

# 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:

$$H = \sum_i H_i + H_{\text{nlloc}} \quad (1)$$

$H_i$  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:

$$H_i = \mu \sum_{\sigma} \hat{n}_{i\sigma} \quad (2)$$

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

$$H_i = U \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} \quad (3)$$

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

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

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

$$H_i |\Psi_i^n\rangle = E_i^n |\Psi_{\text{loc}}^n\rangle \quad (5)$$

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  $\psi_i^n(\vec{r} - \vec{R}_i)$  are very local; that is, they are non-zero only very close to their specific lattice sites ( $\vec{r} - \vec{R}_i \sim 0$ ). More specifically, we assume that  $\psi_i^n(\vec{r})$  becomes zero when  $H_{\text{nlloc}}(\vec{r} - \vec{R}_i)$  is non-zero. In such a situation,  $\psi_i^n(\vec{r} - \vec{R}_i)$  becomes a very good wavefunction of the full Hamiltonian:

$$\begin{aligned} H(\vec{r}) \psi_i^n(\vec{r} - \vec{R}_i) &= \left[ \sum_i H_i(\vec{r}) + H_{\text{nlloc}}(\vec{r}) \right] \psi_i^n(\vec{r} - \vec{R}_i) \\ &= \begin{cases} H_i(\vec{r}) \psi_i^n(\vec{r} - \vec{R}_i) = E_i^n \psi_i^n(\vec{r} - \vec{R}_i) & \text{when } \vec{r} \sim \vec{R}_i \\ H_{\text{nlloc}}(\vec{r}) \psi_i^n(\vec{r} - \vec{R}_i) = 0 & \text{otherwise} \end{cases} \end{aligned} \quad (6)$$

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

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

because it can be rewritten as

$$\phi^n(\vec{k}) = \frac{1}{\sqrt{N}} e^{i\vec{k} \cdot \vec{r}} \sum_i e^{-i\vec{k} \cdot (\vec{r} - \vec{R}_i)} \psi_i^n(\vec{r} - \vec{R}_i) = e^{i\vec{k} \cdot \vec{r}} u_{\vec{k}}^n(\vec{r}) \quad (8)$$

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

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

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

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

This gives

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

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

$$\xi_{\vec{k}} = \alpha + 2\gamma \sum_{i=x,y,\dots} \cos a_i k_i \quad (12)$$

## 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:

$$c_{\vec{k}}, c_{\vec{q}}^\dagger : \{c_{\vec{k}}, c_{\vec{q}}^\dagger\} = \delta_{kq} \quad (13)$$

$i, j$  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

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

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

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

Using this, we can write

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

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

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

This gives

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

with  $\xi_k = -2t (\cos(k_x a_x) + \cos(k_y a_y)) - \mu$ . 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":

