The Tight-Binding Model

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Single-particle Hamiltonian viewpoint

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, $\psi_i^n(\vec{r}-\vec{R}_i)$ becomes a very good wavefunction of the full Hamiltonian:

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

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

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

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

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

$\vec{e}_i$ 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

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

Second-quantized Hamiltonian viewpoint

The tight-binding model can also be developed starting from a second-quantized Hamiltonian. Here we work with field operators:

$$c_{\vec{k}}, c_{\vec{q}}^{\dagger} : \left\{ c_{\vec{k}}, c_{\vec{q}}^{\dagger} \right\} = \delta_{kq} \tag{0.13}$$

i, j are some quantum numbers. For example, $c^{\dagger}(\vec{r})$ creates an electron at position $\vec{r}$.

The assumption of at most nearest neighbour Hamiltonian matrix elements naturally leads to the model

$$H = -t \sum_{\langle ij \rangle, \sigma} \left(c_{i\sigma}^{\dagger} c_{j\sigma} + \text{h.c.} \right) - \mu \hat{N} \tag{0.14}$$

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

$$c_{\vec{k}\sigma}^{\dagger} = \frac{1}{\sqrt{N}} \sum_i e^{\vec{k}\cdot\vec{R}_i} c_{i\sigma}^{\dagger}, \quad c_{i\sigma}^{\dagger} = \frac{1}{\sqrt{N}} \sum_i e^{-\vec{k}\cdot\vec{R}_i} c_{\vec{k},\sigma}^{\dagger} \tag{0.15}$$

Using this, we can write

$$\begin{aligned} H &= -t \frac{1}{N} \sum_{\langle ij \rangle, \sigma} \sum_{\vec{k}\vec{q}} \left(e^{i\left[\vec{k}\cdot\vec{R}_i - \vec{q}\cdot\vec{R}_j\right]} c_{\vec{k}\sigma}^{\dagger} c_{\vec{q}\sigma} + \text{h.c.} \right) - \mu \hat{N} \\ &= -t \frac{1}{N} \frac{1}{2} \sum_i \sum_{j \in \text{NN of i}} \sum_{\vec{k}\vec{q}} \sum_{\sigma} \left(e^{i\left[\vec{k}\cdot\vec{R}_i - \vec{q}\cdot\vec{R}_j\right]} c_{\vec{k}\sigma}^{\dagger} c_{\vec{q}\sigma} + \text{h.c.} \right) - \mu \hat{N} \end{aligned} \tag{0.16}$$

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

$$\begin{aligned} \sum_j e^{-i\vec{q}\cdot\vec{R}_j} &= e^{-i\vec{q}\cdot\left(\vec{R}_i + \vec{a}_x\right)} + e^{-i\vec{q}\cdot\left(\vec{R}_i - \vec{a}_x\right)} + e^{-i\vec{q}\cdot\left(\vec{R}_i + \vec{a}_y\right)} + e^{-i\vec{q}\cdot\left(\vec{R}_i - \vec{a}_y\right)} \\ &= 2e^{-i\vec{q}\cdot\vec{R}_i} \left(\cos(q_x a_x) + \cos(q_y a_y) \right) \end{aligned} \tag{0.17}$$

This gives

$$\begin{aligned} H &= -t \frac{1}{N} \frac{1}{2} \sum_{\vec{k}\vec{q},\sigma} \left[2 \left(\cos(q_x a_x) + \cos(q_y a_y) \right) c_{\vec{k}\sigma}^{\dagger} c_{\vec{q}\sigma} + \text{h.c.} \right] \sum_i e^{i\left(\vec{k}-\vec{q}\right)\cdot\vec{R}_i} - \mu \hat{N} \\ &= -t \frac{1}{N} \sum_{\vec{k}\vec{q},\sigma} \left(\cos(q_x a_x) + \cos(q_y a_y) \right) \left(c_{\vec{k}\sigma}^{\dagger} c_{\vec{q}\sigma} + \text{h.c.} \right) N \delta_{\vec{k},\vec{q}} - \mu \hat{N} \\ &= -2t \sum_{\vec{k},\sigma} \left(\cos(k_x a_x) + \cos(k_y a_y) \right) c_{\vec{k}\sigma}^{\dagger} c_{\vec{k}\sigma} - \mu \hat{N} \\ &= \sum_{k\sigma} \xi_k \hat{n}_{k\sigma} \end{aligned} \tag{0.18}$$

with $\xi_k = -2t \left(\cos(k_x a_x) + \cos(k_y a_y) \right) - \mu$. The bandwidth is $8t$.

