Chapter 3

Tight-binding model

For the numerical calculation of physical quantities, such as the transmission co-efficients in the Landauer-Büttiker formulas, it is convenient to have a numerical representation of the problem that is easy to use and of sufficiently general purpose. In this chapter, a tight-binding representation is seen to fulfill such requirements.

The tight-binding model of a system is obtained by discretizing its Hamiltonian on a lattice. The smaller one chooses the lattice cell size, the better this representation represents the continuum limit. As such, not every lattice site corresponds to an atom as in ab-initio theories; rather a site may represent a region containing many atoms, but this region should be small compared to physically relevant quantities such as the Fermi wavelength.

Although this kind of tight-binding approach is widely used nowadays, some new viewpoints will be presented in this chapter, e.g., considering a gauge for describing inhomogeneous fields, and the description of spin-orbit coupling. The application of the tight-binding approach to spin-dependent transport calculations will be treated in some detail since this is a more recent development, while spin-degenerate systems are only briefly discussed because their treatment can be found in textbooks nowadays (see, e.g., Ref. [2]).

3.1   Spin-degenerate system

3.1.1   Generalities

The Hamiltonian for a spinless electron in a two-dimensional system moving in a magnetic field is given by

$$H = \frac{1}{2m^*} \left(i\hbar\nabla - e\mathbf{A} \right)^2 + V, \tag{3.1}$$

where m^* and $-e$ are the effective mass and the electronic charge respectively. The potential V comprises both the potential that confines the electrons and the one due to impurities (disorder) in the system. The vector potential $\mathbf{A}$ describes the influence of a magnetic field $\mathbf{B} = \nabla \times \mathbf{A}$. Since we are considering a 2D system,

only fields applied perpendicular to the sample will have an influence on the orbit of the electron.

The general scheme for discretizing this Hamiltonian looks as follows. First, one constructs a square lattice with lattice parameter a by defining points $(n, m) = (x = na, y = ma)$ with n and m integer. By approximating the derivative operators on this lattice as $\partial_x f = 1/a[f(x + a/2) - f(x - a/2)]$ (and an equivalent expression for $\partial_y f$), one can show that the Hamiltonian (3.1) can be mapped onto a nearest-neighbor tight-binding Hamiltonian [2]

$$
\begin{aligned}
\mathcal{H} &= \sum_n \sum_m \left[t_{nm}^x \, |n+1, m\rangle\langle n, m| + t_{nm}^y \, |n, m+1\rangle\langle n, m| + \text{H.c.} \right] + \\
&\quad + \sum_n \sum_m \epsilon_{nm} \, |n, m\rangle\langle n, m|,
\end{aligned}
\tag{3.2}
$$

that acts in the discrete space spanned by the states $|n, m\rangle = |x = na, y = ma\rangle$.

The on-site energies ϵ_{nm} in this Hamiltonian are

$$
\epsilon_{nm} = 4t + V_{nm},
\tag{3.3}
$$

with $V_{nm} = V(na, ma)$. They have been shifted up by an amount $4t$ so that the energy band for free electrons ($V = 0$) in an infinite lattice,

$$
\varepsilon = 2t\big(2 - \cos k_x a - \cos k_y a\big),
\tag{3.4}
$$

has a value of zero at the bottom. The k_x and k_y are wavevectors belonging to the first Brillouin zone of the square lattice. It can be seen that the tight-binding model is a good approximation only when $k_x a, k_y a \ll 1$, i.e., when the lattice spacing is smaller than the Fermi wavelength, since the dispersion relation then becomes approximately parabolic like in the continuum case.

The quantities t_{nm}^x and t_{nm}^y in the tight-binding Hamiltonian give the hopping amplitude in the horizontal, respectively vertical direction. In the absence of a magnetic field they are given by:

$$
t_{nm}^x = t_{nm}^y = -t = -\frac{\hbar^2}{2m^* a^2}.
\tag{3.5}
$$

When the vector potential $\mathbf{A}$ is included, the hopping parameters change to

$$
t_{nm}^{x(y)} = -t \, e^{-\mathrm{i}\, e/\hbar \int \mathbf{A} \cdot \mathrm{d}\mathbf{l}},
\tag{3.6}
$$

where $\int \mathbf{A} \cdot \mathrm{d}\mathbf{l}$ is the integral of the vector potential along the hopping path[1]. This is called the Peierls substitution [38, 39]. Given a certain magnetic field distribution, we still have the freedom to choose the gauge for the vector potential that suits best to our needs. One very convenient gauge for representing a homogeneous field $B\mathbf{e_z}$

