Advanced Solid State Physics

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Adiabatic Approximation and Primer on Topology

In this chapter, we develop the basic framework to see how electron-electron (e-e), electron-ion (e-i), and ion-ion (i-i) interactions affect the properties of solids. We first show that the electron and ion degrees of freedom can be decoupled. Such a separation arises because ions and electrons have vastly different velocities in a solid; roughly, electron velocity is 1000 times larger than the ion velocity. As a consequence, the electrons view the ions as providing a static background in which they move. This physical picture is at the heart of the Born-Oppenheimer approximation [BO1927]. We also introduce the basic concepts in topological matter. The relationship with Born-Oppenheimer is the primacy of adiabaticity in the Berry phase.

1.1 Basic Hamiltonian

It useful at the outset to consider the total Hamiltonian to understand how to separate the electronic from the ionic motion. We denote the position and momentum of the i^{th} ion by $\mathbf{R}_i$ and $\mathbf{P}_i$, respectively, and that of the j^{th} electron by $\mathbf{r}_j$ and $\mathbf{p}_j$. We assume that all the ions have mass M and nuclear charge Ze. The total Hamiltonian is then

$$H = \sum_i \frac{\mathbf{P}_i^2}{2M} + \sum_j \frac{\mathbf{p}_j^2}{2m} + \frac{(Ze)^2}{2} \sum_{i,i'} \frac{1}{|\mathbf{R}_i - \mathbf{R}_{i'}|} + \frac{e^2}{2} \sum_{j,j'} \frac{1}{|\mathbf{r}_j - \mathbf{r}_{j'}|} - Ze^2 \sum_{i,j} \frac{1}{|\mathbf{r}_j - \mathbf{R}_i|}. \tag{1.1}$$

This Hamiltonian does not include external electric or magnetic fields or magnetic interactions among the constituents. The last three terms are the i-i, e-e, and e-i interactions, respectively. To progress with this Hamiltonian, we divide the electrons into two groups – the core and the valence or conduction electrons – depending on the degree to which they are bound. This separation is useful because core electrons move with the nuclei. Conduction or valence electrons transport throughout the solid. With this separation in mind, we obtain

$$\begin{aligned} H &= \sum_i \frac{\mathbf{P}_i^2}{2M} + \sum_{j=\text{cond.elec.}} \frac{\mathbf{p}_j^2}{2m} + \sum_{i,i'} V_{i,i'}(|\mathbf{R}_i - \mathbf{R}_{i'}|) \\ &\quad + \frac{e^2}{2} \sum_{j,j'=\text{cond.elec.}} \frac{1}{|\mathbf{r}_j - \mathbf{r}_{j'}|} + \sum_{i,j} V_{ei}(|\mathbf{r}_j - \mathbf{R}_i|) + E_{\text{core}} \end{aligned} \tag{1.2}$$

as the partitioned Hamiltonian. In Eq. (1.2), V_{ii} and V_{ei} represent the effective potential between the ions and the valence electrons with the ions, respectively. The energy of the core electrons is E_{core}. In the example of Na, the total Z is 11, with the orbital filling $1s^2\ 2s^2\ 2p^6\ 3s$. There is only one unpaired valence electron. The effective charge of the ion in this representation is $Z = 1$.

1.2 Adiabatic Approximation

To simplify Eq. (1.2), we separate the nuclear motion from that of the electrons, a separation that makes sense because the ions are much more massive than the electrons. Typically $m/M \sim 1/2000$ to $1/500{,}000$. The small parameter characterizing the expansion is $(m/M)^{1/4}$. We now show that the ion velocity is related to the Fermi velocity by the ratio $(m/M)^{3/4}$. As a result, the ions can be treated as essentially static relative to the electrons. This allows us to solve for the electron motion assuming first that the ions are fixed at their equilibrium positions. The effects of the ion motion can be treated as a perturbation; that is, the electrons adjust adiabatically to the ion motion. From the perspective of the ions, the rapid motion of the electrons creates an overall average electron potential which they feel. This separation is the essence of the Born-Oppenheimer approximation.

To understand the relative orders of magnitude of the ionic and electron velocities and energies, we assume, for the sake of the argument, that

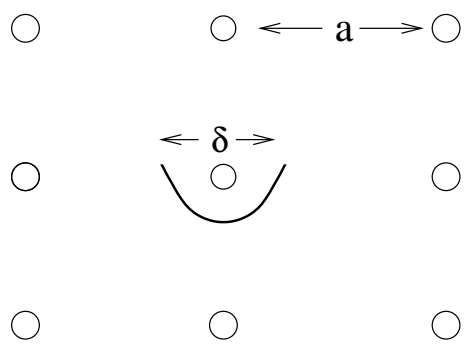

Figure 1.1: Ion lattice with spacing a. Each ion oscillates in a harmonic well with a deviation from its home position that is small relative to the ion spacing. The deviation is roughly $\delta \sim (m/M)^{1/4}a \sim 10^{-4}a$, where m is the electron mass and M the mass of the ions. It is for this reason that the ions can be treated essentially as fixed relative to the electronic degrees of freedom. That the ions comprise a fixed, almost rigid background for the electron motion is the essence of the Born-Oppenheimer approximation.

ions individually move in harmonic wells (see Fig. (1.1)) of the form $V_{\rm osc} = M\omega^2 R^2/2$, where R measures the deviation of an ion from its home (or equilibrium) position. Consider displacing an ion by a lattice spacing, a. The energy required to do so, $\sim M\omega^2 a^2/2$, is essentially that required to distort the electron wavefunction, and thus the energy is of order $\hbar^2/2ma^2$, which in turn is of the order of the electron kinetic energy, $p_F^2/2m$. Thus $M\omega^2 a^2/2 \sim p_F^2/2m$. Solving for ω, we find that

$$\boxed{\omega \sim (m/M)^{1/2}\frac{\hbar}{ma^2}.} \tag{1.3}$$

However, for an ion in a harmonic well, $P^2/2M = \hbar\omega/2$, or equivalently, the square of the ion velocity is $\hbar\omega/M$. Combining this result with those for ω, we see that

$$\boxed{v_{\rm ion} \sim (m/M)^{3/4}v_F \sim (10^{-2} \text{ to } 10^{-3})v_F.} \tag{1.4}$$

