§ 2. HUBBARD MODEL – DERIVATION

Interacting fermions / electrons

$$\boxed{\hat{\mathcal{H}} = \sum_{i=1}^{N} \frac{\hat{\vec{p}}_i^{\,2}}{2m} + V_1(\vec{r}_i) + \frac{1}{2}\sum_{ij} V_2(\vec{r}_i - \vec{r}_j)}$$

Second quantization

$$\left\{ \hat{\Psi}_\sigma(\vec{r}),\ \hat{\Psi}^+_{\sigma'}(\vec{r}\,') \right\} = \delta_{\sigma\sigma'}\,\delta(\vec{r}-\vec{r}\,')$$

etc.

Expand the field operator in a Wannier base

$$\hat{\Psi}_\sigma(\vec{r}) = \sum_i W_i(\vec{r})\,\hat{a}_{i\sigma}$$

$$\hat{\Psi}^+_\sigma(\vec{r}) = \sum_i W_i(\vec{r})^*\,\hat{a}^+_{i\sigma}$$

where

$$\left\{ \hat{a}_{i\sigma},\ \hat{a}^+_{j\sigma'} \right\} = \delta_{ij}\,\delta_{\sigma\sigma'}$$

etc.

One-body part of the Hamiltonian

spin diagonal

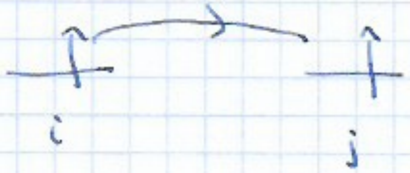
$$\hat{\mathcal{H}}_1 = \sum_{i=1}^{N} \frac{\hat{\vec{p}}_i^{\,2}}{2m} + V_1(\vec{r}_i) = \sum_\sigma \int d_3r\ \hat{\Psi}^+_\sigma(\vec{r}) \left[\frac{\hat{\vec{p}}^{\,2}}{2m} + V_1(\vec{r}) \right] \hat{\Psi}_\sigma(\vec{r}) =$$

$$= \sum_{ij} \sum_\sigma \int d_3r\ \hat{a}^+_{i\sigma}\, W_i(\vec{r})^* \left[\frac{\hat{\vec{p}}^{\,2}}{2m} + V(\vec{r}) \right] W_j(\vec{r})\, \hat{a}_{j\sigma} =$$

$$= \sum_{ij} \sum_\sigma t_{ij}\, \hat{a}^+_{i\sigma}\, \hat{a}_{j\sigma}$$

$$\boxed{t_{ij} = \int d^3r\, w_i^*(\bar r)\left[\frac{\hat{\bar p}^2}{2m} + V_1(\bar r)\right] w_j(\bar r)}$$

↑ hopping amplitude, "kinetic energy" (!?)



$$\hat H_1 = \sum_{ij\sigma} t_{ij}\, \hat a^\dagger_{i\sigma} \hat a_{j\sigma}$$

Two-body part of the Hamiltonian

$$\hat H_2 = \frac{1}{2}\sum_{ij} V_2(\bar r_i - \bar r_j) =$$

$$= \frac{1}{2}\sum_{\sigma\sigma'} \int d^3r \int d^3r'\, \hat\Psi^\dagger_\sigma(\bar r)\, \hat\Psi^\dagger_{\sigma'}(\bar r')\, V_2(\bar r - \bar r')\, \hat\Psi_{\sigma'}(\bar r')\, \hat\Psi_\sigma(\bar r) =$$

$$= \frac{1}{2}\sum_{\sigma\sigma'} \sum_{ijkl} \hat a^\dagger_{i\sigma} \hat a^\dagger_{j\sigma'} \hat a_{l\sigma'} \hat a_{k\sigma} \int d^3r\, d^3r'\, w_i^*(\bar r)\, w_j^*(\bar r')\, V_2(\bar r - \bar r')\, w_k(\bar r')\, w_l(\bar r)$$

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

$$\boxed{U_{ijkl} = \int d^3r \int d^3r'\, w_i^*(\bar r)\, w_j^*(\bar r')\, V_2(\bar r - \bar r')\, w_k(\bar r')\, w_l(\bar r)}$$

↑ interaction matrix elements

"interacting potential"

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

exact representation of the interacting Hamiltonian for a single band ~~with local on-site interaction~~.

<u>Consider a local term</u> $\quad i=j=k=l$

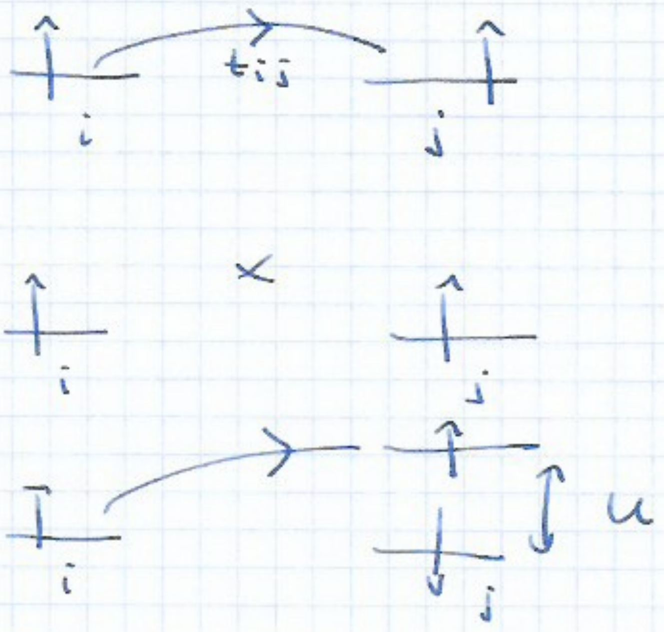
$$\frac{1}{2} \sum_{\sigma\sigma'} \sum_i U_{iiii}\, \hat{a}^\dagger_{i\sigma} \hat{a}^\dagger_{i\sigma'} a_{i\sigma'} a_{i\sigma} =$$

$$= \frac{1}{2} \sum_{i\sigma} a^\dagger_{i\sigma} a^\dagger_{i\sigma} \underbrace{a_{i\sigma} a_{i\sigma}}_{=0} + a^\dagger_{i\sigma} a^\dagger_{i\bar{\sigma}} a_{i\bar{\sigma}} a_{i\sigma} =$$

$$= \frac{1}{2} \sum_{i\sigma} U_{iiii}\, \hat{a}^\dagger_{i\sigma} \hat{a}_{i\sigma} \hat{a}^\dagger_{i\bar{\sigma}} \hat{a}_{i\bar{\sigma}} = \frac{1}{2} \sum_{i\sigma} U_{iiii}\, \hat{n}_{i\sigma} \hat{n}_{i\bar{\sigma}} = \sum_i U_{iiii}\, \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$$

<u>The Hubbard model</u> $\qquad U = U_{iiii}$

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



$[\hat{H}_1, \hat{H}_2] \neq 0$!

non trivial many body Hamiltonian

Pauli exclusion!