# The tight-binding model on the 2D square lattice

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**Abstract**

This is a quick introduction to the tight-binding problem on a 2D square lattice. I describe how it can be obtained from a more general model, its solution and some of its important properties like the isoenergetic contours and van Hove singularities.

## 1 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:

$$H = \sum_i H_i + H_{\text{nloc}} \tag{1}$$

$H_i$ 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:

$$H_i = \mu \sum_\sigma \hat{n}_{i\sigma} \tag{2}$$

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

$$H_i = U \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} \tag{3}$$

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

$$H_{\text{nloc}} = -t \sum_{i\sigma} \left( c^\dagger_{i\sigma} c_{i+1,\sigma} + \text{h.c.} \right) \tag{4}$$

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

$$H_i |\Psi^n_i\rangle = E^n_i |\Psi^n_{\text{loc}}\rangle \tag{5}$$

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:

$$\begin{aligned} H(\vec{r})\psi^n_i(\vec{r} - \vec{R}_i) &= \left[ \sum_i H_i(\vec{r}) + H_{\text{nloc}}(\vec{r}) \right] \psi^n_i(\vec{r} - \vec{R}_i) \\ &= \begin{cases} H_i(\vec{r})\psi^n_i(\vec{r} - \vec{R}_i) = E^n \psi^n_i(\vec{r} - \vec{R}_i) & \text{when } \vec{r} \sim \vec{R}_i \\ H_{\text{nloc}}(\vec{r})\psi^n_i(\vec{r} - \vec{R}_i) = 0 & \text{otherwise} \end{cases} \end{aligned} \tag{6}$$

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

$$\phi^n(\vec{k}) = \frac{1}{\sqrt{N}} \sum_i e^{i\vec{k}\cdot\vec{R}_i} \psi^n_i(\vec{r} - \vec{R}_i) \tag{7}$$

because it can be rewritten as

$$\phi^n(\vec{k}) = \frac{1}{\sqrt{N}} e^{i\vec{k}\cdot\vec{r}} \sum_i e^{-i\vec{k}\cdot(\vec{r} - \vec{R}_i)} \psi^n_i(\vec{r} - \vec{R}_i) = e^{i\vec{k}\cdot\vec{r}} u^n_{\vec{k}}(\vec{r}) \tag{8}$$

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

$$\xi_{\vec{k}} = \langle \Phi_{\vec{k}}^n | \, H \, | \phi_{\vec{k}}^n \rangle = \frac{1}{N} \sum_{ij} e^{i\vec{k}\cdot(\vec{R}_i - \vec{R}_j)} \, \langle \Psi_i^n | \, H \, | \Psi_j^n \rangle \tag{9}$$

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

$$\langle \Psi_i^n | \, H \, | \Psi_j^n \rangle = \alpha \delta_{ij} + \gamma \delta_{|i-j|-1} \tag{10}$$

This gives

$$\xi_{\vec{k}} = \alpha + \gamma \sum_{\vec{e}_i} e^{i\vec{k}\cdot\vec{e}_i} \tag{11}$$

$\vec{e}_i$ 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

$$\xi_{\vec{k}} = \alpha + 2\gamma \sum_{i=x,y,\ldots} \cos a_i k_i \tag{12}$$

# 2 Second-quantized Hamiltonian viewpoint

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

$$c_{\vec{k}}, c_{\vec{q}}^\dagger : \left\{ c_{\vec{k}}, c_{\vec{q}}^\dagger \right\} = \delta_{kq} \tag{13}$$

$i, j$ 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

$$H = -t \sum_{\langle ij \rangle, \sigma} \left( c_{i\sigma}^\dagger c_{j\sigma} + \text{h.c.} \right) - \mu \hat{N} \tag{14}$$

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

$$c_{\vec{k}\sigma}^\dagger = \frac{1}{\sqrt{N}} \sum_i e^{\vec{k}\cdot\vec{R}_i} c_{i\sigma}^\dagger, \quad c_{i\sigma}^\dagger = \frac{1}{\sqrt{N}} \sum_i e^{-\vec{k}\cdot\vec{R}_i} c_{\vec{k},\sigma}^\dagger \tag{15}$$

