Chapter 2
Berry Phase, Chern Number

To describe the theory of topological band insulators we will use the language of adiabatic phases. In this chapter we review the basic concepts: the Berry phase, the Berry curvature, and the Chern number. We further describe the relation between the Berry phase and adiabatic dynamics in quantum mechanics. Finally, we illustrate these concepts using a two-level system as a simple example.

For pedagogical introductions, we refer the reader to Berry's original paper [6], and papers from the American Journal of Physics [14, 18]. For the application to solid state physics, we will mostly build on Resta's lecture note [26], and the review paper [36].

2.1 Discrete Case

The subject of adiabatic phases is strongly related to adiabatic quantum dynamics, when a Hamiltonian is slowly changed in time, and the time evolution of the quantum state follows the instantaneous eigenstate of the Hamiltonian. In that context, as time is a continuous variable and the time-dependent Schrödinger equation is a differential equation, the adiabatic phase and the related concepts are expressed using differential operators and integrals. We will arrive to that point later during this chapter; however, we start the discussion using the language of discrete quantum states. Besides the conceptual simplicity, this language also offers an efficient tool for the numerical evaluation of the Chern number, which is an important topological invariant for two-dimensional electron systems.

J.K. Asbóth et al., *A Short Course on Topological Insulators*, Lecture Notes in Physics 919, DOI 10.1007/978-3-319-25607-8_2

2.1.1 Relative Phase of Two Nonorthogonal Quantum States

In quantum mechanics, the state of a physical system is represented by an equivalence class of vectors in a Hilbert space: a multiplication by a complex phase factor does not change the physical content. A gauge transformation is precisely such a multiplication:

$$|\Psi\rangle \to e^{i\alpha} |\Psi\rangle , \quad \text{with } \alpha \in [0, 2\pi). \tag{2.1}$$

In that sense, the phase of a vector $|\Psi\rangle$ does not represent physical information. We can try to define the relative phase γ_{12} of two nonorthogonal states $|\Psi_1\rangle$ and $|\Psi_2\rangle$ as

$$\gamma_{12} = -\arg \langle \Psi_1 \mid \Psi_2 \rangle , \tag{2.2}$$

where $\arg(z)$ denotes the phase of the complex number z, with the specification that $\arg(z) \in (-\pi, \pi]$. Clearly, the relative phase γ_{12} fulfils

$$e^{-i\gamma_{12}} = \frac{\langle \Psi_1 \mid \Psi_2 \rangle}{|\langle \Psi_1 \mid \Psi_2 \rangle|}. \tag{2.3}$$

However, the relative phase is not invariant under a local gauge transformation,

$$\left|\Psi_j\right\rangle \to e^{i\alpha_j} \left|\Psi_j\right\rangle \qquad\qquad e^{-i\gamma_{12}} \to e^{-i\gamma_{12}+i(\alpha_2-\alpha_1)}. \tag{2.4}$$

2.1.2 Berry Phase

Take $N \geq 3$ states in a Hilbert space, order them in a loop, and ask about the phase around the loop. As we show below, the answer—the *Berry phase*—is gauge invariant. For states $\left|\Psi_j\right\rangle$, with $j = 1, 2, \ldots, N$, and for the ordered list $L = (1, 2, \ldots, N)$ which define the loop, shown in Fig. 2.1, the Berry phase is defined as

$$\gamma_L = -\arg e^{-i(\gamma_{12}+\gamma_{23}+\ldots+\gamma_{N1})} = -\arg \left(\langle \Psi_1 \mid \Psi_2 \rangle \langle \Psi_2 \mid \Psi_3 \rangle \ldots \langle \Psi_N \mid \Psi_1 \rangle\right). \tag{2.5}$$

To show the gauge invariance of the Berry phase, it can be rewritten as

$$\gamma_L = -\arg \mathrm{Tr} \left(|\Psi_1\rangle \langle \Psi_1| \, |\Psi_2\rangle \langle \Psi_2| \ldots |\Psi_N\rangle \langle \Psi_N|\right). \tag{2.6}$$

Here, we expressed the Berry phase γ_L using projectors that are themselves gauge invariant.

Even though the Berry phase is not the expectation value of some operator, it is a gauge invariant quantity, and as such, it can have a direct physical significance. We will find such a significance, but first, we want to gain more intuition about its behaviour.

2.1.3 Berry Flux

Consider a Hilbert space of quantum states, and a finite two-dimensional square lattice with points labelled by $n, m \in \mathbb{Z}$, $1 \leq n \leq N$, and $1 \leq m \leq M$. Assign a quantum state $|\Psi_{n,m}\rangle$ from the Hilbert space to each lattice site. Say you want to know the Berry phase of the loop L around this set,

$$\gamma_L = -\arg\exp\Bigg[-i\Bigg(\sum_{n=1}^{N-1}\gamma_{(n,1),(n+1,1)} + \sum_{m=1}^{M-1}\gamma_{(N,m),(N,m+1)} + \sum_{n=1}^{N-1}\gamma_{(n+1,M),(n,M)} + \sum_{m=1}^{M-1}\gamma_{(1,m+1),(1,m)}\Bigg)\Bigg] \tag{2.7}$$

as shown in Fig. 2.1. Although the Berry phase is a gauge invariant quantity, calculating it according to the recipe above involves multiplying together many gauge dependent complex numbers. The alternative route, via Eq. (2.6), involves multiplying gauge independent matrices, and then taking the trace.

There is a way to break the calculation of the Berry phase of the loop down to a product of gauge independent complex numbers. To each plaquette (elementary square) on the grid, with n, m indexing the lower left corner, we define the

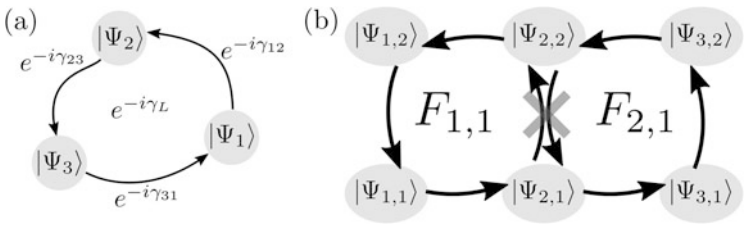

Fig. 2.1 Berry phase, Berry flux and Berry curvature for discrete quantum states. (**a**) The Berry phase γ_L for the loop L consisting of $N = 3$ states is defined from the relative phases γ_{12}, γ_{23}, γ_{31}. (**b**) The Berry phase of a loop defined on a lattice of states can be expressed as the sum of the Berry phases $F_{1,1}$ and $F_{2,1}$ of the plaquettes enclosed by the loop. The plaquette Berry phase $F_{n,m}$ is also called Berry flux

Berry flux $F_{n,m}$ of the plaquette using the sum of the relative phases around its boundary,

$$F_{nm} = -\arg\exp\left[-i\left(\gamma_{(n,m),(n+1,m)} + \gamma_{(n+1,m),(n+1,m+1)} + \gamma_{(n+1,m+1),(n,m+1)} + \gamma_{(n,m+1),(n,m)}\right)\right], \tag{2.8}$$

for $n = 1, \ldots, N$ and $m = 1, \ldots, M$. Note that the Berry flux is itself a Berry phase and is therefore gauge invariant. Alternatively, we can also write

$$F_{nm} = -\arg\left(\langle\Psi_{n,m} \mid \Psi_{n+1,m}\rangle \langle\Psi_{n+1,m} \mid \Psi_{n+1,m+1}\rangle \langle\Psi_{n+1,m+1} \mid \Psi_{n,m+1}\rangle \langle\Psi_{n,m+1} \mid \Psi_{n,m}\rangle\right), \tag{2.9}$$

