The Tight-Binding Model

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This method deals with the situation in which the local atomic orbitals are a good approximation to the full problem, and fairly good solutions can be obtained by adding corrections to the local wavefunctions. We start by separating the full Hamiltonian into a local and a non-local piece:

$$H = \sum_i H_i + H_{\text{nloc}} \tag{0.1}$$

H_i is an operator that acts only very close to the real space lattice site i, and is zero otherwise. A very extreme and simple example would be a chemical potential term:

$$H_i = \mu \sum_\sigma \hat{n}_{i\sigma} \tag{0.2}$$

where $\hat{n}_{i\sigma} = c^\dagger_{i\sigma} c_{i\sigma}$ is thee number operator for the i^{th} site. A more non-trivial example would be an extremely localised Coulomb repulsion term:

$$H_i = U \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} \tag{0.3}$$

The non-local piece H_{nloc} connects multiple sites. A simple example of such a term would be a nearest-neighbour hopping:

$$H_{\text{nloc}} = -t \sum_{i\sigma} \left(c^\dagger_{i\sigma} c_{i+1,\sigma} + \text{h.c.} \right) \tag{0.4}$$

In general, let $\left\{ |\Psi^n_i\rangle \right\}$ be the set of eigenstates of the local Hamiltonian H_i:

$$H_i \, |\Psi^n_i\rangle = E^n_i \, |\Psi^n_{\text{loc}}\rangle \tag{0.5}$$

We will drop the superscript i on the energy eigenvalue because they are actually independent of i on account of translation invariance. We assume that all the $\psi^n_i(\vec{r} - \vec{R}_i)$ are very local; that is, they are non-zero only very close to their specific lattice sites $\left(\vec{r} - \vec{R}_i \sim 0 \right)$. More specifically, we assume that $\psi^n_i(\vec{r})$ becomes zero when $H_{\text{nloc}}(\vec{r} - \vec{R}_i)$ is non-zero. In such a situation, $\psi^n_i(\vec{r} - \vec{R}_i)$ becomes a very good wavefunction of the full Hamiltonian:

$$\begin{aligned} H(\vec{r}) \psi^n_i(\vec{r} - \vec{R}_i) &= \left[\sum_i H_i(\vec{r}) + H_{\text{nloc}}(\vec{r}) \right] \psi^n_i(\vec{r} - \vec{R}_i) \\ &= \begin{cases} H_i(\vec{r}) \psi^n_i(\vec{r} - \vec{R}_i) = E^n \psi^n_i(\vec{r} - \vec{R}_i) & \text{when } \vec{r} \sim \vec{R}_i \\ H_{\text{nloc}}(\vec{r}) \psi^n_i(\vec{r} - \vec{R}_i) = 0 & \text{when } \vec{r} \nsim \vec{R}_i \end{cases} \end{aligned} \tag{0.6}$$

However, these wavefunctions do not satisfy Bloch's theorem. The following linear combination does:

$$\phi^n(\vec{k}) = \frac{1}{\sqrt{N}} \sum_i e^{i\vec{k}\cdot\vec{R}_i} \psi_i^n(\vec{r} - \vec{R}_i) \tag{0.7}$$

because it can be rewritten as

$$\phi^n(\vec{k}) = \frac{1}{\sqrt{N}} e^{i\vec{k}\cdot\vec{r}} \sum_i e^{-i\vec{k}\cdot\left(\vec{r}-\vec{R}_i\right)} \psi_i^n(\vec{r} - \vec{R}_i) = e^{i\vec{k}\cdot\vec{r}} u_{\vec{k}}^n(\vec{r}) \tag{0.8}$$

such that $u_{\vec{k}}^n(\vec{r})$ is translationally-invariant. The energy expectation values are

$$\epsilon_{\vec{k}} = \langle \Phi_{\vec{k}}^n | \, H \, | \phi_{\vec{k}}^n \rangle = \frac{1}{N} \sum_{ij} e^{i\vec{k}\cdot\left(\vec{R}_i - \vec{R}_j\right)} \langle \Psi_i^n | \, H \, | \Psi_j^n \rangle \tag{0.9}$$

At this point we assume that the Hamiltonian has non-zero matrix elements for local and, at the most, nearest-neighbour terms:

$$\langle \Psi_i^n | \, H \, | \Psi_j^n \rangle = \alpha \delta_{ij} + \gamma \delta_{|i-j|-1} \tag{0.10}$$

This gives

$$\epsilon_{\vec{k}} = \alpha + \gamma \sum_{\vec{e}_i} e^{i\vec{k}\cdot\vec{e}_i} \tag{0.11}$$

