Tight-Binding Formalism in the Context of the PythTB Package

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(Updated December 6, 2017)

1 Introduction

The empirical tight-binding (TB) method is a useful tool for constructing and solving simple models of the electronic structure of solid-state systems. Essentially, one parametrizes the Hamiltonian matrix elements connecting localized atomic-like basis orbitals, and uses this to compute the band energies and Bloch eigenvectors. Such TB models can, for example, give a highly informative first-order picture of the electronic structure of the CuO planes in a high-T_c superconductor, or of the π bands in graphene or carbon nanotubes. For basic references about the TB approach, see the Wikipedia article [1], the text by Harrison [2], or almost any standard solid-state physics text.

With the strong development of interest in topological insulators after about 2005, TB models have again played a central role as model systems. Examples include the models of Haldane [3], Kane and Mele [4], and Fu, Kane and Mele [5]. In connection with the topological properties, it also becomes crucial to be able to calculate, within the context of the TB model, various quantities that are related in some way to Berry phases or curvatures, including electric polarization, orbital magnetization, anomalous Hall conductivity, Chern indices, the effects of adiabatic cycling of the Hamiltonian, and the like. The definitions of these quantities and practical methods for calculating them are discussed in several review articles [6–9] and a relevant Wikipedia page [10].

The PythTB package (http://www.physics.rutgers.edu/pythtb) is an open-source software package, written in the Python programming/scripting language, that allows for the construction and solution of simple TB models such as those mentioned above. Moreover, it includes tools for calculating many of the Berry-phase related quantities mentioned above. As such, it can be used as a research tool for determining the behavior of model systems, or as a pedagogical tool at the level of a graduate or upper-level undergraduate solid-state physics course.

The present notes outline the TB formalism as it pertains to the PythTB package, providing needed definitions and basic results. In keeping with the capabilities of the PythTB package, we restrict ourselves here to the *orthogonal tight binding* approach, in which the TB basis orbitals are assumed to be orthonormal. We also emphasize that the code is not currently set up to handle realistic chemical interactions. So for example, the Slater-Koster forms [11] for interactions between s, p and d orbitals are not currently coded, although the addition of such features could be considered for a future release.

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2 Basic definitions

For the case of a 3D crystal, the lattice vectors are

$$\mathbf{R} = n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3 \tag{2.1}$$

and the corresponding reciprocal lattice vectors are

$$\mathbf{G} = m_1\mathbf{b}_1 + m_2\mathbf{b}_2 + m_3\mathbf{b}_3 \tag{2.2}$$

where n_i and m_i are integers, and the primitive real and reciprocal lattice vectors obey

$$\mathbf{a}_i \cdot \mathbf{b}_j = 2\pi\,\delta_{ij} \ . \tag{2.3}$$

It follows that

$$e^{i\mathbf{G}\cdot\mathbf{R}} = 1 \tag{2.4}$$

for any pair of real and reciprocal lattice vectors. A wavevector $\mathbf{k}$ in the Brillouin zone (BZ) can be written either in Cartesian coordinates, $\mathbf{k} = k_x\hat{x} + k_y\hat{y} + k_z\hat{z}$, or in internal coordinates, $\mathbf{k} = k_1\mathbf{b}_1 + k_2\mathbf{b}_2 + k_3\mathbf{b}_3$.

The generalization to d dimensions is obvious. (The PYTHTB code also handles the case of $d{=}0$, corresponding to an isolated molecule, cluster, or finite sample.)

Let μ label the atoms in the primitive cell and α label the orbitals on a given atom, and let the TB basis orbitals be $\varphi_{\mu\alpha}(\mathbf{r} - \mathbf{R} - \mathbf{t}_\mu)$ where $\mathbf{t}_\mu$ is the location of atom μ in the home unit cell. Note that it is possible for $\mathbf{r}$ and $\mathbf{t}$ to live in a higher-dimensional space than $\mathbf{R}$ and $\mathbf{k}$. For example, $\mathbf{R}$ and $\mathbf{k}$ would be one-dimensional for a polymer, and they would be two-dimensional for an infinite slab of finite thickness, while $\mathbf{r}$ and $\mathbf{t}$ would remain three-dimensional in both cases.

