§4. Symmetries of the Hubbard model

SU(2) - symmetry

The hopping part of the Hubbard model is the same for spin up and down, hence the H_1 term is spin rotational invariant

Let $\hat{\Psi}_j = \begin{pmatrix} \hat{a}_{j\uparrow} \\ \hat{a}_{j\downarrow} \end{pmatrix}$, $\hat{\Psi}_i^\dagger = (\hat{a}_{i\uparrow}^\dagger, \hat{a}_{i\downarrow}^\dagger)$

$$\hat{H}_1 = \sum_{ij} \sum_\sigma t_{ij} \hat{a}_{i\sigma}^\dagger \hat{a}_{j\sigma} = \sum_{ij} t_{ij} \hat{\Psi}_i^\dagger \hat{\Psi}_j$$

How about $\hat{H}_2$?

When we rotate the spin ~~axis~~ quantization axis the fermion operator transforms as

$$\hat{\tilde{a}}_{i\sigma} = \sum_\rho \hat{U}_{\sigma\rho} \hat{a}_{i\rho}$$

$$\hat{\tilde{\Psi}} = \hat{U}\hat{\Psi}, \quad \hat{\tilde{\Psi}}^\dagger = \hat{\Psi}^\dagger \hat{U}^\dagger$$

$U_{\sigma\rho}$ - 2×2 SU(2) matrix
$\hat{U}^{-1} = \hat{U}^\dagger$, $\det \hat{U} = 1$

We can parametrize SU(2) matrix $U(\bar{\theta})$ as

$$\hat{U}(\bar{\theta}) = e^{i\bar{\theta}\cdot\bar{\tau}} = \cos\theta\,\mathbb{1} + i\sin\theta \frac{\bar{\theta}\cdot\bar{\tau}}{|\theta|} \qquad \theta = |\bar{\theta}|$$

$$\bar{\tau} = (\tau_x, \tau_y, \tau_z) \qquad \bar{\theta} = (\theta_x, \theta_y, \theta_z)$$

$$\tau_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \tau_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \tau_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

The spin operator $\qquad \hbar = 1$

$$S_i^a = \frac{1}{2} \sum_{\mu\nu} a_{i\mu}^\dagger \tau_{\mu\nu}^a a_{i\nu} = \frac{1}{2} \hat{\Psi}_i^\dagger \tau^a \hat{\Psi}_i$$

under $SU(2)$ transformation the spin operator transforms as

$$\tilde{S}_i^a = \frac{1}{2} \hat{\tilde{\Psi}}^\dagger \tau^a \hat{\tilde{\Psi}} = \frac{1}{2} \hat{\Psi}_i^\dagger (\hat{U}^\dagger \tau^a \hat{U}) \hat{\Psi}_i =$$

$$= \frac{1}{2} \hat{\Psi}_i^\dagger \Big(\sum_{ab} \underbrace{R_{ab}}_{\text{rotation matrix}} \tau^b \Big) \hat{\Psi}_i \qquad (*)$$

On the other hand, using

$$\sum_a \tau^a_{\sigma\rho} \tau^a_{\mu\nu} = 2 \delta_{\sigma\nu} \delta_{\rho\mu} - \delta_{\sigma\rho} \delta_{\mu\nu}$$

one can show that

$$n_{i\uparrow} n_{i\downarrow} = -\frac{2}{3} \vec{S}_i^{\,2} + \frac{1}{2} U \hat{n}_i$$

hence $\qquad \hat{N}_e = \sum_i \hat{n}_i$

$$\hat{H} = \sum_{ij} t_{ij} \hat{\Psi}_i^\dagger \hat{\Psi}_j - \frac{2}{3} U \sum_i \vec{S}_i^{\,2} + \frac{\hat{N}_e U}{2}$$

Since $\vec{S}_i^{\,2}$ is rotationally invariant due to $(*)$

the Hubbard model is ~~rotationally~~

$SU(2)$ invariant up to a constant term.

<u>particle-hole symmetry</u>

particle-hole transformation $\hat{\Gamma}$ for a spinless fermion is defined

$$\boxed{\hat{\Gamma}\,\hat{a}_i\,\hat{\Gamma}^{+} = \hat{a}_i^{+}}$$

antiunitary operator

Naive generalization for spinfull fermions

$$\boxed{\hat{\Gamma}\,\hat{a}_{i\sigma}\,\hat{\Gamma}^{+} = \hat{a}_{i\sigma}^{+}} \qquad (*)$$

gives

$$\hat{\Gamma}\hat{H}\hat{\Gamma}^{+} = +\sum_{ij\sigma} t_{ij}\, a_{i\sigma} a_{j\sigma}^{+} + U\sum_i (1-n_{i\uparrow})(1-n_{i\downarrow}) =$$