Let us estimate how far the ions move from their equilibrium positions. For a displacement δ, $M\omega^2\delta^2/2 \sim \hbar\omega/2$. Substituting $\omega \sim (m/M)^{1/2}\hbar/ma^2$, we find an ion displacement

$$\boxed{\delta \sim a(m/M)^{1/4} \sim 10^{-4}a,} \tag{1.5}$$

which is negligible as illustrated in Fig. (1.1)). As far as the electrons are concerned, the ions are static. We can calculate the role of the electronic degrees of freedom by developing a perturbation series in the small quantity δ/a or $(m/M)^{1/4}$. Note also that because $P^2/2M \sim \hbar\omega/2 \sim \epsilon_F(m/M)^{1/2} \ll \epsilon_F$, the ion kinetic energy is relatively small.

The formal development of the Born-Oppenheimer approximation begins with the assumption that the full wavefunction is a function of the many-electron positions $\mathbf{r} \equiv \{\mathbf{r}_j\}$, and ionic positions $\mathbf{R} \equiv \{\mathbf{R}_i\}$ can be expanded as

$$\Psi\left(\mathbf{r}, \mathbf{R}\right) = \sum_n \Phi_n\left(\mathbf{R}\right) \Psi_{e,n}\left(\mathbf{r}, \mathbf{R}\right), \tag{1.6}$$

where the $\Psi_{e,n}\left(\mathbf{r}, \mathbf{R}\right)$ (indexed by n) are the solutions to the electron-ion problem for a fixed set of ion positions $\mathbf{R}$. The ionic wavefunctions, $\Phi_n(\mathbf{R})$, on the one hand, describe the amplitude for the ions to be found at positions $\mathbf{R}$; on the other hand they can be regarded as expansion coefficients of the electronic wavefunctions. The $\Psi_{e,n}$'s form a complete orthonormal set. Consequently,

$$\int d\mathbf{r} \Psi^*_{e,n}\left(\mathbf{r}, \mathbf{R}\right) \Psi_{e,m}\left(\mathbf{r}, \mathbf{R}\right) = \langle en|em\rangle = \delta_{nm}. \tag{1.7}$$

Coupled with the orthogonality condition on the nuclear wavefunctions

$$\int d\mathbf{R} \Phi^*_n(\mathbf{R}) \Phi_m(\mathbf{R}) = \delta_{nm}, \tag{1.8}$$

the complete electron-ion wavefunction is normalized,

$$\langle \Psi(\mathbf{r}, \mathbf{R}) \mid \Psi(\mathbf{r}, \mathbf{R}) \rangle = 1.$$

We determine each of the expansion coefficients from the equations of motion obeyed by Φ_n and $\Psi_{e,n}$. To proceed, we rewrite Eq. (1.2) as

$$H = T_i + T_e + V_{ii} + V_{ee} + V_{ei} + E_{\text{core}}, \tag{1.9}$$

where there is a one-to-one correspondence between the terms in (1.9) and those in (1.2). The eigenvalue equation for (1.9) is

$$\left(T_i + T_e + V_{ii} + V_{ee} + V_{ei} + E_{\text{core}}\right) \Psi = E\Psi \tag{1.10}$$

$$(T_i + V_{ii} + E_{\text{core}})\Psi + \sum_n \Phi_n (T_e + V_{ee} + V_{ei}) \Psi_{e,n}(\mathbf{r}, \mathbf{R}) = E\Psi. \tag{1.11}$$

We simplify this equation by noting that $T_e + V_{ee} + V_{ei}$ only operates on the electron part of the product wavefunction. Let $E_{e,n}(\mathbf{R})$ be the energy of the electron system for a fixed set of nuclear coordinates. As a consequence, the nuclear and the electronic eigenvalue equations

$$\sum_n \left(T_i + V_{ii} + E_{\text{core}} + E_{e,n} - E\right) \Phi_n \Psi_{e,n} = 0 \tag{1.12}$$

and

$$(T_e + V_{ee} + V_{ei})\Psi_{e,n}(\mathbf{r}, \mathbf{R}) = E_{e,n}(\mathbf{R})\Psi_{e,n} \tag{1.13}$$

can be separated.

Let us multiply the nuclear eigenvalue equation by $\Psi^*_{em} = \langle em|\mathbf{r}, \mathbf{R}\rangle$ and integrate:

$$\sum_n \int d\mathbf{r}\ \Psi^*_{e,m}\left(\mathbf{r}, \mathbf{R}\right) T_i \Phi_n(\mathbf{R})\Psi_{e,n}(\mathbf{r}, \mathbf{R}) + \left(V_{ii} + E_{\text{core}} + E_{e,m}\left(\mathbf{R}\right) - E\right) \Phi_m\left(\mathbf{R}\right) = 0. \tag{1.14}$$

Because the matrix element $\langle en|V_{ii}(\mathbf{R})|em\rangle$ involves purely algebraic operators, it has only diagonal elements. The kinetic energy term, however, has off-diagonal elements; explicitly,

$$\sum_i \left\langle em \left| \frac{\mathbf{P}_i^2}{2M} \Phi_n\left(\mathbf{R}_i\right) \right| en \right\rangle = -\frac{\hbar^2}{2M} \sum_i \int d\mathbf{r} \Psi^*_{e,m}(\mathbf{r}, \mathbf{R}) \Big[\left(\nabla^2_{\mathbf{R_i}} \Phi_n(\mathbf{R})\right) + 2\left(\nabla_{\mathbf{R_i}} \Phi_n(\mathbf{R})\right) \cdot \nabla_{\mathbf{R_i}} + \Phi_n(\mathbf{R}) \nabla^2_{\mathbf{R_i}} \Big] \Psi_{e,n}(\mathbf{r}, \mathbf{R}). \tag{1.15}$$

