Tight Binding

The tight binding model is especially simple and elegant in second quantized notation. A few examples should demonstrate this point

1D Simple Cubic

1 atom 1 orbital per site (nearest neighbor hopping)

The Hamiltonian in localized basis

$$\hat{H} = A \sum_j \left(c_{j+1}^\dagger c_j + c_j^\dagger c_{j+1} \right) \tag{1}$$

Notice by changing to delocalized basis

$$c_j^\dagger = \frac{1}{\sqrt{N}} \sum_q e^{-iqja} c_q^\dagger \tag{2}$$

Any non-diagonal term becomes diagonal through completeness relation [1]

$$
\begin{aligned}
\sum_j c_{j+n}^\dagger c_j &= \sum_j \left(\frac{1}{\sqrt{N}} \sum_q e^{-iq(j+n)a} c_q^\dagger \right) \left(\frac{1}{\sqrt{N}} \sum_{q'} e^{iq'ja} c_{q'} \right) \\
&= \frac{1}{N} \sum_{q,q'} e^{-iqna} c_q^\dagger c_{q'} \left(\sum_j e^{-i(q-q')ja} \right) \\
&= \frac{1}{N} \sum_{q,q'} e^{-iqna} c_q^\dagger c_{q'} \cdot N\delta(q-q') \\
&= \sum_q e^{-iqna} c_q^\dagger c_q \tag{3}
\end{aligned}
$$

Therefore the Hamiltonian is diagonalized

$$\hat{H} = A \sum_q \left(e^{-iqa} + e^{iqa} \right) c_q^\dagger c_q \tag{4}$$

with eigenvalues $E_q = 2A\cos(qa)$ and eigenvectors given by (2). It is conventional to write the Hamiltonian for **j and j+1 sites**, and it's important to use **localized basis set** for c_j.

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[1] This trick works as long as translation symmetry is maintained. In other words, the *complete* set of basis elements go into the transformation

It's interesting to note that (1) represents the hopping back and forth between the j and $j+1$ sites. One may reorder the sum and write it as the hopping from the j to $j-1$ and $j+1$ sites

$$\hat{H} = A \sum_j \left(c_{j-1}^\dagger c_j + c_{j+1}^\dagger c_j \right) \tag{5}$$

use (3) to eyeball the change of basis ($n = \pm 1$) and recover the same result.

$$\begin{aligned} \hat{H} =& A \left((\sum_j c_{j-1}^\dagger c_j) + (\sum_j c_{j+1}^\dagger c_j) \right) \\ =& A \left(\sum_q e^{iqa} c_q^\dagger c_q + \sum_q e^{-iqa} c_q^\dagger c_q \right) \\ =& A \sum_q (e^{-iqa} + e^{iqa}) c_q^\dagger c_q \end{aligned} \tag{6}$$

In general, we can write the Hamiltonian in a number of creative ways as long as we include the correct number of hops per site (2 in this case) and still recover the correct answer. However, only considering two neighboring sites is desirable because (1) can be written as

$$\hat{H} = A \sum_j \left(c_{j+1}^\dagger c_j + h.c. \right) \tag{7}$$

where $h.c.$ stands for hermitian conjugate, whereas (5) cannot.

It's important to realize that implicit in (1) is the assumption that hopping terms between second neighbors and beyond are zero. That is, in general

$$\hat{H} = \sum_j \left(A_1 c_{j+1}^\dagger c_j + A_2 c_{j+2}^\dagger c_j + \cdots + h.c. \right) \tag{8}$$

and the hopping terms depend on the basis elements $\{\psi_j\}$ of $\{c_j\}$

$$A_n = \langle \psi_j \,|\, \Delta \,|\, \psi_{j+n} \rangle = \int \psi(x) \Delta(x) \psi(x + na) dx \tag{9}$$

Therefore, even though there's an analogous transform from c_q to c_j

$$c_q^\dagger = \frac{1}{\sqrt{N}} \sum_j e^{iqja} c_j^\dagger \tag{10}$$

The roles of c_j and c_q cannot be reversed, because $A_n \neq 0$ for $n > 1$ if the delocalized basis of $\{c_q\}$ is used. (What are A_n in this case?)