We now introduce a compound index $j = \{\mu\alpha\}$ that runs over all the L TB orbitals in the primitive cell, and define

$$\phi_{\mathbf{R}j}(\mathbf{r}) = \phi_j(\mathbf{r} - \mathbf{R}) = \varphi_{\mu\alpha}(\mathbf{r} - \mathbf{R} - \mathbf{t}_\mu) \tag{2.5}$$

to be the TB basis orbital of type j in cell $\mathbf{R}$. From now on we drop indices $\mu\alpha$ and work only with j, letting $\mathbf{t}_\mu \to \mathbf{t}_j$.

We now restrict ourselves to a *minimal TB model* having the property that the basis orbitals are orthonormal,

$$\langle\phi_{\mathbf{R}i}|\phi_{\mathbf{R}'j}\rangle = \delta_{\mathbf{R}\mathbf{R}'}\,\delta_{ij} \tag{2.6}$$

and that the position matrix have the simplest possible form,

$$\langle\phi_{\mathbf{R}i}|\mathbf{r}|\phi_{\mathbf{R}'j}\rangle = (\mathbf{R} + \mathbf{t}_j)\,\delta_{\mathbf{R}\mathbf{R}'}\,\delta_{ij} \ . \tag{2.7}$$

The Hamiltonian is assumed to have translational symmetry, so that its matrix elements are defined via

$$H_{ij}(\mathbf{R}) = \langle\phi_{\mathbf{R}'i}|H|\phi_{\mathbf{R}'+\mathbf{R},j}\rangle = \langle\phi_{\mathbf{0}i}|H|\phi_{\mathbf{R},j}\rangle \tag{2.8}$$

and we assume that $H_{ij}(\mathbf{R})$ decays rapidly with increasing $\mathbf{R}$.

3 Transition to the Bloch representation

3.1 Convention I

We construct Bloch-like basis functions

$$\chi_j^{\mathbf{k}}(\mathbf{r}) = \sum_{\mathbf{R}} e^{i\mathbf{k}\cdot(\mathbf{R}+\mathbf{t}_j)} \, \phi_j(\mathbf{r} - \mathbf{R}) \tag{3.1}$$

which we write henceforth in a bra-ket language as

$$|\chi_j^{\mathbf{k}}\rangle = \sum_{\mathbf{R}} e^{i\mathbf{k}\cdot(\mathbf{R}+\mathbf{t}_j)} \, |\phi_{\mathbf{R}j}\rangle \tag{3.2}$$

with the understanding that the normalization is to a single unit cell, i.e.,

$$\langle\chi|\chi'\rangle \equiv \int_{\text{cell}} d^3r \, \chi^*(\mathbf{r}) \, \chi'(\mathbf{r}) \, . \tag{3.3}$$

It follows from Eq. (2.6) that

$$\langle\chi_i^{\mathbf{k}}|\chi_j^{\mathbf{k}}\rangle = \delta_{ij} \, . \tag{3.4}$$

The Bloch eigenstates are then expanded as

$$|\psi_{n\mathbf{k}}\rangle = \sum_j C_j^{n\mathbf{k}} \, |\chi_j^{\mathbf{k}}\rangle \tag{3.5}$$

and the Hamiltonian matrix is constructed as

$$H_{ij}^{\mathbf{k}} = \langle\chi_i^{\mathbf{k}}|H|\chi_j^{\mathbf{k}}\rangle = \sum_{\mathbf{R}} e^{i\mathbf{k}\cdot(\mathbf{R}+\mathbf{t}_j-\mathbf{t}_i)} \, H_{ij}(\mathbf{R}) \, . \tag{3.6}$$

The secular equation to be solved is

$$\mathcal{H}_{\mathbf{k}} \cdot \mathcal{C}_{n\mathbf{k}} = E_{n\mathbf{k}} \, \mathcal{C}_{n\mathbf{k}} \tag{3.7}$$

where $\mathcal{H}_{\mathbf{k}}$ is the $L \times L$ matrix of elements $H_{ij}^{\mathbf{k}}$ and $\mathcal{C}_{n\mathbf{k}}$ is the column vector of elements $C_j^{n\mathbf{k}}$.