Because $\nabla^2_{\mathbf{R}}$ acts exclusively on $\Phi_n(\mathbf{R})$ in the first term in the integral, the resultant matrix element is purely diagonal. For the moment, we ignore the last two terms in the kinetic energy matrix element and obtain

$$\sum_n \left(T_i + V_{ii} + E_{\text{core}} + E_{e,n}\left(\mathbf{R}\right)\right) \Phi_n\left(\mathbf{R}\right) = \sum_n E_n \Phi_n(\mathbf{R}), \tag{1.16}$$

or equivalently,

$$\boxed{\left[T_i + V_{ii} + E_{\text{core}} + E_{e,n}\left(\mathbf{R}\right)\right] \Phi_n(\mathbf{R}) = E_n \Phi_n\left(\mathbf{R}\right),} \tag{1.17}$$

as the eigenvalue equation for the nuclear degrees of freedom. Equations (1.13) and (1.17) are the principal results in the Born-Oppenheimer method.

In the nuclear eigenvalue equation, $E_{e,n}(\mathbf{R})$ serves as the effective nuclear potential that results when the electronic degrees of freedom are integrated out. The solutions to (1.17) will describe the phonon modes of the ions.

To justify this treatment of the ion kinetic energy term, we analyze the relative magnitude of the three contributions in Eq. (1.15). We first need a reasonably accurate form for the nuclear wave functions. For our purposes, the harmonic approximation we made in conjunction with the derivation of the ion velocity is adequate. In this case,

$$\Phi_n \sim e^{-M\omega\left(\mathbf{R}-\mathbf{R}^0\right)^2/2\hbar}, \tag{1.18}$$

where $\mathbf{R}^0$ is the equilibrium position of the ion. Consequently,

$$\begin{aligned} \frac{\hbar^2}{2M}\nabla^2_{\mathbf{R}_i}\Phi_n \cdot \Psi_{e,n} &\sim \frac{\hbar^2}{2M}\left(\frac{M\omega}{\hbar}\delta\right)^2 \Phi_n\Psi_{e,n} \\ &\sim \boxed{\left(\frac{m}{M}\right)^{1/2}\epsilon_F\Phi_n\Psi_{e,n}.} \end{aligned} \tag{1.19}$$

Consider now the second term in Eq. (1.15). The inverse length scale on which the electron wave functions change is $\nabla_R \sim 1/a$. As a consequence

$$\begin{aligned} \frac{\hbar^2}{2M}\nabla_{\mathbf{R}_i}\Phi_n \cdot \nabla_{\mathbf{R}_i}\Psi_{e,n} &\sim \frac{\hbar^2}{2M}\frac{M\omega}{\hbar}\frac{\delta}{a}\Psi_{e,n}\Phi_n \\ &\sim \left(\frac{m}{M}\right)^{3/4}\epsilon_F\Phi_n\Psi_{e,n}, \end{aligned} \tag{1.20}$$

and

$$\frac{\hbar^2}{2M}\Phi_n\nabla^2_{\mathbf{R}_i}\Psi_{e,n} \sim \frac{\hbar^2}{2M}\frac{1}{a^2}\Psi_{e,n}\Phi_n \sim \frac{m}{M}\epsilon_F\Phi_n\Psi_{e,n}. \tag{1.21}$$

As is evident, the largest contribution to the nuclear kinetic energy matrix element arises from $\nabla^2_{\mathbf{R}_i}\Phi_n$. The primary reason why this is so is that gradients of Φ_n exceed those of $\Psi_{e,n}$ by a factor of $(M/m)^{1/4}$. Consequently, dropping the last two terms in Eq. (1.15) incurs a negligible error on the order of $(m/M)^{1/4}$.

To lowest order in m/M, we then neglect the ion kinetic energy and assume $\mathbf{R} = \mathbf{R}^0$. The ground electronic wave function is $\Psi_{e,n=0}(\mathbf{r}, \mathbf{R}^0)$; its corresponding energy, $E_{e,n=0}(\mathbf{R}^0)$, obeys the Schrödinger equation

$$\left[T_e + V_{ee} + V_{ei}(\mathbf{r} - \mathbf{R}^0)\right]\Psi_{e,n=0}(\mathbf{r}, \mathbf{R}^0) = E_{e,n=0}(\mathbf{R}^0)\Psi_{e,n=0}(\mathbf{r}, \mathbf{R}^0). \tag{1.22}$$

The subsequent ground-state nuclear wavefunctions and energies can be found with the effective potential $E_{e,n=0}(\mathbf{R}^0)$. If deviations about the equilibrium ion positions are considered within a simple harmonic oscillator model, the total energy of each low-energy state is given by

$$\begin{aligned} E_n &= E_{e,n}(\mathbf{R}^0) + E_{\rm core} + V_{ii}(\mathbf{R}^0) \\ &\quad + \sum_q \hbar\omega_q(n_q + \frac{1}{2}) + \text{anharmonic terms.} \end{aligned} \tag{1.23}$$

1.3 Berry Phase

The Born-Oppenheimer approximation allows us to separate the fast (electrons) degrees of freedom from the slow ones, the ions. In so doing, we came across in Eq. (1.15) quantities of the form, $\langle\Phi_n(\mathbf{R})\nabla_{\mathbf{R}}|\mathbf{\Phi_n}(\mathbf{R})\rangle$ which closely resembles the Berry phase, in fact the square of it. That is, it is through gradients of the wavefunction for the slow degrees of freedom that the Hamiltonian for the fast sector is modified. This is not a surprise. The Born-Oppenheimer approach invokes the adiabatic approximation which is at the heart of Berry's[BO1927] derivation of his celebrated phase. What adiabaticity ensures is that no sudden transitions are made in the time evolution. The only allowable change is a phase factor.

