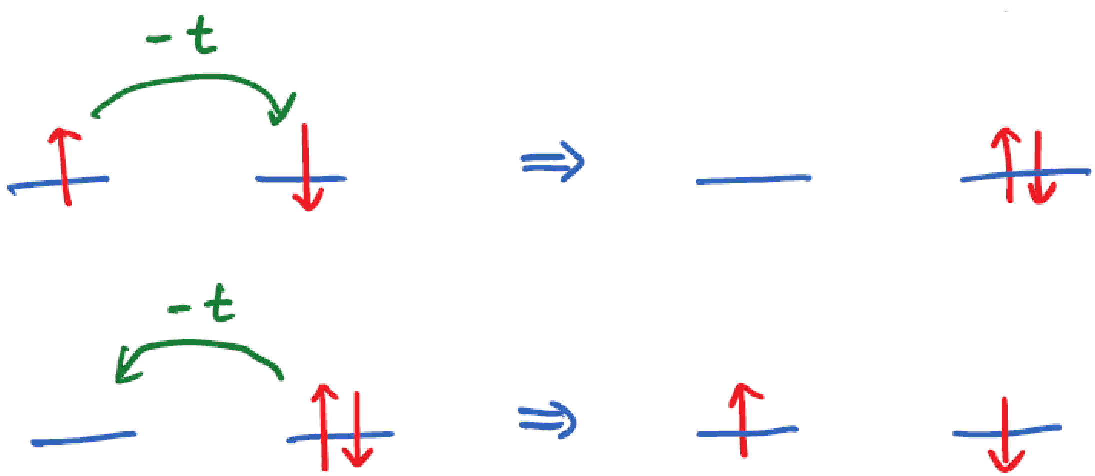
singly-occupied electron

$$J = \frac{4t^2}{U} > 0$$

(AFM interaction)

§ 6.1 Hubbard & Heisenberg models

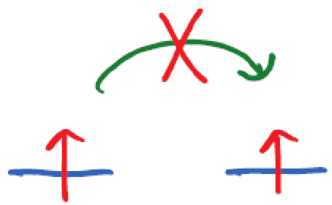
virtual process in second-order perturbation theory:



(gain energy $\sim t^2/U$ when antiparallel)

§ 6.1 Hubbard & Heisenberg models

virtual process in second-order perturbation theory:



forbidden due to Pauli's exclusion principle!

(does not gain energy from hopping when parallel)

§ 6.1 Hubbard & Heisenberg models

- Superexchange interaction:

Two-site low-energy subspace:

$$|\uparrow,\uparrow\rangle,\ |\uparrow,\downarrow\rangle,\ |\downarrow,\uparrow\rangle,\ |\downarrow,\downarrow\rangle$$

$$1 = P_0 + P_1$$

P_0: project onto the singly occupied subspace

P_1: orthogonal complement

§ 6.1 Hubbard & Heisenberg models

$$\underbrace{\langle a|}_{\text{low-energy subspace}} H_{eff}^{(2)} \underbrace{|b\rangle}_{\text{low-energy subspace}} = \langle a| \underbrace{H_t}_{-t(c_{1\sigma}^{\dagger} c_{2\sigma} + c_{2\sigma}^{\dagger} c_{1\sigma})} P_1 \frac{1}{\underbrace{E^{(0)}}_{=0} - \underbrace{H_U}_{=U(n_{1\uparrow} n_{1\downarrow} + n_{2\uparrow} n_{2\downarrow})}} P_1 H_t |b\rangle$$

§ 6.1 Hubbard & Heisenberg models

$$\langle \uparrow\uparrow | H_{eff}^{(2)} | \uparrow\uparrow \rangle = \langle \uparrow\uparrow | -t(C_{1\sigma}^{+}C_{2\sigma} + C_{2\sigma}^{+}C_{1\sigma}) P_1$$

$$\times \frac{-1}{H_U} P_1 (-t) \underbrace{(C_{1\sigma}^{+}C_{2\sigma} + C_{2\sigma}^{+}C_{1\sigma}) C_{1\uparrow}^{+}C_{2\uparrow}^{+}|0\rangle}_{= 0}$$

$$= 0$$

e.g. $C_{1\uparrow}^{+}C_{2\uparrow} C_{1\uparrow}^{+}C_{2\uparrow}^{+}|0\rangle = 0$