Using this, we can write

$$\begin{aligned} H &= -t \frac{1}{N} \sum_{\langle ij \rangle, \sigma} \sum_{\vec{k}\vec{q}} \left( e^{i\left[\vec{k}\cdot\vec{R}_i - \vec{q}\cdot\vec{R}_j\right]} c_{\vec{k}\sigma}^\dagger c_{\vec{q}\sigma} + \text{h.c.} \right) - \mu \hat{N} \\ &= -t \frac{1}{N} \frac{1}{2} \sum_i \sum_{j \in \text{NN of i}} \sum_{\vec{k}\vec{q}} \sum_\sigma \left( e^{i\left[\vec{k}\cdot\vec{R}_i - \vec{q}\cdot\vec{R}_j\right]} c_{\vec{k}\sigma}^\dagger c_{\vec{q}\sigma} + \text{h.c.} \right) - \mu \hat{N} \end{aligned} \tag{16}$$

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

$$\begin{aligned} \sum_j e^{-i\vec{q}\cdot\vec{R}_j} &= e^{-i\vec{q}\cdot\left(\vec{R}_i + \vec{a}_x\right)} + e^{-i\vec{q}\cdot\left(\vec{R}_i - \vec{a}_x\right)} + e^{-i\vec{q}\cdot\left(\vec{R}_i + \vec{a}_y\right)} + e^{-i\vec{q}\cdot\left(\vec{R}_i - \vec{a}_y\right)} \\ &= 2e^{-i\vec{q}\cdot\vec{R}_i} \left( \cos(q_x a_x) + \cos(q_y a_y) \right) \end{aligned} \tag{17}$$

This gives

$$\begin{aligned} H &= -t \frac{1}{N} \frac{1}{2} \sum_{\vec{k}\vec{q},\sigma} \left[ 2 \left( \cos(q_x a_x) + \cos(q_y a_y) \right) c_{\vec{k}\sigma}^\dagger c_{\vec{q}\sigma} + \text{h.c.} \right] \sum_i e^{i\left(\vec{k}-\vec{q}\right)\cdot\vec{R}_i} - \mu \hat{N} \\ &= -t \frac{1}{N} \sum_{\vec{k}\vec{q},\sigma} \left( \cos(q_x a_x) + \cos(q_y a_y) \right) \left( c_{\vec{k}\sigma}^\dagger c_{\vec{q}\sigma} + \text{h.c.} \right) N \delta_{\vec{k},\vec{q}} - \mu \hat{N} \\ &= -2t \sum_{\vec{k},\sigma} \left( \cos(k_x a_x) + \cos(k_y a_y) \right) c_{\vec{k}\sigma}^\dagger c_{\vec{k}\sigma} - \mu \hat{N} \\ &= \sum_{k\sigma} \xi_k \hat{n}_{k\sigma} \end{aligned} \tag{18}$$

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

## 3 Constant-energy contours

The contours of constant energy $E$ are defined by

$$\xi_k = E \tag{19}$$

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

$$\xi_k = 0 \implies \cos(k_x a_x) + \cos(k_y a_y) = -\frac{\mu}{2t} \tag{20}$$

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

$$\begin{aligned} & \cos(k_x a_x) + \cos(k_y a_y) = 0 \\ \implies & \cos(\pm k_x a_x) = \cos(\pi \pm k_y a_y) \\ \implies & \begin{cases} k_x + k_y = \frac{\pi}{a} \\ k_x - k_y = \frac{\pi}{a} \end{cases}, \begin{cases} -k_x + k_y = \frac{\pi}{a} \\ -k_x - k_y = \frac{\pi}{a} \end{cases} \end{aligned} \tag{21}$$