To proceed, we consider a general problem consisting of a fast sector specified by H_f and a slow sector described by H_s. We assume the eigenspectrum of H_f is discrete and that H_s is sufficiently weak so that during a time interval $[0, T]$, no quantum transitions obtain among the eigenstates. This is the essence of adiabaticity: nothing unexpected obtains in the fast sector. Let's assume the system is initially in the $n^{\rm th}$ eigenstate of H_f, ξ_n. The coordinates $\mathbf{R}$ represent the observables of our system. At any time, the state of the system is specified by $|\psi_n(t)\rangle = e^{i\theta(t)}|\xi_n(\mathbf{R})\rangle$. The static state $|\xi_n(\mathbf{R})\rangle$ is assumed to be non-degenerate with eigen-energy $E_n(\mathbf{R})$. What Berry has taught us is that aside from the standard phase factor $E_n t/\hbar$, an additional geometrical phase factor accompanies the time evolution of our system. To uncloak what was overlooked, we focus on the time-dependent Schrödinger equation,

$$i\hbar\frac{d}{dt}e^{i\theta(t)}|\xi_n(\mathbf{R})\rangle = H_{\rm f}e^{i\theta(t)}|\xi_n(\mathbf{R})\rangle, \tag{1.24}$$

which takes the standard form. Carrying out the time derivative,

$$-\hbar\left(\frac{d\theta(t)}{dt}\right)e^{i\theta(t)}|\xi_n(\mathbf{R})\rangle + i\hbar e^{i\hbar\theta(t)}\left(\frac{d}{dt}|\xi_n(\mathbf{R})\rangle\right) = E_n(\mathbf{R})e^{i\theta(t)}|\xi_n(\mathbf{R})\rangle \quad (1.25)$$

leads to three terms. Note the middle term does not reduce to E_n as this is only true for the total derivative of $|\psi_n(t)\rangle$. Taking the inner product with $\langle\xi_n(\mathbf{R})|e^{-i\theta(t)}$ leads to

$$\hbar\frac{d\theta}{dt} = i\hbar\langle\xi_n(\mathbf{R})|\frac{d}{dt}|\xi_n(\mathbf{R})\rangle - \frac{E_n(\mathbf{R})}{\hbar} \quad (1.26)$$

which we solve immediately

$$\frac{d\theta}{dt} = \frac{i}{\hbar}\langle\xi_n(\mathbf{R})|\nabla_R|\xi_n(\mathbf{R})\rangle\cdot\frac{d\mathbf{R}}{dt} - \frac{E_n(\mathbf{R})}{\hbar}. \quad (1.27)$$

Integrating both sides with respect to time,

$$\theta(t) = \gamma_n(t) - \int_0^t \frac{E_n}{\hbar}dt', \quad (1.28)$$

yields two contributions, the standard dynamical (second factor) plus a geometrical term

$$\gamma_n(t) = i\int_0^t \langle\xi_n(\mathbf{R})\nabla_R|\xi_n(\mathbf{R})\rangle\cdot\frac{d\mathbf{R}}{dt'}dt' = i\int_C \langle\xi_n(\mathbf{R}|\nabla_{\mathbf{R}}|\xi_n(\mathbf{R})\rangle\cdot d\mathbf{R} \quad (1.29)$$

known as the Berry phase[BO1927] which depends explicitly on the time-dependent path, C. Although the Berry phase integrated over a closed loop need not be an integer, there is a telling parallel with standard electromagnetism. The inherent redundancy in treating the electrical and magnetic fields as independent quantities is overcome by introducing the vector potential, $\mathbf{A}$. Quantization of the electrical charge, q follows from

$$\frac{q}{\hbar c}\oint d\ell\cdot\mathbf{A} \in \mathbb{Z} \quad (1.30)$$

where $\mathbb{Z}$ are the integers. The restriction to integers obtains because the line integral of the vector potential can be rewritten as a surface integral defining the flux and hence simply counts the total charge enclosed. By analogy, we define the Berry connection

$$A_n(\mathbf{R}) = i\langle\xi_n(\mathbf{R})|\nabla_{\mathbf{R}}|\xi_n(\mathbf{R})\rangle \quad (1.31)$$

in anticipation that the notion of a Berry curvature is as useful as is the 2-form $d\mathbf{A}$ in E&M. But first a preliminary. Note that because of the normalization $\langle\xi_n(\mathbf{R})|\xi_n(\mathbf{R})\rangle = 1$,

$$\langle\nabla_{\mathbf{R}}\xi_n(\mathbf{R})|\xi_{\mathbf{n}}(\mathbf{R})\rangle + \langle\xi_{\mathbf{n}}(\mathbf{R})|\nabla_{\mathbf{R}}\xi_{\mathbf{n}}(\mathbf{R})\rangle = \nabla_{\mathbf{R}}\langle\xi_{\mathbf{n}}(\mathbf{R})|\xi_{\mathbf{n}}(\mathbf{R})\rangle = \mathbf{0}. \quad (1.32)$$

Since the two terms yielding the zero sum are complex conjugates, each must be purely imaginary. Consequently, the Berry connection is purely real as it must be since it enters as a phase. Consider multiplying $|\xi_n(\mathbf{R})\rangle$ by the phase factor $e^{i\chi(\mathbf{R})}$. Carrying the algebra through as before (see Problem 1) leads to the conclusion,

$$A_n(\mathbf{R}) \to A_n(\mathbf{R}) - \nabla_{\mathbf{R}}\chi(\mathbf{R}), \quad (1.33)$$

that χ enters the Berry connection as an effective gauge transformation. Assuming $\chi(\mathbf{R})$ is a smooth single-valued function, then integrating $\nabla_{\mathbf{R}}\chi(\mathbf{R})$ over a closed loop vanishes. Consequently, the Berry connection is gauge invariant when defined on a closed loop. However, there is no guarantee that the Berry phase is an integer. If so, it can be canceled on transport through a closed path. The lack of integer quantization of the Berry phase stems from the fact that it is not about any conservation law. After all, the very form of the Berry phase shows up in the separation of fast and slow degrees of freedom in the Born-Oppenheimer approximation which has nothing to do with a $U(1)$ charge, unlike the vector potential in E&M.

