Chapter 2
Square Lattice with Magnetic Field

Abstract  Electrons moving in a periodic potential experience a quantized energy spectrum, where the discrete energy bands are known as Bloch bands. In a magnetic field the spectrum further splits into highly degenerate Landau levels. The interplay between both effects leads to a complex fractal energy spectrum known as Hofstadter’s butterfly. This chapter provides an introduction into the theoretical description of the system in the absence of interactions in terms of magnetic translation symmetries. The topological properties of the system are further discussed in terms of topological invariants, the Chern numbers, which are directly related to the quantization of the Hall conductivity.

Electrons moving in a periodic potential experience a quantized energy spectrum, where the discrete energy bands are known as Bloch bands. In a magnetic field the spectrum further splits into highly degenerate Landau levels. The interplay between both effects leads to a complex fractal energy spectrum known as Hofstadter’s butterfly [1]. In order to observe related effects experimentally, magnetic fields on the order of one flux quantum per lattice unit cell are required. In solid state setups the lattice constants are rather small, i.e. on the order of a few angstroms. Consequently, unfeasible large magnetic fields would need to be applied to the material to enter this regime. To overcome this limitation artificial materials with larger lattice constants can be designed. Recently this was demonstrated by engineering superlattice structures with graphene placed on hexagonal boron nitride [2–4]. Additionally the same experimental regimes became accessible in photonics [5, 6] and with ultracold atoms [7, 8].

Already the single particle physics in a periodic potential with large magnetic field shows very interesting phenomena. The motion of a charged particle in a magnetic field is accompanied by a geometric phase, the Aharonov-Bohm phase [9]. On a lattice these phases are introduced in the form of so-called Peierls phases that a particle picks up when hopping in the lattice (Sect. 2.1). Unlike the zero-field case the magnetic Hamiltonian is not invariant under the usual translation by a lattice unit vector. Instead one has to consider the magnetic translation symmetries of the Hamiltonian which effectively enlarge the usual lattice unit cell depending on the
magnetic flux. The new unit cell is denoted as magnetic unit cell. Its area is determined by the strength of the flux but its dimensions are not unique (Sect. 2.2). The resulting single-particle energy spectrum shows a fractal structure as a function of the magnetic flux per unit cell, which is known as Hofstadter’s butterfly (Sect. 2.3). Depending on the flux the lowest tight-binding band splits into several subbands, whose topological properties are characterized by topological invariants called Chern numbers, which are directly related to the quantization of the Hall conductivity in the integer QH effect (Sect. 2.4).

2.1 Peierls Phase-Factors

The physics of electrons moving in a periodic potential can be described by the Hubbard model, which was first introduced by John Hubbard in 1963 [10]. This model is a good approximation for systems at low temperatures where all particles occupy the lowest energy band [11, 12]. It is typically characterized by two terms: a kinetic term that describes the hopping of particles between neighboring sites in the potential and an on-site interaction term. For a single electron in a 2D lattice potential the Hamiltonian consists only of the kinetic term and can be written in the following form

\[
\hat{H}_0 = -J \sum_{m,n} \left( \hat{a}^\dagger_{m+1,n} \hat{a}_{m,n} + \hat{a}^\dagger_{m,n+1} \hat{a}_{m,n} + \text{h.c.} \right),
\]  

(2.1)

where \( \hat{a}^\dagger_{m,n} \) and \( \hat{a}_{m,n} \) are the creation and annihilation operators on site \((m, n)\) respectively, \(m\) is the site index along \(x\) and \(n\) the one along \(y\). The model is based on the

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{fig2.1}
\caption{Equivalence between complex tunneling amplitudes on a square lattice and the Aharonov-Bohm phase. a Schematic drawing of a 2D lattice with complex tunneling amplitudes determined by the Peierls phases \(\phi_{m,n}^i, i = \{x, y\}\). The coupling strength along both directions is given by \(J\). An electron that tunnels around the borders of one lattice unit cell (gray shaded area) picks up a phase \(\Phi = \phi_{m,n}^x + \phi_{m+1,n}^y - \phi_{m,n+1}^x - \phi_{m,n}^y\) due to the presence of the vector potential \(A\). b Illustration of an electron moving along a closed path \(C\) in an external magnetic field \(B = \nabla \times A\). The particle picks up a geometric phase \(\Phi_{AB}\) known as Aharonov-Bohm phase.}
\end{figure}
2.1 Peierls Phase-Factors

**tight-binding approximation** where the electrons are assumed to occupy the standard orbitals of the atoms and the overlap between atomic wave functions on neighboring sites is small. The tunneling amplitude for an electron to hop from one atom to the next is determined by the coupling matrix element $J$.

In the presence of an external magnetic field $\mathbf{B} = \nabla \times \mathbf{A}$, where $\mathbf{A}$ is the vector potential, Hamiltonian (2.1) is modified according to the Peierls substitution [13]. As a result the tunneling matrix elements become complex and hopping in the lattice is accompanied by a phase $\phi_{m,n} = -eA_{m,n}^i/h$, $i = \{x, y\}$, which is known as Peierls phase (Fig. 2.1a), $e$ is the electron charge and $\hbar = h/(2\pi)$ the reduced Planck constant. Accordingly, the tight-binding Hamiltonian takes the following form

$$\hat{H} = -J \sum_{m,n} \left( e^{i\phi_{x,m,n}^i} \hat{a}_{m+1,n}^{\dagger} \hat{a}_{m,n} + e^{i\phi_{y,m,n}^i} \hat{a}_{m,n+1}^{\dagger} \hat{a}_{m,n} + \text{h.c.} \right). \quad (2.2)$$