Now consider the product of all plaquette phase factors $e^{-iF_{nm}}$,

$$\prod_{n=1}^{N-1}\prod_{m=1}^{M-1} e^{-iF_{nm}} = \exp\left[-i\sum_{n=1}^{N-1}\sum_{m=1}^{M-1} F_{nm}\right] = \exp\left[-i\sum_{n=1}^{N-1}\sum_{m=1}^{M-1}\left(\gamma_{(n,m),(n+1,m)} + \gamma_{(n+1,m),(n+1,m+1)} + \gamma_{(n+1,m+1),(n,m+1)} + \gamma_{(n,m+1),(n,m)}\right)\right] \tag{2.10}$$

Each internal edge of the lattice is shared between two plaquettes, and therefore occurs twice in the product. However, since we fixed the orientation of the plaquette phases, these two contributions will always be complex conjugates of each other, and cancel each other. Therefore the exponent in the right-hand-side of Eq. (2.10) simplifies to the exponent appearing in Eq. (2.7), implying

$$\exp\left[-i\sum_{n=1}^{N-1}\sum_{m=1}^{M-1} F_{nm}\right] = e^{-i\gamma_L}. \tag{2.11}$$

This result is reminiscent of the Stokes theorem connecting the integral of the curl of a vector field on an open surface and the line integral of the vector field along the boundary of the surface. In Eq. (2.11), the sum of the relative phases, i.e., the Berry phase γ_L, plays the role of the line integral, whereas the double sum of the Berry fluxes plays the role of the surface integral. There is an important difference with respect to the Stokes theorem, namely, the equality of the total Berry flux and the Berry phase is not guaranteed: Eq. (2.11) only tells that they are either equal or have a difference of 2π times an integer.

2.1.4 Chern Number

Consider states in a Hilbert space arranged on a grid as above, $|\Psi_{n,m}\rangle$, with $n, m \in \mathbb{Z}$, $1 \leq n \leq N$, and $1 \leq m \leq M$, but now imagine this grid to be on the surface of a torus. We use the same definition for the Berry flux per plaquette as in (2.9), but now with $n \bmod N + 1$ in place of $n + 1$ and $m \bmod M + 1$ in place of $m + 1$.

The product of the Berry flux phase factors of all plaquettes is now 1,

$$\prod_{m=1}^{M} \prod_{n=1}^{N} e^{-iF_{nm}} = 1. \tag{2.12}$$

The same derivation can be applied as for Eq. (2.11) above, but now every edge is an internal edge, and so all contributions to the product cancel.

The Chern number Q associated to our structure is defined via the sum of the Berry fluxes of all the plaquettes forming the closed torus surface:

$$Q = \frac{1}{2\pi} \sum_{nm} F_{nm}. \tag{2.13}$$

The fact that the Chern number Q is defined via the gauge invariant Berry fluxes ensures that Q itself is gauge invariant. Furthermore, taking the arg of Eq. (2.12) proves that the Chern number Q is an integer.

It is worthwhile to look a little deeper into the discrete formula for the Chern number. We can define modified Berry fluxes $\tilde{F}_{nm}$ as

$$\tilde{F}_{nm} = \gamma_{(n,m),(n+1,m)} + \gamma_{(n+1,m),(n+1,m+1)} + \gamma_{(n+1,m+1),(n,m+1)} + \gamma_{(n,m+1),(n,m)}. \tag{2.14}$$

Since each edge is shared between two neighboring plaquettes, the sum of the modified Berry fluxes over all plaquettes vanishes,

$$\sum_{m=1}^{M} \sum_{n=1}^{N} \tilde{F}_{nm} = 0. \tag{2.15}$$

If $-\pi \leq \tilde{F}_{nm} < \pi$, then we have $\tilde{F}_{nm} = F_{nm}$. However, $\tilde{F}_{nm}$ can be outside the range $[-\pi, \pi)$: then as the logarithm is taken in Eq. (2.8), F_{nm} is taken back into $[-\pi, \pi)$ by adding a (positive or negative) integer multiple of 2π. In that case, we say the plaquette nm contains a number $Q_{nm} \in \mathbb{Z}$ of vortices, with

$$Q_{nm} = \frac{F_{nm} - \tilde{F}_{nm}}{2\pi} \in \mathbb{Z}. \tag{2.16}$$

We have found a simple picture for the Chern number: *The Chern number Q, that is, the sum of the Berry fluxes of all the plaquettes of a closed surface, is the number of vortices on the surface*,

$$Q = \frac{1}{2\pi} \sum_{nm} F_{nm} = \sum_{nm} Q_{nm} \in \mathbb{Z}. \tag{2.17}$$

Although we proved it here for the special case of a torus, the derivation is easily generalized to all orientable closed surfaces. We focused on the torus, because this construction can be used as a very efficient numerical recipe to discretize and calculate the (continuum) Chern number of a 2-dimensional insulator [12], to be defined in Sect. 2.2.4.

2.2 Continuum Case

We now assume that instead of a discrete set of states, $\{|\Psi_j\rangle\}$, we have a continuum, $|\Psi(\mathbf{R})\rangle$, where the $\mathbf{R}$'s are elements of some D-dimensional parameter space $\mathscr{P}$.

2.2.1 Berry Connection

We take a smooth directed path $\mathscr{C}$, i.e., a *curve* in the parameter space $\mathscr{P}$,

$$\mathscr{C} : [0, 1) \to \mathscr{P}, \quad t \mapsto \mathbf{R}(t). \tag{2.18}$$

We assume that all components of $|\Psi(\mathbf{R})\rangle$ are smooth, at least in an open neighborhood of the curve $\mathscr{C}$. The relative phase between two neighbouring states on the curve $\mathscr{C}$, corresponding to the parameters $\mathbf{R}$ and $\mathbf{R} + d\mathbf{R}$, is

$$e^{-i\Delta\gamma} = \frac{\langle \Psi(\mathbf{R}) \mid \Psi(\mathbf{R} + d\mathbf{R})\rangle}{|\langle \Psi(\mathbf{R}) \mid \Psi(\mathbf{R} + d\mathbf{R})\rangle|}; \quad \Delta\gamma = i \langle \Psi(\mathbf{R})| \nabla_{\mathbf{R}} |\Psi(\mathbf{R})\rangle \cdot d\mathbf{R}, \tag{2.19}$$

obtained to first order in $d\mathbf{R} \to 0$. The quantity multiplying $d\mathbf{R}$ on the right-hand side defines the *Berry connection*,

$$\mathbf{A}(\mathbf{R}) = i \langle \Psi(\mathbf{R}) \mid \nabla_{\mathbf{R}} \Psi(\mathbf{R})\rangle = -\mathrm{Im}\ \langle \Psi(\mathbf{R}) \mid \nabla_{\mathbf{R}} \Psi(\mathbf{R})\rangle\,. \tag{2.20}$$

Here $|\nabla_{\mathbf{R}} \Psi(\mathbf{R})\rangle$ is defined by requiring for every Hilbert space vector $|\Phi\rangle$, that

$$\langle \Phi \mid \nabla_{\mathbf{R}} \Psi(\mathbf{R})\rangle = \nabla_{\mathbf{R}} \langle \Phi \mid \Psi(\mathbf{R})\rangle\,. \tag{2.21}$$

The second equality in Eq. (2.20) follows from the conservation of the norm, $\nabla_{\mathbf{R}} \langle \Psi(\mathbf{R}) \mid \Psi(\mathbf{R}) \rangle = 0$.