Nonetheless, we can take the purely mathematical analogy with E&M a step further since any line integral can be written as a surface one by invoking Stokes' theorem. The integrand will now depend on the Berry curvature identified as the curl of the Berry connection, $\nabla \times A_n = dA_n$, d the exterior derivative with components

$$\mathbf{F}_n \equiv dA_n = \partial_{[i}A_{j]n} \quad (1.34)$$

where the subscripts $[i, j]$ stand for antisymmetrization consistent with the curl rule. The components of the Berry curvature are

$$F_{\mu\nu} = \langle\nabla_\mu\xi_n(\mathbf{R})|\nabla_\nu\xi_n(\mathbf{R})\rangle - \mu \leftrightarrow \nu$$

and from Stokes' theorem, we have that

$$\gamma_n = -\mathrm{Im}\int d\mathbf{S}_{\mathbf{i}}\epsilon_{ijk}\mathbf{F}_{jk_n}. \quad (1.35)$$

which pegs the Berry phase to an effective flux. It is the effective flux through the surface S that characterizes much of the topology in condensed matter physics.

In its present form, γ_n requires a spatial derivative of the eigenstates. This requires as locally single-valued basis. This constraint can be removed with a little rewriting. First, we insert a complete set of states at each $\mathbf{R}$ to obtain

$$F_{\mu\nu} = \sum_m \langle \nabla_\mu \xi_n(\mathbf{R}) | m \rangle \langle m | \nabla_\nu \xi_n(\mathbf{R}) \rangle - \mu \leftrightarrow \nu. \tag{1.36}$$

We now note that for any two eigenstates $|m\rangle$ and $|n\rangle$ of a Hamiltonian H enjoy the relationship,

$$E_n \langle m | \nabla n \rangle = \langle m | (\nabla H) | n \rangle = \langle m | (\nabla H) | n \rangle + E_m \langle m | \nabla n \rangle. \tag{1.37}$$

Moving the second term to the left-hand-side of this expression results in the compact form

$$\langle m | \nabla n \rangle = \frac{\langle m | (\nabla H) | n \rangle}{E_n - E_m} \tag{1.38}$$

which removes the derivatives of the eigenstates in lieu of a much easier-to-compute derivative of the Hamiltonian. Of course in applying this expression, we impose the constraint that $m \neq n$. In terms of these derivatives, the Berry phase becomes

$$\gamma_n = -\mathrm{Im} \int_C dS_i \epsilon_{ijk} \sum_{m \neq n} \frac{\langle \xi_n | (\nabla_j H_f) | m(\mathbf{R}) \rangle \langle m(\mathbf{R}) | (\nabla_k H_f) | \xi_n(\mathbf{R}) \rangle}{(\mathbf{E_n} - \mathbf{E_m})^\mathbf{2}} \tag{1.39}$$

which is the standard expression for this surprising geometrical phase for adiabatic evolution.

Consider choosing the surface in Eq. (1.39) to be the Brillouin zone. Herein lies the rub. Because of the boundary condition that all k-points differing by $\delta k = 2\pi/a$, all points on the left boundary are equivalent to those on the right edge. Ditto for those lying on the bottom and the top. As a consequence, the Brillouin zone in 2D is homeomorphic to a torus. A torus, however, has no boundary. Hence, application of Stokes' theorem to the Berry connection should lead to nothing of interest. Consider the simple case of Bloch states. We obtain the k-th component of the Berry connection

by taking the derivative ∂_{k_i} on $e^{i\mathbf{k}\cdot\mathbf{r}}$ or simply ir_i. All the components of the curvature look like $r_{[i}r_{j]}$ which is identically zero. Non-trivial topology is tied then to singularities of the Berry connection in the Brillouin zone. That is, the eigenstates must have a particular structure. We will spell this out when we construct the Haldane[H1988] model.

1.3.1 Topology 101: Two-level System

Before we present the Haldane model, we consider a particle in a magnetic field. The relevant Hamiltonian is simply

$$H = h(\mathbf{R}) \cdot \sigma \tag{1.40}$$

where σ are the Pauli matrices

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{1.41}$$

and $h(\mathbf{R}) = |h|(\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$. There are two eigenstates

$$|u_-\rangle = \begin{pmatrix} e^{-i\phi}\sin\theta/2 \\ -\cos\theta/2 \end{pmatrix} \tag{1.42}$$

and

$$|u_+\rangle = \begin{pmatrix} e^{-i\phi}\cos\theta/2 \\ -\sin\theta/2 \end{pmatrix}, \tag{1.43}$$

with energies $-|h|/2$ and $+|h|/2$, respectively. Consider the points $\theta = 0$ or $\theta = \pi$ which correspond to the magnetic field pointing to the south or north poles, respectively. At $\theta = 0$ or $\theta = \pi$, the coordinates x and y both vanish, thereby rendering ϕ ill-defined. Nonetheless, the upper component of $|u_-\rangle$ is still $e^{-i\phi}$. As a result, the wave function itself is ill-defined even upon an adiabatic excursion in the full coordinate space. That is, the system has no proper mechanism of acquiring a non-zero value of ϕ if both x and y vanish. In essence, ∂_ϕ is singular. It is this singularity which will give rise to a non-zero Berry curvature. To see this, we compute the elements of the Berry connection, which are explicitly

$$\begin{aligned} A_\theta &= \langle u_\pm | i\partial_\theta | u_\pm \rangle = 0 \\ A_\phi &= \langle u_- | i\partial_\phi | u_- \rangle = \sin^2\frac{\theta}{2} \end{aligned} \tag{1.44}$$

which yields immediately,

$$\begin{aligned} F_{\theta\phi} &= \partial_\theta A_\phi - \partial_\phi A_\theta \\ &= \frac{\sin\theta}{2}, \end{aligned} \tag{1.45}$$

a non-zero value for the Berry curvature. The non-zero value here is tied entirely to the fact that the $|u_-\rangle$ eigenstate is not well-defined at $\theta = \pi$ or $\theta = 0$. Shifting the eigenstate by the phase $e^{i\phi}$ which puts the ϕ degree of freedom on the second row of the eigenstates does not alleviate the problem. In fact, we obtain the same answer, implying that the coordinate singularity cannot be gauged away.

