Facultad
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Ciencias

Topological phase transitions in the one dimensional $s - p$ model

(Transiciones de fase topológicas en el modelo $s - p$ unidimensional)

Trabajo de Fin de Grado
para acceder al

GRADO EN FÍSICA

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Junio - 2019

Abstract

In the present work, we shall study the topological phase transition that takes place in the one dimensional $s-p$ model. This transition will be studied in two ways. In the first way, the topological transition takes place in a sudden way. The interactions between the orbitals will depend on a parameter that, when varied continuously, closes the gap and allows the topological transition to take place. The system goes from an atomic-like bonding to a covalent bonding. In the second way, the topological transition is made in a smooth way. The parameter in which the Hamiltonian depends never closes the gap directly. The center of the Wannier functions shift continuously, even shifting a full lattice constant. Finally, we studied the "'bulk-boundary" correspondence, which allows to explain why the second way performs a topological transition if the gap is never directly closed.

Key words: tight-binding model, topological phase transition, topological insulator, Wannier functions.

Resumen

En este trabajo, se estudiará la transición de fase topológica que tiene lugar en el modelo $s-p$ unidimensional. Esta transición será estudiada empleando dos métodos. En el primer método, la transición topológica tine lugar de una manera repentina. Las interacciones entre los orbitales dependerán de un parámetro que, al ser variado de una forma continua, cierra el gap y permite que la transición topológica tenga lugar. El sistema pasa de un enlace tipo atómico a un enlace covalente. En el segundo método, la transición topológica tiene lugar de una manera más suave. El parámetro del que depende el Hamiltoniano del sistema nunca cierra el gap directamente. El centro de las funciones de Wannier se desplaza de una forma continuada, hasta desplazarse una constante de red. Por último, se estudió la correspondencia "bulk-boundary", que permite explicar por qué en el segundo método una transición topológica tiene lugar si el gap nunca se cierra directamente.

Palabras clave: modelo de enlace fuerte, transición de fase topológica, aislante topológico, funciones de Wannier.

CONTENTS

1. Introduction

The combination of the scientific fields of Condensed Matter Physics and Topology is a topic that is generating enormous interest nowadays. Since 2016, when the Nobel Prize was awarded to the British scientists Thouless, Duncan Haldane and Kosterlitz "for theoretical discoveries of topological phase transitions and topological phases of matter", this topic has become more and more popular.

Topology is the branch of mathematics that describes the properties that remain intact when an object is stretched, twisted, bent or, summarizing, deformed. However, not every kind of deformation is valid. The object must not be torn apart or glued together to maintain these properties, which means that no holes can be created or destroyed.

There is a well-known joke that says that a topologist is someone who can not tell the difference between a doughnut and a coffee mug. This joke just makes reference to the fact that these two objects are topologically equivalent, as they both have the same number of holes. One can transform one object into the other, and the other way around, only by continuously deforming them as seen in Fig. 1. Similarly, a beach ball and the computer in which I am writing this work are also topologically equivalent, as none of them have any holes.

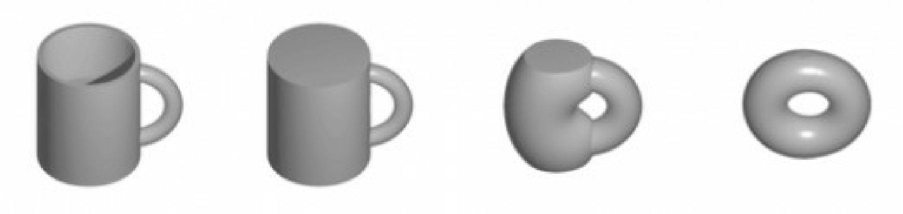

Figure 1: Continuous deformation of a coffee mug into a doughnut.

In the present work, we are going to study the simplest electronic structure model for a system that can vary from an atomic-like to a covalent bonding, taking place a topological phase transition. This model has one atom per unit cell and two orbitals, which are an even-symmetry s orbital and an odd-symmetry p orbital.

As it will be seen from their band structures, both states are insulators, as a gap separates their lower and upper bands. Qualitatively, only by looking at their band structures, no one would be able to tell the difference between them. However, these two states are topologically different.

Two topological insulators are said to belong to the same topological class if their Hamiltonians can be continuously connected in such way that the gap never closes at any point along the connecting path. And why is the closing of the gap associated with a topological transition? This is due to the fact that at the points of the Brillouin zone where the gap closes, the eigenstates become degenerate. The states from the upper and the lower bands can exchange eigenvectors in these points, changing then the way the set of eigenvectors connect in the Brillouin zone.

Similarly to the topology of surfaces, where a "violent event" that creates or destroys a hole in a surface changes its classification, in this particular example the "violent event" that changes the classification of the topological insulator is the closing of the gap.