The Peierls phases are a manifestation of the Aharonov-Bohm phase experienced by a charged particle moving in a magnetic field (Fig. 2.1b)

$$\Phi_{AB} = -\frac{e}{\hbar} \oint_{C} \mathbf{A} \cdot d\mathbf{r} = -2\pi \frac{\Phi_B}{\Phi_0}, \quad (2.3)$$

where $\Phi_B$ is the magnetic flux through the area enclosed by the contour $C$ and $\Phi_0 = h/e$ is the magnetic flux quantum [9]. Equivalently one can define the magnetic flux per lattice unit cell in units of the magnetic flux quantum as

$$\alpha = \frac{1}{2\pi} \Phi = \frac{1}{2\pi} \left( \phi_{m,n}^x + \phi_{m,n+1}^y - \phi_{m+1,n}^x - \phi_{m,n}^y \right). \quad (2.4)$$

In the following $\Phi$ will be denoted as the flux per unit cell of the underlying lattice or simply the flux per plaquette.

**2.2 Magnetic Translation Operators**

In the zero-field case the lattice translation operators $\hat{T}_i^0$ commute with Hamiltonian (2.1) for all Bravais lattice vectors [11, 12],

$$\hat{T}_x^0 = \sum_{m,n} \hat{a}_{m+1,n}^{\dagger} \hat{a}_{m,n}, \quad \hat{T}_y^0 = \sum_{m,n} \hat{a}_{m,n+1}^{\dagger} \hat{a}_{m,n}; \quad (2.5)$$

they further commute with each other $[\hat{T}_x^0, \hat{T}_y^0] = 0$, which allows us to apply the well-known Bloch theorem [11, 12]. In the presence of a vector potential, however, the Hamiltonian is no longer invariant under the translation by one lattice unit vector because the corresponding vector potential $\mathbf{A}_{m,n}$ is not invariant under this discrete translation even though the magnetic field $\mathbf{B}$ itself might be. Hence, the translation
operators $\hat{T}_i^0$ do not commute with Hamiltonian (2.2). For the following discussion it is convenient to write Hamiltonian (2.2) in the following form

$$\hat{H} = \hat{T}_x + \hat{T}_y + \text{h.c.},$$

(2.6)

where $\hat{T}_x$ and $\hat{T}_y$ describe the translation by one lattice constant along the $x$- and $y$-direction in the presence of a vector potential $\mathbf{A}_{m,n}$:

$$\hat{T}_x = \sum_{m,n} \hat{a}^\dagger_{m+1,n} \hat{a}_{m,n} e^{i\phi_{m,n}^x}, \quad \hat{T}_y = \sum_{m,n} \hat{a}^\dagger_{m,n+1} \hat{a}_{m,n} e^{i\phi_{m,n}^y}. \quad (2.7)$$

For simplicity the tunnel coupling is set to $J = -1$. It can be easily verified that in general the operators $\hat{T}_i$ do not commute with each other $[\hat{T}_x, \hat{T}_y] \neq 0$, thus, they neither commute with the Hamiltonian, $[\hat{T}_x, \hat{H}] \neq 0$ and $[\hat{T}_y, \hat{H}] \neq 0$. To find the new symmetries of the lattice Hamiltonian with flux and to recover translational invariance new operators have to be constructed, which form a complete set of commuting operators with Hamiltonian (2.6). These operators are a combination of translation and gauge transformation

$$\hat{T}_M^x = \sum_{m,n} \hat{a}^\dagger_{m+1,n} \hat{a}_{m,n} e^{i\theta_{m,n}^x}, \quad \hat{T}_M^y = \sum_{m,n} \hat{a}^\dagger_{m,n+1} \hat{a}_{m,n} e^{i\theta_{m,n}^y}, \quad (2.8)$$

and are called magnetic translations operators (MTOs) [14–16]. In general the new magnetic translation symmetry will differ from the one of the underlying lattice potential. The phases $\theta_{m,n}^i$ are determined by the formal requirement that the MTOs have to commute with the Hamiltonian, $[\hat{T}_i^M, \hat{H}] = 0$, leading to

$$\theta_{m,n}^x = \phi_{m,n}^x + \Phi_{m,n} n, \quad \theta_{m,n}^y = \phi_{m,n}^y - \Phi_{m,n} m. \quad (2.9)$$

A detailed derivation of these expressions can be found in Appendix A, which closely follows Ref. [17]. The flux per unit cell $\Phi_{m,n}$ is allowed to vary across the lattice and

![Fig. 2.2](image-url) Effective magnetic flux $\Phi_{m,n}$ per plaquette. The vector potential $\mathbf{A}_{m,n}$ gives rise to and effective flux per plaquette (gray shaded area) as defined in Eq. (2.10), with the convention that the magnetic field is pointing along the $+\hat{e}_z$-direction. The arrows illustrate the direction of the tunneling.
its index is determined by the lattice site on the lower left corner (Fig. 2.2)

\[
\Phi_{m,n} = \phi_{m,n}^x + \phi_{m+1,n}^y - \phi_{m,n+1}^x - \phi_{m,n}^y. \tag{2.10}
\]

Although the derivation of Eq. (2.9) was carried out for general flux distributions \(\Phi_{m,n}\), it might not be directly applicable in the case of more complicated configurations such as staggered flux distributions (Chap. 5). However, even in this case the corresponding MTOs can be derived using the methods described in Appendix A. The MTOs obtained in this way do commute with the Hamiltonian by construction but they do not necessarily commute with each other. The value of the commutator \([\hat{T}_x^M, \hat{T}_y^M]\) can be computed using the single-particle state \(\psi_{i,j} = \hat{a}^\dagger_{i,j} |0\rangle\) on lattice site \((i, j)\):

\[
\hat{T}_x^M \hat{T}_y^M \psi_{i,j} = \hat{T}_x^M \psi_{i,j+1} = e^{i\theta_{i,j+1}^y} \psi_{i,j+1} = e^{i(\theta_{i,j+1}^y + \theta_{i,j}^x)} \psi_{i+1,j+1},
\]

\[
\hat{T}_y^M \hat{T}_x^M \psi_{i,j} = \hat{T}_y^M \psi_{i+1,j} = e^{i\theta_{i+1,j}^x} \psi_{i+1,j} = e^{i(\theta_{i+1,j}^x + \theta_{i,j}^y)} \psi_{i+1,j+1}. \tag{2.12}
\]

The specific form of the MTOs depends on the particular form of the vector potential \(A_{m,n}\), which in turn depends on the choice of gauge. However, there is no fundamental reason for the two magnetic translations operators \(\hat{T}_x^M\) and \(\hat{T}_y^M\) defined in Eq. (2.8) to commute with each other.

