§3. Extended Hubbard model

Exact two-body part of the Hamiltonian

$$\hat{H}_2 = \frac{1}{2}\sum_{\sigma\sigma'}\sum_{ijkl} U_{ijkl}\,\hat{a}^\dagger_{i\sigma}\hat{a}^\dagger_{j\sigma'}\hat{a}_{l\sigma'}\hat{a}_{k\sigma}$$

$$U_{ijkl} = \int d^3r \int d^3r'\, w_i^*(r)\, w_j^*(r')\, V(|r-r'|)\, w_k(r')\, w_l(r)$$

In the Hubbard model we used

$\rightarrow$ $i = j = k = l$

Now consider pairwise identical indices:

$\rightarrow$ $i = j \neq k = l$

$i = k \neq j = l$

$i = l \neq j = k$

$$\frac{1}{2}\sum_{\sigma}\sum_{ik}{}' U_{iikk}\Big(\underbrace{\hat{a}^\dagger_{i\sigma}\hat{a}^\dagger_{i\sigma}}_{=0}\underbrace{\hat{a}_{k\sigma}\hat{a}_{k\sigma}}_{=0} + \hat{a}^\dagger_{i\sigma}\hat{a}^\dagger_{i\bar\sigma}\hat{a}_{k\bar\sigma}\hat{a}_{k\sigma}\Big) +$$

$$\frac{1}{2}\sum_{\sigma}\sum_{ij}{}' U_{ijji}\Big(\hat{a}^\dagger_{i\sigma}\hat{a}^\dagger_{j\sigma}\hat{a}_{j\sigma}\hat{a}_{i\sigma} + \hat{a}^\dagger_{i\sigma}\hat{a}^\dagger_{j\bar\sigma}\hat{a}_{j\bar\sigma}\hat{a}_{i\sigma}\Big) +$$

$$\frac{1}{2}\sum_{\sigma}\sum_{ij}{}' U_{ijij}\Big(\hat{a}^\dagger_{i\sigma}\hat{a}^\dagger_{j\sigma}\hat{a}_{i\sigma}\hat{a}_{j\sigma} + \hat{a}^\dagger_{i\sigma}\hat{a}^\dagger_{j\bar\sigma}\hat{a}_{i\bar\sigma}\hat{a}_{j\sigma}\Big) =$$

$$= \sum_{ij}{}' U_{iijj}\, a^\dagger_{i\uparrow}a^\dagger_{i\downarrow}a_{j\downarrow}a_{j\uparrow} +$$

$$\vec{S}_i\cdot\vec{S}_j = \frac{1}{2}\left(S_i^+S_j^- + S_i^-S_j^+\right) + S_i^z S_j^z$$

$$+\frac{1}{2}\sum_{\sigma}\sum_{ij}{}' U_{ijji}\Big(\cancel{n_{i\sigma}n_{j\sigma}} - n_{i\sigma}n_{j\sigma} - s_i^{\sigma}s_j^{\bar\sigma}\Big) +$$

$$+\frac{1}{2}\sum_{\sigma}\sum_{ij}{}' U_{ijij}\Big(n_{i\sigma}n_{j\sigma} + n_{i\sigma}n_{j\bar\sigma}\Big) =$$

$$= \sum_{ij}{}'\Big[U_{iijj}\,\hat{a}^\dagger_{i\uparrow}\hat{a}^\dagger_{i\downarrow}\hat{a}_{j\downarrow}\hat{a}_{j\uparrow} - U_{ijji}\Big(\vec{S}_i\cdot\vec{S}_j + \frac{1}{4}\hat{n}_i\hat{n}_j\Big) + \frac{1}{2}U_{ijij}\,\hat{n}_i\hat{n}_j\Big]$$

$$= \sum_{ij}{}' \Big[U_{iijj}\, a_{i\uparrow}^{+} a_{i\downarrow}^{+} a_{j\downarrow} a_{j\uparrow} +$$

$$+ \frac{1}{2} U_{ijji} (n_{i\sigma} n_{j\sigma} + n_{i\sigma} n_{j\bar\sigma}) +$$

$$+ \frac{1}{2} U_{ijij} (- n_{i\sigma} n_{j\sigma} - S_i^{\sigma} S_j^{\bar\sigma}) \Big]$$

$$\bar{S}_i \cdot \bar{S}_j = \frac{1}{2} (S_i^{+} S_j^{-} + S_i^{-} S_j^{+}) + S_i^{z} S_j^{z}$$

$$S_i^{z} = \frac{1}{2} (n_{i\uparrow} - n_{i\downarrow})$$

$$\mathcal{H}_2 = U \sum_i n_{i\uparrow} \hat{n}_{i\downarrow} +$$

$$+ \sum_{ij}{}' \Big[U_{iijj}\, \hat{a}_{i\uparrow}^{+} \hat{a}_{i\downarrow}^{+} \hat{a}_{j\downarrow} \hat{a}_{j\uparrow} -$$

$$- U_{ijij} (\hat{\bar{S}}_i \cdot \hat{\bar{S}}_j + \frac{1}{4} \hat{n}_i \hat{n}_j) +$$

$$+ \frac{1}{2} U_{ijji}\, \hat{n}_i \hat{n}_j \Big] .$$

$$n_i = \hat{n}_{i\uparrow} + \hat{n}_{i\downarrow}$$

$$U = U_{iiii} = \int dr \int dr' \, |W_i(r)|^2 \, V(r-r') \, |W_i(r')|^2$$

$$\tilde{J}_{ij} = U_{iijj} = \int dr \int dr' \, W_i^*(r) W_i^*(r') \, V(|r-r'|) \, W_j(r') W_j(r)$$

$$K_{ij} = U_{ijji} = \int dr \int dr' \, |W_i(r)|^2 \, V(r-r') \, |W_j(r')|^2$$

$$J_{ij} = U_{ijij} = \int dr \int dr' \, W_i^*(r) W_j^*(r') \, V(r-r') \, W_i(r') W_j(r)$$

$$\hat{H}_2 = U \sum_i n_{i\uparrow} n_{i\downarrow} +$$

$$+ \sum_{ij}{}' \Big[\tilde{J}_{ij} \, \hat{a}^+_{i\uparrow} \hat{a}^+_{i\downarrow} \hat{a}_{j\downarrow} \hat{a}_{j\uparrow} -$$ $|j \uparrow\downarrow\rangle \to |i \uparrow\downarrow\rangle$ – singlet hopping

$$- J_{ij} \left(\hat{\bar{S}}_i \cdot \hat{\bar{S}}_j + \frac{1}{4} \hat{n}_i n_j \right) +$$ – spin – spin (exchange) interaction

$$+ \frac{1}{2} K_{ij} \, \hat{n}_i \hat{n}_j \Big]$$ – Coulomb interaction between i and j sites.

Extended Hubbard model

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

$$+ \sum_{ij}{}' \Big[\tilde{J}_{ij} \, a^+_{i\uparrow} a^+_{i\downarrow} a_{j\downarrow} a_{j\uparrow} -$$

$$- J_{ij} \left(\bar{S}_i \cdot \bar{S}_j + \frac{1}{4} n_i n_j \right) +$$

$$+ \frac{1}{2} K_{ij} \, n_i n_j \Big]$$