In our example, when continuously varying the Hamiltonian of the system, the gap will close in a particular point. This is the point where the exchange of eigenvectors happens, and the system becomes metallic due to the degeneracy of the eigenstates at the closing points.

This topological phase transition can be observed in where the Wannier functions, which give the position of the center of the bands, are centered. In the initial situation, there is an atomic bonding, as the Wannier functions are centered in the positions of the atoms. Immediately after the topological transition happens, right after the gap closes and the system becomes metallic, there is a covalent bonding. In this state, the Wannier functions are not centered anymore in the atoms. Instead, they are centered in the bonding between them.

This work is closely related with three subjects that I coursed in this degree. The first one is *Física Cuántica y Estructura de la Materia III: Física del Estado Sólido.* In this subject, I studied the basic physical concepts in which this work is based, such as the tight-binding model. In addition to this, two other subjects were specially useful in this work. These subjects are *Métodos Numéricos* and *Advanced Computation.* These two subjects played a key role in the development of the code used in this work, which can be found in the CD and was written in *MATLAB. Métodos Numéricos* was extremely helpful in the learning of the programming language in which the code was written, while *Advanced Computation* helped me to understand how to relate a physics problem with the coding of a program to solve it.

2. Method: Tight-Binding model

The tight-binding model is a theory developed by the Swiss physicist Felix Bloch in 1928. This model is an approach to the calculation of the electronic band structure that introduces a number of approximations, but none of them are so severe that they modify the physical forces that determine structural and dynamical properties.

The first assumption that is made in the tight-binding model is that next to each lattice point, the crystal hamiltonian can be approximated by the hamiltonian of a single atom located at that lattice point. In addition, it is also assumed that the bound states of the atomic Hamiltonian are well localized. This means that if $\phi_\mu(\vec{r}-\vec{R}_I)$ is the wavefunction for an electron in a bound state in the lattice position $\vec{R}_I$ with energy E_μ (being μ a coefficient that can run over every atomic orbital of a given atom), then

$$\hat{H}_{\text{at}}(\vec{r}-\vec{R}_{\text{I}})\phi_\mu(\vec{r}-\vec{R}_{\text{I}}) = E_\mu\phi_\mu(\vec{r}-\vec{R}_{\text{I}}), \tag{1}$$

where $\hat{H}_{\text{at}}$ is the hamiltonian for a free atom in the lattice position $\vec{R}_{\text{I}}$. The set of functions $\phi_\mu(\vec{r})$, each associated with an atom in the unit cell at the position $\vec{R}_{\text{I}}$, will form a basis of localized functions.

The problem is now to solve the time-independent Schrödinger equation for a single electron, described below in Eq. (2). It is also assumed that the potential in which the electron is found is a periodic potential. This means that $V(\vec{r}) = V(\vec{r}+\vec{T})$, where $\vec{T}$ is the translation vector that reproduces the periodicity of the lattice.

$$\hat{H}\psi(\vec{r}) = \left[-\frac{\hbar^2}{2m}\nabla^2 + V(\vec{r})\right]\psi(\vec{r}) = E\psi(\vec{r}). \tag{2}$$

Due to the periodicity of the potential, the eigenfunctions of the hamiltonian must comply with the Bloch theorem, which affirms that these solutions can be expressed as the product of a plane wave times a function with the periodicity of the lattice

$$\psi_{n\vec{k}} = e^{i\vec{k}\cdot\vec{r}} u_{n\vec{k}}(\vec{r}), \tag{3}$$

where $u_{n\vec{k}}(\vec{r}+\vec{T}) = u_{n\vec{k}}(\vec{r})$. These solutions are characterized by two quantum numbers: n, which is discrete and provides the band index, and $\vec{k}$, which is a continuum wave vector.

Since the eigenfunctions of the Hamiltonian must comply with the Bloch theorem, a good starting point is to construct from the localized atomic orbitals $\phi_\mu(\vec{r}-\vec{R}_I)$ a delocalized basis for each $\vec{k}$-point already compliant with this theorem,

$$\phi_{\mu\vec{k}}(\vec{r}) = \sum_{\vec{T}} e^{i\vec{k}\cdot(\vec{T}+\vec{R}_I)}\phi_\mu(\vec{r}-\vec{R}_I), \tag{4}$$

and then, as a good approximation, assume that the eigenfunctions can be expressed as a linear combination of these Bloch-like atomic orbitals

$$\psi_{n\vec{k}}(\vec{r}) \approx \Phi_{n\vec{k}}(\vec{r}) = \sum_{\mu} c_{\mu n}(\vec{k})\phi_{\mu\vec{k}}(\vec{r}). \tag{5}$$