§ 6.1 Hubbard & Heisenberg models

$$\langle \uparrow\downarrow | H_{eff}^{(2)} | \uparrow\downarrow \rangle = \underbrace{\langle 0 | c_{2\downarrow} c_{1\uparrow} (-t) (c_{1\sigma}^{+} c_{2\sigma} + c_{2\sigma}^{+} c_{1\sigma})}_{(-t)\left(\langle 0 | c_{2\downarrow} c_{2\uparrow} + \langle 0 | c_{1\downarrow} c_{1\uparrow} \right)} P_1$$

$$\times \frac{-1}{H_U} P_1 (-t) \underbrace{(c_{1\sigma}^{+} c_{2\sigma} + c_{2\sigma}^{+} c_{1\sigma}) c_{1\uparrow}^{+} c_{2\downarrow}^{+} | 0 \rangle}_{c_{1\uparrow}^{+} c_{1\downarrow}^{+} | 0 \rangle + c_{2\uparrow}^{+} c_{2\downarrow}^{+} | 0 \rangle}$$

$$= - \frac{2t^2}{U}$$

§ 6.1 Hubbard & Heisenberg models

$$\langle \uparrow\downarrow | H_{eff}^{(2)} | \downarrow\uparrow \rangle = \underbrace{\langle 0 | c_{2\downarrow} c_{1\uparrow} (-t) \left(c_{1\sigma}^{+} c_{2\sigma} + c_{2\sigma}^{+} c_{1\sigma} \right)}_{= (-t)\left(\langle 0 | c_{2\downarrow} c_{2\uparrow} + \langle 0 | c_{1\downarrow} c_{1\uparrow} \right)} P_1$$

$$\times \frac{-1}{H_U} P_1 (-t) \underbrace{\left(c_{1\sigma}^{+} c_{2\sigma} + c_{2\sigma}^{+} c_{1\sigma} \right) c_{1\downarrow}^{+} c_{2\uparrow}^{+} | 0 \rangle}_{= - c_{1\uparrow}^{+} c_{1\downarrow}^{+} | 0 \rangle - c_{2\uparrow}^{+} c_{2\downarrow}^{+} | 0 \rangle}$$

$$= + \frac{2t^2}{U}$$

§ 6.1 Hubbard & Heisenberg models

$$\Rightarrow \quad H_{eff}^{(2)} = \frac{2t^2}{U} \begin{array}{c} \begin{array}{cccc} |\uparrow\uparrow\rangle & |\uparrow\downarrow\rangle & |\downarrow\uparrow\rangle & |\downarrow\downarrow\rangle \end{array} \\ \left(\begin{array}{c|cc|c} 0 & 0 & 0 & 0 \\ \hline 0 & -1 & 1 & 0 \\ 0 & 1 & -1 & 0 \\ \hline 0 & 0 & 0 & 0 \end{array}\right) \end{array} \begin{array}{c} |\uparrow\uparrow\rangle \\ |\uparrow\downarrow\rangle \\ |\downarrow\uparrow\rangle \\ |\downarrow\downarrow\rangle \end{array}$$

$$= \frac{t^2}{U} \left(\sigma^x \otimes \sigma^x + \sigma^y \otimes \sigma^y + \sigma^z \otimes \sigma^z - \mathbb{1}_{2\times 2} \otimes \mathbb{1}_{2\times 2} \right)$$

$$= \frac{4t^2}{U} \left(\vec{S}_1 \cdot \vec{S}_2 - \frac{1}{4} \right) \quad \checkmark$$

§ 6.1 Hubbard & Heisenberg models

Single-band Hubbard model :

$$H = -t \sum_{\langle i,j \rangle} \left(c_{i\sigma}^{+} c_{j\sigma} + c_{j\sigma}^{+} c_{i\sigma} \right) + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

$$\Big\downarrow \quad U \gg t \,, \quad \text{half filling} \ (N_e = N)$$

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

single site : $S = 1/2$ $\quad \uparrow \quad \downarrow$

Antiferromagnetic super-exchange interaction : $J = \frac{4t^2}{U} > 0$

§ 6.1 Hubbard & Heisenberg models

- Heisenberg interaction for two spin-1/2's:

$$H = J\,\vec{S}_1 \cdot \vec{S}_2$$

$$= \frac{J}{2}\left[\underbrace{(\vec{S}_1+\vec{S}_2)^2}_{\vec{S}^2 = (\vec{S}_1+\vec{S}_2)^2} - \vec{S}_1^{\,2} - \vec{S}_2^{\,2}\right]$$

$$\vec{S}_1^{\,2} = \vec{S}_2^{\,2} = s(s+1) = \frac{1}{2}\left(\frac{1}{2}+1\right) = \frac{3}{4}$$