We have seen in the discrete case that the relative phase of two states is not gauge invariant; neither is the Berry connection. Under a gauge transformation, it changes as

$$|\Psi(\mathbf{R})\rangle \to e^{i\alpha(\mathbf{R})} |\Psi(\mathbf{R})\rangle : \qquad \mathbf{A}(\mathbf{R}) \to \mathbf{A}(\mathbf{R}) - \nabla_{\mathbf{R}} \alpha(\mathbf{R}). \tag{2.22}$$

2.2.2 Berry Phase

Consider a closed directed curve $\mathscr{C}$ in parameter space. The Berry phase along the curve is defined as

$$\gamma(\mathscr{C}) = -\arg \exp \left[-i \oint_{\mathscr{C}} \mathbf{A} \cdot d\mathbf{R} \right] \tag{2.23}$$

The Berry phase of a closed directed curve is gauge invariant, since it can be interpreted as a limiting case of the discrete Berry phase, via Eqs. (2.20), (2.19), and (2.5), and the latter has been shown to be gauge invariant.

2.2.3 Berry Curvature

As in the discrete case above, we would like to express the gauge invariant Berry phase as a surface integral of a gauge invariant quantity. This quantity is the *Berry curvature*. Similarly to the discrete case, we consider a two-dimensional parameter space, and for simplicity denote the parameters as x and y. We take a simply connected region $\mathscr{F}$ in this two-dimensional parameter space, with the oriented boundary curve of this surface denoted by $\partial\mathscr{F}$, and consider the continuum Berry phase corresponding to the boundary.

2.2.3.1 Smoothness of the Manifold of States

Before relating the Berry phase to the Berry curvature, an important note on the manifold $|\Psi(\mathbf{R})\rangle$ of considered states is in order. From now on, we consider a manifold of states, living in our two-dimensional parameter space, that is smooth, in the sense that the map $\mathbf{R} \mapsto |\Psi(\mathbf{R})\rangle \langle\Psi(\mathbf{R})|$ is smooth. Importantly, this condition does not necessarily imply that that the function $\mathbf{R} \mapsto |\Psi(\mathbf{R})\rangle$, also referred to as a *gauge* describing our manifold, is smooth. (For further discussion and examples, see Sect. 2.5.1.) Nevertheless, even if the gauge $\mathbf{R} \mapsto |\Psi(\mathbf{R})\rangle$ is not smooth in a

point $\mathbf{R}_0$ of the parameter space, one can always find an alternative gauge $|\Psi'(\mathbf{R})\rangle$ which is (i) locally smooth, that is, smooth in the point $\mathbf{R}_0$, and (ii) locally generates the same map as $|\Psi(\mathbf{R})\rangle$, that is, for which $|\Psi'(\mathbf{R})\rangle\langle\Psi'(\mathbf{R})| = |\Psi(\mathbf{R})\rangle\langle\Psi(\mathbf{R})|$ in an infinitesimal neighborhood of $\mathbf{R}_0$. Let us formulate an intuitive argument supporting the latter claim using quantum-mechanical perturbation theory. Take the Hamiltonian $\hat{H}(\mathbf{R}) = -|\Psi(\mathbf{R})\rangle\langle\Psi(\mathbf{R})|$, which can be substituted in the infinitesimal neighborhood of $\mathbf{R}_0$ with $\hat{H}(\mathbf{R}_0 + \Delta\mathbf{R}) = \hat{H}(\mathbf{R}_0) + \Delta\mathbf{R}\cdot(\nabla\hat{H})(\mathbf{R}_0)$. According to first-order perturbation theory, the ground state of the latter is given by

$$\left|\Psi'(\mathbf{R}_0 + \Delta\mathbf{R})\right\rangle = |\Psi(\mathbf{R}_0)\rangle - \sum_{n=2}^{D} |\Psi_n(\mathbf{R}_0)\rangle\langle\Psi_n(\mathbf{R}_0)|\,\Delta\mathbf{R}\cdot(\nabla\hat{H})(\mathbf{R}_0)\,|\Psi(\mathbf{R}_0)\rangle\,, \tag{2.24}$$

where the states $|\Psi_n(\mathbf{R}_0)\rangle$ ($n = 2, 3, \ldots, D$), together with $|\Psi(\mathbf{R}_0)\rangle$, form a basis of the Hilbert space. On the one hand, Eq. (2.24) defines a function that is smooth in $\mathbf{R}_0$, hence the condition (i) above is satisfied. On the other hand, as $|\Psi'(\mathbf{R}_0 + \Delta\mathbf{R})\rangle$ is the ground state of $\hat{H}(\mathbf{R}_0 + \Delta\mathbf{R})$, condition (ii) is also satisfied.

2.2.3.2 Berry Phase and Berry Curvature

Now return to our original goal and try to express the Berry phase as a surface integral of a gauge invariant quantity. We start by relating the Berry phase to its discrete counterpart:

$$\oint_{\partial\mathscr{F}} \mathbf{A}\cdot d\mathbf{R} = \lim_{\Delta x,\Delta y\to 0} \gamma_{\partial\mathscr{F}}, \tag{2.25}$$

where we discretize the parameter space using a square grid of steps Δx, Δy, and express the integral as the discrete Berry phase $\gamma_{\partial\mathscr{F}}$ of a loop approximating $\partial\mathscr{F}$, in the limit of an infinitesimally fine grid. Then, from Eq. (2.25) and the Stokes-type theorem in Eq. (2.11), we obtain

$$\exp\left[-i\oint_{\partial\mathscr{F}} \mathbf{A}\cdot d\mathbf{R}\right] = \lim_{\Delta x,\Delta y\to 0} e^{-i\sum_{nm} F_{nm}}, \tag{2.26}$$

where the nm sum goes for the plaquettes forming the open surface $\mathscr{F}$. Furthermore, let us take a gauge $|\Psi'(\mathbf{R})\rangle$ and the corresponding Berry connection $\mathbf{A}'$ that is smooth in the plaquette nm; this could be $|\Psi(\mathbf{R})\rangle$ and $\mathbf{A}$ if that was already smooth. Then, due to the gauge invariance of the Berry flux we have

$$e^{-iF_{nm}} = e^{-iF'_{nm}}, \tag{2.27}$$

where F'_{nm} is the Berry flux corresponding to the locally smooth gauge. Furthermore, in the limit of an infinitely fine grid it holds that

$$F'_{nm} = A'_x\left(x_n + \frac{\Delta x}{2}, y_m\right)\Delta x + A'_y\left(x_{n+1}, y_m + \frac{\Delta y}{2}\right)\Delta y - A'_x\left(x_n + \frac{\Delta x}{2}, y_{m+1}\right)\Delta x - A'_y\left(x_n, y_m + \frac{\Delta y}{2}\right)\Delta y. \tag{2.28}$$

Taylor expansion of the Berry connection around $\mathbf{R}_{nm} = \left(x_n + \frac{\Delta x}{2}, y_n + \frac{\Delta y}{2}\right)$ to first order yields

$$F'_{nm} = \left[\partial_x A'_y(\mathbf{R}_{nm}) - \partial_y A'_x(\mathbf{R}_{nm})\right]\Delta x \Delta y. \tag{2.29}$$

Thereby, with the definition of the *Berry curvature* as

$$B = \lim_{\Delta x, \Delta y \to 0} \frac{F'_{nm}}{\Delta x \Delta y}, \tag{2.30}$$

we obtain a quantity that is gauge invariant, as it is defined via the gauge invariant Berry flux, and is related to the Berry connection via

$$B = \partial_x A'_y(\mathbf{R}_{nm}) - \partial_y A'_x(\mathbf{R}_{nm}). \tag{2.31}$$

We can rephrase Eq. (2.29) as follows: the Berry flux for the *nm* plaquette is expressed as the product of the Berry curvature on the plaquette and the surface area of the plaquette.