Constant-energy contours

The contours of constant energy E are defined by

$$\xi_k = E \tag{0.19}$$

The Fermi surface is defined as the set of points in $k-$space on the contour at zero energy:

$$\xi_k = 0 \implies \cos(k_x a_x) + \cos(k_y a_y) = -\frac{\mu}{2t} \tag{0.20}$$

The case of $\mu = 0$ results in a "diamond-shaped Fermi surface":

$$\begin{aligned} & \cos(k_x a_x) + \cos(k_y a_y) = 0 \\ \implies & \cos(\pm k_x a_x) = \cos(\pi \pm k_y a_y) \\ \implies & \begin{cases} k_x + k_y = \frac{\pi}{a} \\ k_x - k_y = \frac{\pi}{a} \\ -k_x + k_y = \frac{\pi}{a} \\ -k_x - k_y = \frac{\pi}{a} \end{cases} \end{aligned} \tag{0.21}$$

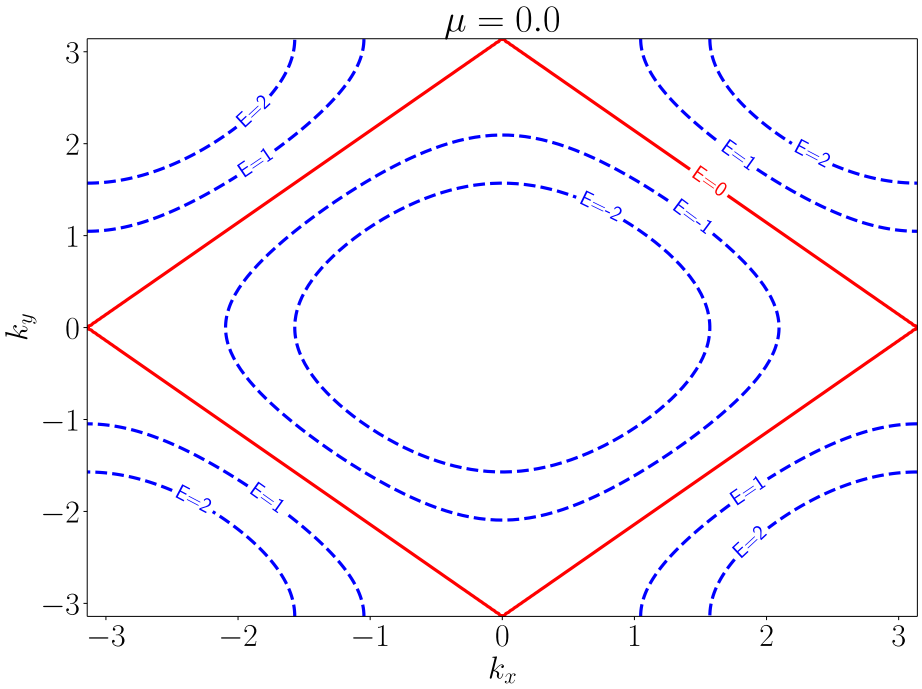


Figure 1: Contours of constant energy on the 2D tight-binding lattice model, at half-filling ($\mu = 0$). The red lines form the Fermi surface, while the blue lines form other contours.

Half-filling

The case of $\mu = 0$ is often referred to as half-filling, because at this parameter value, the Hamiltonian is particle-hole symmetric. This means that the Hamiltonian remains invariant under a particle-hole transformation. To see this on the 2D lattice, we visualize the lattice as the sum of two sub-lattices, A and B. A site on sublattice A (pink in figure) only has sites of sublattice B (green in figure) as its nearest-neighbour, and vice-versa. We will represent the Fermionic operators for sublattice A with $a, a^\dagger$ ad those of sublattice B with $b, b^\dagger$.

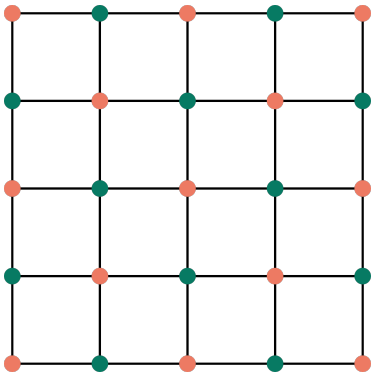


Figure 2: 2D lattice composed of two sublattices. Pink indicates sites on sublattice A and green indicates sites on sublattice B.