### 2.2.1 Homogeneous Magnetic Fields

Let us consider a homogeneous magnetic field with \(\Phi_{m,n} \equiv \Phi = 2\pi \alpha\) per plaquette (Fig. 2.3a). Inserting Eq. (2.9) into the expressions given in Eqs. (2.11) and (2.12) leads to the following result

![Fig. 2.3](image-url) Magnetic translation operators for a homogeneous magnetic field. a Schematic drawing of a square lattice with lattice constant \(a\) and homogeneous flux \(\Phi\) per plaquette. b Action of the magnetic translation operators along a closed path around one lattice unit cell, \((\hat{T}_y^M)^\dagger (\hat{T}_x^M)^\dagger \hat{T}_x^M \hat{T}_y^M \psi_{i,j} = \exp(-i\Phi)\psi_{i,j}\). c If the path shown in (b) is enlarged around a super-cell of dimension \(k \times l\) the action of the MTOs along that path corresponds to a phase shift of \(-k\Phi = -2\pi \alpha \cdot kl\)
Consequently, the commutator vanishes only if \( \Phi \) is an integer multiple of \( 2\pi \). Such a flux configuration is however gauge-equivalent to the trivial case of zero flux per plaquette and does not correspond to the situation we are interested in. Nevertheless equation (2.13) does provide us with an intuitive picture of the MTOs by acting with them on a single-particle state \( \psi_{i,j} \) around the borders of one lattice unit cell that is pierced by a flux \( \Phi \). Choosing the direction illustrated in Fig. 2.3b the single particle state \( \psi_{i,j} \) picks up a phase \( -e^{-i/\Phi} \), which corresponds to a flux pointing in the opposite direction.

For flux values different from \( \Phi = \nu \times 2\pi, \nu \in \mathbb{Z} \), this intuitive picture suggests that commuting magnetic translation operators can be constructed if they enclose a super-cell on the lattice pierced by a magnetic flux equal to an integer multiple of \( 2\pi \). For a super-cell of dimension \( k \times l \) one obtains

\[
\left( \hat{T}_x^M \right)^{k} \left( \hat{T}_y^M \right)^{l} \psi_{i,j} = \left( \hat{T}_x^M \right)^{k} \exp \left( i \sum_{v=0}^{l-1} \theta_{i,j+v}^y \right) \psi_{i,j} \]

\[
= \exp \left( i \sum_{\mu=0}^{k-1} \theta_{i+\mu,j+l}^x + i \sum_{v=0}^{l-1} \theta_{i,j+v}^y \right) \psi_{i+k,j+l}, \quad (2.14)
\]

\[
\left( \hat{T}_y^M \right)^{l} \left( \hat{T}_x^M \right)^{k} \psi_{i,j} = \left( \hat{T}_y^M \right)^{l} \exp \left( i \sum_{\mu=0}^{k-1} \theta_{i+\mu,j}^x \right) \psi_{i,j} \]

\[
= \exp \left( i \sum_{v=0}^{l-1} \theta_{i+k,j+v}^y + i \sum_{\mu=0}^{k-1} \theta_{i+\mu,j}^x \right) \psi_{i+k,j+l}. \quad (2.15)
\]

Hence, the phase acquired by the single-particle state \( \psi_{i,j} \) which was translated along the borders of the super-cell by acting on it with the MTOs is simply given by the sum of the corresponding phase terms \( \theta_{m,n}^i \) along the borders of the super-cell. This sum can be decomposed in \( k \cdot l \) lattice unit cells, for which the phase term was determined in Eq. (2.13), and one obtains

\[
e^{-i\Phi} \left( \hat{T}_x^M \right)^{k} \left( \hat{T}_y^M \right)^{l} = \left( \hat{T}_y^M \right)^{l} \left( \hat{T}_x^M \right)^{k}, \quad (2.16)
\]

as illustrated in Fig. 2.3c. For rational values of \( \alpha = p/q \) \( (p, q \in \mathbb{Z}) \) the commutator vanishes if

\[
k\ell \Phi = 2\pi p \frac{k\ell}{q} = 2\pi \times \nu, \quad \nu \in \mathbb{Z}. \quad (2.17)
\]
The smallest possible super-cell for which \([\hat{T}_x^M, (\hat{T}_y^M)^\dagger] = 0\) is given by \(kl = q\) and is called magnetic unit cell. The area of the magnetic unit cell \(A_{MU}\) is \(q\) times larger than the area of the normal lattice unit cell and contains \(q\) sites. The new operators \((\hat{T}_x^M)^k \equiv \hat{M}_x^k\) and \((\hat{T}_y^M)^l \equiv \hat{M}_y^l\) together with \(\hat{H}\) (2.6) form a complete set of commuting operators such that one can find simultaneous eigenstates \(\Psi_{m,n}\) by formulating a generalized Bloch theorem based on the magnetic translation symmetries:

\[
\hat{M}_x^k \Psi_{m,n} = e^{i\mu_{m,n}} \Psi_{m+k,n} = e^{ik_x ka} \Psi_{m,n},
\]

\[
\hat{M}_y^l \Psi_{m,n} = e^{i\mu_{m,n}} \Psi_{m,n+l} = e^{ik_y la} \Psi_{m,n}. \tag{2.18}
\]

with \(kl = q\), \(a\) the lattice constant and \(k = (k_x, k_y)\) defined within the first magnetic Brillouin zone (FBZ): \(-\pi/(ka) \leq k_x < \pi/(ka), -\pi/(la) \leq k_y < \pi/(la)\). An explicit form of the eigenstates will be derived in the following section for \(\alpha = 1/4\). Note that the area of the magnetic unit cell is fixed by the strength of the magnetic flux \(\alpha = p/q\), its dimensions, however, are not.

