The Tight-Binding Model on the 2D Lattice

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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, $\psi^n_i(\vec{r} - \vec{R}_i)$ 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

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

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:

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

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

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

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

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

Using this, we can write

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

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

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

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":

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

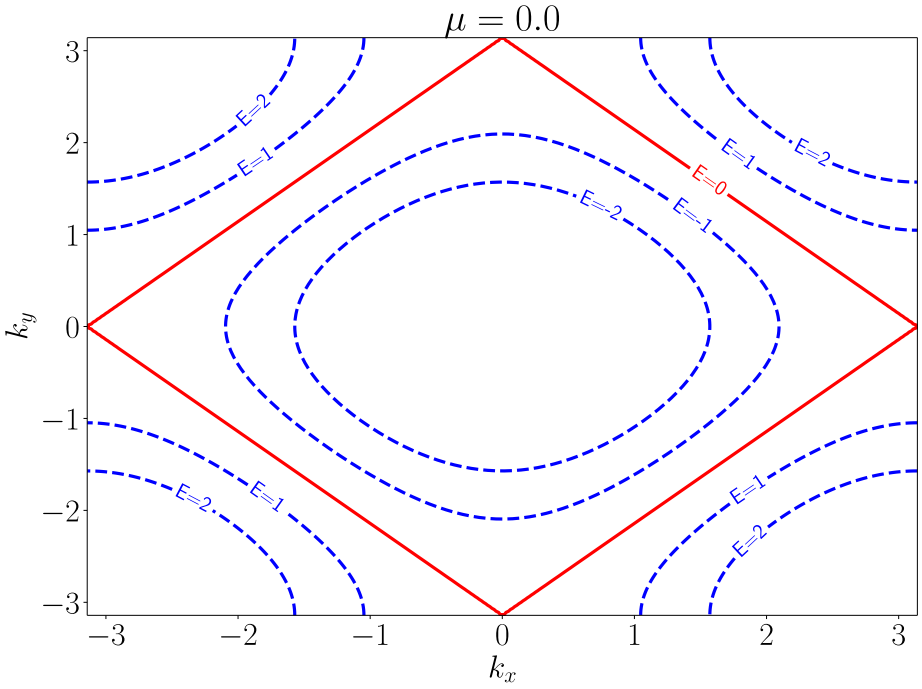


Figure 1: Contours of constant energy on the 2D tight-binding lattice model, at half-filling ($\mu = 0$). The red lines form the Fermi surface, while the blue lines form other contours.

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 $b, b^\dagger$.

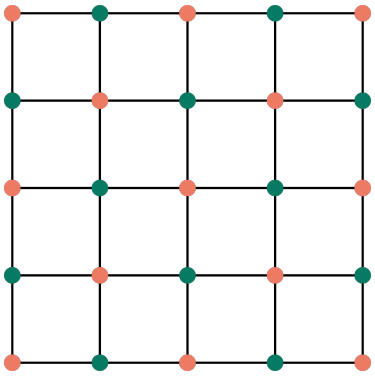


Figure 2: 2D lattice composed of two sublattices. Pink indicates sites on sublattice A and green indicates sites on sublattice B.

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

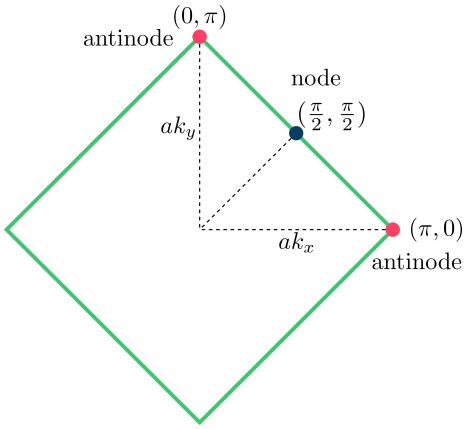
$$\mu \hat{N} = \mu \left(\sum_{i \in A, \sigma} a^\dagger_{i\sigma} a_{i\sigma} + \sum_{j \in B, \sigma} b^\dagger_{j\sigma} b_{j\sigma} \right) \to -\mu \hat{N} + \text{constant} \tag{0.24}$$

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

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

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.