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[1]A lucid discussion on the physics of Eq. (3.6) is given in Ref. [37] on page 21-2.

is the Landau gauge: $\mathbf{A} = -By\mathbf{e_x}$. In this gauge, the hopping parameters found from Eq. (3.6) are explicitly given by

$$
\begin{aligned}
t_{nm}^x &= -t\,e^{\mathrm{i}2\pi(m-1)\Phi/\Phi_0}, & \text{(3.7a)} \\
t_{nm}^y &= -t, & \text{(3.7b)}
\end{aligned}
$$

where we have defined $\Phi = Ba^2$ as the magnetic flux per lattice cell, and $\Phi_0 = h/e$ the magnetic flux quantum. This gauge is particularly interesting for describing fields in the leads because it conserves translational invariance along the X axis. Choosing in every lead a coordinate system with the local X axis pointing along the longitudinal direction[2], the conservation of translational invariance along this axis assures that one is still able to speak of in- and outgoing waves in the leads, which is necessary to define the transmission coefficients in the Landauer-Büttiker formalism [see Eq. (2.3) and the discussion thereafter].

3.1.2 Inhomogeneous fields

The Peierls substitution method gives a very convenient way of dealing with magnetic fields in a tight-binding model. However, although the Landau gauge proved to be very convenient for describing homogeneous fields, it is not always clear what gauge to choose for more exotic field distributions. It is for instance not obvious how the vector potential $\mathbf{A}$ should look like when one has a completely random magnetic field in the device.

Nevertheless, we have found a convenient gauge for any possible field distribution, as will be explained with the help of Fig. 3.1. Suppose that one has a perpendicular magnetic field with strength B that is localized on a single lattice cell. The influence of this local field can be described by changing all the hopping parameters t_{mn}^x *above* the flux tube as follows:

$$
t_{nm}^x \to -t\,e^{\mathrm{i}2\pi\Phi_1/\Phi_0}, \quad \text{for } m > m_1, \tag{3.8}
$$

where Φ_1 is the magnetic flux enclosed by the unit cell: $\Phi_1 = B_1 a^2$. An electron traveling along any closed path around the flux tube will then pick up a phase $2\pi\Phi_1/\Phi_0$, thus giving a correct description of the field. A second localized flux tube in the same column will contribute another phase change Φ_2, but again only to the hopping parameters *above* the second flux tube. The total change of the hopping parameters is then the sum of both contributions (see Fig. 3.1):

$$
t_{nm}^x \to \begin{cases} -t & ,m < m_1 < m_2 \\ -t\,e^{\mathrm{i}2\pi\Phi_1/\Phi_0} & ,m_1 < m \le m_2 \\ -t\,e^{\mathrm{i}2\pi(\Phi_1+\Phi_2)/\Phi_0} & ,m_1 < m_2 < m \end{cases} \tag{3.9}
$$

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[2]A proof that the gauge for the vector potential can indeed always be chosen to be Landau-like in every lead is given in Ref. [40].
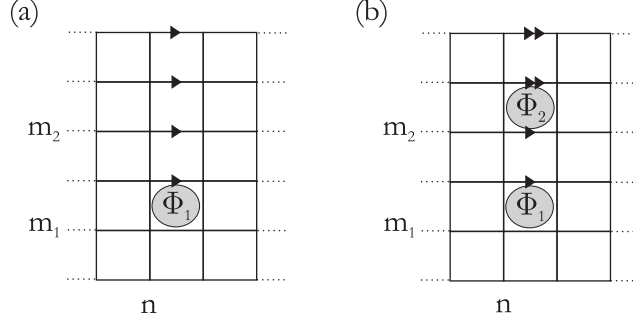
Figure 3.1: An arbitrary magnetic field is composed of flux tubes localized on single lattice cells. For a single flux tube, all hopping parameters above it change their phase by ϕ_1 [single arrow in (a)]. If a second flux tube is included above the first one, hopping parameters located above both cells will change their phase by $\phi_1 + \phi_2$ [double arrows in (b)].