### 2.2.2 Magnetic Translation Operators for \(\alpha = 1/4\)

In this section the MTOs for \(\alpha = 1/4\) are introduced. According to Eq. (2.17) the magnetic unit cell consists of four lattice unit cells, such that its area is given by \(A_{MU} = 4a^2\). For this value of the flux there are three different possibilities to choose its dimensions (Fig. 2.4). The specific form of the MTOs is gauge dependent, therefore the following example is carried out choosing the Landau gauge \(\phi_{m,n} = (-2\pi \alpha n, 0)\).

The non-commuting magnetic translation operators in this gauge are
\[
\hat{T}_x^M = \sum_{m,n} \hat{a}_{m+1,n}^\dagger \hat{a}_{m,n} , \quad \hat{T}_y^M = \sum_{m,n} \hat{a}_{m,n+1}^\dagger \hat{a}_{m,n} e^{-i2\pi am} , \quad (2.19)
\]

and the commuting ones are given by

\[
\hat{M}_x^k = \sum_{m,n} \hat{a}_{m+k,n}^\dagger \hat{a}_{m,n} , \quad \hat{M}_y^l = \sum_{m,n} \hat{a}_{m,n+l}^\dagger \hat{a}_{m,n} e^{-i2\pi aml} , \quad (2.20)
\]

with \(kl = 4\). In the following explicit forms of the eigenfunctions for the different choices of the magnetic unit cell are determined.

**Rectangular magnetic unit cell oriented along y (Fig. 2.4a):** In the literature this is the most common choice for the magnetic unit cell in the Landau gauge because the MTOs take the form of usual lattice translation operators

\[
\hat{M}_x^1 = \sum_{m,n} \hat{a}_{m+1,n}^\dagger \hat{a}_{m,n} , \quad \hat{M}_y^4 = \sum_{m,n} \hat{a}_{m,n+4}^\dagger \hat{a}_{m,n} , \quad (2.21)
\]

and the eigenfunctions satisfying the generalized Bloch’s theorem in Eq. (2.18) can be written in the following form

\[
\Psi_{m,n} = e^{ik_x a} e^{ik_y n} \psi_n , \quad \psi_{n+4} = \psi_n , \quad (2.22)
\]

where \(\Psi_{m,n}\) is expanded in single-particle on-site wave functions; \(\psi_i, i = \{0, 1, 2, 3\}\), is the complex amplitude of the wave function on the four sites of the magnetic unit cell and \(k\) is defined within the FBZ: \(-\pi/a \leq k_x < \pi/a, -\pi/(4a) \leq k_y < \pi/(4a)\).

One can verify that this ansatz fulfills the generalized form of Bloch’s theorem (2.18)

\[
\hat{M}_x^1 \Psi_{m,n} = \Psi_{m+1,n} = e^{ik_x a} \Psi_{m,n} , \quad \hat{M}_y^4 \Psi_{m,n} = \Psi_{m,n+4} = e^{4ik_y a} \Psi_{m,n} . \quad (2.23)
\]

**Symmetric magnetic unit cell (Fig. 2.4b):** For the square symmetric magnetic unit cell the MTO along \(y\) is slightly more complicated. It is a combination of a usual translation by two lattice sites and an additional phase factor,

\[
\hat{M}_x^2 = \sum_{m,n} \hat{a}_{m+2,n}^\dagger \hat{a}_{m,n} , \quad \hat{M}_y^2 = \sum_{m,n} \hat{a}_{m,n+2}^\dagger \hat{a}_{m,n} e^{-i\pi m} . \quad (2.24)
\]

In this case the wave function has to fulfill the following relations

\[
\hat{M}_x^2 \Psi_{m,n} = \Psi_{m+2,n} = e^{2ik_x a} \Psi_{m,n} , \quad \hat{M}_y^2 \Psi_{m,n} = e^{-i\pi m} \Psi_{m,n+2} = e^{2ik_y a} \Psi_{m,n} . \quad (2.25)
\]
For $m$ even the eigenfunctions take the usual form Bloch functions; for $m$ odd, however, additional phase terms have to be introduced. The combined solution can be written as

$$\Psi_{m,n} = e^{ik_x m a} e^{ik_y n a} \begin{cases} 
\psi_0, & \text{for } m, n \text{ even} \\
\psi_1 e^{-in\pi/2}, & \text{for } m \text{ odd, } n \text{ even} \\
\psi_2, & \text{for } m \text{ even, } n \text{ odd} \\
\psi_3 e^{-in\pi/2}, & \text{for } m, n \text{ odd}
\end{cases} \quad (2.26)$$

with $k$ defined within the FBZ, $-\pi/(2a) \leq k_x < \pi/(2a)$ and $-\pi/(2a) \leq k_y < \pi/(2a)$.