This secular equation can be straightforwardly diagonalized to give the TB solution for the energy eigenvalues and eigenvectors. Of course, this TB solution only produces L bands, where L is the number of TB basis orbitals per cell, representing an approximation to the L bands of the crystal that are built from these TB orbitals (usually these are the L lowest valence and conduction bands).

3.2 Convention II

In this convention the phase factor $e^{i\mathbf{k}\cdot\mathbf{t}_j}$ is not included in the definition of the Bloch-like basis functions. Using tilde'd quantities to denote objects defined in Convention II, we get

$$|\widetilde{\chi}_j^{\mathbf{k}}\rangle = \sum_{\mathbf{R}} e^{i\mathbf{k}\cdot\mathbf{R}} \, |\phi_{\mathbf{R}j}\rangle \, , \tag{3.8}$$

$$|\psi_{n\mathbf{k}}\rangle = \sum_j \widetilde{C}_j^{n\mathbf{k}} \, |\widetilde{\chi}_j^{\mathbf{k}}\rangle \, , \tag{3.9}$$

$$\widetilde{H}_{ij}^{\mathbf{k}} = \langle\widetilde{\chi}_i^{\mathbf{k}}|H|\widetilde{\chi}_j^{\mathbf{k}}\rangle = \sum_{\mathbf{R}} e^{i\mathbf{k}\cdot\mathbf{R}} \, H_{ij}(\mathbf{R}) \, . \tag{3.10}$$

$$\widetilde{\mathcal{H}}_{\mathbf{k}} \cdot \widetilde{\mathcal{C}}_{n\mathbf{k}} = E_{n\mathbf{k}} \, \widetilde{\mathcal{C}}_{n\mathbf{k}} \, . \tag{3.11}$$

3.3 Relationship between the two conventions

The quantities in the two conventions are related via

$$\widetilde{H}_{ij}^{\mathbf{k}} = e^{i\mathbf{k}\cdot(\mathbf{t}_i - \mathbf{t}_j)} H_{ij}^{\mathbf{k}} \tag{3.12}$$

and

$$\widetilde{C}_j^{n\mathbf{k}} = e^{i\mathbf{k}\cdot\mathbf{t}_j} C_j^{n\mathbf{k}} . \tag{3.13}$$

The two conventions are essentially just related by a unitary rotation in the L-dimensional space.

When reading the literature, it is a good idea to be careful to determine which convention the authors are using. Convention II is probably the more common one, because the extra factors of $e^{i\mathbf{k}\cdot\mathbf{t}_j}$ can be ignored. However, Convention I is in many ways more natural, especially in connection with the calculation of electric polarization and related Berry-phase quantities, and is the convention adopted in the PYTHTB code.

One way of seeing this is to draw an analogy between the Bloch function $\psi_{n\mathbf{k}}(\mathbf{r})$ and $\widetilde{C}_j^{n\mathbf{k}}$, and between the cell-periodic Bloch function $u_{n\mathbf{k}}(\mathbf{r})$ and $C_j^{n\mathbf{k}}$. Recalling that

$$\psi_{n\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} u_{n\mathbf{k}}(\mathbf{r}) , \tag{3.14}$$

and temporarily adopting the change of notation $C_j^{n\mathbf{k}} \to C_{n\mathbf{k}}(j)$ and similarly for $\widetilde{C}$, we can write

$$|\psi_{n\mathbf{k}}\rangle = \sum_{\mathbf{R}} \int_{\text{cell}} d^3r\, \psi_{n\mathbf{k}}(\mathbf{r})\, e^{i\mathbf{k}\cdot\mathbf{R}} |\mathbf{R} + \mathbf{r}\rangle ,$$

$$\tag{3.15}$$

$$= \sum_{\mathbf{R}} \sum_{j} \widetilde{C}_{n\mathbf{k}}(j)\, e^{i\mathbf{k}\cdot\mathbf{R}} |\phi_{\mathbf{R}j}\rangle , \tag{3.16}$$

