

Invariance and quantization of charges and currents

The theoretical framework of solid state physics is built on the two principal pillars of electromagnetism and quantum mechanics. The former is needed to specify the microscopic (mainly Coulomb) forces acting between electrons and nuclei, while the latter provides the framework for describing states of the system. The close marriage of electromagnetism and quantum mechanics is taken for granted at this fundamental level.

However, there is another, more macroscopic level at which electromagnetism and quantum mechanics become intimately intertwined in the physics of materials. Here there are subtleties that are not often emphasized in the standard texts. For example, virtually all elementary electrodynamics texts discuss the electrical and magnetic properties of material media and introduce the concepts of macroscopic electric polarization and magnetization. However, this discussion is usually carried out in the context of a simplified model in which solids are assembled out of non-overlapping classical charge or current distributions representing “atoms” or “molecules,” with little real attention paid to the quantum nature of the sources of polarization and magnetization.

Indeed, in real polarized solids, as for example in ferroelectric BaTiO_3 , the electrons are distributed throughout the crystal according to the Bloch solutions of the Schrodinger equation. The resulting electron charge distribution peaks around the atomic positions, of course, but it does not fall to zero between atoms. As a result, there is no natural way to decompose the electron charge into “polarized units.” Similar problems exist for the orbital currents that give rise to macroscopic magnetization. The puzzle of how properly to define polarization and magnetization, and how to compute their responses to external fields and strains, has been a recurrent theme of theoretical and computational condensed-matter theory, with important new developments continuing to occur even into the present decade.

But there is yet another sense in which electromagnetism and quantum mechanics can combine to produce effects – sometimes surprising and beautiful effects – at the macroscopic scale, especially for insulating systems. The quintessential example of this is the quantum Hall effect, discovered in 1980, in which a two-dimensional electron gas is subjected to a perpendicular magnetic field at low temperature. If the Fermi level lies in a mobility gap between a pair of adjacent Landau levels, then a transverse conductivity appears that is quantized to an integer multiple of e^2/h , where e is the charge quantum and h is Planck’s constant.

This brings us to the theme of the present chapter. The discovery of the quantum Hall effect provided one of the first hints that concepts of quantization, invariance, and topology may play an important role in condensed-matter theory. There were, of course, many other hints. The most obvious was the phenomenology of superconductivity, where quantization appears prominently in such properties as the magnetic flux in vortices and the Josephson-junction response. The discovery of the fractional quantum Hall effect in 1982 demonstrated that such quantization concepts could also play a central role in strongly correlated systems. More recently, the blossoming of interest in so-called “topological insulators,” which will be discussed in Ch. 6, has led to a renewed interest in, and understanding of, the role of topology in classifying phases of matter.

The purpose of this chapter is to introduce and describe a class of phenomena in which concepts of topology and quantization play an important role, beginning with “ordinary” electric and magnetic responses of conventional materials, but especially including the anomalous Hall conductivity, and eventually connecting with the physics of topological insulators.

The emphasis in this first chapter will be on general physical arguments; the introduction of the formalism needed for a proper discussion of these phenomena will be deferred to later chapters. Nevertheless, the physical arguments to be presented here constrain the form of any candidate theory. For example, it will become clear in Sec. 1.1 that any proposed definition of electric polarization that does not allow for an ambiguity modulo a quantum must necessarily be incorrect, while the same statement does not apply to orbital magnetization. Similarly, strong arguments will be given as to why the anomalous Hall conductivity of a two-dimensional insulator must be quantized, suggesting a connection to some kind of topological index. As we shall see, these expectations are indeed satisfied by the detailed developments that will be presented in the later chapters.

The concept of adiabatic evolution of a crystalline insulating system as a function of one or more external parameters will play an important role in

many of the arguments to be given below. Moreover, in most cases we will argue that the conclusions can be extended from noninteracting to interacting systems, as long as an adiabatic connection exists between them. By a *non-interacting* system we mean one whose electronic Hamiltonian is built entirely out of one-particle operators. Typically these include the electronic kinetic energy $\sum_i p_i^2/2m$ and potential energy $\sum_i V(\mathbf{r}_i)$, where \mathbf{r}_i and \mathbf{p}_i are the coordinates and momenta of the i 'th electron and $V(\mathbf{r})$ is the crystal potential, but it may also be augmented to account for spinor electrons, external fields, or relativistic corrections. The eigenstates of such a system can be regarded as a single Slater determinant constructed from the occupied one-particle orbitals. On the other hand, *interacting* systems are those that also have two-particle or higher interactions in the Hamiltonian, such as the all-important Coulomb interaction $\sum_{ij} e^2/|\mathbf{r}_i - \mathbf{r}_j|$ involving the inverse of the distance between pairs of electrons. While the physical arguments to follow will mostly be formulated in the noninteracting context, they usually apply equally well to any interacting system that can be reduced to a noninteracting one along an adiabatic path that takes the interaction strength to zero, provided the system remains insulating everywhere along the path. In such cases we shall say that the properties in question are “robust against interactions.”

Of course, in real insulating materials such as Si or MgO or BaTiO₃, the two-particle Coulomb interaction is enormously important, and a theory in which it is neglected would be a disaster. Instead, we almost invariably start from a mean-field approximation in which each electron feels an electrostatic potential coming from the nuclei and the *average* charge cloud of the other electrons. In most cases, this non-interacting mean-field Hamiltonian is sufficiently close (in some physical sense) to the true interacting one that an adiabatic path can in principle connect them. The mean-field theory may be Hartree-Fock theory, or more commonly, density-functional theory, in which the mean-field potential contains Hartree, exchange, and correlation terms that approximate the effects of the true two-body Coulomb interactions. However, it should be kept in mind that for some strongly-interacting systems, e.g., displaying superconductivity or the fractional quantum Hall effect, no such path exists and the conclusions may have to be modified. In such cases, if one imagines turning up the interaction strength from zero, there is typically a critical interaction strength at which some kind of phase transition occurs; beyond this point the system has changed qualitatively, so that arguments based on an adiabatic connection no longer apply.

The concept of “robustness against interactions” described above has a counterpart in “robust against disorder.” Here one imagines starting with

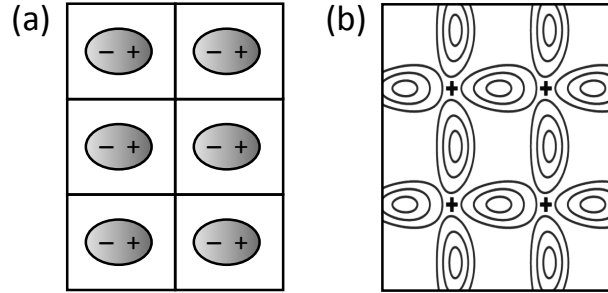


Figure 1.1 (a) Sketch of charge distribution in an idealized classical insulating crystal. Charges are decomposed into isolated packages well separated by charge-free interstitial regions. (b) The charge distribution in a realistic insulator in which the electrons are treated quantum-mechanically. No such interstitial regions exist.

a perfect crystal and smoothly tuning the strength of the disorder up from zero. If the Fermi energy stays in a mobility gap, one may be able to argue that some claimed properties persist, at least up to some critical disorder strength at which the behavior changes qualitatively. We shall see examples of such arguments later in this chapter.

Finally, let me add a word of encouragement. Throughout this chapter, the presentation is targeted at the level of a physics colloquium. You may encounter concepts that have not yet been adequately introduced or arguments that you cannot follow in detail. The arguments may sometimes have a hand-waving character, and subtleties are often swept under the rug. The reader is encouraged to push ahead, even if only to catch the flavor of the arguments and get a feel for the motivations. The specifics should eventually become clearer when we get into the details in the subsequent chapters.

1.1 Polarization, adiabatic currents, and surface charge

The macroscopic electric polarization \mathbf{P} , which carries the physical meaning of dipole moment per unit volume, is one of the central concepts of the electrodynamics of material media. However, the proper definition of polarization for a crystalline insulator becomes far from obvious when the electrons in the solid are treated quantum-mechanically.

To illustrate the problem, consider the sketch in Fig. 1.1(a), which typifies the discussion in most electromagnetism textbooks. The solid is considered to be decomposable into polarized entities, perhaps atoms or molecules, which are well separated by vacuum regions in which the charge density falls to zero. In this case the obvious choice is to define $\mathbf{P} = \mathbf{d}/V_{\text{cell}}$, where

\mathbf{d} is the dipole moment of the entity and V_{cell} is the unit cell volume. On the other hand, Fig. 1.1(b) shows what a charge-density contour plot might look like in a real polarized crystal. The charge does not come subdivided into convenient packages; on the contrary, the quantum charge cloud extends throughout the unit cell.

In this case, how are we to define a dipole per unit cell? An approach that may seem reasonable at first sight is to make some choice of unit cell and let

$$\mathbf{P} = \frac{1}{V_{\text{cell}}} \int_{\text{cell}} \mathbf{r} \rho(\mathbf{r}) d^3r, \quad (1.1)$$

that is, compute the dipole moment of the (nuclear and electronic) charge density $\rho(\mathbf{r})$ inside this cell and divide by the cell volume. Unfortunately, as we shall see later in Sec. 4.1, this does not lead to a unique answer; different choices of unit cell boundaries lead to different results for \mathbf{P} . Of course, for a centrosymmetric crystal it is natural to choose a cell centered at an inversion center, which will give zero as it should, but what should we do for a noncentrosymmetric crystal? This is, after all, precisely the case where \mathbf{P} matters.

It turns out that the problem goes quite deep. According to the “modern theory of polarization,” developed in the 1990s, we now understand that even if the periodic charge density $\rho(\mathbf{r})$ is perfectly known, this information *is not enough, even in principle*, to determine \mathbf{P} . Some other ingredients are needed. We seek a *bulk* definition of \mathbf{P} , so the answer is not to use information about the surfaces; instead we must find some deeper way of characterizing the ground state in the interior of the crystal that goes beyond the information carried in $\rho(\mathbf{r})$.