Physically, a non-zero Berry curvature for a spin tells us that transport along x followed by a pathway along y does not commute. As this non-commutativity is intrinsic, integration of the Berry curvature over the relevant phase space should define a unique number. In this case, this integral

$$\frac{1}{2\pi}\int F_{\theta\phi} d\theta d\phi = \frac{1}{2\pi}\int_0^\pi \frac{\sin\theta}{2} d\theta d\phi = 1 \equiv C \tag{1.46}$$

yields unity. What is being enumerated here is topology, in particular the first Chern number (C), which we will see plays a crucial role in quantum Hall physics. Quantization of the conductance in this problem arises because the integral of the Berry curvature over the Brillouin zone is always an integer modulo 2π. The first Chern number is a fundamental topological invariant in the physics of solids.

1.4 Tight-binding Approximation

Before we evaluate the Berry connection for a non-trivial system, we need to introduce the tight-binding approximation. From our presentation on the Born-Oppenheimer approximation, the effective electron problem is

$$H_e = T_e + V_{ee} + V_{\text{ion}}(\mathbf{r}), \tag{1.47}$$

where

$$V_{\text{ion}}(\mathbf{r}) = \sum_{i,j} V_{ei}(\mathbf{r}_j - \mathbf{R}_i^0). \tag{1.48}$$

Here $V_{\rm ion}(\mathbf{r})$ is the potential felt by the electrons produced by the ions in their equilibrium positions. To a good approximation, this potential is periodic. Let us group all the one-body terms together as $h_e(\mathbf{r}) = T_e + V_{\rm ion}(\mathbf{r})$. The reduced electronic Hamiltonian is then

$$H_e = h_e + V_{ee}. \tag{1.49}$$

It is this Hamiltonian that we will primarily discuss in the remainder of this book.

A closer look at the 1-body part of our Hamiltonian is warranted. In the previous chapter, we treated the electrons in a metal as if they were free particles not tethered to any ions. Of course this is wrong. Electrons know about the ions and interact strongly with them. Why then is it possible to regard the electrons as being free? It turns out that had we started with the localized picture advanced by Wannier, we would still end up with the same answer. The solution to the 1-body part of the Hamiltonian is described by a set of periodic Bloch waves,

$$u_{n\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} c_{n\mathbf{k}}(\mathbf{r}), \tag{1.50}$$

for the n^{th} band with momentum $\mathbf{k}$. Here $c_{\mathbf{k}}(\mathbf{r})$ is a function that has the periodicity of the lattice. Since the Bloch functions are complete, we can form a state localized on a particular lattice site $\mathbf{R}$,

$$\boxed{w_n(\mathbf{R},\mathbf{r}) = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} e^{-i\mathbf{k}\cdot\mathbf{R}} u_{n\mathbf{k}}(\mathbf{r}),} \tag{1.51}$$

by expanding appropriately. Because the Bloch states are orthonormal, so are the Wannier [W1937] states,

$$\begin{aligned} \langle \mathbf{R}'|\mathbf{R}\rangle \equiv \int d\mathbf{r} w_n(\mathbf{R},\mathbf{r}) w_m^*(\mathbf{R}',\mathbf{r}) &= \frac{1}{N}\sum_{\mathbf{k},\mathbf{k}'} \int d\mathbf{r} e^{-i\mathbf{k}\cdot\mathbf{R}+i\mathbf{k}'\cdot\mathbf{R}'} u_{n\mathbf{k}}(\mathbf{r}) u^*_{m\mathbf{k}'}(\mathbf{r}) \\ &= \frac{1}{N}\sum_{\mathbf{k},\mathbf{k}'} e^{-i\mathbf{k}\cdot\mathbf{R}+i\mathbf{k}'\cdot\mathbf{R}'} \delta_{m,n}\delta_{\mathbf{k},\mathbf{k}'} \\ &= \delta_{\mathbf{R},\mathbf{R}'}\delta_{m,n} \end{aligned} \tag{1.52}$$

as can be seen from a direct calculation. The statement that Wannier states form an orthonormal basis is somewhat problematic. If we were to rewrite

h_e in terms of the Wannier states,

$$\boxed{h_e = \sum_{\mathbf{R},\mathbf{R}'} |\mathbf{R}'\rangle\langle\mathbf{R}'|h_e|\mathbf{R}\rangle\langle\mathbf{R}|,} \tag{1.53}$$

by using the completeness relationship on the state vectors associated with the Wannier states, $|\mathbf{R}\rangle$, we would have to conclude that there are no off-diagonal matrix elements of our Hamiltonian. That is, if the Wannier states on two neighbouring sites do not have any overlap, any matrix element with the Hamiltonian should be zero. The statement that the Wannier basis forms an orthornomal basis in practice means that beyond nearest neighbours, the wavefunctions have no appreciable amplitude. This is the tight-binding approximation and the Hamiltonian that results is termed the tight-binding (TB) Hamiltonian. Restricting ourselves to nearest neighbours, we define the parameters in our TB model as

$$\langle\mathbf{R}|h_e|\mathbf{R}\rangle \equiv E_0 \tag{1.54}$$

and the nearest-neighbour matrix element as

$$\langle\mathbf{R}|h_e|\mathbf{R}+\boldsymbol{\delta}\rangle \equiv -t \tag{1.55}$$

where δ is a unit vector from site $\mathbf{R}$ to the nearest neighbours. Our Hamiltonian simplifies to

$$\boxed{H^{\mathrm{TB}} = -t\sum_{\mathbf{R},\boldsymbol{\delta}} |\mathbf{R}\rangle\langle\mathbf{R}+\boldsymbol{\delta}| + E_0\sum_{\mathbf{R}} |\mathbf{R}\rangle\langle\mathbf{R}|.} \tag{1.56}$$

Regardless of the form of the underlying lattice, the tight-binding model can be solved exactly by Fourier transforming,

$$|\mathbf{R}\rangle = \frac{1}{\sqrt{N}}\sum_{\mathbf{k}} e^{-i\mathbf{k}\cdot\mathbf{R}}|\mathbf{k}\rangle. \tag{1.57}$$