Substituting Eqs. (2.27) and (2.29) into Eq. (2.26) yields

$$\exp\left[-i \oint_{\partial \mathscr{F}} \mathbf{A} \cdot d\mathbf{R}\right] = \exp\left[-i \int_{\mathscr{F}} B(x, y) dx dy\right], \tag{2.32}$$

which is the continuum version of the result (2.11). Equation (2.32) can also be rephrased as

$$\gamma(\partial \mathscr{F}) = -\arg e^{-i \int_{\mathscr{F}} B(x,y) dx dy}. \tag{2.33}$$

2.2.3.3 A Special Case Where the Usual Stokes Theorem Works

A shortcut towards a stronger result than Eq. (2.32) is offered in the special case when $|\Psi(\mathbf{R})\rangle$ is smooth on the open surface $\mathscr{F}$. Then, a direct application of the two-dimensional Stokes theorem implies

$$\oint_{\partial \mathscr{F}} \mathbf{A} \cdot d\mathbf{R} = \int_{\mathscr{F}} (\partial_x A_y - \partial_y A_x) dx dy = \int_{\mathscr{F}} B dx dy \tag{2.34}$$

Summarizing Eqs. (2.32) and (2.34), we can say that line integral of the Berry connection equals the surface integral of the Berry curvature if the set of states $|\Psi(\mathbf{R})\rangle$ is smooth on $\mathscr{F}$, but they might differ with an integer multiple of 2π otherwise.

2.2.3.4 The Case of the Three-Dimensional Parameter Space

Let us briefly discuss also the case of a three-dimensional parameter space. This will be particularly useful in the context of two-level systems. Starting with the case when the gauge $|\Psi(\mathbf{R})\rangle$ on the two-dimensional open surface $\mathscr{F}$ embedded in the three-dimensional parameter space is smooth in the neighborhood of $\mathscr{F}$, we can directly apply the three-dimensional Stokes theorem to convert the line integral of $\mathbf{A}$ to the surface integral of the curl of $\mathbf{A}$ to obtain

$$\oint_{\partial\mathscr{F}} \mathbf{A}\cdot d\mathbf{R} = \int_{\mathscr{F}} \mathbf{B}\cdot d\mathbf{S}, \tag{2.35}$$

where the Berry curvature is defined as the vector field $\mathbf{B}(\mathbf{R})$ via

$$\mathbf{B}(\mathbf{R}) = \nabla_{\mathbf{R}} \times \mathbf{A}(\mathbf{R}), \tag{2.36}$$

which is gauge invariant as in the two-dimensional case. Even if $|\Psi(\mathbf{R})\rangle$ is not smooth on $\mathscr{F}$, the relation

$$\gamma(\partial\mathscr{F}) = -\arg e^{-i\oint_{\partial\mathscr{F}} \mathbf{A}\cdot d\mathbf{R}} = -\arg e^{-i\int_{\mathscr{F}} \mathbf{B}\cdot d\mathbf{S}} \tag{2.37}$$

holds, similarly to the two-dimensional result Eq. (2.32).

Note furthermore that the Berry phase $\gamma(\partial\mathscr{F})$ for a fixed boundary curve $\partial\mathscr{F}$ is not only gauge invariant, but also invariant against continuous deformations of the two-dimensional surface $\mathscr{F}$ embedded in three dimensions, as long as the Berry curvature is smooth everywhere along the way.

We also remark that although we used the three-dimensional notation here, but the above results can be generalized for any dimensionality of the parameter space.

The notation $\mathbf{A}$ and $\mathbf{B}$ for the Berry connection and Berry curvature suggest that they are much like the vector potential and the magnetic field. This is a useful analogy, for instance, $\nabla_{\mathbf{R}}\mathbf{B} = 0$, from the definition (2.36). Nevertheless, it is not true that in every problem where the Berry curvature is nonzero, there is a physical magnetic field.

2.2.4 Chern Number

In the discrete case, we defined the Chern number as a sum of Berry fluxes for a square lattice living on a torus (or any other orientable closed surface). Here, we take a continuum parameter space that has the topology of a torus. The motivation is that certain physical parameter spaces in fact have this torus topology, and the corresponding Chern number does have physical significance. One example will be the Brillouin zone of a two-dimensional lattice representing a solid crystalline material, where the momentum vectors (k_x, k_y), $(k_x + 2\pi, ky)$, and $(k_x, k_y + 2\pi)$ are equivalent.

Quite naturally, in the continuum definition of the Chern number, the sum of Berry fluxes is replaced by the surface integral of the Berry curvature over the whole of the parameter space $\mathscr{P}$,

$$Q = -\frac{1}{2\pi}\int_{\mathscr{P}} B dx dy. \tag{2.38}$$

As this can be interpreted as a continuum limit of the discrete Chern number, it inherits the properties of the latter: the continuum Chern number is a gauge invariant integer.

For future reference, let us lay down the notation to be used for calculating the Chern numbers of electronic energy bands in two-dimensional crystals. Consider a square lattice for simplicity, which has a square-shaped Brillouin zone as well. Our parameter space $\mathscr{P}$ is the two-dimensional Brillouin zone now, which has a torus topology as discussed above. The parameters are the Cartesian components $k_x, k_y \in [-\pi, \pi)$ of the momentum vector $\mathbf{k}$. The electronic energy bands and the corresponding electron wavefunctions can be obtained from the bulk momentum-space Hamiltonian $\hat{H}(k_x, k_y)$. The latter defines the Schrödinger equation

$$\hat{H}(\mathbf{k})\,|u_n(\mathbf{k})\rangle = E_n(\mathbf{k})\,|u_n(\mathbf{k})\rangle\,, \tag{2.39}$$

where $n = 1, 2, \ldots$ is the band index, which has as many possible values as the dimension of the Hilbert space of the internal degree of freedom of our lattice model. Note that defining the Berry connection, the Berry curvature and the Chern number for the nth band is possible only if that band is separated from other bands by energy gaps. The Berry connection of the nth band, in line with the general definition (2.20), reads

$$A_j^{(n)}(\mathbf{k}) = i\,\langle u_n(\mathbf{k})|\,\partial_{k_j}\,|u_n(\mathbf{k})\rangle\,, \quad \text{for} \quad j = x, y. \tag{2.40}$$

The Chern number of the nth band, in correspondence with Eqs. (2.38) and (2.31), reads

$$Q^{(n)} = -\frac{1}{2\pi}\int_{BZ} dk_x dk_y \left(\frac{\partial A_y^{(n)}}{\partial k_x} - \frac{\partial A_x^{(n)}}{\partial k_y}\right). \tag{2.41}$$

Certain approximations of the band structure theory of electrons provide low-dimensional momentum-space Hamiltonians that can be diagonalized analytically, allowing for an analytical derivation of the Chern numbers of the electronic bands. More often, however, the electronic wave functions are obtained from numerical techniques on a finite-resolution grid of (k_x, k_y) points in the Brillouin zone. In that case, the Chern number of a chosen band can still be effectively evaluated using the discrete version of its definition (2.13).