**Rectangular magnetic unit cell oriented along x (Fig. 2.4c):** The third possible choice is a rectangular magnetic unit cell oriented along $x$, where the corresponding MTOs are

$$\hat{M}_x^4 = \sum_{m,n} \hat{a}_{m+4,n} \hat{a}_{m,n}, \quad \hat{M}_y^1 = \sum_{m,n} \hat{a}_{m,n+1} \hat{a}_{m,n} e^{-i\pi m/2}. \quad (2.27)$$

For this choice of the magnetic unit cell, the translation along $x$ is again of the usual form but the one along $y$ is not. For every site $m$ an additional phase term has to be introduced in $\Psi_{m,n}$ to fulfill Bloch’s theorem (2.18)

$$\hat{M}_x^4 \Psi_{m,n} = \Psi_{m+4,n} = e^{4ik_x a} \Psi_{m,n}, \quad \hat{M}_y^1 \Psi_{m,n} = e^{-i\pi m/2} \Psi_{m,n+1} = e^{ik_y a} \Psi_{m,n}. \quad (2.28)$$

The form of the eigenfunctions involves an additional phase factor that depends on the site index $(m, n)$ and can be written as

$$\Psi_{m,n} = e^{ik_x m a} e^{ik_y n a} e^{i\pi mn/2} \psi_m, \quad \psi_{m+4} = \psi_m. \quad (2.29)$$

where $k$ is defined in the range $-\pi/(4a) \leq k_x < \pi/(4a)$ and $-\pi/a \leq k_y < \pi/a$.

### 2.3 Harper-Hofstadter Hamiltonian

The theoretical description of a lattice Hamiltonian with flux depends on the choice of the gauge since the explicit form of the MTOs depends on the particular form of the vector potential as was shown above. The physical observables investigated in the following (energy spectrum, topological invariants) are gauge independent and one can choose a vector potential where the calculations are particularly simple. As in the previous section the vector potential will be written in the Landau gauge $\phi_{m,n} = (-\Phi n, 0)$, which corresponds to a uniform magnetic field with flux $\Phi = 2\pi \alpha$ per plaquette.
\[ \hat{H} = -J \sum_{m,n} \left( e^{-i\Phi_n} \hat{a}_{m+1,n}^\dagger \hat{a}_{m,n} + \hat{a}_{m,n+1}^\dagger \hat{a}_{m,n} + \text{h.c.} \right) \] \hspace{1cm} (2.30)

In this gauge only tunneling along the \( x \)-direction is complex while tunneling along the \( y \)-direction is real. This Hamiltonian is known as the famous Harper-Hofstadter Hamiltonian [1, 18, 19], whose single-particle energy spectrum exhibits a fractal self-similar structure as a function of the flux \( \alpha \), known as Hofstadter’s butterfly [1].

### 2.3.1 Single-Particle Energy Spectrum

In order to solve the Schrödinger equation first the commuting magnetic translation operators need to be constructed using the MTOs given in Eq. (2.19), which were derived in the same gauge. For rational values of the flux \( \alpha = p/q \) one can always choose a magnetic unit cell oriented along the \( y \)-direction with dimensions \( (1 \times q) \cdot a^2 \) (see also Fig. 2.4a for \( \alpha = 1/4 \)). For this particular choice of the magnetic unit cell the commuting MTOs can be written in the following form,

\[ \hat{M}_x^1 = \sum_{m,n} \hat{a}_{m+1,n}^\dagger \hat{a}_{m,n} \, , \quad \hat{M}_y^q = \sum_{m,n} \hat{a}_{m,n+q} \hat{a}_{m,n} \] \hspace{1cm} (2.31)

Both operators are equivalent to the usual lattice translation operators as defined in Eq. (2.5), where the one along \( x \) corresponds to a translation by one lattice constant and the one along \( y \) by \( q \) lattice constants. The magnetic unit cell contains a flux \( \Phi_{MU} = p \times 2\pi \). In order to solve the Schrödinger equation one can make the following ansatz for the wave function

\[ \psi_{m,n} = e^{ik_x a} e^{ik_y a} \psi_n \, , \quad \psi_{n+q} = \psi_n \] \hspace{1cm} (2.32)

where \( k_x, k_y \) are defined in the range \(-\pi/a \leq k_x < \pi/a \) and \(-\pi/(qa) \leq k_y < \pi/(qa)\). As shown above, this ansatz fulfills the generalized Bloch theorem (2.18)

\[ \hat{M}_x^1 \psi_{m,n} = \psi_{m+1,n} = e^{ik_x a} \psi_{m,n} \, , \quad \hat{M}_y^q \psi_{m,n} = \psi_{m,n+q} = e^{ik_y qa} \psi_{m,n} \] \hspace{1cm} (2.33)

By inserting Eq. (2.32) into the Schrödinger equation associated with the Harper-Hofstadter Hamiltonian (2.30)

\[ E \psi_{m,n} = -J (e^{-i\Phi_n} \psi_{m+1,n} + e^{i\Phi_n} \psi_{m-1,n} + \psi_{m,n+1} + \psi_{m,n-1}) \] \hspace{1cm} (2.34)

one obtains the following simplified equation

\[ E \psi_n = -J \left[ 2 \cos(k_x a - \Phi n) \psi_n + e^{ik_x a} \psi_{n+1} + e^{-ik_x a} \psi_{n-1} \right] \] \hspace{1cm} (2.35)
Consequently, the problem reduces to a \( q \)-dimensional eigenvalue equation

\[
E(k) \begin{pmatrix} \psi_0 \\ \psi_1 \\ \vdots \\ \psi_{q-1} \end{pmatrix} = H(k) \begin{pmatrix} \psi_0 \\ \psi_1 \\ \vdots \\ \psi_{q-1} \end{pmatrix}, \tag{2.36}
\]