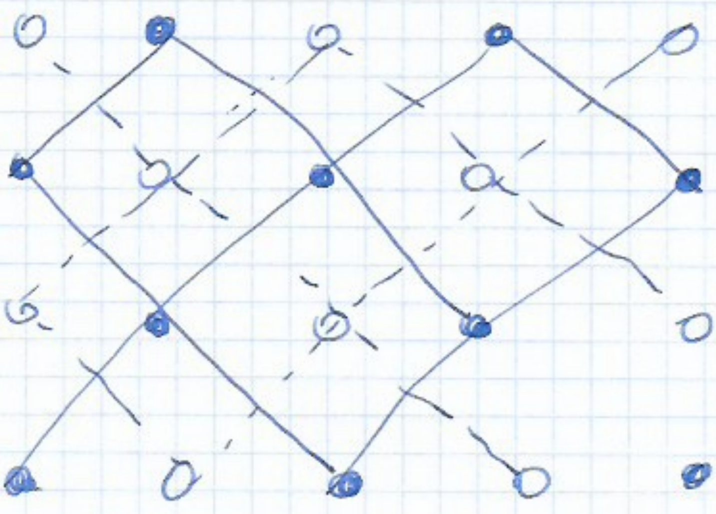
$$= -\sum_{ij} t_{ij}\, a_{i\sigma}^{+} a_{j\sigma} + U\sum_i n_{i\uparrow} n_{i\downarrow} + \text{const.}$$

!

After this transformation the hopping term is changed! No particle-hole symmetry of type $(*)$

<u>Geometric symmetry</u>

On a <u>bipartite lattices</u> we change the definition of particle-hole transformation



o – sublattice A or B

$$t_{ij} = \begin{cases} t_{ij} & \\ 0 & \text{same} \end{cases}$$

● – sublattice B

$$\cancel{t_{ij} = \begin{cases} t_{ij}^{A} & i,j \in A \\ t_{ij}^{B} & i,j \in B \\ 0 & i\in A, j\in B \end{cases}}$$

p-h transformation

$$\hat{\Gamma}\, \hat{a}_{i\sigma}\, \hat{\Gamma}^{+} = \begin{cases} \hat{a}^{+}_{i\sigma} & \text{if } i \in A \\ -\hat{a}^{+}_{i\sigma} & \text{if } i \in B \end{cases}$$

$$\hat{\Gamma}\, \hat{H}\, \hat{\Gamma}^{+} = -\sum_{ij\sigma} t_{ij}\, \hat{a}_{i\sigma}\, \hat{a}^{+}_{j\sigma} + U \sum_i (1-n_{i\uparrow})(1-n_{i\downarrow}) =$$

$$= \sum_{ij\sigma} t_{ij}\, \hat{a}_{i\sigma}\, \hat{a}_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} + \text{const.}$$

now, the Hubbard model is symmetric under p-h transformation.

→ The phase diagram is symmetric under the half-filling

U(1) gauge symmetry

$$a_{i\sigma} \to a_{i\sigma}\, e^{-i\theta}$$

$$a^{+}_{i\sigma} \to a^{+}_{i\sigma}\, e^{i\theta}$$

$$\sum_{ij}\sum_{\sigma} t_{ij}\, a^{+}_{i\sigma} a_{j\sigma} \to \sum_{ij} t_{ij}\, a^{+}_{i\sigma} a_{j\sigma} \underbrace{e^{i\theta} e^{-i\theta}}_{1}$$

$$\sum_i n_{i\uparrow} n_{i\downarrow} \to \sum_i a^{+}_{i\uparrow} a_{i\uparrow}\, a^{+}_{i\downarrow} a_{i\downarrow}\, \underbrace{e^{i\theta} e^{-i\theta}}_{1}\, \underbrace{e^{i\theta} e^{-i\theta}}_{1}$$

$\hat{H} = \hat{H}_1 + \hat{H}_2$ – charge conservation

Particle-hole symmetry

$$\hat{a}^{+}_{i\sigma} \to (-1)^{i}\, \hat{a}_{i\sigma}$$

$$\hat{a}_{i\sigma} \to (-1)^{i}\, \hat{a}^{+}_{i\sigma}$$

$$\hat{n}_{i\sigma} = \hat{a}^{+}_{i\sigma}\hat{a}_{i\sigma} \to (-1)^{2i}\,\hat{a}_{i\sigma}\hat{a}^{+}_{i\sigma} = 1 - \hat{a}^{+}_{i\sigma}\hat{a}_{i\sigma} = 1-\hat{n}_{i\sigma}$$

$$\hat{H} = \sum_{ij\sigma} t_{ij}\,\hat{a}^{+}_{i\sigma}\hat{a}_{j\sigma} + U\sum_i n_{i\uparrow}n_{i\downarrow}\,.$$