1 atom 2 orbitals per site (n.n. hopping and interaction)

Per convention, we only consider j and j+1 sites. Here we have 4 states to include: s and p orbitals on site j along with s and p orbitals on site j+1. In the most general consideration, there are 16 hopping terms (js to js, jp, js+1, jp+1, etc.) the hopping matrix in its full glory

$$
\left\langle \hat{H} \right\rangle = \sum_j
\begin{array}{c}
{}_{\text{to}/}{}^{\text{from}} \\
js \\
jp \\
j+1s \\
j+1p
\end{array}
\begin{array}{cccc}
js & jp & j+1s & j+1p
\end{array}
\left[
\begin{array}{cccc}
E_s & \sim 0 & V_{ss\sigma} & V_{sp\sigma} \\
\sim 0 & E_p & V_{ps\sigma} & V_{pp\sigma} \\
V_{ss\sigma}^* & V_{sp\sigma}^* & E_s & \sim 0 \\
V_{ps\sigma}^* & V_{pp\sigma}^* & \sim 0 & E_p
\end{array}
\right]
\tag{11}
$$

where each term is the coupling between the states by the background potential. That's why s and p orbitals almost have no coupling, since they are eigenstates of the atomic potential. And similar to the previous problem, hopping from j+1 to j involve terms that are complex conjugate of the terms for hopping from j to j+1 by (9).

The Hamiltonian is much cleaner in second quantization notation as we utilize the symmetry of the problem

$$
\hat{H} = \sum_{j,\alpha,\beta} \left(c_{j+1,\alpha}^\dagger T_{\alpha,\beta} c_{j,\beta} + c_{j,\alpha}^\dagger T_{\alpha,\beta}^\dagger c_{j+1,\beta} + c_{j,\alpha}^\dagger M_{\alpha,\beta} c_{j,\beta} \right)
\tag{12}
$$

Where the hopping and on-site matrices are

$$
T_{\alpha,\beta} = \begin{pmatrix} V_{ss\sigma} & V_{sp\sigma} \\ V_{ps\sigma} & V_{pp\sigma} \end{pmatrix}
\tag{13}
$$

$$
M_{\alpha,\beta} = \begin{pmatrix} E_s & 0 \\ 0 & E_p \end{pmatrix}
\tag{14}
$$

eyeball the change of basis from j to q

$$
\hat{H} = \sum_{q,\alpha,\beta} c_{q,\alpha}^\dagger \left((e^{-iqa} + e^{iqa}) T_{\alpha,\beta} + M_{\alpha,\beta} \right) c_{q,\beta}
\tag{15}
$$

now one only has to diagonalize a two-by-two matrix for each q to get the eigenvalues and eigenvectors in the c_q basis.

2 atoms per site 1 orbital per atom

(a) 1 atom per site, 2 orbitals per atom   (b) 2 atoms per site, 1 orbital per atom

Figure 1: Viewed at the unit cell level, these two models are very similar

The same picture from above still applies with the different levels on each site being atoms rather than orbitals

$$\hat{H} = \sum_{j,\alpha,\beta} \left(c_{j+1,\alpha}^{\dagger} T_{\alpha,\beta} c_{j,\beta} + c_{j,\alpha}^{\dagger} T_{\alpha,\beta}^{\dagger} c_{j+1,\beta} + c_{j,\alpha}^{\dagger} M_{\alpha,\beta} c_{j,\beta} \right) \tag{16}$$

$$T_{\alpha,\beta} = \begin{pmatrix} 0 & W_{AB} \\ 0 & 0 \end{pmatrix} \tag{17}$$

$$M_{\alpha,\beta} = \begin{pmatrix} E_A & \Gamma_{AB} \\ \Gamma_{AB}^{*} & E_B \end{pmatrix} \tag{18}$$