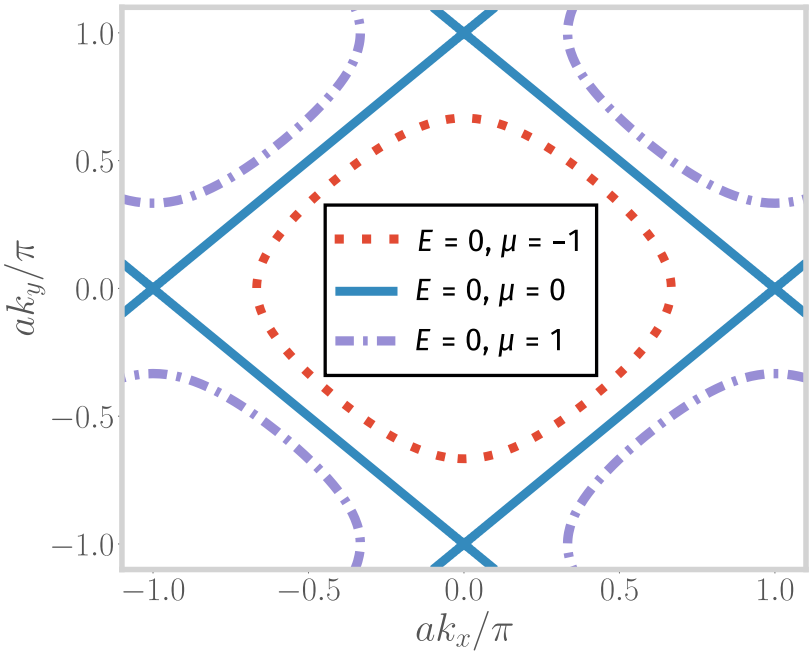



Figure 1: Contours of zero energy (Fermi surface) on the 2D tight-binding lattice model, at multiple values of the filling.

## 4 The case of 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 $b, b^\dagger$. With this in mind, the tight-binding Hamiltonian can be written as

$$H = -t \sum_{i \in A} \sum_{j \in \text{NN of i}} \sum_{\sigma} \left( a_{i\sigma}^\dagger b_{j\sigma} + \text{h.c.} \right) - \mu \hat{N} \tag{22}$$

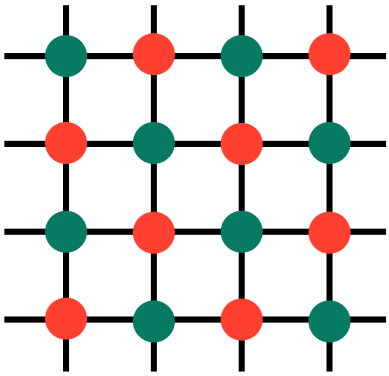


Figure 2: 2D lattice composed of two sublattices.

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

$$a^\dagger_{i\sigma} b_{j\sigma} + b^\dagger_{j\sigma} a_{i\sigma} \to -a_{i\sigma} b^\dagger_{j\sigma} - b_{j\sigma} a^\dagger_{i\sigma} = a^\dagger_{i\sigma} b_{j\sigma} + b^\dagger_{j\sigma} a_{i\sigma} \tag{23}$$

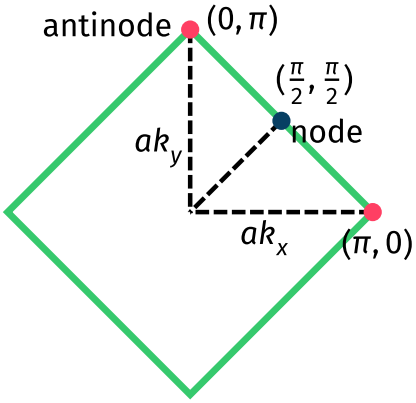
The total number part transforms as

$$\mu \hat{N} = \mu \left( \sum_{i \in A, \sigma} a^\dagger_{i\sigma} a_{i\sigma} + \sum_{j \in B, \sigma} b^\dagger_{j\sigma} b_{j\sigma} \right) \to -\mu \hat{N} + \text{constant} \tag{24}$$

This term will be invariant when

$$\mu \hat{N} = -\mu \hat{N} \implies \mu = 0 \tag{25}$$

# 5 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.

$$\text{antinodes} \to (ak_x, ak_y) = \begin{cases} (0, \pi), (\pi, 0) \\ (0, -\pi), (-\pi, 0) \end{cases} \quad , \quad \text{nodes} \to (ak_x, ak_y) = \begin{cases} \left(\frac{\pi}{2}, \frac{\pi}{2}\right), \left(-\frac{\pi}{2}, -\frac{\pi}{2}\right) \\ \left(\frac{\pi}{2}, -\frac{\pi}{2}\right), \left(-\frac{\pi}{2}, \frac{\pi}{2}\right) \end{cases}$$