The Chern number of a band of an insulator is a topological invariant in the following sense. One can imagine that the Hamiltonian describing the electrons on the lattice is deformed adiabatically, that is, continuously and with the energy gaps separating the nth band from the other bands kept open. In this case, the Berry curvature varies continuously, and therefore its integral for the Brillouin zone, which is the Chern number, cannot change as the value of the latter is restricted to integers. If the deformation of the crystal Hamiltonian is such that some energy gaps separating the nth band from a neighboring band is closed and reopened, that is, the deformation of the Hamiltonian is not adiabatic, then the Chern number might change. In this sense, the Chern number is a similar topological invariant for two-dimensional lattice models as the winding number is for the one-dimensional SSH model.

2.3 Berry Phase and Adiabatic Dynamics

In most physical situations of interest, the set of states whose geometric features (Berry phases) we are interested in are eigenstates of some Hamiltonian $\hat{H}$. Take a physical system with D real parameters that are gathered into a formal vector $\mathbf{R} = (R_1, R_2, \ldots, R_D)$. The Hamiltonian is a smooth function $\hat{H}(\mathbf{R})$ of the parameters, at least in the region of interest. We order the eigenstates of the Hamiltonian according to the energies $E_n(\mathbf{R})$,

$$\hat{H}(\mathbf{R})\,|n(\mathbf{R})\rangle = E_n(\mathbf{R})\,|n(\mathbf{R})\rangle\,. \tag{2.42}$$

We call the set of eigenstates $|n(\mathbf{R})\rangle$ the *snapshot basis*.

The definition of the snapshot basis involves *gauge fixing*, i.e., specifying the otherwise arbitrary phase prefactor for every $|n(\mathbf{R})\rangle$. This can be a tricky issue: even in cases where a gauge exists where all elements of the snapshot basis are smooth functions of the parameters, this gauge might be very challenging to construct.

We consider the following problem. We assume that the system is initialized with $\mathbf{R} = \mathbf{R}_0$ and in an eigenstate $|n(\mathbf{R}_0)\rangle$ that is in the discrete part of the spectrum, i.e., $E_n(\mathbf{R}) - E_{n-1}(\mathbf{R})$ and $E_{n+1}(\mathbf{R}) - E_n(\mathbf{R})$ are nonzero. At time $t = 0$ we thus have

$$\mathbf{R}(t=0) = \mathbf{R}_0; \qquad |\psi(t=0)\rangle = |n(\mathbf{R}_0)\rangle\,. \tag{2.43}$$

Now assume that during the time $t = 0 \to T$ the parameter vector $\mathbf{R}$ is slowly changed: $\mathbf{R}$ becomes $\mathbf{R}(t)$, and the values of $\mathbf{R}(t)$ define a continuous directed curve $\mathscr{C}$. Also, assume that $|n(\mathbf{R})\rangle$ is smooth along the curve $\mathscr{C}$. The state of the system evolves according to the time-dependent Schrödinger equation:

$$i\frac{d}{dt}|\psi(t)\rangle = \hat{H}(\mathbf{R}(t))\,|\psi(t)\rangle\,. \tag{2.44}$$

Further, assume that $\mathbf{R}$ is varied in such a way that at all times the energy gaps around the state $|n(\mathbf{R}(t))\rangle$ remain finite. We can then choose the rate of variation of $\mathbf{R}(t)$ along the path $\mathscr{C}$ to be slow enough compared to the frequencies corresponding to the energy gap, so the *adiabatic approximation* holds In that case, the system remains in the energy eigenstate $|n(\mathbf{R}(t))\rangle$, only picking up a phase. We are now going to find this phase.

By virtue of the adiabatic approximation, we take as Ansatz

$$|\psi(t)\rangle = e^{i\gamma_n(t)}e^{-i\int_0^t E_n(\mathbf{R}(t'))dt'}\,|n(\mathbf{R}(t))\rangle\,. \tag{2.45}$$

For better readability, in the following we often drop the t argument where this leads to no confusion. The time derivative of Eq. (2.45) reads

$$i\frac{d}{dt}|\psi(t)\rangle = e^{i\gamma_n}e^{-i\int_0^t E_n(\mathbf{R}(t'))dt'}\left(-\frac{d\gamma_n}{dt}\,|n(\mathbf{R})\rangle + E_n(\mathbf{R})\,|n(\mathbf{R})\rangle + i\left|\tfrac{d}{dt}n(\mathbf{R})\right\rangle\right). \tag{2.46}$$

To show what we mean by $\left|\frac{d}{dt}n(\mathbf{R}(t))\right\rangle$, we write it out explicitly in terms of a fixed basis, that of the eigenstates at $\mathbf{R} = \mathbf{R}_0$:

$$|n(\mathbf{R})\rangle = \sum_m c_m(\mathbf{R})\,|m(\mathbf{R}_0)\rangle\,; \tag{2.47}$$

$$\left|\tfrac{d}{dt}n(\mathbf{R}(t))\right\rangle = \frac{d\mathbf{R}}{dt}\cdot|\nabla_{\mathbf{R}}n(\mathbf{R})\rangle = \frac{d\mathbf{R}}{dt}\sum_m \nabla_{\mathbf{R}}c_m(\mathbf{R})\,|m(\mathbf{R}_0)\rangle\,. \tag{2.48}$$

We insert the Ansatz (2.45) into the right hand side of the Schrödinger equation (2.44), use the snapshot eigenvalue relation (2.42), simplify and reorder the Schrödinger equation, and obtain

$$-\frac{d\gamma_n}{dt}\,|n(\mathbf{R})\rangle + i\left|\tfrac{d}{dt}n(\mathbf{R})\right\rangle = 0. \tag{2.49}$$

Multiplying from the left by $\langle n(\mathbf{R})|$, and using Eq. (2.48), we obtain

$$\frac{d}{dt}\gamma_n(t) = i\left\langle n(\mathbf{R}(t))\,\middle|\,\tfrac{d}{dt}n(\mathbf{R}(t))\right\rangle = \frac{d\mathbf{R}}{dt}i\,\langle n(\mathbf{R})\,|\,\nabla_{\mathbf{R}}n(\mathbf{R})\rangle\,. \tag{2.50}$$

We have found that for the directed curve $\mathscr{C}$ in parameter space, traced out by $\mathbf{R}(t)$, there is an adiabatic phase $\gamma_n(\mathscr{C})$, which reads

$$\gamma_n(\mathscr{C}) = \int_{\mathscr{C}} i \langle n(\mathbf{R}) \mid \nabla_{\mathbf{R}} n(\mathbf{R}) \rangle \, d\mathbf{R}. \tag{2.51}$$

A related result is obtained after a similar derivation, if the parameter space of the $\mathbf{R}$ points is omitted and the snapshot basis $|n(t)\rangle$ is parametrized directly by the time variable. Then, the adiabatic phase is

$$\gamma_n(t) = \int_0^t i \left\langle n(t') \,\middle|\, \partial_{t'} n(t') \right\rangle dt'. \tag{2.52}$$

Equation (2.51) allows us to formulate the key message of this section as the following. Consider the case of an adiabatic and *cyclic* change of the Hamiltonian, that is, when the curve $\mathscr{C}$ is closed, implying $\mathbf{R}(T) = \mathbf{R}_0$. In this case, the adiabatic phase reads

$$\gamma_n(\mathscr{C}) = \oint_{\mathscr{C}} i \langle n(\mathbf{R}) \mid \nabla_{\mathbf{R}} n(\mathbf{R}) \rangle \, d\mathbf{R}. \tag{2.53}$$

Therefore, the adiabatic phase picked up by the state during a cyclic adiabatic change of the Hamiltonian is equivalent to the Berry phase corresponding to the closed oriented curve representing the Hamiltonian's path in the parameter space.