while

$$|\psi_{n\mathbf{k}}\rangle = \sum_{\mathbf{R}} \int_{\text{cell}} d^3r\, u_{n\mathbf{k}}(\mathbf{r})\, e^{i\mathbf{k}\cdot(\mathbf{R}+\mathbf{r})} |\mathbf{R} + \mathbf{r}\rangle ,$$

$$\tag{3.17}$$

$$= \sum_{\mathbf{R}} \sum_{j} C_{n\mathbf{k}}(j)\, e^{i\mathbf{k}\cdot(\mathbf{R}+\mathbf{t}_j)} |\phi_{\mathbf{R}j}\rangle . \tag{3.18}$$

To summarize, then, the analogy is

$$\psi_{n\mathbf{k}}(\mathbf{r}) \Leftrightarrow \widetilde{C}_j^{n\mathbf{k}} \qquad \text{and} \qquad u_{n\mathbf{k}}(\mathbf{r}) \Leftrightarrow C_j^{n\mathbf{k}}$$

As we shall see in Sec. 4, it is the cell-periodic functions $u_{n\mathbf{k}}(\mathbf{r})$ that play a central role in the formulation of Berry-phase quantities such as electric polarization. It is largely for this reason that we have adopted Convention I for our PYTHTB implementation, and this convention is assumed for the remainder of these notes.

3.4 Spinor models

Up to this point, the formalism has been written as though for a TB model for "spinless electrons." However, it is easy to generalize to the case of spinors by doubling each TB orbital. That is, we now take the label 'j' (in, e.g., $C_j^{n\mathbf{k}}$) be a condensed notation $j = \{\mu\alpha s\}$ for spin s (up or down along z) and orbital α on atom μ, with $j = 1, ..., 2L$. The real-space Hamiltonian becomes $H_{ij,ss'}(\mathbf{R}) = \langle \phi_{0is}|H|\phi_{\mathbf{R}js'}\rangle$ and $H_{ij,ss'}^{\mathbf{k}}$ is constructed from it in analogy with Eq. (3.6). From the Bloch solutions, spin densities

$$n_{i,ss'} = \frac{1}{N}\sum_{n\mathbf{k}}^{\text{occ}} (C_{is}^{n\mathbf{k}})^* C_{is'}^{n\mathbf{k}} \tag{3.19}$$

can also be constructed, where N is the number of $\mathbf{k}$-points in the BZ. The particle density n_i is the trace of the corresponding spin density matrix.

Clearly the Hamiltonian can be regarded as an $L \times L$ matrix of 2×2 blocks. An alternative notation (either in real or reciprocal space) is

$$H_{ij,ss'} = \sum_a h_{ij,a}\sigma_{a,ss'} \tag{3.20}$$

where $a = \{0, 1, 2, 3\}$, $\sigma_0 = E$ (the 2×2 identity), and σ_a is the Pauli spin matrix for $a \neq 0$. A similar notation can be adopted for spin densities.

The PYTHTB code package has features to allow the user to define a spinor TB Hamiltonian and to set spin-independent or spin-dependent onsite energies and intersite hoppings. Spin-dependent terms can be input either as 2×2 matrices or using the $\sum_a h_{ij,a}\sigma_{a,ss'}$ four-vector notation.

4 Berry potential, Berry curvature, and Berry phase

In this section we concentrate on establishing the definitions of, and basic relations among, the various quantities related to Berry phases. The reader is referred to the references [6–10] mentioned in the Introduction for derivations and for explanations of the physical significance of the various quantities.