where the \( q \times q \) matrix is defined as

\[
H(k) = -J \begin{pmatrix} h_0 & e^{ik_y a} & 0 & \ldots & e^{-ik_y a} \\ e^{-ik_y a} & h_1 & e^{ik_y a} & \ldots & 0 \\ 0 & e^{-ik_y a} & h_2 & \ldots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ e^{ik_y a} & 0 & 0 & \ldots & h_{q-1} \end{pmatrix}, \tag{2.37}
\]

with \( h_q = 2 \cos(k_x a - q\Phi) \). Without magnetic field, or more generally for \( \alpha \in \mathbb{Z} \), one obtains a single energy band with dispersion relation

\[
E(k) = -2J \cos(k_x a) - 2J \cos(k_y a), \tag{2.38}
\]

where the corresponding bandwidth is given by \( E_{bw} = 2 \times 4J \). In the presence of a rational flux per plaquette \( \alpha = p/q \) this band splits into \( q \) subbands (Fig. 2.5) with dispersion relations \( E_\mu(k), \mu = \{1, \ldots, q\} \). This leads to the famous fractal structure of the Hofstadter butterfly which displays the single-particle energy as a function of the magnetic flux \( \alpha \). In Fig. 2.6 two examples of such a spectrum are shown for \( \alpha = 1/5 \) and \( \alpha = 1/6 \), which were computed using Eqs. (2.36) and (2.37).

**Fig. 2.5** Single-particle energy spectrum of an electron in a periodic potential exposed to large magnetic fields, known as Hofstadter’s butterfly. Energy spectrum of the lowest tight-binding band as a function of the flux per unit cell \( \alpha = \Phi/(2\pi) \) displaying a fractal, self-similar structure. The number of energy bands depends crucially on the value of the flux per lattice unit cell. (Data taken from Ref. [1])
Fig. 2.6 Single-particle energy spectrum and Chern number distribution of the Hofstadter model for $\alpha = 1/5$ (a) and $\alpha = 1/6$ (b). For $\alpha = 1/5$ the spectrum splits into five subbands, while for $\alpha = 1/6$ it splits into six. The Hamiltonian is particle-hole symmetric, which manifests itself in certain symmetries between the dispersion relations of the individual subbands (Sect. 2.3.2). It further leads to a symmetric Chern number distribution around $E = 0$.

For irrational values of the flux the spectrum splits into an infinite number of energy levels forming a Cantor set [1]. Similar spectra were further computed for graphene-type lattices [20, 21]. The nature of the single-particle energy spectrum is determined by rational and irrational values of $\alpha$ respectively. In a Penrose lattice two kinds of elementary tilings may exist such that one of them is pierced by a rational flux $\alpha$ while the second one is pierced by an irrational one. It has been shown that such a configuration can lead to interesting electronic properties and the spectrum is butterfly-like with a periodicity that is characteristic of the underlying quasicrystal [22].

### 2.3.2 Particle-Hole Symmetry

An important property of the Hofstadter model is the particle-hole symmetry, which gives rise to certain symmetries in the energy spectrum and the Chern number distribution of the energy bands (Sect. 2.4). Let us consider the following transformation

$$\Psi_{m,n} \rightarrow \tilde{\Psi}_{m,n} = (-1)^{m+n} \Psi_{m,n}.$$  \hspace{1cm} (2.39)

The new wave function $\tilde{\Psi}_{m,n}$ satisfies the Harper equation (2.34)

$$-E\tilde{\Psi}_{m,n} = -J(e^{-i\Phi_n} \tilde{\Psi}_{m+1,n} + e^{i\Phi_n} \tilde{\Psi}_{m-1,n} + \tilde{\Psi}_{m,n+1} + \tilde{\Psi}_{m,n-1}),$$ \hspace{1cm} (2.40)

which is similar to Eq. (2.34) but with different energy $E \rightarrow -E$. This means that if there exists a state $\Psi_{m,n}$ with energy $E$ there necessarily also exists a state $\tilde{\Psi}_{m,n}$.
with opposite energy $-E$. This result illustrates the particle-hole symmetry present in the system. The state can be also written in the following way

$$\tilde{\Psi}_{m,n} = e^{ik_x ma} e^{ik_y na} \tilde{\psi}_n, \quad \tilde{\psi}_{n+q} = \tilde{\psi}_n.$$  \quad (2.41)

Inserting this state into Eq. (2.40) leads to an eigenvalue equation for the new periodic function $\tilde{\psi}_n$, which can be written as follows

$$E \tilde{\psi}_n = -J \left[ 2 \cos (k_x a + \pi - \Phi n) \tilde{\psi}_n + e^{i(k_x a + \pi)} \tilde{\psi}_{n+1} + e^{-i(k_x a + \pi)} \tilde{\psi}_{n-1} \right].$$  \quad (2.42)

Comparing this result with Eq. (2.35) shows that the eigenstate associated with the band $E(k)$ located at positive energies is related to the state in the lower band at negative energies through the relation

$$\psi_n(k_x, k_y) = \tilde{\psi}_n(k_x + \pi/a, k_y + \pi/a).$$  \quad (2.43)

Consequently the particle-hole transformation (2.39) maps a state at energy $+E$ to a state at energy $-E$. Additionally this transformation corresponds to a shift in momentum space $(k_x, k_y) \to (k_x + \pi/a, k_y + \pi/a)$. Hence, the dispersion relation of a band $\mu$ which is located around a mean energy $\bar{E}_\mu > 0$ is related to the dispersion relation of a band $\tilde{\mu}$ located around a mean value $\bar{E}_{\tilde{\mu}} < 0$ according to

$$E_\mu(k_x, k_y) = -E_{\tilde{\mu}}(k_x + \pi/a, k_y + \pi/a).$$  \quad (2.44)

In addition the particle-hole symmetry has important consequences for the Chern number distribution as will be discussed in the following section.