In Sec. 4.2 we shall derive a proper bulk expression for \mathbf{P} , but the focus of our present interest is to ask a different question. Here we inquire: based on physical principles, what properties must any hypothetical bulk definition of electric polarization have, in order to have a chance of being correct? For example, we expect the polarization to be constrained by the symmetry of the crystal in an obvious way, but this is only qualitative. What can we say quantitatively?

First, consider a crystalline insulator that is changing slowly in time, but in such a way that it remains unit-cell periodic. This might, for example, result from the application of a weak external electric or magnetic field, or from the slow motion of a zone-center optical phonon. If this causes \mathbf{P} to change, then we expect there to be a macroscopic current density \mathbf{J} flowing

in the interior of the crystal¹ and satisfying

$$\mathbf{J} = \frac{d\mathbf{P}}{dt}. \quad (1.2)$$

In general, a part of this current will be given by the displacements of the positively-charged nuclei, but certainly the electrons must contribute as well.

Second, consider a static situation in which there is a slow *spatial* variation of the crystal Hamiltonian, such that the crystal Hamiltonian H , and the resulting \mathbf{P} , vary slowly with a macroscopic spatial coordinate \mathbf{r} that is regarded as being defined only on length scales much larger than the atomic one. Then we expect a macroscopic charge density

$$\rho(\mathbf{r}) = -\nabla \cdot \mathbf{P}(\mathbf{r}) \quad (1.3)$$

to appear. This is what is referred to as a “bound” charge density in elementary electrostatics texts. Note that Eqs. (1.2) and (1.3) are consistent with each other in the case that the system varies slowly in both space and time, since then the charge conservation condition $\dot{\rho} = -\nabla \cdot \mathbf{J}$ is evidently satisfied.

Third, consider a static situation in which a crystalline insulator with polarization \mathbf{P} has a surface normal to $\hat{\mathbf{n}}$. We expect bound charge to accumulate at the surface, and if the surface is insulating such that free charge is absent, we expect a relation of the form

$$\sigma_{\text{surf}} = \mathbf{P} \cdot \hat{\mathbf{n}}, \quad (1.4)$$

where σ_{surf} is the macroscopic surface charge. As we shall see shortly, Eq. (1.4) is not quite correct as written, but we expect that some relation like Eq. (1.4) must hold.

Eqs. (1.2-1.4) provide powerful constraints on any bulk theory of electric polarization. For example, they provide strong hints that the polarization \mathbf{P} cannot be uniquely defined; instead, it is only well defined modulo a “quantum,” in a sense that will be made precise shortly. This remarkable result is at the heart of the modern theory of polarization. Let us see how this comes about.

1.1.1 Surface charge

Figure 1.2(a) shows a toy model of an ionic crystal such as NaCl; we can take the filled and open circles to represent cations and anions respectively, which form an ideal checkerboard lattice in the bulk. However, atoms typically

¹ The macroscopic \mathbf{J} is by definition the unit-cell average of the microscopic current density $\mathbf{J}(\mathbf{r})$ deep in the bulk.

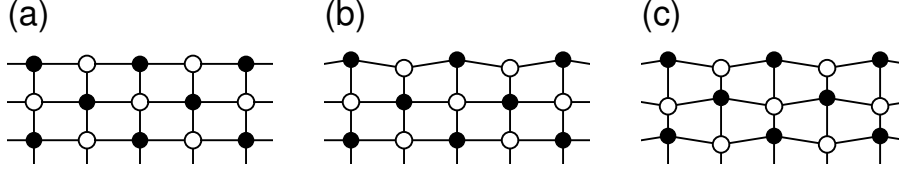


Figure 1.2 (a) Initial configuration of the surface of an ionic crystal composed, with cations and anions indicated by filled and open circles respectively. (b) Relaxed surface configuration, but with no change of bulk structure. (c) Surface structure after a bulk polar distortion has also been applied.

relax at the surface, as for example in Fig. 1.2(b) where the cations are shown relaxing outward relative to the anions. We imagine computing the fully quantum-mechanical electron charge densities for cases (a) and (b), and then extracting the macroscopic surface charge σ_{surf} in both cases. We now ask: What is the change of σ_{surf} as the atoms relax, taking the system from (a) to (b)?

The answer is exactly zero!

Before defending this remarkable statement, we have to add some conditions, namely that the surface and bulk are both insulating, with the Fermi level falling in a gap common to both the bulk and surface. Also, this “experiment” has to be done in complete vacuum, so that no charge can arrive at the surface from above.

The argument runs as follows. Imagine slowly moving the surface atoms from configuration (a) to configuration (b), and ask what current flows into the surface region. None can come from the vacuum, and none can travel laterally along the surface, because of the conditions specified in the previous paragraph. Moreover, the atoms do not move deep in the bulk during this surface distortion, so the current \mathbf{J} , and in particular its component J_z normal to the surface, remain exactly zero there. So if no current flows into the surface region, the net surface charge cannot change, i.e., the surface charge density σ_{surf} is exactly invariant. This argument can be tightened up by introducing a “pillbox” with in-plane radius R extending from a height H above the surface to a depth D below it, where R , H and D are all much larger than the atomic length scale a , and relating the macroscopic currents flowing into the pillbox with the change of surface charge density inside.

This argument is only valid so long as the surface remains insulating, since otherwise the current flowing into the pillbox at the surface is uncontrolled. There is also another, very important, implicit assumption: that the charge $\rho(\mathbf{r})$ and adiabatic current $\mathbf{J}(\mathbf{r})$ in an insulator depend only on the local

Hamiltonian and its (slow) time variation. This is often referred to as the “nearsightedness principle,” a phrase coined by Kohn (1996) and elaborated by Prodan and Kohn (2005), who have argued that it is a universal property of all insulators, even with interactions and disorder. The basic concept is that if one makes a local perturbation, as for example a Ge substitution in a Si crystal, the resulting change in charge density decays exponentially away from the site of the perturbation with a decay length ξ characteristic of the insulator.² Strictly speaking, this statement is only true when charge self-consistency is neglected; clearly a charged impurity in Si would generate a long-range electric field that polarizes the medium far away, so that the change in the microscopic $\rho(\mathbf{r})$ would have a longer power-law decay. In many cases, however, the conclusions can be shown to remain unchanged when charge self-consistency is carefully taken into account.³

Returning to our main line of argument, we have seen that the surface charge density σ_{surf} of an insulator is exactly unchanged by a variation of the surface Hamiltonian, provided that the surface remains insulating along the path of variation. But this is also what we should expect based on Eq. (1.4), since the polarization \mathbf{P} deep in the bulk is unchanged by the adiabatic variation at the surface. Furthermore, we can consider making some slow variation of the *bulk* Hamiltonian instead, as shown in Fig. 1.2(c) for the case in which the bulk atoms have been displaced according to the pattern of a polar zone-center phonon. In this case, a macroscopic current $\mathbf{J} \cdot \hat{\mathbf{n}}$ flows across the lower boundary of the pillbox, so that $dQ_{\text{in}}/dt = \pi R^2 \mathbf{J} \cdot \hat{\mathbf{n}}$ and, using Eq. (1.2), $d\sigma_{\text{surf}}/dt = \hat{\mathbf{n}} \cdot d\mathbf{P}/dt$. Integrating with respect to time, we again conclude that a relation like Eq. (1.4) should be correct.

However, Eq. (1.4) cannot quite be correct as written! That is, if we assume that Eq. (1.4) is correct for any insulating surface of a crystalline insulator, and if we assume that \mathbf{P} is a unique local property of the bulk Hamiltonian, we arrive at a contradiction. For, consider a case like that shown in Fig. 1.3. The sketch shows the local density of states (LDOS) at the surface of an insulating crystal, with the shaded region at left and the unshaded region on the right corresponding to the occupied bulk valence band (VB) and empty bulk conduction band (CB) respectively. We also assume that there is a surface-state band whose bandwidth is small enough that

² Roughly speaking, ξ is determined by the exponential decay of the Green’s function $G(\mathbf{r}, \mathbf{r}'; E)$ with $|\mathbf{r} - \mathbf{r}'|$ for E deep in the gap.

³ For example, to argue that the change in the surface charge $\Delta\sigma$ between Figs. 1.2(a-b) vanishes, one can use a 2D Fourier analysis of the Poisson equation to show that if $\Delta\sigma=0$, the microscopic charge variations produce a Coulomb perturbation that decays exponentially into the bulk; and if, beyond this decay length scale, the bulk is unperturbed, then no current can flow to the surface. Having found a self-consistent solution with $\Delta\sigma=0$, one then invokes uniqueness to conclude that this is *the* solution.

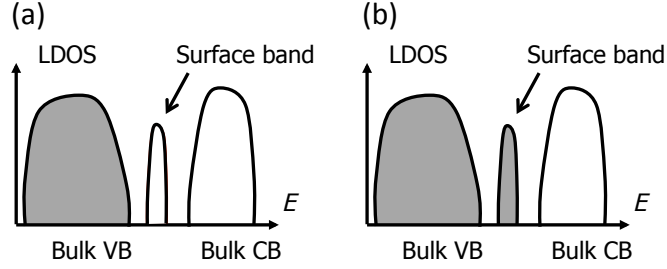


Figure 1.3 (a) Sketch of the local density of states (LDOS) at the surface of an insulating crystal, where there is a surface band (center) that lies entirely within the bulk gap between the valence band (VB) and conduction band (CB). An insulating surface results when the surface band is either (a) entirely empty, or (b) completely filled.

it fits entirely inside the bulk gap, as shown. In this case we can fulfill the insulating-surface condition in two ways: we can either put the surface Fermi level E_F in the lower gap, leaving the surface band empty, as in Fig. 1.3(a), or we can raise E_F until the surface band is filled as in Fig. 1.3(b). The surface charge density clearly differs by $-e/A_{\text{surf}}$ (or by $-2e/A_{\text{surf}}$ for spin-paired electrons), where $e > 0$ is the charge quantum and A_{surf} is the surface unit-cell area for a surface normal to $\hat{\mathbf{n}}$.