Two further remarks are in order. First, on the face of it, our derivation seems to do too much. It seems that we have produced an exact solution of the Schrödinger equation. Where did we use the adiabatic approximation? In fact, Eq. (2.50) does not imply Eq. (2.49). For the more complete derivation, showing how the nonadiabatic terms appear, see [15].

The second remark concerns the measurability of the Berry phase. The usual way to experimentally detect phases is by an interferometric setup. This means coherently splitting the wavefunction of the system into two parts, taking them through two adiabatic trips in parameter space, via $\mathbf{R}(t)$ and $\mathbf{R}'(t)$, and bringing the parts back together. The interference only comes from the overlap between the states: it is maximal if $|n(\mathbf{R}(T))\rangle = |n(\mathbf{R}'(T))\rangle$, which is typically ensured if $\mathbf{R}(T) = \mathbf{R}'(T)$. The difference in the adiabatic phases γ_n and γ_n' is the adiabatic phase associated with the closed loop $\mathscr{C}$, which is the path obtained by going forward along $t = 0 \to T : \mathbf{R}(t)$, then coming back along $t = T \to 0 : \mathbf{R}'(t)$.

2.4 Berry's Formulas for the Berry Curvature

Berry provided [6] two practical formulas for the Berry curvature. Here we present them in a form corresponding to a three-dimensional parameter space. To obtain the two-dimensional case, where the Berry curvature B is a scalar, one can identify the latter with the component B_z of the three-dimensional case treated below; for generalization to higher than 3 dimensions, see the discussion in Berry's paper [6]. First,

$$B_j = -\mathrm{Im}\ \epsilon_{jkl}\, \partial_k \langle n \mid \partial_l n \rangle = -\mathrm{Im}\ \epsilon_{jkl}\, \langle \partial_k n \mid \partial_l n \rangle + 0, \tag{2.54}$$

where the second term is 0 because $\partial_k \partial_l = \partial_l \partial_k$ but $\epsilon_{jkl} = -\epsilon_{jlk}$.

To obtain Berry's second formula, inserting a resolution of identity in the snapshot basis in the above equation, we obtain

$$\mathbf{B}^{(n)} = -\mathrm{Im} \sum_{n' \neq n} \left\langle \nabla n \,\middle|\, n' \right\rangle \times \left\langle n' \,\middle|\, \nabla n \right\rangle, \tag{2.55}$$

where the parameter set $\mathbf{R}$ is suppressed for brevity. The term with $n' = n$ is omitted from the sum, as it is zero, since because of the conservation of the norm, $\langle \nabla n \mid n \rangle = -\langle n \mid \nabla n \rangle$. To calculate $\langle n' \mid \nabla n \rangle$, start from the definition of the eigenstate $|n\rangle$, act on both sides with ∇, and then project unto $|n'\rangle$:

$$\hat{H} \,|n\rangle = E_n \,|n\rangle\,; \tag{2.56}$$

$$(\nabla \hat{H}) \,|n\rangle + \hat{H} \,|\nabla n\rangle = (\nabla E_n) \,|n\rangle + E_n \,|\nabla n\rangle\,; \tag{2.57}$$

$$\left\langle n' \right| \nabla \hat{H} \,|n\rangle + \left\langle n' \right| \hat{H} \,|\nabla n\rangle = 0 + E_n \left\langle n' \,\middle|\, \nabla n \right\rangle. \tag{2.58}$$

Act with $\hat{H}$ towards the left in Eq. (2.58), rearrange, substitute into (2.55), and you obtain the second form of the Berry curvature, which is manifestly gauge invariant:

$$\mathbf{B}^{(n)} = -\mathrm{Im} \sum_{n' \neq n} \frac{\langle n| \nabla \hat{H} \,|n'\rangle \times \langle n'| \nabla \hat{H} \,|n\rangle}{(E_n - E_{n'})^2}. \tag{2.59}$$

This shows that the monopole sources of the Berry curvature, if they exist, are the points of degeneracy.

A direct consequence of Eq. (2.59), is that the sum of the Berry curvatures of all eigenstates of a Hamiltonian is zero. If all the spectrum of $\hat{H}(\mathbf{R})$ is discrete

along a closed curve $\mathscr{C}$, then one can add up the Berry phases of all the energy eigenstates.

$$\begin{aligned}\sum_n \mathbf{B}^{(n)} &= -\mathrm{Im}\sum_n \sum_{n'\neq n} \frac{\langle n|\nabla_{\mathbf{R}}\hat{H}|n'\rangle \times \langle n'|\nabla_{\mathbf{R}}\hat{H}|n\rangle}{(E_n - E_{n'})^2} \\ &= -\mathrm{Im}\sum_n \sum_{n'<n} \frac{1}{(E_n - E_{n'})^2}\Big(\langle n|\nabla_{\mathbf{R}}\hat{H}|n'\rangle \times \langle n'|\nabla_{\mathbf{R}}\hat{H}|n\rangle \\ &\quad + \langle n'|\nabla_{\mathbf{R}}\hat{H}|n\rangle \times \langle n|\nabla_{\mathbf{R}}\hat{H}|n'\rangle \Big) = 0. \end{aligned} \tag{2.60}$$

The last equation holds because $\mathbf{a}\times\mathbf{b} = -\mathbf{b}\times\mathbf{a}$ for any two vectors $\mathbf{a}, \mathbf{b}$.

2.5 Example: The Two-Level System

So far, most of the discussion on the Berry phase and the related concepts have been kept rather general. In this section, we illustrate these concepts via the simplest nontrivial example, that is, the two-level system.

2.5.1 No Continuous Global Gauge

Consider a Hamiltonian describing a two-level system:

$$\hat{H}(\mathbf{d}) = d_x\hat{\sigma}_x + d_y\hat{\sigma}_y + d_z\hat{\sigma}_z = \mathbf{d}\cdot\hat{\boldsymbol{\sigma}}, \tag{2.61}$$

with $\mathbf{d} = (d_x, d_y, d_z) \in \mathbb{R}^3\backslash\{0\}$. Here, the vector $\mathbf{d}$ plays the role of the parameter $\mathbf{R}$ in of preceding sections, and the parameter space is the punctured three-dimensional Euclidean space $\mathbb{R}^3\backslash\{0\}$, to avoid the degenerate case of the energy spectrum. Note the absence of a term proportional to σ_0: this would play no role in adiabatic phases. Because of the anticommutation relations of the Pauli matrices, the Hamiltonian above squares to a multiple of the identity operator, $\hat{H}(\mathbf{d})^2 = \mathbf{d}^2\sigma_0$. Thus, the eigenvalues of $\hat{H}(\mathbf{d})$ have to have absolute value $|\mathbf{d}|$.