The resultant Hamiltonian,

$$H^{\mathrm{TB}} = \sum_{\mathbf{k}} E(\mathbf{k})|\mathbf{k}\rangle\langle\mathbf{k}|, \tag{1.58}$$

depends on a single parameter, namely the band structure

$$\boxed{E(\mathbf{k}) = E_0 - t\sum_{\boldsymbol{\delta}} e^{i\mathbf{k}\cdot\boldsymbol{\delta}}.} \tag{1.59}$$

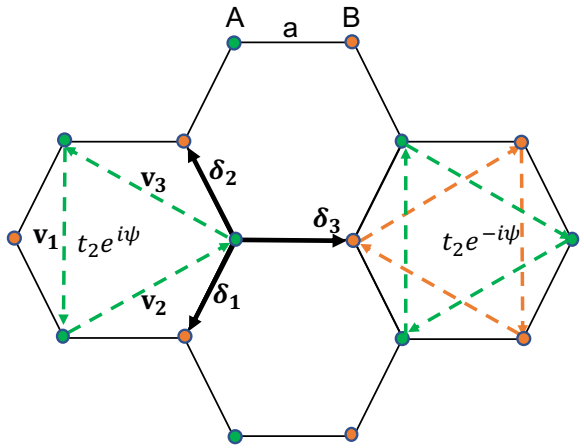

Figure 1.2: Tight-binding structure of the Haldane model. The lattice vectors $\delta_\mathbf{i}$ and $\mathbf{v_i}$ denote nearest and next-nearest neibhbors, respectively. In addition to nearest-neighbour (of magnitude t_1, next-nearest hoppping exists as well with a complex matrix element, $t_2e^{i\psi}$. The flux vanishes in each plaquette as a result of the two counter-rotating loops. Nonetheless, for $\psi \neq 0$, the model breaks time-reversal symmetry.

The energy band, $E(\mathbf{k})$, defines the energy of a non-interacting particle with momentum $\mathbf{k}$ and hence is the TB analogue of the free-particle dispersion. The TB model can be viewed as the lattice analogue of the free-particle problem.

1.5 Primer on Topology: Haldane Model

In retrospect, that transport along x followed by a y-excursion yields a non-zero Chern number for the two-level system studied previously is not surprising as a magnetic field is present. The question arises: Is non-trivial topology possible without an external magnetic field? Haldane provided the definitive answer to this question with a seemingly artificial model depicted in Fig.(1.62) which we can now introduce with the TBM in tow. The underlying lattice is a honeycomb as in graphene with an added twist of a complex nearest-neighbour hopping $t_2e^{i\psi}$. Each plaquette has two nearest-neighbour loops of opposite parity. Hence, there is net flux in each plaquette but no net

external field. Nonetheless, the model breaks time-reversal symmetry. As I have assigned the band structure of graphene as problem 2, I will use the same notation in this problem to elucidate the band structure. The key here is to note that for the honeycomb lattice, two distinct atoms exist, denoted by A and B in the figure. To obtain the TBM band structure for this model, we introduce the nearest ($\boldsymbol{\delta}_i$) and nearest-neighbour lattice $\mathbf{v}_i$,

$$\boldsymbol{\delta}_1 = a(0,1), \quad \boldsymbol{\delta}_2 = \frac{a}{2}(-1,\sqrt{3}), \quad \boldsymbol{\delta}_3 = \frac{a}{2}(-1,-\sqrt{3}) \tag{1.60}$$

$$\mathbf{v}_1 = a\sqrt{3}(0,1), \quad \mathbf{v_2} = a\frac{\sqrt{3}}{2}(-\sqrt{3},-1), \quad \mathbf{v_3} = a\frac{\sqrt{3}}{2}(\sqrt{3},-1) \tag{1.61}$$

with a the lattice constant. The nearest-neighbour lattice vectors connect A to B sites whereas the v_i's connect sites on the same sublattice. The Haldane model also contains an on-site potential with magnitude, M. Consequently, the Hamiltonian for the Haldane model on graphene,

$$\begin{aligned} H_{\rm HM}(\mathbf{k}) &= t_1 \sum_i [\sigma_x \cos(\mathbf{k}\cdot\boldsymbol{\delta}_i) - \sigma_y \sin(\mathbf{k}\cdot\boldsymbol{\delta}_i)] + M\sigma_z \\ &\quad -2t_2 \sin\psi \sum_i \sigma_z \sin(\mathbf{k}\cdot\mathbf{v}_i)] \\ &= d(\mathbf{R})\cdot\sigma, \end{aligned} \tag{1.62}$$

contains three terms and the last equality emphasizes that it is of the two-level system form and hence a similar topological structure should emerge for certain parameter regimes. The first two terms in the Hamiltonian represent nearest-neighbour hopping between the graphene A and B sublattices. The third term is the sub-lattice potential (of magnitude M) which breaks the inversion symmetry, controlled by M. The last term is the next-nearest neighbour hopping process that explicitly breaks time-reversal symmetry (TRS). This can be seen from the fact that under time reversal, $k \to -k$ and $i \to -i$. Only the last term breaks this symmetry as $\sin k \cdot\ v_i$ is odd but σ_z is even. The last two terms are required for the non-trivial topological phase of the model. To tease out the topology, we write the Hamiltonian in matrix form,

$$H(\mathbf{k}) = \begin{pmatrix} M - 2t_2 \sin\psi h_z(\mathbf{k}) & t_1(h_x(\mathbf{k}) + ih_y(\mathbf{k})) \\ t_1(h_x(\mathbf{k}) - ih_y(\mathbf{k})) & -M + 2t_2 \sin\psi h_z(\mathbf{k}) \end{pmatrix}, \tag{1.63}$$

where

$$h_x(\mathbf{k}) = \sum_i \cos(\mathbf{k}\cdot\boldsymbol{\delta}_i), \quad h_y(\mathbf{k}) = \sum_i \sin(\mathbf{k}\cdot\boldsymbol{\delta}_i), \quad h_z(\mathbf{k}) = \sum_i \sin(\mathbf{k}\cdot\mathbf{v}_i) \tag{1.64}$$