How can two different values of σ_{surf} be consistent with a unique \mathbf{P} in Eq. (1.4)? It seems we either have to give up on the notion of a bulk definition of electric polarization entirely, or else we have to broaden the notion such that different “branch choices,” differing from one another by an integer multiple of some “quantum,” are equally valid. While the latter point of view may seem surprising and unnatural at first sight, in what follows we give several further arguments designed to show that it is, in fact, the correct approach.

The conclusion to be drawn from the above argument is that we have to modify Eq. (1.4) to become

$$\sigma_{\text{surf}} = \mathbf{P} \cdot \hat{\mathbf{n}} \mod \frac{e}{A_{\text{surf}}}, \quad (1.5)$$

where we admit to an uncertainty as to which is the correct “branch choice” for $\mathbf{P} \cdot \hat{\mathbf{n}}$ as indicated by the modulo at the end of the equation. Even this way of writing things runs a danger of being misleading, since it could be read as suggesting that $\mathbf{P} \cdot \hat{\mathbf{n}}$ has a definite value, as σ_{surf} really does, and that these differ by the modulo. To be more precise, we can adopt a notation similar to that introduced by Vanderbilt and Resta (2006) and Resta and

Vanderbilt (2007) in which Eq. (1.5) is written as

$$\sigma_{\text{surf}} := \mathbf{P} \cdot \hat{\mathbf{n}}. \quad (1.6)$$

Here the special notation ‘:=’ means that the object on the left-hand side is equal to *one of the values* on the right hand side when $\mathbf{P} \cdot \hat{\mathbf{n}}$ is regarded as a multivalued object whose values are separated by the lattice of values e/A_{surf} . Clearly $\hat{\mathbf{n}}$ is uniquely defined, so this implies that \mathbf{P} carries the branch-choice uncertainty. For this argument to work on any surface facet, we must have that \mathbf{P} is only defined modulo a 3D lattice of values separated by

$$\Delta \mathbf{P} = \frac{e \mathbf{R}}{V_{\text{cell}}} \quad (1.7)$$

where \mathbf{R} is a lattice vector, since then $\Delta \mathbf{P} \cdot \hat{\mathbf{n}} = e(\hat{\mathbf{n}} \cdot \mathbf{R})/V_{\text{cell}} = me/A_{\text{cell}}$ (m an integer) as required. An equation such as (1.6) does not pretend to specify *which* branch choice of \mathbf{P} gives the correct value; only that *one of them* does.

Before proceeding, it is useful to generalize the above 3D discussion to 2D and 1D. The current density \mathbf{J} that has units of C/m²s in 3D acquires units of C/ms in 2D (sometimes denoted as a sheet current \mathbf{K}), and becomes a simple current I with units of C/s in 1D. Correspondingly, the polarization \mathbf{P} has units of C/m², C/m, and C in 3D, 2D, and 1D respectively. The “quantum of surface charge” $\Delta \sigma_{\text{surf}} = e/A_{\text{surf}}$ in 3D becomes a quantum of edge charge $\Delta \lambda_{\text{edge}} = e/b_{\text{edge}}$ in 2D, where b_{edge} is the edge lattice constant, and a quantum of end charge $\Delta Q_{\text{end}} = e$ for a 1D chain. In 3D or 2D the quantum of surface charge is consistent with an uncertainty of the polarization

$$\Delta \mathbf{P} = e \mathbf{R} / \Omega_{\text{cell}} \quad (1.8)$$

where \mathbf{R} is a lattice vector and Ω_{cell} is the cell volume V_{cell} in 3D or the cell area A_{cell} in 2D. In 1D we have $R = \Omega_{\text{cell}} = a$, the lattice constant, so that the quantum of polarization is just the charge quantum e . The arguments given in the previous paragraphs can then be generalized to 2D or 1D in an obvious way.⁴

As a precaution, it is useful to point out that the distinction between “bound” and “free” charge, while intuitive in certain simplified contexts, is not always clean in practice. For example, either of Figs. 1.3(a-b) could be used as a reference for the absence of free charge at the surface, and in the

⁴ Actually, the essential physics described here is 1D physics, and the generalization to 2D or 3D can be regarded as being accomplished by introducing one or two orthogonal dimensions over which averages are taken in a standard way.

case of a one-third-filled surface band, we could say with equal justification that the free charge is $-e/3A_{\text{surf}}$ or $+2e/3A_{\text{surf}}$. Some additional sources of charge, such as those arising from charged defects or stoichiometric variations, are not easily classified as “bound” or “free.” Thus, these terms should be regarded as useful and intuitive in certain situations, but not as fundamental concepts that can be put on a rigorous footing in general.

1.1.2 Adiabatic loop and charge pumping

From Eq. (1.2) it follows that an adiabatic evolution of a bulk crystalline insulator leads to a change of polarization

$$\Delta \mathbf{P} = \int_i^f \mathbf{J}(t) dt. \quad (1.9)$$

If \mathbf{P} were uniquely defined, it would follow that $\Delta \mathbf{P} = 0$ for any cyclic evolution, i.e., along a loop in parameter space that returns the crystalline Hamiltonian to its starting point at the end of the loop – provided, as always, that the system remains insulating along the path. But it is not hard to find counterexamples to show that this is not always the case. For example, Fig. 1.4 shows a sketch of a sliding charge-density wave in an insulating 1D crystal. In Fig. 1.4(a-c) this is modeled in extreme simplicity by the 1D electronic Hamiltonian

$$H = \frac{p^2}{2m} - V_0 \cos(2\pi x/a - \lambda) \quad (1.10)$$

where a is the lattice constant and λ is a cyclic parameter which returns the Hamiltonian to itself after running from 0 to 2π . For a sufficiently large value of V_0 it seems clear that the electron of charge $-e$ is semiclassically localized around the minimum of the potential at $x = a\lambda/2\pi$, so that a charge of $-e$ is pumped by $+a\hat{x}$ during one cycle.

Figure 1.4(d-f) shows a slightly more sophisticated model of the same phenomenon, in which a simple 1D tight-binding model of (spinless) s orbitals at one-third filling is modulated by a sliding cosine potential,

$$H = -t_0 \sum_j (c_j^\dagger c_{j+1} + \text{h.c.}) - V_0 \sum_j \cos(2\pi j/3 - \lambda) c_j^\dagger c_j, \quad (1.11)$$

so that the actual period is a if the spacing between sites is $a/3$. Here the uniform nearest-neighbor hopping $-t_0$ plays the role of a kinetic energy. Again, if V_0 is large, our intuition tells us that the electron will be confined primarily to one or two sites at any given λ , as shown in Fig. 1.4(b), such

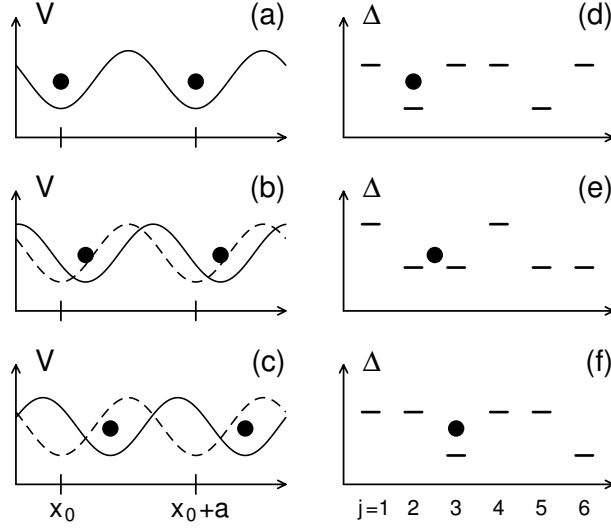


Figure 1.4 (a-c) Evolution of the model described by Eq. (1.10) at three increasing values of the parameter λ . (d-f) Same but for the model of Eq. (1.11), where the site energy Δ is $V_0 \cos(2\pi j/3 - \lambda)$. Both cases result in the transport of electrons, indicated semiclassically as black dots, to the right.

that it would be transported by a over the course of one cycle. We can write this as

$$\Delta P_{\text{cyc}} \equiv \oint J(t) dt = Ne \quad (1.12)$$

where N is an integer (-1 in our example) and ‘ \oint ’ indicates a line integral around a closed cycle.

This result – a pumping of one electron by one lattice vector during one cycle – is thus inconsistent with the notion of a completely well defined electric polarization P ! On the other hand, it is fully consistent with Eq. (1.7) (recall that the quantum of polarization is just $\Delta P = e$ in 1D), which was obtained from an entirely different surface-charge argument!