A practical graphical representation of $\hat{H}(\mathbf{d})$ is the Bloch sphere, shown in Fig. 2.2. The spherical angles $\theta \in [0, \pi)$ and $\varphi \in [0, 2\pi)$ are defined as

$$\cos\theta = \frac{d_z}{|\mathbf{d}|}; \qquad e^{i\varphi} = \frac{d_x + id_y}{\sqrt{d_x^2 + d_y^2}}. \tag{2.62}$$

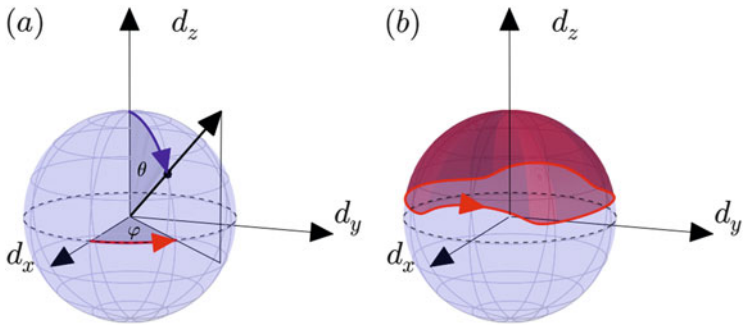

Fig. 2.2 The Bloch sphere. A generic traceless gapped two-level Hamiltonian is a linear combination of Pauli matrices, $\hat{H}(\mathbf{d}) = \mathbf{d} \cdot \hat{\boldsymbol{\sigma}}$. This can be identified with a point in $\mathbb{R}^3 \backslash \{0\}$. The eigenenergies are given by the distance of the point from the origin, the eigenstates depend only on the direction of the vector $\mathbf{d}$, i.e., on the angles θ and φ, as defined in subfigure (**a**) and in Eq. (2.62) The Berry phase of a closed curve $\mathscr{C}$ is half the area enclosed by the curve when it is projected onto the surface of the Bloch sphere

We denote the two eigenstates of the Hamiltonian $\hat{H}(\mathbf{d})$ by $|+_{\mathbf{d}}\rangle$ and $|-_{\mathbf{d}}\rangle$, with

$$\hat{H}(\mathbf{d}) \, |\pm_{\mathbf{d}}\rangle = \pm |\mathbf{d}| \, |\pm_{\mathbf{d}}\rangle \, . \tag{2.63}$$

These eigenstates depend on the direction of the 3-dimensional vector $\mathbf{d}$, but not on its length. The eigenstate with $E = +|\mathbf{d}|$ of the corresponding Hamiltonian is:

$$|+_{\mathbf{d}}\rangle = e^{i\alpha(\theta,\varphi)} \begin{pmatrix} e^{-i\varphi/2} \cos\theta/2 \\ e^{i\varphi/2} \sin\theta/2 \end{pmatrix}, \tag{2.64}$$

while the eigenstate with $E = -|\mathbf{d}|$ is $|-_{\mathbf{d}}\rangle = e^{i\beta(\mathbf{d})} \, |+_{-\mathbf{d}}\rangle$. The choice of the phase factors α and β above corresponds to fixing a gauge. We will now review a few gauge choices.

Consider fixing $\alpha(\theta, \varphi) = 0$ for all θ, φ. This is a very symmetric choice, in this way in formula (2.64), we find $\theta/2$ and $\varphi/2$. There is problem, however, as you can see if you consider a full circle in parameter space: at any fixed value of θ, let $\varphi = 0 \to 2\pi$. We should come back to the same Hilbert space vector, and we do, but we also pick up a phase of π. We can either say that this choice of gauge led to a discontinuity at $\varphi = 0$, or that our representation is not single-valued. We now look at some attempts at fixing these problems, to find a gauge that is both continuous and single valued.

As a first attempt, let us fix $\alpha = \varphi/2$; denoting this gauge by subscript S, we have

$$|+_{\mathbf{d}}\rangle_S = \begin{pmatrix} \cos\theta/2 \\ e^{i\varphi} \sin\theta/2 \end{pmatrix}. \tag{2.65}$$

The phase prefactor now gives an additional factor of -1 as we make the circle in φ at fixed θ, and so it seems we have a continuous, single valued representation. There are two tricky points, however: the North Pole, $\theta = 0$, and the South Pole, $\theta = \pi$. At the North Pole, $|(0, 0, 1)\rangle_S = (1, 0)$ no problems. This gauge is problematic at the South Pole, however (which explains the choice of subscript): there, $|(0, 0, -1)\rangle_S = (0, e^{i\varphi})$, the value of the wavefunction depends on which direction we approach the South Pole from.

We can try to solve the problem at the South Pole by choosing $\alpha = -\varphi/2$, which gives us

$$|+_{\mathbf{d}}\rangle_N = \begin{pmatrix} e^{-i\varphi}\cos\theta/2 \\ \sin\theta/2 \end{pmatrix}. \tag{2.66}$$

As you can probably already see, this representation runs into trouble at the North Pole: $|(0, 0, 1)\rangle_N = (e^{-i\varphi}, 0)$.

We can try to overcome the problems at the poles by taking linear combinations of $|+_{\mathbf{d}}\rangle_S$ and $|+_{\mathbf{d}}\rangle_N$, with prefactors that vanish at the South and North Poles, respectively. A family of options is:

$$|+_{\mathbf{d}}\rangle_\chi = e^{i\chi}\sin\frac{\theta}{2}|+_{\mathbf{d}}\rangle_S + \cos\frac{\theta}{2}|+_{\mathbf{d}}\rangle_N \tag{2.67}$$

$$= \begin{pmatrix} \cos\frac{\theta}{2}(\cos\frac{\theta}{2} + \sin\frac{\theta}{2}e^{i\chi}e^{-i\varphi}) \\ \sin\frac{\theta}{2}e^{i\varphi}(\cos\frac{\theta}{2} + \sin\frac{\theta}{2}e^{i\chi}e^{-i\varphi}) \end{pmatrix}. \tag{2.68}$$

This is single valued everywhere, solves the problems at the Poles. However, it has its own problems: somewhere on the Equator, at $\theta = \pi/2$, $\varphi = \chi \pm \pi$, its norm disappears.

It is not all that surprising that we could not find a well-behaved gauge: there is none. By the end of this chapter, it should be clear, why.

2.5.2 Calculating the Berry Curvature and the Berry Phase

Consider the two-level system as defined in the previous section. Take a closed curve $\mathscr{C}$ in the parameter space $\mathbb{R}^3\backslash\{0\}$. We are going to calculate the Berry phase γ_- of the $|-_{\mathbf{d}}\rangle$ eigenstate on this curve:

$$\gamma_-(\mathscr{C}) = \oint_{\mathscr{C}} \mathbf{A}(\mathbf{d})d\mathbf{d}, \tag{2.69}$$

with the Berry vector potential defined as

$$\mathbf{A}(\mathbf{d}) = i\,\langle -_{\mathbf{d}}|\,\nabla_{\mathbf{d}}\,|-_{\mathbf{d}}\rangle\,. \tag{2.70}$$

The calculation becomes straightforward if we use the Berry curvature,

$$\mathbf{B}(\mathbf{d}) = \nabla_{\mathbf{d}} \times \mathbf{A}(\mathbf{d}); \tag{2.71}$$

$$\gamma_-(\mathscr{C}) = \int_{\mathscr{S}} \mathbf{B}(\mathbf{d}) d\mathscr{S}, \tag{2.72}$$

where $\mathscr{S}$ is any surface whose boundary is the loop $\mathscr{C}$. (Alternatively, it is a worthwhile exercise to calculate the Berry phase directly in a fixed gauge, e.g., one of the three gauges introduced above.)