In view of the comments in Sec. 3.3, we now change notation and write the column vector of coefficients $C_j^{\mathbf{k}}$ as a ket vector $|u_n(\mathbf{k})\rangle$,

$$\begin{pmatrix} C_1^{\mathbf{k}} \\ \vdots \\ C_d^{\mathbf{k}} \end{pmatrix} \quad \Rightarrow \quad |u_n(\mathbf{k})\rangle \tag{4.1}$$

and the corresponding row vector of conjugated elements as $\langle u_n(\mathbf{k})|$. We also consider that the Bloch states may be functions of a set of g parameters $\lambda_1, ..., \lambda_g$ in addition to the d elements of $\mathbf{k} = k_1, ..., k_d$. In fact, we further generalize the notation so that $\mathbf{\Lambda} = \{\Lambda_1, ..., \Lambda_{d+g}\} = \{k_1, ..., k_d, \lambda_1, ..., \lambda_g\}$. (In special cases it is possible to have $g = 0$, signifying no external parameters, or to have $d=0$, as for a molecule subjected to a set of external fields.) We assume that the state (or band) n remains non-degenerate with neighboring states (or bands) throughout the relevant region of $\mathbf{\Lambda}$-space.

The Schrödinger equation is then

$$H_{\mathbf{\Lambda}}|u_n(\Lambda)\rangle = E_n(\Lambda)|u_n(\Lambda)\rangle \tag{4.2}$$

5

where $H_\mathbf{\Lambda} = H_\mathbf{k}(\lambda_1, ..., \lambda_g)$. In what follows we will typically drop the explicit argument $\mathbf{\Lambda}$, letting it be understood that all quantities (including A and Ω to be defined shortly) are functions of Λ as well. We also henceforth adopt the notation that $\partial_a = \partial/\partial\Lambda_a$.

4.1 Single band

For a single isolated band n (i.e., one that does not touch a higher or lower band anywhere in the BZ) we define the Berry connection

$$A_{n,a} = i\langle u_n | \partial_a u_n \rangle \; , \tag{4.3}$$

and the Berry curvature

$$\begin{aligned}\Omega_{n,ab} &= \partial_a A_{n,b} - \partial_b A_{n,a} \\ &= i\langle \partial_a u_n | \partial_b u_n \rangle - i\langle \partial_b u_n | \partial_a u_n \rangle = -2\,\mathrm{Im}\,\langle \partial_a u_n | \partial_b u_n \rangle \; ,\end{aligned} \tag{4.4}$$

where a and b run over the $(d+g)$-dimensional generalized parameter space. A Berry phase ϕ_n is associated with the phase evolution of the n'th state over a closed curve $\mathcal{C}$ in this space via

$$\phi_n = \oint_\mathcal{C} \mathbf{A}_n \cdot d\mathbf{\Lambda} = \oint_\mathcal{C} A_{n,a}\, d\Lambda_a \; , \tag{4.5}$$

where an implied sum notation is used on the right side of the second equality and similarly in other equations to follow. If $\mathcal{C}$ is the boundary of a surface S, then by Stokes's theorem we may also write

$$\phi_n = \int_\mathcal{S} \varepsilon_{abc}\,\Omega_{n,ab}\, dS_c \; . \tag{4.6}$$

In the special case that S is a closed surface, the integral of its Berry curvature is guaranteed to be 2π times an integer index knows as the Chern number (or, more precisely, the "first Chern index"). That is,

$$\oint_\mathcal{S} \varepsilon_{abc}\,\Omega_{n,ab}\, dS_c = 2\pi c_n \tag{4.7}$$

where c_n is the Chern number.

There is a $\mathcal{U}(1)$ "gauge freedom" in the choice of the phases of the Bloch functions. That is, given a manifold $|u_n(\mathbf{\Lambda})\rangle$, one can define a physically identical manifold

$$|\tilde{u}_n(\mathbf{\Lambda})\rangle = e^{i\beta(\mathbf{\Lambda})}\,|u_n(\mathbf{\Lambda})\rangle \tag{4.8}$$

where $\beta(\mathbf{\Lambda})$ is a smooth and continuous real function of $\mathbf{\Lambda}$. The Berry potential $A_{n,a}(\mathbf{\Lambda})$ is gauge-dependent; the Berry phase ϕ_n is gauge-invariant modulo 2π;[1] and the Berry curvature $\Omega_{n,ab}(\mathbf{\Lambda})$ (and therefor the Chern number c_n) is fully gauge-invariant.