Consider now what happens to either of the models shown in Fig. 1.4 as the magnitude of V_0 is gradually reduced. We might expect that some “leakage” would occur as V_0 becomes comparable to the scale of the kinetic energy, such that the total transport of charge as given by Eq. (1.9) would fall below e . However, if \mathbf{P} is to have any meaning at all, this cannot be the case! In fact, it turns out that the pumped charge remains exactly quantized and does not fall as V_0 is reduced.⁵ This fundamentally quantized nature of

⁵ This requires that the adiabatic condition must remain satisfied, which requires that the rate

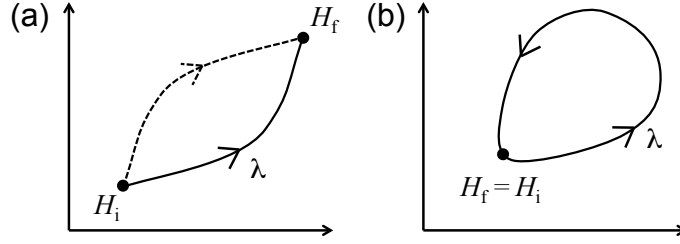


Figure 1.5 (a) In a space of insulating crystal Hamiltonians H , the system is carried adiabatically along two different paths connecting the same initial H_i at λ_i to the same H_f at λ_f . (b) Same but for a closed path, such that λ_i and λ_f label the same Hamiltonian.

adiabatic charge transport, which was derived in a seminal paper of Thouless (1983) and subsequently shown to be robust against interactions and disorder (Niu and Thouless, 1984; Niu, 1986, 1991), provides the essential physical underpinning for the modern theory of polarization.⁶

An important aspect of Eq. (1.12) is that time is a passive variable in the following sense. Let us return to 3D, and for the moment consider an *open* path such that the system is carried from λ_i with Hamiltonian H_i at initial time t_i to λ_f with Hamiltonian H_f at final time t_f , as shown by the solid path in Fig. 1.5(a). We interpret $\mathbf{J} = d\mathbf{P}/dt$ in Eq. (1.2) by noting that even if \mathbf{P} is ill-defined modulo the quantum $e\mathbf{R}/V_{\text{cell}}$, its derivative with respect to the parameter λ describing the Hamiltonian is fully well defined since $e\mathbf{R}/V_{\text{cell}}$ is just a constant,⁷ so that it doesn't matter which branch choice of \mathbf{P} is used. Now the temporal variation of \mathbf{P} really comes about via λ , i.e., $\mathbf{P}(t) = \mathbf{P}(\lambda(t))$, and the analog of Eq. (1.9) becomes

$$\Delta\mathbf{P}_{i \rightarrow f} \equiv \int_i^f \mathbf{J}(t) dt = \int_i^f \frac{d\mathbf{P}}{d\lambda} \frac{d\lambda}{dt} dt = \int_i^f \left(\frac{d\mathbf{P}}{d\lambda} \right) d\lambda \quad (1.13)$$

upon invoking the chain rule. We see that time has dropped out! For a full cycle Eq. (1.12) becomes, in 3D,

$$\Delta\mathbf{P}_{\text{cyc}} = \oint \left(\frac{d\mathbf{P}}{d\lambda} \right) d\lambda = \frac{e\mathbf{R}}{V_{\text{cell}}} \quad (1.14)$$

which is again our quantum of polarization. If \mathbf{P} were uniquely defined, the

of traversal of the loop has to become slower and slower as V_0 is reduced and the gap becomes small. Nevertheless, for any given V_0 , the adiabatic charge transport goes to the quantized value in the limit of a sufficiently slow evolution around the loop.

⁶ While the discussion in these papers was not framed in terms of “polarization,” the essential physics of the modern theory of polarization was already contained there.

⁷ Strictly speaking, we require that elastic strains are not occurring as a function of time, so that \mathbf{R} is constant; otherwise, subtleties associated with the distinction between “proper” and “improper” piezoelectric responses enter in (see, e.g., Vanderbilt, 2000).

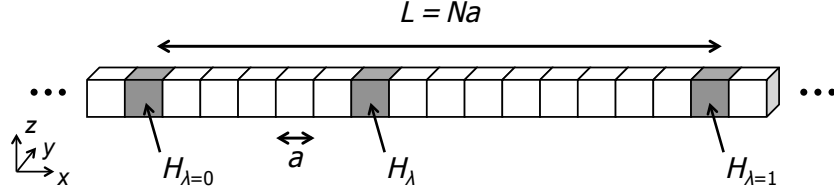


Figure 1.6 Supercell with long repeat distance along $L = Na$ arranged such that the local Hamiltonian H_{λ} undergoes a cyclic variation as x cycles from $x=0$ to $x=L$.

usual rules of calculus would lead us to rewrite the open-path expression in Eq. (1.13) as $\Delta \mathbf{P}_{i \rightarrow f} = \mathbf{P}_f - \mathbf{P}_i$, but this is inappropriate here.⁸ It is safer to adopt the notation of Eq. (1.6) and write that

$$\Delta \mathbf{P}_{i \rightarrow f} := \mathbf{P}_f - \mathbf{P}_i. \quad (1.15)$$

Here the left-hand side has a definite value for a definite path, and we claim that this is equal to *one* of the multiple values given by regarding \mathbf{P} as a lattice-valued quantity on the right-hand side.

This logic also implies that if we consider following two different paths connecting H_i to H_f , such as those indicated by the solid and dashed lines in Fig. 1.5(a), we should get the same result modulo the quantum. This is really just the same as saying that the change in polarization around a closed loop, as shown in Fig. 1.5(b), must be zero or a multiple of the quantum. After all, the difference between the two paths is the same as following one path and then the other in reverse, which is itself a closed path.

To summarize, at this point we have two strong arguments for the notion that electric polarization \mathbf{P} has to be understood as being well defined only modulo the quantum of Eq. (1.7) in crystalline insulators. We shall now give two more.

1.1.3 Slow spatial variation in a supercell

In the previous section, we considered a slow temporal variation of a periodic bulk crystal and arrived at Eq. (1.14), expressing the notion of quantized adiabatic charge transport. We now consider a slow *spatial* variation of the Hamiltonian instead, and show that we can arrive at the same conclusion.

The argument goes as follows. Consider an orthorhombic crystal with lattice constants a , b and c along \hat{x} , \hat{y} and \hat{z} respectively, and construct an $N \times 1 \times 1$ supercell, i.e., a large unit cell of size $L = Na$ along \hat{x} and of primitive

⁸ For example, it would seem to imply that $\Delta \mathbf{P}$ must vanish for any closed cycle.

dimensions along \hat{y} and \hat{z} . Furthermore, arrange that the local Hamiltonian at position x varies slowly along a closed cycle as x runs from 0 to its periodic image at Na . This time we shall let the closed loop be parametrized by λ going from 0 to 1, so that $H_{\lambda=0} = H_{\lambda=1}$, which is a convention we shall frequently adopt later. The situation is sketched in Fig. 1.6. Now since the primitive cells are neutral for any given value of λ , the total charge inside the supercell is given by integrating the “bound” charge $-\nabla \cdot \mathbf{P}$, yielding

$$Q = bc \int_0^{Na} (-\nabla \cdot \mathbf{P}) dx = -bc \int_0^{Na} \frac{dP_x(\lambda(x))}{dx} dx = -\frac{V_{\text{cell}}}{a} \int_0^1 \left(\frac{dP_x}{d\lambda} \right) d\lambda \quad (1.16)$$

where x is now seen to be a passive variable, just as time was in Eq. (1.13). But it is a simple consequence of Bloch’s theorem that filling one band in the bandstructure contributes exactly $-e$ to the charge in the unit cell. Applying this to our supercell, which after all is just a crystal with a strangely shaped unit cell, we argue that $Q = -Ne$ on the left-hand side of Eq. (1.16) for some integer N . This leads directly to

$$\Delta P_{x,\text{cyc}} = \oint \left(\frac{dP_x}{d\lambda} \right) d\lambda = \frac{Nea}{V_{\text{cell}}} \quad (1.17)$$

which is just Eq. (1.14) specialized to the x component of \mathbf{P} .

Thus we see that an argument based on a static crystal Hamiltonian with slow spatial variation yields the same result as one based on a spatially uniform crystal Hamiltonian that varies slowly in time: the polarization \mathbf{P} , if it is well defined at all, is only well defined modulo a quantum of polarization $e\mathbf{R}/V_{\text{cell}}$.

1.1.4 Fictitious physics of classical point charges

In the previous three subsections, arguments based on quantum-mechanical electronic charge densities and currents were invoked to argue that \mathbf{P} is only well defined modulo a quantum. But do we really need to invoke quantum mechanics? Here we see that purely classical considerations can lead to the same conclusion!

In our real world it is a good approximation to treat crystals as composed of classical positively-charged nuclei and distributed electron charge clouds, as sketched in Fig. 1.7(a). But imagine that we live in a fictitious world in which matter is composed entirely of classical point particles of charge Ze (Z an integer) connected by springs or similar two- or three-body forces.⁹

⁹ These need to be stronger than the Coulomb force at short distances to prevent the collapse of opposite charges onto one another.

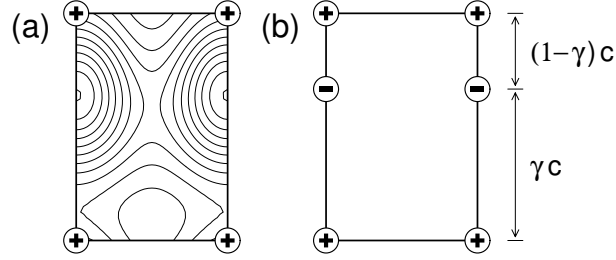


Figure 1.7 (a) A realistic crystal in which a quantum-delocalized electron charge cloud (shown by density contours) coexists with positive classical point charges. (b) An imaginary crystal composed of positive and negative classical point charges.

Figure 1.7(b) shows a typical crystal built out of two particles of charge $\pm e$, where the symmetry is such that we expect a nonzero polarization along the \hat{z} direction. One might expect that all the subtleties discussed above should disappear in such a simple world, but this is not at all the case. For how shall we decide what electric polarization P_z to assign to the crystal shown in Fig. 1.7(b)?