Specifically, we make use of Berry's gauge invariant formulation (2.59) of the Berry curvature, derived in the last chapter. In the case of the generic two-level Hamiltonian (2.61), Eq. (2.59) gives

$$\mathbf{B}^{\pm}(\mathbf{d}) = -\mathrm{Im}\, \frac{\langle \pm | \nabla_{\mathbf{d}} \hat{H} | \mp \rangle \times \langle \mp | \nabla_{\mathbf{d}} \hat{H} | \pm \rangle}{4\mathbf{d}^2}, \tag{2.73}$$

with

$$\nabla_{\mathbf{d}} \hat{H} = \hat{\boldsymbol{\sigma}}. \tag{2.74}$$

To evaluate (2.73), we choose the quantization axis parallel to $\mathbf{d}$, thus the eigenstates simply read

$$|+_{\mathbf{d}}\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}; \qquad |-_{\mathbf{d}}\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}. \tag{2.75}$$

The matrix elements can now be computed as

$$\langle - | \hat{\sigma}_x | + \rangle = \begin{pmatrix} 0 & 1 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = 1, \tag{2.76}$$

and similarly,

$$\langle - | \sigma_y | + \rangle = i; \tag{2.77}$$

$$\langle - | \sigma_z | + \rangle = 0. \tag{2.78}$$

So the cross product of the vectors reads

$$\langle - | \hat{\boldsymbol{\sigma}} | + \rangle \times \langle + | \hat{\boldsymbol{\sigma}} | - \rangle = \begin{pmatrix} 1 \\ i \\ 0 \end{pmatrix} \times \begin{pmatrix} 1 \\ -i \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 2i \end{pmatrix}. \tag{2.79}$$

This gives us for the Berry curvature,

$$\mathbf{B}^{\pm}(\mathbf{d}) = \pm\frac{\mathbf{d}}{|\mathbf{d}|}\frac{1}{2\mathbf{d}^2}. \tag{2.80}$$

We can recognize in this the field of a pointlike monopole source in the origin. Alluding to the analog between the Berry curvature and the magnetic field of electrodynamics (both are derived from a "vector potential") we can refer to this field, as a "magnetic monopole". Note however that this monopole exists in the abstract space of the vectors $\mathbf{d}$ and not in real space.

The Berry phase of the closed loop $\mathscr{C}$ in parameter space, according to Eq. (2.72), is the flux of the monopole field through a surface $\mathscr{S}$ whose boundary is $\mathscr{C}$. It is easy to convince yourself that this is half of the solid angle subtended by the curve,

$$\gamma_-(\mathscr{C}) = \frac{1}{2}\Omega_{\mathscr{C}}. \tag{2.81}$$

In other words, the Berry phase is half of the area enclosed by the image of $\mathscr{C}$, projected onto the surface of the unit sphere, as illustrated in Fig. 2.2.

What about the Berry phase of the other energy eigenstate? From Eq. (2.73), the corresponding Berry curvature $\mathbf{B}_+$ is obtained by inverting the order of the factors in the cross product: this flips the sign of the cross product. Therefore the Berry phases of the ground and excited state fulfil the relation

$$\gamma_+(\mathscr{C}) = -\gamma_-(\mathscr{C}). \tag{2.82}$$

One can see the same result on the Bloch sphere. Since $\langle + | - \rangle = 0$, the point corresponding to $|-\rangle$ is antipodal to the point corresponding to $|+\rangle$. Therefore, the curve traced by the $|-\rangle$ on the Bloch sphere is the inverted image of the curve traced by $|+\rangle$. These two curves have the same orientation, therefore the same area, with opposite signs.

2.5.3 Two-Band Lattice Models and Their Chern Numbers

The simplest case where a Chern number can arise is a two-band system. Consider a particle with two internal states, hopping on a two-dimensional lattice. The two internal states can be the spin of the conduction electron, but can also be some sublattice index of a spin polarized electron. In the translation invariant bulk, the wave vector $\mathbf{k} = (k_x, k_y)$ is a good quantum number, and the Hamiltonian reads

$$\hat{H}(\mathbf{k}) = \mathbf{d}(\mathbf{k})\hat{\boldsymbol{\sigma}}, \tag{2.83}$$

with the function $\mathbf{d}(\mathbf{k})$ mapping each point of the Brillouin Zone to a three-dimensional vector. Since the Brillouin zone is a torus, the endpoints of the vectors $\mathbf{d}(\mathbf{k})$ map out a deformed torus in $\mathbb{R}^3\backslash\{0\}$. This torus is a directed surface: its inside can be painted red, its outside, blue.

The Chern number of $|-\rangle$ (using the notation of Sect. 1.2, of $|u_1(\mathbf{k})\rangle$) is the flux of $\mathbf{B}_-(\mathbf{d})$ through this torus. We have seen above that $\mathbf{B}_-(\mathbf{d})$ is the magnetic field of a monopole at the origin $\mathbf{d} = 0$. If the origin is on the inside of the torus, this flux is $+1$. If it is outside of the torus, it is 0. If the torus is turned inside out, and contains the origin, the flux is -1. The torus can also intersect itself, and therefore contain the origin any number of times.

One way to count the number of times the torus contains the origin is as follows. Take any line from the origin to infinity, and count the number of times it intersects the torus, with a $+1$ for intersecting from the inside, and a -1 for intersecting from the outside. The sum is independent of the shape of the line, as long as it goes all the way from the origin to infinity.

Problems

2.1 Discrete Berry phase and Bloch vectors

Take an ordered set of three arbitrary, normalized states of a two-level system. Evaluate the corresponding discrete Berry phase. Each state is represented by a vector on the Bloch sphere. Show analytically that if two of the vectors coincide, then the discrete Berry phase vanishes.

2.2 Two-level system and the Berry connection

Consider the two-level system defined in Eq. (2.61), and describe the excited energy eigenstates using the gauge $|+_{\mathbf{d}}\rangle_S$ defined in Eq. (2.65). Using this gauge, evaluate and visualize the corresponding Berry connection vector field $\mathbf{A}(\mathbf{d})$. Is it well-defined in every point of the parameter space? Complete the same tasks using the gauge $|+_{\mathbf{d}}\rangle_N$ defined in Eq. (2.66).

2.3 Massive Dirac Hamiltonian

Consider the two-dimensional *massive Dirac Hamiltonian* $\hat{H}(k_x, k_y) = m\hat{\sigma}_z + k_x\hat{\sigma}_x + k_y\hat{\sigma}_y$, where $m \in \mathbb{R}$ is a constant and the parameter space is $\mathbb{R}^2 \ni (k_x, k_y)$. (a) Take a circular loop with radius κ in the parameter space, centered around the origin. Calculate the Berry phase associated to this loop and the ground-state manifold of the Hamiltonian: $\gamma_-(m, \kappa) =?$. (b) Calculate the Berry connection $B_-(k_x, k_y)$ for the ground-state manifold. (c) Integrate the Berry connection for the whole parameter space. How does the result depend on m?

2.4 Absence of a continuous global gauge

In Sect. 2.5.1, we have shown example gauges for the two-level system that were not globally smooth on the parameter space. Prove that such globally smooth gauge does not exist.

2.5 Chern number of two-band models

Consider a two-band lattice model with the Hamiltonian $\hat{H}(\mathbf{k}) = \mathbf{d}(\mathbf{k}) \cdot \hat{\boldsymbol{\sigma}}$. Express the Chern number of the lower-energy band in terms of $\mathbf{d}(\mathbf{k})/|\mathbf{d}(\mathbf{k})|$.