With this in mind, the tight-binding Hamiltonian can be written as

$$H = -t \sum_{i \in A} \sum_{j \in \text{NN of i}} \sum_{\sigma} \left(a^\dagger_{i\sigma} b_{j\sigma} + \text{h.c.} \right) - \mu \hat{N} \tag{0.22}$$

Now we define a particle-hole transformation $a \to a^\dagger, b \to -b^\dagger$. The hopping part remains unchanged by this transformation:

$$a^\dagger_{i\sigma} b_{j\sigma} + b^\dagger_{j\sigma} a_{i\sigma} \to -a_{i\sigma} b^\dagger_{j\sigma} - b_{j\sigma} a^\dagger_{i\sigma} = a^\dagger_{i\sigma} b_{j\sigma} + b^\dagger_{j\sigma} a_{i\sigma} \tag{0.23}$$

The total number part transforms as

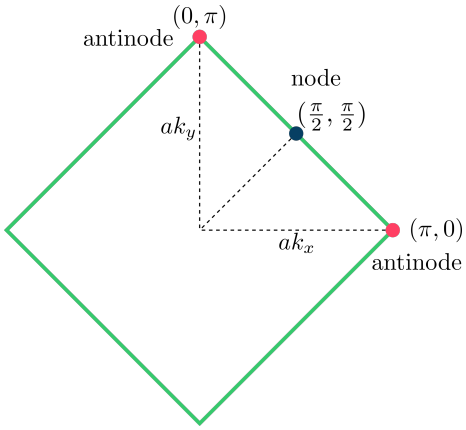
$$\mu \hat{N} = \mu \left(\sum_{i \in A, \sigma} a^\dagger_{i\sigma} a_{i\sigma} + \sum_{j \in B, \sigma} b^\dagger_{j\sigma} b_{j\sigma} \right) \to -\mu \hat{N} + \text{constant} \tag{0.24}$$

This term will be invariant when

$$\mu \hat{N} = -\mu \hat{N} \implies \mu = 0 \tag{0.25}$$

Electronic differentiation and nesting at half-filling

The half-filled Fermi surface has two sets of high-symmetry points. The points at the four corners are referred to as the *antinodal points*, while those at the centers of the four arms are referred to as the *nodal points*. The dispersion behaves differently near the two sets of points: near the nodes, it is massless Dirac-like, while near the antinodes, it becomes hyperbolic.



$$\text{antinodes} \;\rightarrow \Big(ak_x, ak_y\Big) = \begin{cases} \big(0,\pi\big)\,, \big(\pi,0\big) \\ \big(0,-\pi\big)\,, \big(-\pi,0\big) \end{cases}$$

$$\text{nodes} \;\rightarrow \Big(ak_x, ak_y\Big) = \begin{cases} \Big(\frac{\pi}{2},\frac{\pi}{2}\Big)\,, \Big(-\frac{\pi}{2},-\frac{\pi}{2}\Big) \\ \Big(\frac{\pi}{2},-\frac{\pi}{2}\Big)\,, \Big(-\frac{\pi}{2},\frac{\pi}{2}\Big) \end{cases}$$

The dispersion $\epsilon_k = -2t\Big(\cos(k_x a_x) + \cos(k_y a_y)\Big)$ near the nodes and antinodes can be obtained by expanding the cosines in Taylor series about those points. Near the nodes, we have

$$ak \sim \frac{\pi}{2} \implies \cos(ak) \sim \left(ak - \frac{\pi}{2}\right)(-1) \tag{0.26}$$

which gives

$$\epsilon_k|_{\text{node}} \sim 2t\Big(a_x k_x + a_y k_y\Big) \tag{0.27}$$

The dispersion becomes linear near the nodes. Near one of the antinodes, we have $k_x a_x \sim \pi, k_y a_y \sim 0$, so

$$\begin{aligned} \cos(a_x k_x) &\sim -1 + \frac{1}{2}\big(\pi - a_x k_x\big)^2 \\ \cos(a_y k_y) &\sim 1 - \frac{1}{2}\Big(a_y k_y\Big)^2 \end{aligned} \tag{0.28}$$

such that

$$\epsilon_k|_{\text{antinode}} \sim t\left[\Big(a_y k_y\Big)^2 - \big(\pi - a_x k_x\big)^2\right] \tag{0.29}$$

which shows that the *dispersion becomes hyperbolic near the antinodal points.*

Nesting refers to the situation where a single vector in the reciprocal lattice vector space (momentum space) connects large patches of the Fermi surface. For the case of a half-filled Fermi surface, the momentum vector $\vec{Q} = \frac{1}{a}\Big(\frac{\pi}{2},\frac{\pi}{2}\Big)$ connects

two whole arms of the Fermi surface. If there is some scattering mechanism in the theory that connects states lying at momenta k and $k+Q$, there will be terms in perturbation theory that go as

$$\frac{1}{\xi_{\vec{k}} - \xi_{\vec{k}+\vec{Q}}} \tag{0.30}$$

Since $\vec{Q}$ connects a large number of points on the Fermi surface, there will be many choices such that $\vec{k}$ and $\vec{k}+\vec{Q}$ lie on the Fermi surface, and are hence degenerate states. The presence of the nesting vector $\vec{Q}$ thus leads to a very high static structure factor for such scattering processes between degenerate states.