The problem is that we have to decide upon a “basis” to describe the contents of the unit cell, i.e., a list of the charges eZ_j and their coordinates $\boldsymbol{\tau}_j$, chosen such that a periodic repetition of this basis “tiles” the space and reproduces the crystal in question. Figure 1.7(b) is sketched for the case of a 3D tetragonal crystal with charges $Z_1=+1$ and $Z_2=-1$. We can choose their locations to be $\boldsymbol{\tau}_1 = \mathbf{0}$ and $\boldsymbol{\tau}_2 = \gamma c \hat{z}$ (‘-’ above ‘+’ by γc), but an equally valid choice of basis is $\boldsymbol{\tau}_1 = c \hat{z}$ and $\boldsymbol{\tau}_2 = \gamma c \hat{z}$ (‘+’ above ‘-’ by $(1 - \gamma)c$). The polarization is the dipole per unit cell

$$\mathbf{P} = \frac{e}{V_{\text{cell}}} \sum_j Z_j \boldsymbol{\tau}_j, \quad (1.18)$$

which gives $-\gamma e \hat{z}/A$ or $(1 - \gamma)e \hat{z}/A$ respectively for the two choices of basis, where A is the basal cell area. In fact, an infinite number of choices is possible, as for example with $\boldsymbol{\tau}_1 = \mathbf{0}$ and $\boldsymbol{\tau}_2 = \mathbf{R} + \gamma c \hat{z}$ for any lattice vector \mathbf{R} ; this correctly tiles the space to give the specified crystal, regardless of the choice of \mathbf{R} , but the inferred polarization is then only well defined modulo $e\mathbf{R}/V_{\text{cell}}$.

This is exactly the indeterminacy that we arrived at from the quantum-mechanical arguments given earlier! So, even if we lived in this fictitious world, our physicists would still have to argue about a proper definition of polarization, and would still arrive at the notion that only a definition “modulo a quantum” makes sense.

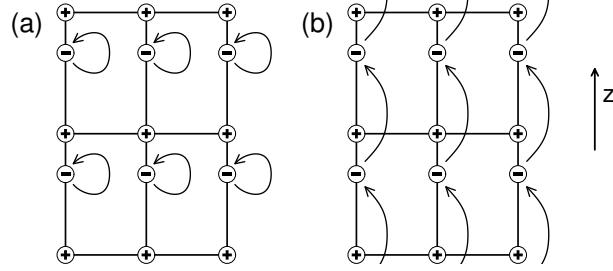


Figure 1.8 Fictitious classical crystal undergoing a cyclic evolution. (a) Negative charges return to themselves such that $\Delta \mathbf{P} = \mathbf{0}$. (b) Negative charges replace partners in the next cell such that $\Delta \mathbf{P} = -e\hat{\mathbf{z}}/A$.

In fact, the arguments given in the previous three subsections all have their counterparts in this fictitious world. The arguments given in Sec. 1.1.1, that an adiabatic adjustment of the coordinates of surface “atoms” (here “charges”) does not change the macroscopic surface charge, are equally valid here. We found there that we could change the macroscopic surface charge by Ne/A_{surf} (integer N), which we can do here by simply adding or removing a layer of charges at the surface. We would again conclude that Eq. (1.6) is valid, i.e., $\sigma_{\text{surf}} = \mathbf{P} \cdot \hat{\mathbf{n}}$ for one of the many possible values of \mathbf{P} . Similarly, the kind of adiabatic loop discussed in Sec. 1.1.2 would correspond here just to the motion of the charges. Figure 1.8 shows two possible cycles, in which the positive charges remain fixed but the negative charges migrate as a function of the loop parameter. The first results in $\Delta \mathbf{P} = \mathbf{0}$ while the second results in a change by our now-familiar quantum $\Delta \mathbf{P} = e\mathbf{R}/V_{\text{cell}}$, here with $\mathbf{R} = -c\hat{\mathbf{z}}$. Finally, we can also consider a supercell with a long repeat period along $\hat{\mathbf{z}}$, with a spatial variation chosen according to the same loop; if built from N primitive cells, this will result in the presence of N positive and $N - 1$ negative charges in the supercell, and arguments parallel to those in Sec. 1.1.3 apply.

To summarize, all of the above arguments are consistent with a viewpoint in which the polarization \mathbf{P} should be regarded as well defined only modulo $e\mathbf{R}/V_{\text{cell}}$, or equivalently, as a *multivalued* quantity whose equally valid values are separated by $e\mathbf{R}/V_{\text{cell}}$. We shall refer to such a mathematical object as *lattice-valued*. For physical statements that can be expressed in differential form, as for example $\rho = -\nabla \cdot \mathbf{P}$ or $\mathbf{J} = d\mathbf{P}/dt$, this uncertainty modulo the quantum introduces no difficulty, as long as we insist on staying on the same branch while carrying out the derivative. On the other hand, some questions such as “What is the macroscopic surface charge σ_{surf} on *this* facet of the crystal?” or “How much net current $\int \mathbf{J} dt$ flowed during *this* adiabatic

evolution?” can only be *partially* answered by a knowledge of the (lattice-valued) bulk polarization. We can say that the answers are respectively $\sigma_{\text{surf}} = \mathbf{P} \cdot \hat{\mathbf{n}}$ or $\int \mathbf{J} dt = \mathbf{P}_f - \mathbf{P}_i$ for one of the valid values of \mathbf{P} or $\mathbf{P}_f - \mathbf{P}_i$, but without knowing more about the particular surface or the particular path, we cannot say which one is correct.

1.1.5 Robustness against weak interactions

The above arguments were framed in the context of a non-interacting description of the electrons. The interacting Hamiltonian is of the form

$$H_{\text{full}} = \sum_i \left[\frac{p_i^2}{2m} + V_{\text{bare}}(\mathbf{r}_i) \right] + \sum_{\langle ij \rangle} \frac{e^2}{|\mathbf{r}_i - \mathbf{r}_j|} \quad (1.19)$$

where V_{bare} is the unscreened attraction of the electrons to the nuclei, but we typically approximate this with a mean-field (MF) Hamiltonian

$$H_{\text{MF}} = \sum_i \left[\frac{p_i^2}{2m} + V_{\text{MF}}(\mathbf{r}_i) \right] \quad (1.20)$$

where V_{MF} includes terms that approximately describe the interaction of an individual electron with the collective electron cloud. Because only one-electron operators appear in Eq. (1.20), its overall ground state is just a single Slater determinant of all of the occupied one-particle eigenfunctions of $p^2/2m + V_{\text{MF}}(\mathbf{r})$, i.e., the Bloch states $\psi_{n\mathbf{k}}(\mathbf{r})$. Typically H_{MF} is constructed using some variety of density-functional theory, and this works quite well for ordinary insulators such as Si, GaAs, and BaTiO₃.

However, we have made various exact claims in the previous subsections: that the surface charge is exactly unchanged by a surface perturbation, that the charge pumped by an adiabatic cycle is exactly e times a lattice vector, etc. It is then natural to ask: Do these statements remain exactly true in the context of the full interacting Hamiltonian of Eq. (1.19)? If so, we say that these statements are “robust against interactions.” This is not to say that the polarization \mathbf{P} of a certain crystal is the same according to Eqs. (1.19) and (1.20); only that the quantum of polarization $e\mathbf{R}/V_{\text{cell}}$ plays exactly the same role, and has the same value, in both cases.

In some situations, the answer is a simple “yes.” For example, when discussing Figs. 1.2(a-b) we argued earlier that the change in the macroscopic surface charge $\Delta\sigma$ resulting from an adiabatic modification of the surface Hamiltonian must vanish exactly if the surface gap does not close. The arguments given there go through equally well for the case of the full many-body Hamiltonian. Similarly, the argument given in Sec. 1.1.3 works equally well

if we just accept that the number of electrons per cell remains quantized to an integer even in the many-body case. But is this true? Here the answer is a qualified “yes.” One can show that it *is* true for any many-body system that can be adiabatically connected to a non-interacting mean-field one. To clarify what is meant by this, consider the Hamiltonian

$$H = (1 - \mu) \mathbf{H}_{\text{MF}} + \mu \mathbf{H}_{\text{full}} \quad (1.21)$$

where μ plays the role of an adiabatic parameter that “turns on” the interacting piece of the Hamiltonian as it runs from 0 to 1. Assuming the crystal remains insulating along this path, which is almost certainly true for most “not too strongly interacting” materials,¹⁰ it can be shown that the macroscopic charge density does not change as μ is varied, i.e., the number of electrons per unit cell remains quantized to an integer.¹¹ The argument of Sec. 1.1.3 then again leads to the quantization of adiabatic charge transport expressed by Eq. (1.14), as was demonstrated by other methods by Niu and Thouless (1984) (see also Niu, 1986, 1991).

We know, however, that there are some strongly-interacting gapped phases that *cannot* be adiabatically connected to a single-particle insulator. An example is the 1/3 fractional quantum Hall state, discovered by Tsui et al. (1982), where the quantized adiabatic charge transport comes in units of $e/3$ because of the existence of quasiparticles with charge $\pm e/3$. Something similar happens for certain spin liquids and other topological phases. Typically these phases are characterized by multiple degenerate ground states, so that arguments based on a unique ground state do not necessarily apply.

This is a fascinating subject, but we shall have little more to say about it here. We shall content ourselves with observing that most “not too strongly” interacting systems, i.e., those that can be adiabatically connected to a mean-field single-particle description, obey the same rules as described in Secs. 1.1.1-1.1.4. In this sense, the conclusions in those sections are “robust against interactions.” Some of them are also “robust against disorder” when this is carefully defined, but a discussion of this interesting topic also falls outside the scope of the present work.

¹⁰ As long as H_{MF} is well chosen, the change to the electronic structure resulting from turning on μ is “weak” in some sense, and the gap remains robust. This would not be the case at all if one were to start from the bare Hamiltonian given by the bracketed term in Eq. (1.19).

