

Tight binding model

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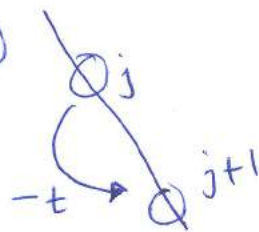
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$$\hat{H} = -t \sum_j \hat{c}_{j+1}^\dagger \hat{c}_j \quad (1)$$

This conforms to our general



form

$$\hat{H} = \sum_{\alpha, \beta} \langle \alpha | \hat{H} | \beta \rangle \hat{c}_\alpha^\dagger \hat{c}_\beta$$

for single particle Hamiltonians. In (2), we assume only interactions between neighboring sites.

Now to the Fourier space :

$$\hat{c}_j = \frac{1}{\sqrt{N}} \sum_{\vec{k}} e^{+ikja} \hat{d}_{\vec{k}} ; \quad \hat{c}_j^\dagger = \frac{1}{\sqrt{N}} \sum_{\vec{k}} e^{-ikja} \hat{d}_{\vec{k}}^\dagger$$

$$\begin{aligned} \hat{H} &= -t \sum_j \sum_{\vec{k}, \vec{k}'} e^{-ik'(j+1)a} \hat{d}_{\vec{k}'}^\dagger e^{+ikja} \hat{d}_{\vec{k}} \\ &= -\frac{t}{N} \sum_j \sum_{\vec{k}, \vec{k}'} e^{-ik'a} e^{-i(k'-k)ja} \hat{d}_{\vec{k}'}^\dagger \hat{d}_{\vec{k}} \\ &= -t \sum_{\vec{k}, \vec{k}'} e^{-ik'a} \left\{ \frac{1}{N} \sum_j e^{-i(k'-k)ja} \right\} \hat{d}_{\vec{k}'}^\dagger \hat{d}_{\vec{k}} \end{aligned}$$

$$\boxed{\hat{H} = -t \sum_{\vec{k}} e^{-ika} \hat{d}_{\vec{k}}^\dagger \hat{d}_{\vec{k}}} \quad \delta_{\vec{k}', \vec{k}}$$

Some variations

interaction with forward and backward spins - a chain

$$\hat{H} = -t \sum_j \left(\hat{c}_{j+1}^\dagger \hat{c}_j + \hat{c}_{j-1}^\dagger \hat{c}_j \right)$$

$$= -2t \sum_{\vec{k}} (\cos ka) \hat{d}_{\vec{k}}^\dagger \hat{d}_{\vec{k}}$$

+ In 2D w 3D, τ neighboring ~~spins~~ sites:

$$\hat{H} = -t \sum_{\vec{k}} \sum_{\tau} e^{-i\vec{k} \cdot \vec{a}_\tau} \hat{d}_{\vec{k}}^\dagger \hat{d}_{\vec{k}}$$

Hubbard model

$$\hat{H} = \sum_{\substack{i,j \\ \text{sites} \\ \sigma = \text{spin}}} \underbrace{\langle i | H_0 | j \rangle}_{\substack{\uparrow \\ \text{single particle} \\ \text{Hamiltonian}}} \hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma} + \sum_{\substack{i,j,l,k \rightarrow \text{sites} \\ \sigma, \sigma' \rightarrow \text{spins}}} \langle lk | V | ij \rangle \hat{c}_{l\sigma}^\dagger \hat{c}_{k\sigma'}^\dagger \hat{c}_{j\sigma'} \hat{c}_{i\sigma}$$

Let's rewrite it clearly

$$\hat{H} = \sum_{i,j,\sigma} \langle i | H_0 | j \rangle \hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma} + \frac{1}{2} \sum_{\substack{i,j,k,l \\ \sigma, \sigma'}} \langle lk | V | ij \rangle \hat{c}_{l\sigma}^\dagger \hat{c}_{k\sigma'}^\dagger \hat{c}_{j\sigma'} \hat{c}_{i\sigma} \quad \text{--- (2)}$$

We assume that ~~spin~~ ^{particle}-hopping (destruction followed by creation in some other state) does not

change the spins.

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Let $\langle i | \hat{H}_0 | j \rangle = E_0 \delta_{i,j} - t \delta_{i,j \pm 1}$

e.g. For a 2 site case, a matrix form,

$$\hat{H}_0 = \begin{pmatrix} E_0 & -t \\ -t & E_0 \end{pmatrix}.$$

Hence the first term in ② becomes:

$$\begin{aligned} & \sum_{i, \sigma} E_0 \hat{c}_{i\sigma}^\dagger \hat{c}_{i\sigma} - t \sum_{j, \sigma} \hat{c}_{j\sigma}^\dagger \hat{c}_{j \pm 1, \sigma} \\ &= E_0 \sum_{i, \sigma} \hat{c}_{i\sigma}^\dagger \hat{c}_{i\sigma} - t \sum_{j, \sigma} \hat{c}_{j\sigma}^\dagger \hat{c}_{j \pm 1, \sigma} \end{aligned}$$

Let $\langle \ell k | V | i j \rangle = U \delta_{\ell, k} \delta_{k, i} \delta_{i, j}$

\Rightarrow i.e., interaction is non-zero when the particles are on the same site. \Rightarrow they must have opposite spins.

I now focus only on the third term = ②.

$$\begin{aligned} & \frac{1}{2} U \sum_j \hat{c}_{j\uparrow}^\dagger \hat{c}_{j\uparrow}^\dagger \hat{c}_{j\downarrow} \hat{c}_{j\downarrow} \\ &= \frac{U}{2} \sum_j \hat{c}_{j\uparrow}^\dagger \hat{c}_{j\downarrow}^\dagger \hat{c}_{j\downarrow} \hat{c}_{j\uparrow} \end{aligned}$$

The quanta state is defined by (j, σ) , i.e. (j, \uparrow) or (j, \downarrow) .
Say $(j, \uparrow) = a$ and $(j, \downarrow) = b$ (quantum numbers).

The term becomes

$$\frac{U}{2} \sum_{\substack{a, b, j \\ a \neq b}} \hat{c}_a^\dagger \hat{c}_b^\dagger \hat{c}_b \hat{c}_a$$

hop

$$= \frac{U}{2} \sum_j - \hat{c}_b^\dagger \hat{c}_a^\dagger \hat{c}_b \hat{c}_a$$

hop

Using $\{\hat{c}_a^\dagger, \hat{c}_b^\dagger\} = 0$

$$= \frac{U}{2} \sum_j \hat{c}_b^\dagger \hat{c}_b \hat{c}_a^\dagger \hat{c}_a$$

$$= \frac{U}{2} \sum_j \hat{c}_{j\downarrow}^\dagger \hat{c}_{j\downarrow} \hat{c}_{j\uparrow}^\dagger \hat{c}_{j\uparrow}$$

$$= \frac{U}{2} \sum_j \hat{n}_{j\downarrow} \hat{n}_{j\uparrow}$$