This line of reasoning can be easily generalized to a situation where every unit cell encompasses a single flux tube. One just changes the hopping parameters as:

$$t_{nm}^x \rightarrow -t \, e^{\mathrm{i}2\pi \sum_{m'<m} \Phi_{nm'}/\Phi_0},\tag{3.10}$$

where $\Phi_{nm'}$ is the flux through the lattice cell above the link connecting site (n, m') with site $(n + 1, m')$. As such, one can describe an arbitrary magnetic field in the device by choosing the appropriate flux tube distribution through the different lattice cells.

From comparison with Eq. (3.6), the description above corresponds to choosing the following gauge for the vector potential:

$$\begin{aligned} A_{n\leftrightarrow n+1,m}^x &= -\tfrac{1}{a} \sum_{l<m} \Phi_{nl} \\ A^y &= 0 \end{aligned},\tag{3.11}$$

where $A_{n\leftrightarrow n+1,m}^x$ is the vector potential at the vertex connecting sites (n, m) and $(n + 1, m)$. Note that for a homogeneous field where all lattice cells comprise the same flux $\Phi_{nm} = \Phi = Ba^2$, the gauge choice above corresponds to the Landau gauge.

3.2 Including spin degrees of freedom

When including spin in the problem, the state space will be extended: it is now spanned by product states $|n, m, \sigma\rangle = |n, m\rangle \otimes |\sigma\rangle$, where $|\sigma\rangle$ defines the spin state of the electron. In a matrix representation of the Hamiltonian, this means that every element of the "spinless" representation now becomes a 2×2 spin matrix itself.

When treating the spin-independent terms in the Hamiltonian, this spin matrix is proportional to the identity matrix. In other words, the Hamiltonian $\mathcal{H}$ in

Eq. (3.2) can be written to act in the extended space by just putting $\mathcal{H} \rightarrow \mathcal{H} \otimes \mathbf{1}$ with $\mathbf{1}$ the identity matrix, and no extra work is needed for finding a tight-binding description for the spin-degenerate Hamiltonian. For operators acting on the spin degrees of freedom however, we still have to derive a tight-binding representation. In the next sections, this will be done for both the Zeeman (or exchange) splitting and spin-orbit coupling terms.

3.2.1 Zeeman/exchange splitting

In a preceding section we discussed the influence of a magnetic field on the orbit of the electron and described it by the Peierls substitution. However, the effect of the field on the spin of the electron was neglected. In fact, an extra term

$$H_S = -\frac{1}{2} g^* \mu_B \, \mathbf{B}_{\text{eff}} \cdot \boldsymbol{\sigma}, \qquad (3.12)$$

should be added to the Hamiltonian, where g^* is the effective Landé factor for the electron and μ_B is the Bohr magneton, while $\boldsymbol{\sigma}$ is a vector containing the Pauli spin matrices: $\boldsymbol{\sigma} = (\sigma^x, \sigma^y, \sigma^z)$. We have written the field as an effective field $\mathbf{B}_{\text{eff}}$, to make it clear that it can be due to an externally applied field, an exchange field (in a ferromagnet, e.g.), or a combination of both. This Hamiltonian will split the energy bands: a spin-up state (with respect to $\mathbf{B}_{\text{eff}}$) will be shifted down in energy by $1/2 \, g^* \mu_B \|\mathbf{B}_{\text{eff}}\|$, while a spin-down state will be shifted up by the same amount.

Since it only acts in spin space, this operator will lead to an on-site term in the tight-binding Hamiltonian:

$$\mathcal{H}_S = -\frac{1}{2} g^* \mu_B \sum_{n,m} |n, m\rangle\langle n, m| \otimes \left(\mathbf{B}_{nm}^{\text{eff}} \cdot \boldsymbol{\sigma} \right), \qquad (3.13)$$

with $\mathbf{B}_{nm}^{\text{eff}} = \mathbf{B}_{\text{eff}}(x = na, y = ma)$. It should be noted that the orbit of the electron is only influenced by the component of the magnetic field perpendicular to the 2D sample, while the spin splitting of course depends on all three components of the field.

3.2.2 Spin-orbit coupling

When a particle with spin moves in an electric field, its spin and orbital degrees of freedom will be coupled. This so-called spin-orbit interaction is essentially a relativistic effect, and gives rise to a Hamiltonian of the form

$$H_{\text{SO}} = \lambda \, \mathbf{P} \cdot \left(\nabla V \times \boldsymbol{\sigma} \right), \qquad (3.14)$$

where V is the electrostatic potential felt by the electron, and $\mathbf{P}$ the mechanical momentum operator. The parameter λ is a material constant describing the strength of the coupling.