¹¹ This is essentially Luttinger’s theorem, which states that the non-integer part of the number of electrons per cell in a metal is proportional to the k -space volume under the Fermi surface, specialized to the case of an insulator for which this volume vanishes. See also Ex. 1.1.2.

Exercises

Exercise 1.1.1 Regarding the argument leading to Eq. (1.17), why is it necessary to assume that the crystal is insulating everywhere along the path – i.e., for all values of λ ? Is this condition sufficient, as well as necessary, to insure an insulating supercell?

Exercise 1.1.2 Give an argument to show that the charge per unit cell does not change at all when the parameter μ controlling the strength of interactions in Eq. (1.21) is varied. Hint: consider varying μ in a localized region in the interior of the sample, and consider the current flowing into this region during the variation.

Exercise 1.1.3 [\[More needed.\]](#)

1.2 Orbital magnetization and surface currents

In elementary electromagnetism we learn that the polarization \mathbf{P} and magnetization \mathbf{M} are the corresponding electric and magnetic order parameters that couple to external electric and magnetic fields. Our focus here is on the spontaneous magnetization \mathbf{M} in magnetic materials, in analogy to the spontaneous polarization \mathbf{P} discussed above. \mathbf{M} has two components, $\mathbf{M} = \mathbf{M}_{\text{spin}} + \mathbf{M}_{\text{orb}}$. In most ferromagnetic materials \mathbf{M}_{spin} is the dominant component describing the excess population of spin-up over spin-down electrons, and is straightforward to describe theoretically. More subtle is the orbital component \mathbf{M}_{orb} , which we can think of as arising from circulating currents on the atoms that make up the crystal as roughly sketched in Fig. 1.9. This is typically induced by the spin-orbit coupling (SOC), which takes the effective form $H_{\text{SOC}} = \xi \mathbf{L} \cdot \mathbf{S}$ on a given atomic site, where \mathbf{S} and \mathbf{L} are the spin and orbital angular momentum operators on this site respectively. Since the SOC is a relativistic effect, its strength ξ tends to be largest for heavy atoms at the bottom of the periodic table.

From elementary electromagnetism we know that just as the electric polarization \mathbf{P} is related to surface charges through Eq. (1.4), an orbital magnetization \mathbf{M}_{orb} manifests itself in the form of a surface current

$$\mathbf{K}_{\text{surf}} = \mathbf{M}_{\text{orb}} \times \hat{\mathbf{n}}, \quad (1.22)$$

where $\hat{\mathbf{n}}$ is the surface normal. But we argued above that \mathbf{P} can only be well defined as a bulk quantity modulo some quantum, leading to the replacement of Eq. (1.4) by Eq. (1.6). We may now ask: is \mathbf{M}_{orb} uniquely defined as a bulk quantity, or does it too suffer from a similar kind of ambiguity?

This time the answer is comforting; the orbital magnetization is indeed

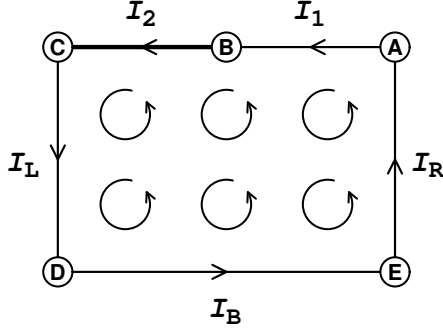


Figure 1.9 Sketch of a rectangular sample cut from a 2D insulating ferromagnet. The edge currents I are argued to be identical (see text) despite different surface cuts and terminations.

well defined in the conventional sense. To see this we can invoke Eq. (1.22), which says that if \mathbf{M}_{orb} is well defined, then all surface currents are determined by this equation. Turning this around, we argue that if it is impossible to modify the surface current by any local surface treatment, then the surface current can be regarded as the manifestation of a unique bulk property.

Consider a finite sample, such as the rectangular one cut from a 2D insulating¹² magnet as shown in Fig. 1.9. In general the manner of truncation may be different on the left (L), bottom (B), and right (R) sides, and just to elaborate the situation, we also imagine that the top surface is broken into two surface patches with different surface terminations labeled by ‘1’ and ‘2’. If we can argue that the edge currents are all identical, $I_L = I_B = I_R = I_1 = I_2$, then it follows that these are all reflections of a unique bulk \mathbf{M}_{orb} . But this immediately follows from conservation of charge. For example, if $I_R \neq I_1$, then there would be a buildup of charge $dQ_A/dt = I_R - I_1$ at point A, and similarly for the other junctions at B, C, D, and E. But we are trying to describe a “stationary state,” i.e., the ground state of this rectangular sample, and it is a basic postulate of quantum mechanics that observables such as these junction charges are independent of time in any stationary state. In other words, such a charge accumulation would have nowhere to go, and is therefore impossible. So all surface currents are the same, and equal to a unique bulk magnetization \mathbf{M}_{orb} . The argument is easily generalized to the surface currents \mathbf{K}_{surf} of a 3D sample.

Note the asymmetry between the physics of $\mathbf{P} \leftrightarrow \sigma_{\text{surf}}$ and $\mathbf{M}_{\text{orb}} \leftrightarrow \mathbf{K}_{\text{surf}}$. In the former case we argued that we could change the surface charge of an

¹² The argument also applies to a metallic sample, although with some elaboration to rule out the role of bulk currents.

insulator by a quantum (one electron per surface cell) via some local change in the surface treatment, so that \mathbf{P} is only well defined modulo a quantum. Here, we find that there is no way to modify \mathbf{K}_{surf} by any local change of the surface, so that we can regard \mathbf{M}_{orb} as being absolutely well defined.¹³

The surface currents \mathbf{K}_{surf} are examples of *dissipationless currents*. Ohm's law plays no role; the currents run forever without slowing down. Moreover, they occur even when the bulk material and its surfaces are all insulating. The existence of dissipationless currents is taken for granted in elementary quantum mechanics, as for example in the $|nlm\rangle = |211\rangle$ state of the H atom,¹⁴ but they seem a little more “creepy” when they occur at the macroscopic scale, and in an insulating system. On the other hand, these are really just “bound currents,” which from another point of view can be regarded as a book-keeping fiction. That is, even if each individual current loop is entirely confined to its own unit cell, so that no “free current” flows at the surface, we claim the existence of a surface current $\mathbf{K} = \mathbf{K}_{\text{bound}}$. This current is “real” in the sense that it generates macroscopic magnetic fields, e.g., contributing to the discontinuity in the surface-parallel component of the macroscopic \mathbf{B} at the surface of a ferromagnet. Dissipationless currents will play a role in many of the phenomena to be discussed later.

Finally, we point out that the arguments given above are generally robust against interactions and disorder. For example, in Fig. 1.9 we can imagine that the many-body terms, controlled by μ in Eq. (1.21), are turned off in surface region 1 but not in surface region 2, or that disorder is introduced to one region but not the other. We still must have $dQ_B/dt = 0$ etc., so all surface currents are identical, and the concept of a bulk \mathbf{M}_{orb} is still allowed. It may seem especially surprising that the presence of surface disorder does not reduce the surface current at all; this is typical of dissipationless currents.

Exercises

Exercise 1.2.1 [\[Exercises needed.\]](#)

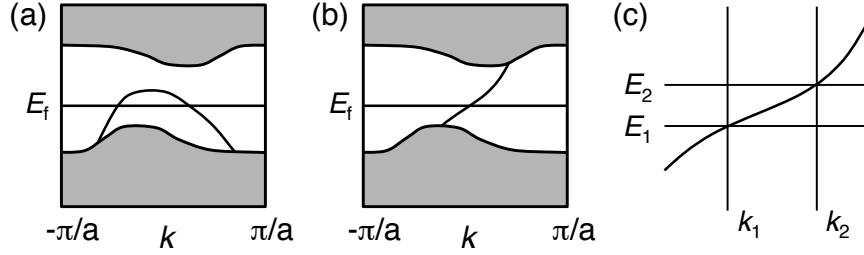


Figure 1.10 (a-b) Possible edge bandstructures of a 2D insulating ferromagnet. Shaded regions are projected bulk bands; isolated curves are edge states. The Fermi energy is at E_f . (c) Close-up of an edge state in the vicinity of E_f .

1.3 Edge channels and anomalous Hall conductivity

1.3.1 Edge channels

It is not too surprising that we cannot modify the edge currents I in Fig. 1.9 by changing the surface properties if the surface is insulating, but it is less obvious if the surface is metallic. Consider again a two-dimensional insulating crystal, but now we study a metallic edge. Figure 1.10 shows what the “edge bandstructure” may look like. We have assumed unit-cell periodicity with the bulk lattice constant a along the edge, so that the edge wavevector k is a good quantum number.¹⁵ Bulk states can be labeled by $(\mathbf{k}n) = (k; k_{\perp}n)$ where k_{\perp} is in the surface-normal direction; allowing k_{\perp} and the bulk band index n to run over all possible values for a given k generates the shaded regions in Figs. 1.10(a-b), which are associated with the occupied bulk valence bands (lower region) and empty bulk conduction bands (upper region). In addition to the bulk bands, there may be edge states (“surface states” in 3D) that are exponentially localized to the vicinity of the edge (or surface); examples of such edge states are shown in the figure. We are again considering a ferromagnetic bulk material; since time-reversal symmetry is absent, there is no reason to expect left-right symmetry in the bandstructures of Figs. 1.10(a-b).¹⁶

In the vicinity of a crossing of an edge band through E_f , the energy position of E_f will clearly influence the contribution of that edge state to the

¹³ This argument that \mathbf{M}_{orb} , and therefore \mathbf{M} , is absolutely well defined rests on an implicit assumption that magnetic monopoles do not exist in nature. If they did, then \mathbf{M} would have to join \mathbf{P} as being multivalued in principle (although not in practice).