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[1]If the loop $\mathcal{C}$ is continuously contractible to zero in an obvious way, then a unique Berry phase can be assigned by assuming ϕ_n to vanish for the zero-size loop. This may not be possible, however, if the loop surrounds a region of degeneracy with neighboring bands, or if it is defined on a topologically nontrivial space with uncontractible cycles (see, e.g., Sec. 4.4).

4.2 Two and three dimensions

In two dimensions, it is convenient to treat $\Omega_n = -2\text{Im}\,\langle\partial_1 u_n|\partial_2 u_n\rangle$ as a scalar, and the Berry phase is just $\phi_n = \oint_{\mathcal{C}} \Omega_n\, dS$.

In three dimensions, it is a common practice to use the axial vector notation for the Berry curvature, i.e.,

$$\Omega_{n,a} = \frac{1}{2}\varepsilon_{abc}\,\Omega_{n,bc} \qquad \Leftrightarrow \qquad \Omega_{n,bc} = \varepsilon_{abc}\Omega_{n,a} \tag{4.9}$$

in which case the Berry phase is just $\phi_n = \int_{\mathcal{S}} \mathbf{\Omega}_n \cdot d\mathbf{S}$.

4.3 Multiband case

It is often the case that one wants to treat all the N_b occupied bands of an insulator as a joint band manifold. This is sometimes referred to as the "non-Abelian" case, because the formalism involves $N_\text{b} \times N_\text{b}$ matrices that do not necessarily commute. We now assume that this group of bands does not touch with those below or above in energy in the relevant region of $\mathbf{\Lambda}$-space; assuming the bands of interest are the occupied valence bands of a crystalline solid, this follows if the crystal is an insulator. The appropriate generalizations of the above equations are as follows.

$$A_{mn,a} = i\langle u_m|\partial_a u_n\rangle\,, \tag{4.10}$$

$$
\begin{aligned}
\Omega_{mn,ab} &= \partial_a A_{mn,b} - \partial_b A_{mn,a} - i[A_a, A_b]_{mn}\\
&= i\langle\partial_a u_m|\partial_b u_n\rangle - i\langle\partial_b u_m|\partial_a u_n\rangle\,,
\end{aligned}
\tag{4.11}
$$

$$
\begin{aligned}
\phi &= \oint_{\mathcal{C}} \text{Tr}\,[A_a]\, d\Lambda_a \tag{4.12}\\
&= \int_{\mathcal{S}} \varepsilon_{abc}\,\text{Tr}\,[\Omega_{ab}]\, dS_c\,. \tag{4.13}
\end{aligned}
$$

and

$$\oint_{\mathcal{S}} \varepsilon_{abc}\,\text{Tr}\,[\Omega_{ab}]\, dS_c = 2\pi c \tag{4.14}$$

where Tr denotes a trace over an $N_\text{b} \times N_\text{b}$ matrix.

There is now a $\mathcal{U}(N_\text{b})$ gauge freedom in the choice of the Bloch functions. That is, given a manifold $|u_m(\Lambda)\rangle$, one can define a physically identical manifold

$$|\tilde{u}_n(\mathbf{\Lambda})\rangle = \sum_m U_{mn}(\mathbf{\Lambda})\,|u_m(\mathbf{\Lambda})\rangle \tag{4.15}$$

where $U_{mn}(\mathbf{\Lambda})$ is an $N_\text{b} \times N_\text{b}$ unitary matrix that depends smoothly and continuously on $\mathbf{\Lambda}$. The Berry potential $A_{mn,a}(\mathbf{\Lambda})$ is gauge-dependent; the Berry phase ϕ is gauge-invariant modulo 2π; the Berry curvature $\Omega_{mn,ab}(\mathbf{\Lambda})$ is gauge-covariant; and its trace, and therefore the Chern number c, are fully gauge-invariant.