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

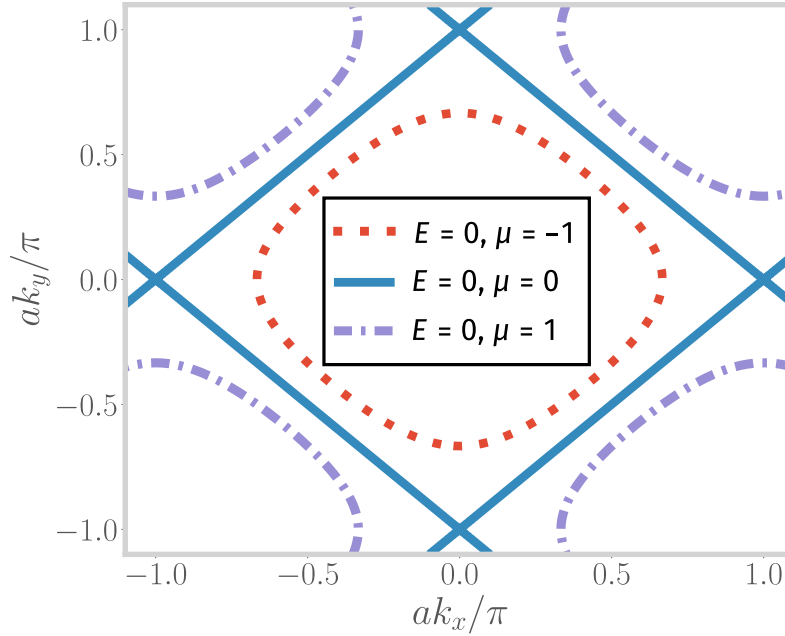


Figure 1: Contours of zero energy (Fermi surface) on the 2D tight-binding lattice model, at multiple values of the filling.

## 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  $a, a^\dagger$  and those of sublattice B with  $b, b^\dagger$ . With this in mind, the tight-binding Hamiltonian can be written as

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

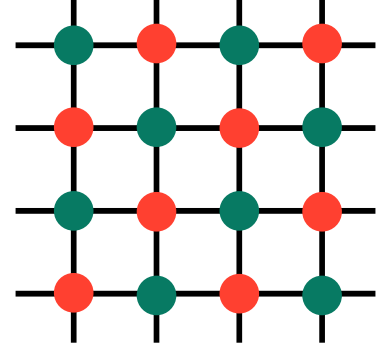


Figure 2: 2D lattice composed of two sublattices. Pink indicates sites on sublattice A and green indicates sites on sublattice B.

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

$$a_{i\sigma}^\dagger b_{j\sigma} + b_{j\sigma}^\dagger a_{i\sigma} \rightarrow -a_{i\sigma} b_{j\sigma}^\dagger - b_{j\sigma} a_{i\sigma}^\dagger = a_{i\sigma}^\dagger b_{j\sigma} + b_{j\sigma}^\dagger a_{i\sigma} \quad (23)$$

The total number part transforms as

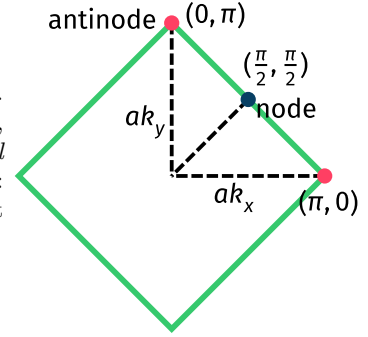
$$\mu \hat{N} = \mu \left( \sum_{i \in A, \sigma} a_{i\sigma}^\dagger a_{i\sigma} + \sum_{j \in B, \sigma} b_{j\sigma}^\dagger b_{j\sigma} \right) \rightarrow -\mu \hat{N} + \text{constant} \quad (24)$$

This term will be invariant when

$$\mu \hat{N} = -\mu \hat{N} \implies \mu = 0 \quad (25)$$

## 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.



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

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

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

which gives

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

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

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

such that

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

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

$$\frac{1}{\xi_{\vec{k}} - \xi_{\vec{k}+\vec{Q}}} \quad (30)$$

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

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

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

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

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

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

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

$$k_y = R \sinh \phi, \quad \pi - k_x = R \cosh \phi \quad (34)$$

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

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

and the arc length can be written as

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

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

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

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

$$k_y = -R \sinh \phi, \quad \pi - k_x = R \cosh \phi \quad (38)$$

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.

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

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  $-\pi \rightarrow \pi$ , such that  $\phi$  ranges from

$$\phi_0 = \sinh^{-1} \frac{-\pi}{R} = -\sinh^{-1} \frac{\pi}{R} \rightarrow \phi_1 = \sinh^{-1} \frac{\pi}{R} \quad (40)$$

This gives

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

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

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

For the DOS, this means

$$\rho(E \rightarrow 0^+) \sim \frac{1}{2t\pi^2} \ln \sqrt{\frac{4t\pi^2}{E}} = \frac{1}{4t\pi^2} (\ln 4t\pi^2 - \ln E) \quad (43)$$

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 instabilities 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*