¹⁴ A better example might be the $1s^2 2s^2 2p^1$ configuration of the boron atom with $m=1$, which is a ground, not an excited, state.

¹⁵ As a matter of convention we let k be in the direction of positive circulation, so that $+k$ points to the *left* on the top surface.

¹⁶ We assume the absence of mirror symmetry parallel to the edge.

total edge current I . Doesn't this suggest that a local modification at the edge – as, for example, by raising E_f slightly at the edge – will allow us to modify the edge current, in contradiction to what was claimed in Sec. 1.2?

Let's see how I depends on E_f . Suppose we raise the Fermi energy from $E_f = E_1$ to E_2 in a rigid-band picture (i.e., the Hamiltonian remains unchanged). Then the additional current coming from an upward-crossing band like that shown in Fig. 1.10(c) is

$$\begin{aligned}\Delta I &= \int_{k_1}^{k_2} \left(\frac{dk}{2\pi} \right) (-ev_g) \\ &= \frac{-e}{2\pi\hbar} \int_{k_1}^{k_2} \frac{dE}{dk} dk = \frac{-e}{h} (E_2 - E_1).\end{aligned}\quad (1.23)$$

Here $1/2\pi$ is the fundamental density of states (number per unit length per unit wavevector), $-e$ is the charge associated with each newly occupied state, and $v_g = \hbar^{-1}dE/dk$ is the group velocity of the state. This is a remarkable result, indicating that the additional current carried by the edge channel is only a function of the energy shift, independent of the shape of the edge bandstructure curve. In other words, the conductance associated with an up-going edge crossing is

$$G = \frac{dI}{d\phi} = -e \frac{dI}{dE_f} = \frac{e^2}{h}, \quad (1.24)$$

a universal constant of nature, where $E_f = -e\phi$ has been reexpressed in terms of the electrostatic potential ϕ .

Up-going crossings correspond to edge channels that propagate in the positive sense of circulation around the crystal boundary. A similar argument shows that the corresponding contribution of a down-going crossing, like the one shown further to the right in Fig. 1.10(a), is $-e^2/h$. When both contributions are taken into account in Fig. 1.10(a), they cancel such that $dI/dE_f = 0$. That is, the contributions from edge channels with positive and negative sense of circulation cancel each other, and we again conclude that a modification of the edge bandstructure has no influence on the edge current, consistent with a unique definition of orbital magnetization.¹⁷

We are then left with the perplexing question of whether a situation like that shown in Fig. 1.10(b) is possible. It has one edge channel in the direction of positive circulation, but none in the opposite direction. Such a situation is clearly impossible if the system has time-reversal symmetry, but

¹⁷ If E_f had different values at the two crossings, this would indicate that the system is out of equilibrium, and is therefore not in a stationary ground state. In practice, charge flow and scattering between edge channels would eventually reestablish a globally uniform E_f .

we remind the reader that we are interested here in magnetic systems where time reversal symmetry has been broken.

One strange property of a system like that in Fig. 1.10(b) is that, despite the bulk being insulating, the orbital magnetization depends on the Fermi-level position through $dM_{\text{orb}}/dE_f = e^2/h$. Because the charge accumulation at junction points like those in Fig. 1.9 must vanish before and after a global rise of E_f , it follows that the excess number $\Delta n_j \equiv n_j^{\text{up}} - n_j^{\text{down}}$ of up-crossings (n^{up}) relative to down-crossings (n^{down}) on edge j must be the same on all edges of this crystal, i.e.,

$$\Delta n_j = C \quad (1.25)$$

for all edges j .

Of course, the number of up-going or down-going edge channels is intrinsically an integer; there can be no such thing as 1.43 up-going edge channels. So, if crystals with this behavior are allowed in nature, the scenario must play out something like this:

- Every 2D insulating crystal is characterized by an integer C which characterizes the excess number Δn of up-crossings on any vacuum-terminated surface.
- Those belonging to the class with $C=0$, as in Fig. 1.10(a), will be referred to as “normal” or “trivial,” with the others denoted as “nontrivial.” As a special case, the vacuum is classified as a trivial insulator.
- Any vacuum-exposed surface of a sample with integer C has $\Delta n = C$ more up-going than down-going edge channels (as measured for k defined in the sense of positive circulation).
- Any interface between crystals A and B has $\Delta n = C_A - C_B$ excess edge channels (as measured for k defined in the sense of positive circulation about region A).
- Every vacuum surface of a non-trivial insulator, and every interface between non-equivalent insulators (as classified by their C) is necessarily metallic.
- The circulating edge current, or equivalently, the orbital magnetization of a nontrivial insulator varies according to $dM_{\text{orb}}/d\phi = C(e^2/h)$.¹⁸
- An adiabatic variation of the bulk crystal Hamiltonian that does not close the gap cannot result in a change of C .

¹⁸ We argued at the end of Sec. 1.1.1 that the distinction between “bound” and “free” charges is not always sharp. In the present context we see that the same is true of “bound” and “free” currents, since it is equally valid to regard the edge current here as resulting from the addition of free carriers, or from a change of the bulk magnetization.

We have here the seeds of a notion of a “topological classification” of insulators. To attach physical significance to our integer index C , however, we need to introduce a physical observable, namely the anomalous Hall conductivity, that will turn out to be closely related to it.

1.3.2 Anomalous Hall conductivity

We have argued that a 2D ferromagnetic insulator is characterized by a bulk integer index C that controls the number of edge channels that must occur on every face through Eq. (1.25). Is this index C related to some measurable physical quantity? We shall show that it is directly related to the anomalous Hall conductivity (AHC), and indeed, the fact that edge channels are intrinsically quantized implies that the AHC of an insulator is also quantized.

The Hall conductivity and its close cousin, the AHC, will be introduced more systematically in Ch. 5. For now, we simply define the conductivity tensor of a 2D system as the 2×2 matrix $\sigma_{ij} = dK_i/d\mathcal{E}_j$, where \mathbf{K} is the sheet current induced to first order by an in-plane electric field \mathcal{E} . But if the system is gapped, then we must have that the rate of dissipation $\mathbf{K} \cdot \mathcal{E} = 0$, since there are no low-energy excitations to carry away the energy. Thus, the symmetric part of this matrix vanishes, and the only freedom left is the antisymmetric AHC part $\sigma_{\text{AHC}} = \sigma_{yx} = -\sigma_{xy}$,¹⁹ so that

$$\sigma_{ij} = -\epsilon_{ij} \sigma_{\text{AHC}} \quad (1.26)$$

where ϵ_{ij} is the 2×2 antisymmetric tensor.

Intuitively we may expect that σ_{yx} should also be zero, since we would not normally expect any current to be flowing in an insulator. But there are other cases where it does. For example, consider a 2D sample with some gradient of chemical composition or other variable along x , such that $M_{\text{orb}}(x)$ varies with x ; then there is a dissipationless sheet current $K_y(x) = -dM_{\text{orb}}/dx$ running in the y direction. So we should take the possibility seriously and ask: what conditions must be satisfied if an AHC is present in an insulator?

A severe constraint arises when we consider possible charge accumulation at surfaces and interfaces. Consider a situation like that shown in Fig. 1.11(a), which shows a finite rectangular sample of material A adjoined to material B (still in 2D). A small electric field $\mathcal{E} = \mathcal{E}_0 \hat{x}$ is applied, such that a current $K_A = \sigma_{\text{AHC}}^A \mathcal{E}_0$ flows upward in region A and $K_B = \sigma_{\text{AHC}}^B \mathcal{E}_0$ flows

¹⁹ The convention adopted here is that $\sigma^{\text{AHC}} = \sigma_{yx} = -\sigma_{xy}$ so that the current response is rotated in the positive sense of circulation relative to the driving \mathcal{E} -field, but beware that both conventions are commonly used in the literature.

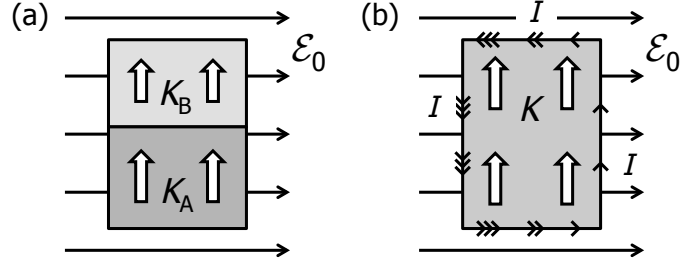


Figure 1.11 Behavior of sheet currents \mathbf{K} and edge currents I for samples subjected to a uniform electric field \mathcal{E}_0 in the x direction. (a) A sample consisting of two adjoined materials A and B having two different values of σ_{AHC} . (b) A detailed view of the edge currents around a single sample.

upward in region B. We also insure that \mathcal{E}_0 is small enough that the induced potential drop from left to right of the sample is much less than the band gap, which is always possible since we are discussing just the linear response to a first-order-small \mathcal{E} . Thus, the system has a well-defined ground state with a Fermi energy in a global gap, and we can consider the stationary ground state of the system. In a stationary state, all observable expectation values must be independent of time, and in particular the charge density at the top edge cannot be changing with time. This is inconsistent with the arrival of charge from the sheet current if the edge is insulating, and we conclude that a non-zero σ_{AHC} requires a metallic edge. Conversely, the presence of an insulating surface implies that σ_{AHC} vanishes in the bulk. A similar argument allows us to show that, if a boundary such as the horizontal AB boundary in Fig. 1.11(a) is insulating, then we must have $\sigma_{\text{AHC}}^{\text{A}} = \sigma_{\text{AHC}}^{\text{B}}$, since otherwise charge would be accumulating at this boundary.