$\vec{S}^2 = (\vec{S}_1+\vec{S}_2)^2$

total spin : $1/2 \times 1/2 \rightarrow 0 + 1$

$$= \frac{J}{2}\left(\vec{S}^2 - \frac{3}{2}\right)$$

$\vec{S}^2 \to S_{tot}(S_{tot}+1)$, $S_{tot} = 0$ or 1

§ 6.1 Hubbard & Heisenberg models

$$H = \frac{J}{2}\left(\vec{S}^2 - \frac{3}{2}\right)$$

$\vec{S}^2 \rightarrow S_{tot}(S_{tot}+1)$, $S_{tot} = 0$ or 1

$$\Rightarrow \quad E = \begin{cases} -\frac{3}{4}J , & S_{tot} = 0 \\ \frac{1}{4}J , & S_{tot} = 1 \end{cases}$$

Energy splitting : J

§ 6.1 Hubbard & Heisenberg models

$$H = \frac{J}{2}\left(\vec{S}^2 - \frac{3}{2}\right)$$

$S_{tot}(S_{tot}+1)$, $S_{tot} = 0$ or 1

Ground state for $J>0$: $S_{tot} = 0$ (antiferromagnetic)

AFM

$$|s\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\rangle_1 |\downarrow\rangle_2 - |\downarrow\rangle_1 |\uparrow\rangle_2\right)$$

singlet

$$H|s\rangle = -\frac{3}{4}J\,|s\rangle$$

§ 6.1 Hubbard & Heisenberg models

$$H = \frac{J}{2}\left(\vec{S}^2 - \frac{3}{2}\right)$$

$\vec{S}^2 \rightarrow S_{tot}(S_{tot}+1)$, $S_{tot} = 0$ or 1

Ground state for $J<0$: $S_{tot} = 1$ (ferromagnetic)

FM

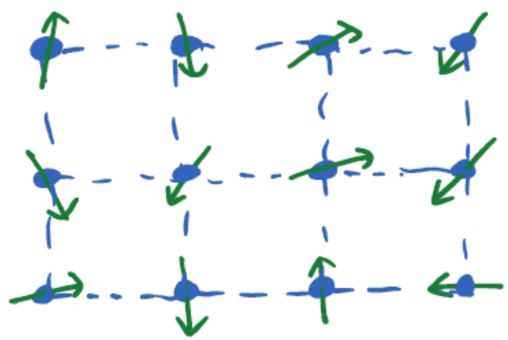
$$|t_1\rangle = |\uparrow\rangle_1 |\uparrow\rangle_2$$

$$|t_0\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\rangle_1 |\downarrow\rangle_2 + |\downarrow\rangle_1 |\uparrow\rangle_2 \right)$$

$$|t_{-1}\rangle = |\downarrow\rangle_1 |\downarrow\rangle_2$$

$$H|t_a\rangle = \frac{1}{4}J|t_a\rangle \qquad (a = \pm 1, 0)$$

§ 6.1 Hubbard & Heisenberg models



$$H = \sum_{i,j} J_{ij} \vec{S}_i \cdot \vec{S}_j$$

Ground state ? Low-energy excitations ? ...

depend on dimensionality, lattice geometry, spin, sign/strength of interactions, temperature ...

§ 6.1 Hubbard & Heisenberg models

Simplification: Heisenberg model

$$H = \frac{J}{2} \sum_{\vec{r}, \vec{\delta}} \vec{S}_{\vec{r}} \cdot \vec{S}_{\vec{r}+\vec{\delta}}$$

all nearest neighbors of site $\vec{r}$

$J < 0$: ferromagnetic (FM)

$J > 0$: antiferromagnetic (AFM)

§ 6.1 Hubbard & Heisenberg models

Simplification: Heisenberg model

$$H = \frac{J}{2} \sum_{\vec{r}, \vec{\delta}} \vec{S}_{\vec{r}} \cdot \vec{S}_{\vec{r}+\vec{\delta}}$$

all nearest neighbors of site $\vec{r}$

spin-S: $\vec{S}_{\vec{r}} = (S^x_{\vec{r}}, S^y_{\vec{r}}, S^z_{\vec{r}})$, $\quad \vec{S}_r^{\,2} = S(S+1)$

$$[S^a_{\vec{r}}, S^b_{\vec{r}'}] = \underbrace{\delta_{\vec{r}\vec{r}'}}_{\text{spin operators at different sites commute with each other}} \cdot \underbrace{i \varepsilon_{abc} S^c_{\vec{r}}}_{\text{standard commutation relation of angular momentum}}$$