### 2.4 Chern Number

The topology of an energy band is robust against continuous deformations of the underlying Hamiltonian and is characterized by topological invariants. These topological properties can have important physical consequences. It has been shown that the quantization of the Hall conductance discovered by Klaus von Klitzing et al. in 1980 [23] is directly related to an integer topological invariant known as the Chern number [24].

In solid-state experiments the quantization of the Hall conductance $\sigma_H$ is observed by sending a constant current through the sample and measuring the voltage difference in the transverse direction. At low temperatures all energy bands below the Fermi energy $E_F$ are filled. If the Fermi energy lies within a spectral gap the Hall conductance is determined by
\[ \sigma_H = \frac{e^2}{h} \sum_{E_\mu < E_F} v_\mu, \quad (2.45) \]

where \( v_\mu \) is the Chern number of the \( \mu \)th band \( E_\mu \) and the sum runs over all occupied bands below the Fermi energy \( E_F < E_F \).

A QH device is insulating in the bulk if the Fermi energy is located in an energy gap and the value of the Hall conductivity is determined by the number of gapless chiral edge states, that are contributing to the current. The existence of these modes can be seen as a manifestation of the topological order of the bulk. The connection between the topological properties of the bulk energy bands and the quantization of the Hall conductance was first identified in the work by Thouless, Kohmoto, Nightingale, den Nijs [24]. The corresponding topological invariant, the Chern number of the \( \mu \)th energy band can be expressed in terms of the periodic eigenfunctions \( \langle u_\mu(k) \rangle \), which are solutions of the eigenvalue equation (2.36) given above,

\[
v_\mu = \frac{i}{2\pi} \int_{FBZ} \frac{1}{\Omega_\mu(k)} \left( \frac{\partial u_\mu(k)}{\partial k_x} \frac{\partial u_\mu(k)}{\partial k_y} - \frac{\partial u_\mu(k)}{\partial k_y} \frac{\partial u_\mu(k)}{\partial k_x} \right) d^2k, \quad (2.46)
\]

where \( \Omega_\mu(k) \) is known as the Berry curvature of the \( \mu \)th band [25] and the integral is carried out over the first magnetic Brillouin zone. This invariant was derived for an infinite system without edges. Using this expression the topological role of the edge states is not yet clear. The relation between the topological properties of the edge modes and the bulk is commonly denoted as bulk-edge correspondence [26–28]. In particular, it was shown by Hatsugai, that the topology of the edge states is characterized by an integer, which is equal to the bulk topological invariant [26, 27].

In Chap. 8 we are going to present an experimental observation of the Chern number of the lowest Hofstadter band for \( \alpha = 1/4 \) with bosonic atoms [29]. In these measurements the topological properties of the bulk were probed through measurements of the anomalous Hall velocity, which occurs transverse to an applied force and is proportional to the Berry curvature defined above [25].

### 2.4.1 Distribution in the Hofstadter Model

The particle-hole symmetry (Sect. 2.3.2) inherent to the Hofstadter model has important consequences on the Chern number distribution \( v_\mu \) of the Hofstadter bands. Taking into account the symmetry properties of the wave-function amplitudes \( \psi_n \) in equation (2.43) leads to an equivalent relation for the eigenfunctions

\[
|u_\mu(k_x, k_y)\rangle = |u_\tilde{\mu}(k_x + \pi/a, k_y + \pi/a)\rangle.
\]

(2.47)
As a consequence the Berry curvature of the $\mu$th band is related the Berry curvature of the opposite band $\tilde{\mu}$ according to

$$\Omega_\mu(k_x, k_y) = \Omega_{\tilde{\mu}}(k_x + \pi/a, k_y + \pi/a). \quad (2.48)$$

Hence, both bands share the same Berry curvature shifted in momentum space by $(\delta k_x, \delta k_y) = (\pi/a, \pi/a)$. The characteristic Chern number $\nu_\mu$ of the band defined in Eq. (2.46) is obtained by integrating the Berry curvature over the first magnetic Brillouin zone. As a result the two bands share the same Chern number $\nu_\mu = \nu_{\tilde{\mu}}$ and the distribution is symmetric around $E = 0$ (Fig. 2.6). Note, that the Chern number of the total tight-binding band necessarily vanishes, i.e.

$$\sum_\mu \nu_\mu = 0. \quad (2.49)$$

### 2.4.2 Diophantine Equation

It has been shown that the fractal structure of the Hofstadter butterfly follows a simple relation, which allows for an analytical computation of the Chern number. For a rational flux $\alpha = p/q$ the energy gaps are characterized by two integers $s_r$ and $t_r$, which are determined by a Diophantine equation [30, 31]

$$r = qs_r + pt_r, \quad |t_r| \leq \frac{q}{2}, \quad s_r, t_r \in \mathbb{Z}, \quad (2.50)$$

where $r$ denotes the $r$th energy gap of the Hofstadter spectrum. Since the spectrum is split into $q$-subbands, $r$ can only take values in the interval $0 \leq r \leq q$. The solutions of equation Eq. (2.50) are uniquely defined and the two numbers $s_r, t_r$ are topological numbers characterizing the gap, where the integer $t_r$ determines the value of the Hall conductivity [24, 32, 33] according to

$$\sigma_H = -\frac{e^2}{h} t_r. \quad (2.51)$$

Thus, $t_r$ is given by the sum of the Chern numbers $\sum_{1}^{r} \nu_r$ of all occupied bands and the $r$th band, which lies between the $r$th and the $(r-1)$st energy gap, carries an integral Hall conductance determined by the Chern number of the $r$th band $\nu_r$ which is a solution of the following Diophantine equation

$$-1 = q(s_{r-1} - s_r) + p(t_{r-1} - t_r) = q\sigma_r + p\nu_r, \quad \sigma_r \in \mathbb{Z}. \quad (2.52)$$

For generic values of the flux with $p = 1$ one can show that the bands with $r < q/2$ exhibit a Chern number $\nu_r = -1$. 
For \( r \) even, the middle two bands touch at \( q \) Dirac cones (Fig. 2.6b) and the Diophantine equation above can only predict the sum of the two Chern numbers \( \nu_r = q - 2 \). For \( r \) odd, the middle band carries a Chern number \( \nu_r = q - 1 \). These analytical results are in agreement with the numerical calculations depicted in Fig. 2.6.