You will diagonalize this matrix in Problem 3 and obtain the eigenvalues

$$E(\mathbf{k})_{\pm} = \pm\sqrt{(M - 2t_2 \sin\psi h_z(\mathbf{k}))^2 + t_1^2(h_x(\mathbf{k})^2 + h_y(\mathbf{k})^2)} \tag{1.65}$$

and the eigenvectors

$$u_{\pm} = \begin{pmatrix} i\frac{(M-2t_2\sin\psi)\pm E(\mathbf{k})}{h_y(\mathbf{k})+ih_x(\mathbf{k})} \\ 1 \end{pmatrix}. \tag{1.66}$$

The Berry connection and thus the Chern number (the integrated Berry curvature) can now be calculated from the eigenvectors using the definitions presented earlier. That is, simply plug the eigenstates into Eq. (1.35) and compute the momentum space derivatives. This would of course require that we explicitly construct $d(\mathbf{R})$ and then construct the Jacobian relating $\mathbf{R}$ to polar coordinates; this is particularly cumbersome. It is best to do the whole problem numerically as is usually done to identify topological structures of any non-trivial model. The results shown in Fig. (1.3) illustrates the rich topological structure of the Haldane model as a function of M and ψ. As is evident, $\psi = \pm\pi/2$ maximizes the topological structure, and the parameter space where the Chern number is unity is demarcated. As we will in Chap. 15, the field of topological insulators arises from two copies of the Haldane model, with a spin-dependent phase, $\psi \to \sigma\psi$. This change reinstates TRS and as a result the Chern number will vanish. However, a non-zero spin Chern number emerges as a result of the underlying $SU(2)$ spin structure. Keep tuned.

Problems

1. Show that by changing the phase in Eq. (1.24) to $\theta \to \theta + \chi(\mathbf{R})$ changes the Berry phase according to Eq. (1.33).

2. This problem concerns the band structure of a single sheet of carbon, graphene (see Fig. (1.4)). Nearest neighbour atoms are connected by the set of vectors,

$$\delta_1 = \frac{a}{2}\left(-1, \sqrt{3}\right), \quad \delta_2 = \frac{a}{2}\left(-1, -\sqrt{3}\right), \quad \delta_3 = a\,(1, 0) \tag{1.67}$$

and the primitive lattice vectors are

$$\mathbf{a}_1 = \frac{a}{2}\left(3, \sqrt{3}\right), \quad \mathbf{a}_2 = \frac{a}{2}\left(3, -\sqrt{3}\right) \tag{1.68}$$

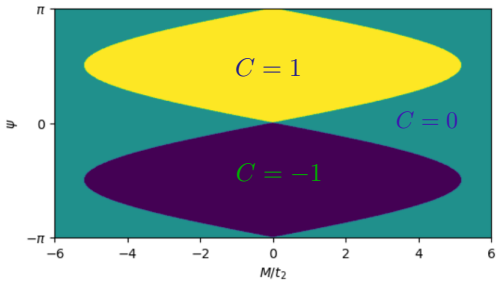

Figure 1.3: Phase diagram of the Haldane model as a function of the on-site potential, M, and the phase ψ associated with the complexified hopping. Throughout the shaded regime, the Chern number is either ± 1 as indicated. What is surprising is that although no net magnetic field is present, the Chern number does not vanish. That band structure can have inherently topological features in the absence of a net magnetic field is the key advance made by the Haldane model.

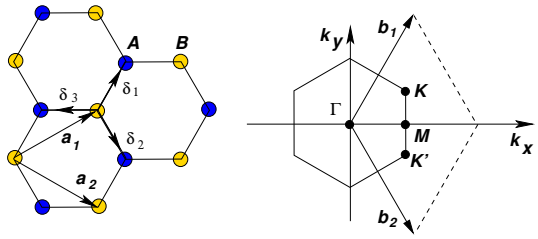

Figure 1.4: Graphene lattice. The panel on the left shows the primitive lattice vectors, $\mathbf{a}_i$, and nearest-neighbour lattice vectors, $\boldsymbol{\delta}_i$. The labels A and B refer to the two kinds of carbon atoms in graphene. The panel on the right shows the first Brillouin zone spanned by the lattice vectors $\mathbf{b_i}$.

where $a = 1.42\mathbf{r}A$, the nearest-neighbour carbon-carbon spacing. The first Brillouin zone shown in Fig. (1.4) is spanned by the reciprocal vectors,

$$\mathbf{b}_1 = \frac{2\pi}{3a}\left(1, \sqrt{3}\right), \quad \mathbf{b}_2 = \frac{2\pi}{3}\left(1, -\sqrt{3}\right). \tag{1.69}$$

The corners of the first Brillouin zone are located at

$$\mathbf{K} = \frac{2\pi}{3a}\left(1, \frac{1}{\sqrt{3}}\right), \quad \mathbf{K}' = \frac{2\pi}{3a}\left(1, -\frac{1}{\sqrt{3}}\right). \tag{1.70}$$

You are to a) write down the tight-binding Hamiltonian for this system and solve it for the energy bands, b) determine the values (there are two) of $\mathbf{k}$ for which the energy dispersion vanishes, c) show that the dispersion can be written as

$$E(\mathbf{q}) = \pm\hbar v_F |\mathbf{q}| \tag{1.71}$$

where $v_F = 3t/2\hbar a \approx 10^6 m/s$ and q is the deviation from the value of the momentum at the zero crossing, and d) show that the effective Hamiltonian near the zero crossings can be written as

$$H \equiv \hbar v_F \begin{pmatrix} 0 & q_x + iq_y \\ q_x - iq_y & 0 \end{pmatrix} = \hbar v_F \sigma \cdot \mathbf{q}.$$

3. Compute the band structure for the Haldane model shown in Fig.(1.62). Show that you end up with Eq. (1.63. Verify numerically that the phase diagram has the structure shown in Fig. (1.3).

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