4.4 Periodic gauge in k-space and cycles in the BZ

The Bloch solutions $\psi_{n,\mathbf{k}+\mathbf{G}}(\mathbf{r})$ and $\psi_{n,\mathbf{k}}(\mathbf{r})$ represent the same physical state, since they obey the same Schrödinger equation and the same boundary conditions $\psi_{n,\mathbf{k}}(\mathbf{r}+\mathbf{R}) = e^{i\mathbf{k}\cdot\mathbf{r}}\psi_{n,\mathbf{k}}(\mathbf{r})$, as follows from Eq. (2.4). It follows that $\psi_{n,\mathbf{k}+\mathbf{G}}(\mathbf{r})$ and $\psi_{n,\mathbf{k}}(\mathbf{r})$ can differ only by a phase. By convention, we normally take them to be exactly equal,

$$\psi_{n,\mathbf{k}+\mathbf{G}}(\mathbf{r}) = \psi_{n,\mathbf{k}}(\mathbf{r}) \ , \tag{4.16}$$

a conditions that is knows as the "periodic gauge" condition. It then follows from Eq. (3.14) that

$$u_{n,\mathbf{k}+\mathbf{G}}(\mathbf{r}) = e^{-i\mathbf{G}\cdot\mathbf{r}}\,u_{n\mathbf{k}}(\mathbf{r}) \tag{4.17}$$

Reversing the notation of Eq. (4.1) back into the explicit TB language, this means that

$$C_j^{n,\mathbf{k}+\mathbf{G}} = e^{-i\mathbf{G}\cdot\mathbf{t}_j}\,C_j^{n\mathbf{k}} \ . \tag{4.18}$$

Because of this periodicity, the BZ in d dimensional $\mathbf{k}$-space can be regarded as a d-torus. We are often interested in calculating the Berry phase as we go around a loop in $\mathbf{k}$-space that cycles around the torus. For example, the component of the electric polarization in the direction of primitive lattice vector $\mathbf{a}_j$ is computed by considering cycles in which $\mathbf{k} \to \mathbf{k} + \mathbf{b}_j$ from beginning to end. When closing the loop and identifying $\mathbf{k}$ with $\mathbf{k} + \mathbf{b}_j$, it is important to remember to use Eq. (4.18). The Berry phase associated with the electric polarization has an intrinsic ambiguity modulo 2π, since the loop on which it is defined is not contractible to zero.

4.5 Discretized formulas for Berry quantities

Practical calculations are done on a mesh of $\mathbf{k}$-points or parameter values. For example, to compute the Berry phase associated with a given loop in $\boldsymbol{\Lambda}$-space, the loop $\mathcal{C}$ is discretized into a large number of closely spaced points $\boldsymbol{\Lambda}_i$, and the integrand of Eq. (4.12) is approximated by the discretized formula for the (traced) Berry connection

$$\mathrm{Tr}\,[\mathbf{A}]\cdot\Delta\boldsymbol{\Lambda} = -\mathrm{Im}\,\ln\det M^{(\boldsymbol{\Lambda}_i,\boldsymbol{\Lambda}_{i+1})} \tag{4.19}$$

where M is a $N_\mathrm{b} \times N_\mathrm{b}$ matrix defined as

$$M_{mn}^{(\boldsymbol{\Lambda}_i,\boldsymbol{\Lambda}_{i+1})} = \langle u_m^{(\boldsymbol{\Lambda}_i)}|u_n^{(\boldsymbol{\Lambda}_{i+1})}\rangle \tag{4.20}$$

and $\Delta\boldsymbol{\Lambda} = \boldsymbol{\Lambda}_{i+1} - \boldsymbol{\Lambda}_i$. The expression for the Berry phase then becomes

$$\phi = -\sum_i \mathrm{Im}\,\ln\det M^{(\boldsymbol{\Lambda}_i,\boldsymbol{\Lambda}_{i+1})} = -\mathrm{Im}\,\ln\prod_i \det M^{(\boldsymbol{\Lambda}_i,\boldsymbol{\Lambda}_{i+1})} \ . \tag{4.21}$$

The discretized approximation to the local Berry curvature is obtained by considering a loop around a small plaquette with vertices $\boldsymbol{\Lambda}_i$, computing the Berry phase around this loop as above, and dividing by the area of the plaquette.

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