$\vec{e}_i$ runs over all vectors that connect a lattice site to its nearest neighbours. For a hypercubic lattice with spacings $a_1, a_2, ...$, the expression becomes

$$\epsilon_{\vec{k}} = \alpha + 2\gamma \sum_{i=x,y,...} \cos a_i k_i \tag{0.12}$$

This can also be motivated from a second-quantized Hamiltonian. The assumption of at most nearest neighbour Hamiltonian matrix elements naturally leads to the model

$$H = -t \sum_{\langle ij \rangle, \sigma} \left(c_{i\sigma}^\dagger c_{j\sigma} + \text{h.c.} \right) - \mu \hat{N} \tag{0.13}$$

$c_{i\sigma}^\dagger$ is the Fermionic field operator that creates an electron with spin σ at $\vec{R}_i$. Defining the Foureir transforms as

$$c_{\vec{k}\sigma}^\dagger = \frac{1}{\sqrt{N}} \sum_i e^{\vec{k}\cdot\vec{R}_i} c_{i\sigma}^\dagger, \quad c_{i\sigma}^\dagger = \frac{1}{\sqrt{N}} \sum_i e^{-\vec{k}\cdot\vec{R}_i} c_{\vec{k},\sigma}^\dagger \tag{0.14}$$

Using this, we can write

$$\begin{aligned} H &= -t \frac{1}{N} \sum_{\langle ij \rangle, \sigma} \sum_{\vec{k}\vec{q}} \left(e^{i\left[\vec{k}\cdot\vec{R}_i - \vec{q}\cdot\vec{R}_j\right]} c_{\vec{k}\sigma}^\dagger c_{\vec{q}\sigma} + \text{h.c.} \right) - \mu \hat{N} \\ &= -t \frac{1}{N} \frac{1}{2} \sum_i \sum_{j \in \text{NN of i}} \sum_{\vec{k}\vec{q}} \sum_\sigma \left(e^{i\left[\vec{k}\cdot\vec{R}_i - \vec{q}\cdot\vec{R}_j\right]} c_{\vec{k}\sigma}^\dagger c_{\vec{q}\sigma} + \text{h.c.} \right) - \mu \hat{N} \end{aligned} \tag{0.15}$$

We assume here that we are on a 2D lattice. Since j sums over all NN of i, we can substitute

$$\begin{aligned}\sum_j e^{-i\vec{q}\cdot\vec{R}_j} &= e^{-i\vec{q}\cdot\left(\vec{R}_i+\vec{a}_x\right)} + e^{-i\vec{q}\cdot\left(\vec{R}_i-\vec{a}_x\right)} + e^{-i\vec{q}\cdot\left(\vec{R}_i+\vec{a}_y\right)} + e^{-i\vec{q}\cdot\left(\vec{R}_i-\vec{a}_y\right)} \\ &= 2e^{-i\vec{q}\cdot\vec{R}_i}\left(\cos(q_x a_x)+\cos(q_y a_y)\right)\end{aligned} \tag{0.16}$$

This gives

$$\begin{aligned}H &= -t\frac{1}{N}\frac{1}{2}\sum_{\vec{k}\vec{q},\sigma}\left[2\left(\cos(q_x a_x)+\cos(q_y a_y)\right)c^\dagger_{\vec{k}\sigma}c_{\vec{q}\sigma}+\text{h.c.}\right]\sum_i e^{i\left(\vec{k}-\vec{q}\right)\cdot\vec{R}_i} - \mu\hat{N} \\ &= -t\frac{1}{N}\sum_{\vec{k}\vec{q},\sigma}\left(\cos(q_x a_x)+\cos(q_y a_y)\right)\left(c^\dagger_{\vec{k}\sigma}c_{\vec{q}\sigma}+\text{h.c.}\right)N\delta_{\vec{k},\vec{q}} - \mu\hat{N} \\ &= -2t\sum_{\vec{k},\sigma}\left(\cos(k_x a_x)+\cos(k_y a_y)\right)c^\dagger_{\vec{k}\sigma}c_{\vec{k}\sigma} - \mu\hat{N} \\ &= \sum_{k\sigma}\epsilon_k\hat{n}_{k\sigma}\end{aligned} \tag{0.17}$$

with $\epsilon_k = -2t\left(\cos(k_x a_x)+\cos(k_y a_y)\right) - \mu$.

$$\eta_{1 \text{ to } 2} = \frac{2t}{\sqrt{t^2 + U^2/16}}$$
$$\eta_{1 \text{ to } 3 \text{ to } 2} = \frac{2t}{t^2 + \omega^2 \sqrt{\frac{U}{4t}}}$$