Instead of deriving this Hamiltonian explicitly by making an expansion in v/c of the Dirac equation, we will give some physical arguments as to why a Hamiltonian of the form above can be expected. Suppose an electron moves with velocity $\mathbf{v}$ in an electric field $\mathbf{E}$. Doing a Lorentz transformation to its rest frame, the electron feels a magnetic field (to first order in v/c)

$$\mathbf{B} = -\frac{1}{c^2}(\mathbf{v} \times \mathbf{E}). \tag{3.15}$$

The magnetic moment of the electron can interact with this field, giving rise to a Zeeman-like term

$$H_{\text{SO}} = -\frac{1}{2}\, g^* \,\mu_B\, \mathbf{B} \cdot \boldsymbol{\sigma}. \tag{3.16}$$

Substituting the magnetic field in this expression with Eq. (3.15), and using that $\mathbf{v} = \mathbf{P}/m^*$, one obtains finally

$$H_{\text{SO}} = g^* \frac{e\hbar}{4m^{*2}c^2}\big(\mathbf{P} \times \mathbf{E}\big) \cdot \boldsymbol{\sigma}. \tag{3.17}$$

Writing the electric field as $\mathbf{E} = \nabla V/e$, with V the electrostatic potential, this indeed leads to a spin-orbit Hamiltonian of the form (3.14), with the parameter λ given by[3]

$$\lambda = \frac{g^*\hbar}{4m^{*2}c^2}. \tag{3.18}$$

In a strictly 2D system, the electrostatic potential V depends only on the coordinates (x, y). In this case, we can write the spin-orbit Hamiltonian (3.14) as

$$H_{\text{SO}} = \lambda\, \sigma^z \left[\left(\frac{\hbar}{\mathrm{i}}\partial_x + eA^x\right)\partial_y V - \left(\frac{\hbar}{\mathrm{i}}\partial_y + eA^y\right)\partial_x V \right], \tag{3.19}$$

where we used $\mathbf{P} = \mathbf{p} + e\mathbf{A} = \frac{\hbar}{\mathrm{i}}\nabla + e\mathbf{A}$ for the mechanical momentum. For deriving the tight-binding version of the Hamiltonian (3.19), we need to discretize this operator on a lattice. Since this involves quite a few technical operations, we have shifted such a discussion into Appendix A. The end result is:

$$\mathcal{H}_{\text{SO}} = \frac{\lambda\hbar}{2a} \sum_{n,m} \left\{ [\partial_x V]_{n,m\leftrightarrow m+1} \left(|n,m\rangle\langle n, m+1| \otimes \mathrm{i}\sigma^z \right) \right. \tag{3.20}$$

$$\left. -[\partial_y V]_{n\leftrightarrow n+1,m}\; e^{-\mathrm{i}\,2\pi \sum_{l<m} \frac{\Phi_{n,l}}{\Phi_0}} \left(|n,m\rangle\langle n+1, m| \otimes \mathrm{i}\sigma^z \right) + \text{H.c.} \right\},$$

---

[3]In our naive derivation, we did not treat the Lorentz transformation between the lab frame and the electron's rest frame completely correctly. An electron moving in an electric field that has a component perpendicular to the electron's velocity describes a curved trajectory. The transformation between the lab frame and the electron's rest frame therefore involves two noncollinear Lorentz transformations. As a consequence, an observer in the electron's rest frame will find that an additional rotation is necessary to align his axes with the axes obtained by just boosting the labframe using the instantaneous velocity of the electron. This results in an extra precession of the electron spin, called Thomas precession. The effect changes the magnitude of the interaction in Eq. (3.16), and will introduce a factor of 1/2 in the expression for λ. We will assume this factor to be absorbed in the definition of g^*. For a more thorough discussion, see, e.g., Ref. [41].

with the derivatives of the potential on the vertices defined as

$$[\partial_y V]_{n \leftrightarrow n+1,m} \approx \frac{1}{2a} \left[\frac{1}{2} \Big(V_{n,m+1} + V_{n+1,m+1} \Big) - \frac{1}{2} \Big(V_{n,m-1} + V_{n+1,m-1} \Big) \right]$$

$$[\partial_x V]_{n,m \leftrightarrow m+1} \approx \frac{1}{2a} \left[\frac{1}{2} \Big(V_{n+1,m} + V_{n+1,m+1} \Big) - \frac{1}{2} \Big(V_{n-1,m} + V_{n-1,m+1} \Big) \right].$$

This Hamiltonian describes a spin-dependent hopping to nearest neighbor sites, clearly illustrating the coupling between spin and orbital degrees of freedom. Upon hopping in the X direction to a neighboring site, the electron will pick up the same phase factor that was due to the presence of a magnetic field (see Sec. 3.1.2).