$\downarrow$ on bipartite

$$\hat{H} = -\sum_{ij\sigma} t_{ij}\,\hat{a}_{i\sigma}\hat{a}^{+}_{j\sigma} + U\sum_i (1-n_{i\uparrow})(1-n_{i\downarrow}) =$$

$$= \sum_{ij\sigma} t_{ij}\,\hat{a}^{+}_{i\sigma}\hat{a}_{j\sigma} + U\sum_i n_{i\uparrow}n_{i\downarrow} + U N_L - U\sum_i (n_{i\uparrow}+n_{i\downarrow})$$

$$\hat{H}_\mu = \hat{H} - \mu\hat{N} \to \cancel{\hat{H}_{-\mu}\,\hat{N}\,U\hat{N}}$$

$$\| $$

$$\sum_{ij\sigma} t_{ij}\,a^{+}_{i\sigma}a_{j\sigma} - \mu\sum_{i\sigma} n_{i\sigma} + U\sum_i n_{i\uparrow}n_{i\downarrow}$$

$$\downarrow$$

$$\sum_{ij\sigma} t_{ij}\,a^{+}_{i\sigma}a_{j\sigma} - \mu\sum_{i\sigma}(1-n_{i\sigma}) + U\sum_i (1-n_{i\uparrow})(1-n_{i\downarrow}) =$$

$$= \sum_{ij\sigma} t_{ij}\,a^{+}_{i\sigma}a_{j\sigma} + \mu\sum_{i\sigma} n_{i\sigma} - 2\mu N_L + U N_L + U\sum_i n_{i\uparrow}n_{i\downarrow} - U\sum_{i\sigma} n_{i\sigma} =$$

$$= \hat{H}_{-\mu} - 2\mu N_L + U N_L - U\sum_{i\sigma} n_{i\sigma} =$$

$$= \hat{H}_{-\mu} - (\cancel{2\mu}\,U)\sum_{i\sigma} n_{i\sigma} + U N_L - 2\mu N_L$$

$$\Xi_h = \mathrm{Tr}\left[e^{-\beta(\hat{H} + \mu\hat{N} - U\hat{N} + U N_L - 2\mu N_L)}\right] = \qquad \mu = \frac{U}{2}$$

$$= \mathrm{Tr}\left[e^{-\beta(\hat{H} - \mu\hat{N} + (2\mu - U)\hat{N} + U N_L - 2\mu N_L}\right] \stackrel{\downarrow}{=} \Xi_p$$

$$\Xi_h(T, \mu, N_L) = \Xi_p(T, U-\mu, N_L)$$

$$\Xi_p(T,\mu,N_L) = \mathrm{Tr}\left[e^{-\beta(\hat{H}-\mu\hat{N})}\right]$$

$$\boxed{n(\mu,T)} = \frac{1}{N_L}\left[\langle \hat{n}_\uparrow\rangle + \langle \hat{n}_\downarrow\rangle\right] =$$

$$= \frac{1}{N_L}\,\frac{\mathrm{Tr}\left[\overbrace{\sum_i(\hat{n}_{i\uparrow}+\hat{n}_{i\downarrow})}^{\hat{N}}\, e^{-\beta(\hat{H}-\mu\hat{N})}\right]}{\mathrm{Tr}\left[e^{-\beta(\hat{H}-\mu\hat{N})}\right]} = \frac{1}{N_L}\frac{1}{\beta}\frac{\partial \ln\Xi}{\partial\mu}$$

$$\frac{1}{N_L}\frac{1}{\beta}\frac{\partial\ln\Xi}{\partial\mu} \xrightarrow[ph]{} \frac{1}{N_L}\frac{1}{\beta}\frac{\partial}{\partial\mu}\ln \mathrm{Tr}\Big[e^{-\beta\left(\sum_{ij\sigma} t_{ij}\, a^\dagger_{i\sigma} a_{j\sigma} + \mu\sum_{i\sigma} n_{i\sigma} + U\sum_i n_{i\uparrow}n_{i\downarrow} + UN_L - 2\mu N_L - U\sum_{i\sigma} n_{i\sigma}\right)}\Big] =$$

$$= \frac{1}{N_L}\,\frac{\mathrm{Tr}\left[(-\hat{N}+2N_L)\,e^{-\beta(\cdots)}\right]}{\mathrm{Tr}\left[e^{-\beta(\hat{H}+\mu\hat{N}-U\hat{N}+UN_L-2\mu N_L)}\right]} =$$

$$\boxed{= 2 - n(U-\mu, T)}$$

at half-filling, $n=1$, $\mu = U-\mu \rightarrow \boxed{\mu = \frac{U}{2}}$