Similar reasoning can be used to demonstrate that a continuous change in the crystal Hamiltonian of an insulator cannot change σ_{AHC} at all. For, let this change be parametrized by λ , and let materials A and B in Fig. 1.11(a) correspond to parameter values λ_0 and $\lambda_0 + \Delta\lambda$ respectively. For small enough $\Delta\lambda$ the AB boundary will certainly be insulating, so $\sigma_{\text{AHC}}^{\text{B}}$ is exactly equal to $\sigma_{\text{AHC}}^{\text{A}}$. Since any insulating path in λ can be discretized into small steps of this kind, it follows that σ_{AHC} must be independent of λ along the path.

So we seem to be left with the possibility that all 2D insulators can be categorized into a discrete set of classes depending on their σ_{AHC} values. A physical boundary between members of two different classes can never be insulating. One class is the class of “normal insulators” (which includes the vacuum) having $\sigma_{\text{AHC}} = 0$; these are the only ones that can have insulating edges.

If there are any insulators that do not fall into this “normal” class, then their metallic edge states must be able to carry off just the right amount of current to cancel the effects of the arriving sheet current and prevent any charge accumulation at the edge. This suggests a connection to edge channels, so it is time to recall the discussion of the previous Sec. 1.3.1, where we found that a given 2D insulator is characterized by an integer C that expresses the net number of positively vs. negatively circulating edge channels through Eq. (1.25). Clearly the “normal” insulators are those with $C = 0$ and $\sigma_{\text{AHC}} = 0$. We now show that everything falls into place if we assume that σ_{AHC} is required to be an integer multiple of e^2/h , where the integer is just C . That is, we can sort all 2D insulators into classes labeled by an integer C and having $\sigma_{\text{AHC}} = Ce^2/h$. Those having $C \neq 0$ are known as “quantum anomalous Hall” (QAH) insulators.

Let’s see how this works out. Consider a rectangular sample of a QAH material immersed in a small uniform electric field \mathcal{E} as shown in Fig. 1.11(b). Since we are considering a system in its stationary ground state, the charge density must everywhere be independent of time, so that the current must be divergence-free. The \mathcal{E} -induced current arriving at a segment of length dx on the top edge of the sample is $K_y dx$, so this will only be drained off if the left-going (i.e., positively circulating) edge current $I(x)$ on the top edge of the sample is x -dependent with $dI/dx = -K_y$. But using Eq. (1.24) and Eq. (1.25) we have

$$K_y = -\frac{dI}{dx} = -\frac{dI}{d\phi} \frac{d\phi}{dx} = C \frac{e^2}{h} \mathcal{E}_x \quad (1.27)$$

or, in short,

$$\sigma_{\text{AHC}} = C \frac{e^2}{h}. \quad (1.28)$$

This demonstrates the quantization of the AHC in a 2D insulator.

Of course, we have still not shown that insulators with non-zero C , or equivalently, with unbalanced right- and left-going edge channels, actually exist in nature – only that they are a logical possibility, consistent with charge conservation in a stationary state. The possibility of the existence of such states began to be taken seriously after 1988, when Haldane (1988) wrote down an explicit model Hamiltonian having $C = \pm 1$ in some regions of its parameter space. In 2013, a first experimental synthesis of a QAH system was demonstrated by the group of Qi-Kun Xue at Tsinghua University (Chang et al., 2013). Furthermore, the physics here is very similar to that of the quantum Hall state discovered in 1980; in that case the insulating state and the broken time-reversal symmetry are both delivered by an external

magnetic field, but the quantization of σ_{AHC} in units of e^2/h and the presence of chiral edge channels (see, e.g., Beenakker, 1990) are just like what has been described above. In fact, there is no doubt that such states *can* exist.

Once again, notice that the arguments given above are quite general, and should be robust against the presence of interactions and/or disorder. For example, if we let regions A and B in Fig. 1.11(a) correspond to a certain system with and without interactions ($\mu=1$ and $\mu=0$ respectively in Eq. (1.21)), then a first-order \mathcal{E} -field applied parallel to the boundary is only consistent with charge conservation if the two regions have identical σ_{AHC} values. So, with the possible exception of highly correlated states that cannot be adiabatically connected to a noninteracting insulating ground state, such as the $1/3$ fractional quantum Hall state mentioned on p. 19, we conclude that σ_{AHC} is quantized to integer multiples of e^2/h even in the presence of interactions.

Exercise 1.3.1 (a) Argue that the current carried by an edge channel remains exactly e^2/h in the presence of weak interactions and/or disorder. (b) Argue that Eq. (1.25) remains true in the presence of weak interactions and/or disorder. You may construct arguments in which the strength of interactions or disorder is turned on or off in various regions of the sample.

Exercise 1.3.2 At the end of Sec. 1.3 it is stated that “an adiabatic variation of the bulk crystal Hamiltonian that does not close the gap cannot result in a change of C .” Justify this statement.

Exercise 1.3.3 In a rigid-band picture (constant H), show that the orbital magnetization in a QAH insulator depends linearly on the Fermi-level position (as long as it remains in the gap, and assuming that the electrostatic potential ϕ is kept constant) according to $dM_{\text{orb}}/dE_{\text{f}} = Ce/h$. Then suppose E_{f} is fixed but ϕ is varied; show that $dM_{\text{orb}}/d\phi = Ce^2/h$. That is, M_{orb} is linearly proportional to the difference $E_{\text{f}} - \bar{V}$, where $\bar{V} = -e\phi$ is the macroscopic electric potential energy.

Exercise 1.3.4 Figure [Figure needed] shows a contour plot of the electrostatic potential in a certain 2D sample of a QAH insulator.

(a) Show that the currents induced by σ_{AHC} always run parallel to the contour lines, and that the total current carried by the ribbon between contour ϕ_0 and contour $\phi_0 + \Delta\phi$ is $C(e^2/h)\Delta\phi$.

(b) Using Eqs. (1.24) and (1.25), show that the edge current I flowing at point B exceeds that at point A by the same amount $C(e^2/h)\Delta\phi$, thus conserving charge at the edge.

1.4 Discussion

In this chapter we have conducted a brief survey of some physical phenomena, mostly connected with the physics of crystalline insulators, that have a topological character and sometimes lead to quantization of certain observables. This includes electric polarization and its relation to surface charges and adiabatic currents, the quantization of charge pumping over an adiabatic loop, orbital magnetization and its relation to surface currents, and the quantized anomalous Hall conductivity and associated chiral edge channels.

It turns out that these physical properties are closely related to a cluster of mathematical concepts revolving around Berry phases, Berry curvatures, and Chern numbers. At least at the single-particle level, the phenomena described above are all represented most naturally in this language. For example, we shall see that the quantization of the adiabatic charge transport in a 1D insulator and of the AHC in a 2D insulator are both a consequence of the Chern theorem, which asserts the quantization of the integral of the Berry curvature over any closed 2D manifold.

The purpose of this book is to introduce these mathematical concepts in a pedagogical fashion, and to explain how they are related to the physical phenomena discussed earlier in this chapter. The Berry phase is named after Michael Berry who, while not exactly responsible for inventing the concept, systematized and popularized it in the 1980s. Essentially, a Berry phase describes the phase evolution of a vector in a complex vector space as a function of some parameter or set of parameters. The connection to the physics discussed in this book arises when the vectors are associated with occupied Bloch functions $|\psi_{n\mathbf{k}}\rangle$ of a crystalline insulator and the parameter space corresponds to the wavevector \mathbf{k} in the BZ, possibly augmented by adiabatic parameters describing the slow evolution of the system. The topological nature of the problem emerges because the BZ can be regarded as a closed manifold, i.e., a loop, 2-torus, or 3-torus in one, two, or three dimensions, respectively. This fact is at the heart of the theory of topological insulators, which will be discussed in one of the later chapters.

As has been emphasized above, many of the physical phenomena under discussion, such as the quantization of charge transport or AHC, are robust against the presence of interactions and disorder, at least if these are sufficiently weak that they do not destroy the insulating state or otherwise cause a phase transition. This strongly suggests that some principles must be at work that transcend the single-particle restriction. An alternative viewpoint, and one that more naturally encompasses interactions and disorder, is the field-theory approach. Electromagnetism, being a gauge field

theory, automatically conserves charge, so that many of the arguments relying on charge conservation given earlier in this chapter follow automatically. The 2D QAH state can be described by augmenting the usual electromagnetic field theory with a Chern-Simons action term, and the quantization of the AHC and other properties then follow naturally from the resulting Lagrangian. Even in cases where the microscopic Hamiltonian is too complex to solve, or for experimental systems for which the microscopic Hamiltonian is poorly known, we may be able to argue that the system is characterized at the macroscopic level by an effective field theory such as the Chern-Simons one. While this field-theory viewpoint is an enormously powerful one, it is not the focus of the present book. For some introduction to this interesting subject, the reader is referred to a foundational paper by Qi et al. (2008), the review by Qi and Zhang (2011), or the book by Bernevig (2013).

Having provided some motivation and physical context in this chapter, we are now ready to begin our journey on the road to understanding how the physical properties introduced above can be understood in terms of mathematical concepts related to Berry phases and curvatures. We begin by going back to basics, starting with Bloch's theorem, and introduce the tight-binding approach to electronic structure theory in Ch. 2. Next, the definitions and basic development of the theory of Berry phases, and its application to Bloch functions in the BZ, will be presented in Ch. 3, where Wannier functions will also be introduced. Chapter 4 is then devoted to the Berry-phase theory of polarization, a subject of broad importance and interest in modern computational electronic structure theory. Chapter 5 deals with the anomalous Hall conductivity, leading into the theory of topological insulators presented in Ch. 6. The theory of orbital magnetization and orbital magnetoelectric coupling will then be the subject of the remaining Chs. 7 and 8.