van Hove singularity: Logarithmic divergence of the density of states

We will now demonstrate how the density of states (DOS) diverges logarithmically near the antinodes. The DOS at an energy E is given by

$$\rho(E) = \frac{1}{4\pi^2} \int_{S(E)} \frac{dS}{|\vec{\nabla}\epsilon_{\vec{k}}|} \tag{0.31}$$

The integral is over the surface $S(E)$ of constant energy E. Henceforth, for simplicity, we will assume $a = 1$. Near the antinodal point $\big(\pi, 0\big)$, we can approximate the dispersion as

$$\epsilon_{\vec{k}} = t\left[k_y^2 - \big(\pi - k_x\big)^2\right] \tag{0.32}$$

Since we are integrating over a constant energy surface E, we can write

$$k_y^2 - \big(\pi - k_x\big)^2 = \frac{E}{2t} = R^2 \tag{0.33}$$

We assumed here that $E > 0$. The hyperbolic nature of the equation suggests a parametrization of the form

$$k_y = R\sinh\phi, \quad \pi - k_x = R\cosh\phi \tag{0.34}$$

This allows us to parametrize the integral using just one variable ϕ. The gradient of the dispersion is

$$|\vec{\nabla}\epsilon_{\vec{k}}| = \sqrt{\left(\frac{\partial\epsilon_{\vec{k}}}{\partial k_x}\right)^2 + \left(\frac{\partial\epsilon_{\vec{k}}}{\partial k_y}\right)^2} = 2t\sqrt{\big(\pi - k_x\big)^2 + k_y^2} = 2tR\sqrt{\cosh^2\phi + \sinh^2\phi} \tag{0.35}$$

and the arc length can be written as

$$dS = \sqrt{(dk_x)^2 + (dk_y)^2} = Rd\phi\sqrt{\cosh^2\phi + \sinh^2\phi} \tag{0.36}$$

The integral can now be written purely in terms of ϕ:

$$\rho(E) = \frac{1}{4\pi^2}\frac{1}{2t}\int d\phi = \frac{1}{4\pi^2}\frac{1}{2t}\big[\phi_1 - \phi_0\big] \tag{0.37}$$

Note that we have accounted for only half of the integration space currently. To see this, consider the case when we are integrating over the half-filled Fermi surface, so we can assume $\sinh\phi = \pi - \cosh\phi$. This however, would just produce the top half of the diamond, because $\sinh\phi$ is always positive here. To get the other half, we need the other parametrization choice of

$$k_y = -R\sinh\phi, \quad \pi - k_x = R\cosh\phi \tag{0.38}$$

Since both dS and the gradient involve only even functions, they will not be affected and the total integral will just be twice of what we currently have.

$$\rho(E) = \frac{1}{4\pi^2}\frac{1}{t}\big[\phi_1 - \phi_0\big] \tag{0.39}$$

We now need to figure out the integration limits ϕ_1 and ϕ_0. Since we are integrating over the first Brillouin zone, k_y ranges from $-\pi \to \pi$, such that ϕ ranges from

$$\phi_0 = \sinh^{-1} \frac{-\pi}{R} = -\sinh^{-1} \frac{\pi}{R} \to \phi_1 = \sinh^{-1} \frac{\pi}{R} \tag{0.40}$$

This gives

$$\rho(E) = \frac{1}{2t\pi^2} \sinh^{-1} \sqrt{\frac{2t\pi^2}{E}} \tag{0.41}$$

We are interested in $E \to 0^+$, so the term in the square root will be very large. This allows us to approximate the sinh inverse as a logarithm:

$$\sinh^{-1}(x) = \ln\left(x + \sqrt{x^2+1}\right) \implies \lim_{x\to\infty} \sinh^{-1}(x) = \ln 2x \tag{0.42}$$

For the DOS, this means

$$\rho(E \to 0^+) \sim \frac{1}{2t\pi^2} \ln \sqrt{\frac{4t\pi^2}{E}} = \frac{1}{4t\pi^2} \left(\ln 4t\pi^2 - \ln E\right) \tag{0.43}$$

The logarithmic divergence in the density of states is visible now. The presence of a large number of states, specially close to the Fermi surface, results in increased correlation between the electrons and might lead to instablities because of the increased scattering near the singularity.

References

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- The Oxford Solid State Basics, *Steven H. Simon*
- An Introduction to the Hubbard Hamiltonian, *Richard T. Scalettar*