A Chern number of the lowest band larger than one \( |\nu_1| > 1 \) can be achieved e.g. with a flux \( \alpha = 4/9 \), where the Chern number of the lowest band is \( \nu_1 = 2 \).

### 2.4.3 Numerical Calculation of the Chern Number

An efficient way to calculate the Berry curvature and the Chern number of non-degenerate bands was proposed by Fukui et al. [34] and will be briefly reviewed here. For the sake of simplicity the band index \( \mu \) is omitted in the following discussion. The fundamental idea is to compute the Berry curvature numerically by discretizing the Brillouin zone using a grid in momentum space defined according to

\[
\mathbf{k}_\alpha = (k_x, k_y), \quad k_x = \frac{2\pi\alpha_1}{N_1}, \quad (\alpha_1 = 0, \ldots, N_1 - 1),
\]

\[
k_y = \frac{2\pi\alpha_2}{qN_2}, \quad (\alpha_2 = 0, \ldots, N_2 - 1),
\]

(2.53)

where \( \alpha = (1, \ldots, N_1 N_2) \) and \( N_1, N_2 \) define the size of the unit cell of the grid. The unit vectors of the grid in momentum space along the two directions are

\[
\hat{e}_1 = \frac{2\pi}{N_1} (1, 0), \quad \hat{e}_2 = \frac{2\pi}{qN_2} (0, 1).
\]

(2.54)

Using this notation the discrete distribution of the Berry curvature \( \tilde{\Omega}_{12}(\mathbf{k}_\alpha) \) in the FBZ is determined by

\[
\tilde{\Omega}_{12}(\mathbf{k}_\alpha) \equiv \ln \mathcal{U}_1(\mathbf{k}_\alpha) \mathcal{U}_2(\mathbf{k}_\alpha + \hat{e}_1) \mathcal{U}_1(\mathbf{k}_\alpha + \hat{e}_2)^{-1} \mathcal{U}_2(\mathbf{k}_\alpha)^{-1},
\]

(2.55)

where \( \mathcal{U}_{1,2} \) is defined as the link variable

\[
\mathcal{U}_1(\mathbf{k}_\alpha) = \frac{\langle \mathbf{u}(\mathbf{k}_\alpha) | \mathbf{u}(\mathbf{k}_\alpha + \hat{e}_1) \rangle}{\langle \mathbf{u}(\mathbf{k}_\alpha + \hat{e}_1) | \mathbf{u}(\mathbf{k}_\alpha) \rangle}, \quad \mathcal{U}_2(\mathbf{k}_\alpha) = \frac{\langle \mathbf{u}(\mathbf{k}_\alpha) | \mathbf{u}(\mathbf{k}_\alpha + \hat{e}_2) \rangle}{\langle \mathbf{u}(\mathbf{k}_\alpha + \hat{e}_2) | \mathbf{u}(\mathbf{k}_\alpha) \rangle}.
\]

(2.56)

From this distribution the Chern number can be simply computed by taking the sum over all possible momenta \( \mathbf{k}_\alpha \)

\[
\bar{\nu} = \frac{1}{2\pi i} \sum_\alpha \tilde{\Omega}_{12}(\mathbf{k}_\alpha).
\]

(2.57)
The numerical determination of the Chern number using the above equations is accurate already for very coarse grids as demonstrated in Ref. [34]. The Chern numbers of the different bands illustrated in Fig. 2.6 were evaluated using this method.

The Case of Band Touching Points

For bands that are not well separated as it is the case for the two middle bands in Fig. 2.6b the method described above cannot be applied directly but it can be generalized as shown in Ref. [34]. Assuming that there are M touching bands $E_1(k), E_2(k), \ldots, E_M(k)$, the link variables can be substituted by determinants of $M \times M$ matrices associated with the multiplet $\psi = (|u_1\rangle, |u_2\rangle, \ldots, |u_M\rangle)$

$$\tilde{U}_\gamma(k_\alpha) = \frac{\det U_\gamma(k_\alpha)}{\left|\det U_\gamma(k_\alpha)\right|}, \quad \gamma = \{1, 2\}. \quad (2.58)$$

The $M$-dimensional matrices $U_\gamma(k_\alpha)$ are defined as

$$U_\gamma(k_\alpha) = \begin{pmatrix}
\langle u_1(k_\alpha) | u_1(k_\alpha + \hat{e}_\gamma) \rangle & \cdots & \langle u_1(k_\alpha) | u_M(k_\alpha + \hat{e}_\gamma) \rangle \\
\vdots & \ddots & \vdots \\
\langle u_M(k_\alpha) | u_1(k_\alpha + \hat{e}_\gamma) \rangle & \cdots & \langle u_M(k_\alpha) | u_M(k_\alpha + \hat{e}_\gamma) \rangle
\end{pmatrix}. \quad (2.59)$$

The corresponding field strength and Chern number of the multiband is defined according to Eqs. (2.55) and (2.57). The Chern number of the middle band in Fig. 2.6b was evaluated for $\alpha = 1/6$ using this technique. The result is in agreement with the analytical solution obtained using the Diophantine equation given in the previous section: $\nu_3 + \nu_4 = q - 2 = 4$.

References

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