3.2.3 Rashba spin-orbit coupling

Experimentally, a two-dimensional electron gas is often created at the interface of a semiconductor heterostructure. Electrons are then confined by an approximately triangular potential well $V(z)$ in the growth direction (see Fig. 3.2). If this well is narrow enough electrons will only occupy the lowest eigenstate and the movement along the Z direction is effectively frozen out so that electrons are only free to move in a two-dimensional plane.
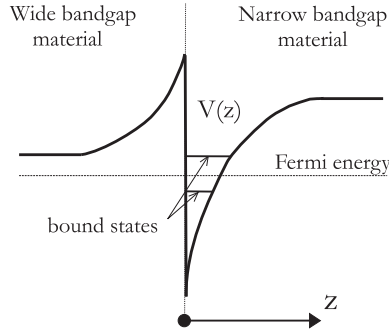
Figure 3.2: Conduction band at the interface of a semiconductor heterostructure. Band bending creates a potential well $V(z)$ confining the electrons to the XY plane. The asymmetry of this well leads to Rashba spin-orbit coupling.

However, the influence of the triangular potential well goes further than confining the electrons in a plane: it can give rise to the so-called the Rashba spin-orbit interaction [42, 43]. Indeed, the potential well $V(z)$ has a nonzero gradient and it will give rise to a spin-orbit coupling according to Eq. (3.14):

$$H_{\text{RSO}} = \lambda \frac{\mathrm{d}V}{\mathrm{d}z} \mathbf{P} \cdot \big(\mathbf{e}_z \times \boldsymbol{\sigma} \big). \tag{3.21}$$

When the well is not exactly triangular, the gradient $\frac{\mathrm{d}V}{\mathrm{d}z}$ is not constant and one has to calculate an average, using the density distribution for electrons in the Z direction

as a weight function. Writing out the cross-product in Eq. (3.21), one obtains an expression for the Rashba term of the form

$$H_{\text{RSO}} = \frac{\alpha}{\hbar}\left(P_y\sigma^x - P_x\sigma^y\right),\qquad(3.22)$$

where $\alpha = \lambda\hbar\langle dV/dz\rangle$ is a material parameter that contains the details of the averaging procedure described above. It is clear that α will only be different from zero when the confining potential is not symmetric. In real heterostructures, α can take on typical values in the range of 1 to 10×10^{-10} eVcm for a large variety of systems (mostly used are GaAs/AlGaAs and InAs/InAlAs heterostructures), depending on the exact shape of the confining potential well. It should be noted that the shape of the confining well, and thus the coupling strength α can be varied by applying a voltage on an electrostatic gate mounted on top of the electron gas [44, 45]. This gives some control on the strength of the spin-orbit interaction and it has lead to proposals for a variety of devices based upon controlling the spin degrees of freedom electrically (rather than with magnetic fields) via the Rashba spin-orbit coupling. Most famous among these is the spin field effect transistor [22].

The tight-binding representation for the Rashba Hamiltonian in Eq. (3.22) is derived in full detail in Appendix A. We only state the end result here:

$$\mathcal{H}_{\text{RSO}} = -t_{\text{SO}}\sum_{n,m}\left\{e^{-i2\pi\sum_{l<m}\Phi_{n,l}/\Phi_0}\left(|n,m\rangle\langle n+1,m|\otimes i\sigma^y\right)\right.$$
$$\left. -\left(|n,m\rangle\langle n,m+1|\otimes i\sigma^x\right) + \text{H.c.}\right\},\qquad(3.23)$$

where we have defined $t_{\text{SO}} = \alpha/2a$. The Rashba Hamiltonian thus describes a hopping between neighboring sites paired with a spin flip. Again, a phase factor is picked up when hopping in the X direction in the presence of a magnetic flux.