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

$$ak \sim \frac{\pi}{2} \implies \cos(ak) \sim \left(ak - \frac{\pi}{2}\right)(-1) \tag{26}$$

which gives

$$\epsilon_k|_{\text{node}} \sim 2t \left(a_x k_x + a_y k_y\right) \tag{27}$$

*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

$$\begin{aligned} \cos(a_x k_x) &\sim -1 + \frac{1}{2}(\pi - a_x k_x)^2 \\ \cos(a_y k_y) &\sim 1 - \frac{1}{2}(a_y k_y)^2 \end{aligned} \tag{28}$$

such that

$$\epsilon_k|_{\text{antinode}} \sim t \left[(a_y k_y)^2 - (\pi - a_x k_x)^2\right] \tag{29}$$

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 $\vec{Q} = \frac{1}{a}(\pi, \pi)$ 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

$$\frac{1}{\xi_{\vec{k}} - \xi_{\vec{k}+\vec{Q}}} \tag{30}$$

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.

# 6 van Hove singularity: Logarithmic divergence of the density of states

The DOS at an energy $E$ is given by

$$\rho(E) = \frac{1}{4\pi^2} \int_{S(E)} \frac{dS}{|\vec{\nabla}\epsilon_{\vec{k}}|} \tag{31}$$

The integral is over the surface $S(E)$ of constant energy $E$. Henceforth, for simplicity, we will assume $\mu = 0$ and $a = 1$.

Near the antinodal point $(\pi, 0)$, we can approximate the dispersion as

$$\epsilon_{\vec{k}} = t\left[k_y^2 - (\pi - k_x)^2\right] \tag{32}$$

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

$$k_y^2 - (\pi - k_x)^2 = \frac{E}{t} = R^2 \tag{33}$$

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

$$k_y = R\sinh\phi, \quad \pi - k_x = R\cosh\phi \tag{34}$$

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

$$|\vec{\nabla}\epsilon_{\vec{k}}| = \sqrt{\left(\frac{\partial\epsilon_{\vec{k}}}{\partial k_x}\right)^2 + \left(\frac{\partial\epsilon_{\vec{k}}}{\partial k_y}\right)^2} = 2t\sqrt{(\pi - k_x)^2 + k_y^2} = 2tR\sqrt{\cosh^2\phi + \sinh^2\phi} \tag{35}$$

and the arc length can be written as

$$dS = \sqrt{(dk_x)^2 + (dk_y)^2} = Rd\phi\sqrt{\cosh^2\phi + \sinh^2\phi} \tag{36}$$

The integral can now be written purely in terms of $\phi$:

$$\rho(E) = \frac{1}{4\pi^2}\frac{1}{2t}\int d\phi = \frac{1}{4\pi^2}\frac{1}{2t}\left[\phi_1 - \phi_0\right] \tag{37}$$

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

$$k_y = -R\sinh\phi, \quad \pi - k_x = R\cosh\phi \tag{38}$$

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.

$$\rho(E) = \frac{1}{4\pi^2}\frac{1}{t}\left[\phi_1 - \phi_0\right] \tag{39}$$

We now need to figure out the integration limits $\phi_1$ and $\phi_0$. Since we are integrating over the first Brillouin zone, $k_y$ ranges from $-\pi \to \pi$, such that $\phi$ ranges from

$$\phi_0 = \sinh^{-1}\frac{-\pi}{R} = -\sinh^{-1}\frac{\pi}{R} \to \phi_1 = \sinh^{-1}\frac{\pi}{R} \tag{40}$$

This gives

$$\rho(E) = \frac{1}{2t\pi^2}\sinh^{-1}\sqrt{\frac{2t\pi^2}{E}} \tag{41}$$

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:

$$\sinh^{-1}(x) = \ln\left(x + \sqrt{x^2+1}\right) \implies \lim_{x\to\infty}\sinh^{-1}(x) = \ln 2x \tag{42}$$

For the DOS, this means

$$\rho(E \to 0^+) \sim \frac{1}{2t\pi^2}\ln\sqrt{\frac{4t\pi^2}{E}} = \frac{1}{4t\pi^2}\left(\ln 4t\pi^2 - \ln E\right) \tag{43}$$

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.

# 7 References


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