§ 6.1 Hubbard & Heisenberg models

Simplification: Heisenberg model

$$H = \frac{J}{2} \sum_{\vec{r},\vec{\delta}} \vec{S}_{\vec{r}} \cdot \vec{S}_{\vec{r}+\vec{\delta}}$$

all nearest neighbors of site $\vec{r}$

$$S^{\pm}_{\vec{r}} = S^{x}_{\vec{r}} \pm i S^{y}_{\vec{r}}$$

$$\Rightarrow \quad [S^{\pm}_{\vec{r}}, S^{z}_{\vec{r}'}] = \mp S^{\pm}_{\vec{r}} \delta_{\vec{r},\vec{r}'}$$

$$[S^{+}_{\vec{r}}, S^{-}_{\vec{r}'}] = 2 S^{z}_{\vec{r}} \delta_{\vec{r},\vec{r}'}$$

§ 6.1 Hubbard & Heisenberg models

single-site basis :

$$|s, m\rangle$$

spin quantum number

magnetic quantum number

$$\begin{cases} \vec{S}_{\vec{r}}^{\,2} |s, m\rangle = s(s+1) |s, m\rangle \\ S_{\vec{r}}^{z} |s, m\rangle = m |s, m\rangle \end{cases}$$

$\longrightarrow m = -s, -s+1, \ldots, s$

$2s+1$ states in a single site

§ 6.1 Hubbard & Heisenberg models

N-site basis: (tensor product of single-site basis)

$$\cdots |s, m\rangle_{\vec{r}} \, |s, m'\rangle_{\vec{r}+\vec{\delta}} \cdots$$

$(2s+1)^N$-dimensional Hilbert space!

We will simplify notation below: $|s, m\rangle \rightarrow |m\rangle$

§ 6.1 Hubbard & Heisenberg models

- Classical limit: $S \to \infty$

$$\left[\underbrace{\frac{\hat{S}^a}{S}}, \frac{\hat{S}^b}{S}\right] = \underbrace{\frac{1}{S}}_{\to\, 0 \text{ for } S \to \infty} \cdot i\epsilon_{abc}\frac{\hat{S}^c}{S}$$

$$\langle S | \frac{\hat{S}^z}{S} | S \rangle = 1 \Rightarrow \left\langle \frac{\hat{S}^z}{S} \right\rangle \le 1$$

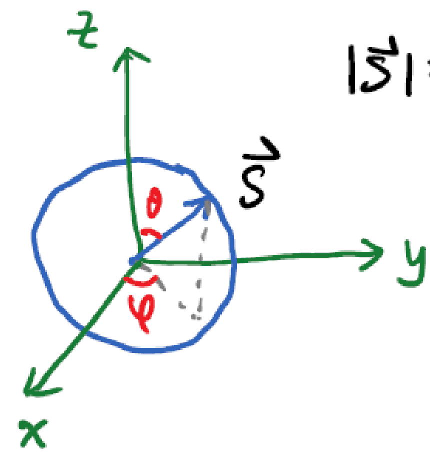
Rescaled spin operators commute in the large-S limit!

§ 6.1 Hubbard & Heisenberg models

Classical spin: unit vectors

$$\vec{S}_j = (S_j^x, S_j^y, S_j^z)$$

$$\begin{cases} S_j^x = \sin\theta_j \cos\varphi_j \\ S_j^y = \sin\theta_j \sin\varphi_j \\ S_j^z = \cos\theta_j \end{cases}$$

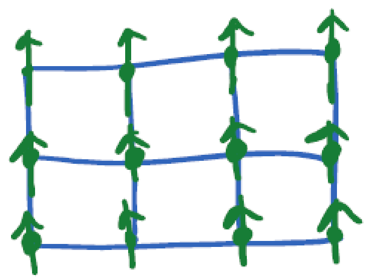


$|\vec{S}| = 1$

§ 6.1 Hubbard & Heisenberg models

Ground state: minimize the energy functional H
(T = 0) with respect to (θ_j, φ_j)

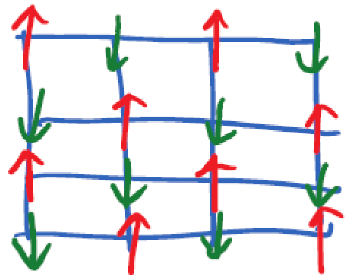
FM:



$\theta_j = 0$
(or rotate every spin by the same angle)

§ 6.1 Hubbard & Heisenberg models

AFM:



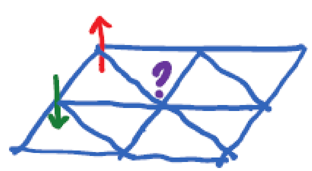
↑ $\theta_j = 0$

↓ $\theta_j = \pi$

bipartite lattice : A-sublattice ↑ Néel order

B-sublattice ↓

nonbipartite lattice : ?



frustration !