With this approximation, the problem has now become into how to compute the coefficients of the expansion $c_{\mu n}(\vec{k})$ and the discrete set of eigenvalues $E_n(\vec{k})$. In order to do this, this expansion is introduced in the Schrödinger equation [Eq. (2)], and it arrives to

$$\sum_{\mu} c_{\mu n}(\vec{k})\hat{H}\phi_{\mu\vec{k}}(\vec{r}) = E_n(\vec{k})\sum_{\mu} c_{\mu n}(\vec{k})\phi_{\mu\vec{k}}(\vec{r}). \tag{6}$$

If this expression is now multiplied at the left by $\phi^*_{\nu\vec{k}}(\vec{r})$ and is integrated all over the space, we obtain

$$\sum_{\mu} c_{\mu n}(\vec{k})\int \phi^*_{\nu\vec{k}}(\vec{r})\hat{H}\phi_{\mu\vec{k}}(\vec{r})d\vec{r} = E_n(\vec{k})\sum_{\mu} c_{\mu n}(\vec{k})\int \phi^*_{\nu\vec{k}}(\vec{r})\phi_{\mu\vec{k}}(\vec{r})d\vec{r}. \tag{7}$$

This expression can then be rewritten as

$$\sum_{\mu} c_{\mu n}(\vec{k})H_{\nu\mu}(\vec{k}) = E_n(\vec{k})\sum_{\mu} c_{\mu n}(\vec{k})S_{\nu\mu}(\vec{k}), \tag{8}$$

where

$$H_{\nu\mu}(\vec{k}) = \int \phi^*_{\nu\vec{k}}(\vec{r})\hat{H}\phi_{\mu\vec{k}}(\vec{r})d\vec{r}, \tag{9a}$$

$$S_{\nu\mu}(\vec{k}) = \int \phi^*_{\nu\vec{k}}(\vec{r})\phi_{\mu\vec{k}}(\vec{r})d\vec{r}, \tag{9b}$$

are known, respectively, as the Hamiltonian and Overlap matrices. If Eq. (8) is reordered by transposing all the terms to the left-hand side, the so-called secular equation is obtained

$$\sum_{\mu}\left[H_{\nu\mu}(\vec{k}) - E_n(\vec{k})S_{\nu\mu}(\vec{k})\right]c_{\mu n}(\vec{k}) = 0. \tag{10}$$

The secular equation can be expressed in a matricial notation, which is

$$\left(H(\vec{k})\right)\left(c_n(\vec{k})\right) = E_n(\vec{k})\left(S(\vec{k})\right)\left(c_n(\vec{k})\right), \tag{11}$$

where the dimensions of the Hamiltonian and the Overlap matrices are $N \times N$, and the dimensions of the coefficients matrix are $N \times 1$ (a column vector), being N the number of atomic orbitals in the unit cell.

Both the Hamiltonian and the Overlap matrices in Eq. (11) are in the reciprocal space. However, their matrix elements can be computed from the sums of the Hamiltonian and the Overlap matrices in real space modulated by a phase by using the expressions

$$H_{\nu\mu}(\vec{k}) = \langle\phi_\nu(\vec{k})|\hat{H}|\phi_\mu(\vec{k})\rangle = \sum_{\vec{T}} e^{i\vec{k}\cdot\vec{T}}H_{\nu\mu}(\vec{T}), \tag{12}$$

and

$$S_{\nu\mu}(\vec{k}) = \langle\phi_\nu(\vec{k})|\phi_\mu(\vec{k})\rangle = \sum_{\vec{T}} e^{i\vec{k}\cdot\vec{T}}S_{\nu\mu}(\vec{T}), \tag{13}$$

where

$$H_{\nu\mu}(\vec{T}) = \int \phi^*_{\nu}(\vec{r})\hat{H}\phi_{\mu}(\vec{r}-\vec{T})d\vec{r}, \tag{14a}$$

$$S_{\nu\mu}(\vec{T}) = \int \phi^*_{\nu}(\vec{r})\phi_{\mu}(\vec{r}-\vec{T})d\vec{r}, \tag{14b}$$

Standard numerical packages can easily be used to solve the generalized eigenvalue problem given in Eq. (11), which amounts to diagonalizing the Hamiltonian $H(\vec{k})$, thereby giving the tight-binding solution for the energy eigenvalues and eigenvectors. This tight-binding solution produces only N bands, representing an approximation to the N bands of the crystal that are built from the tight-binding orbitals. [1]

Different philosophies may be applied during the implementation of these ideas. On the one hand we can find accurate methods, known as *ab-initio linear combination of atomic orbitals*, where the matrix elements of the Hamiltonian and Overlap matrix that appear in Eqs. (14a)-(14b) are computed explicitly, usually at the level of the Density Functional Theory (DFT). That is the case of the SIESTA code [2]. On the other hand, there are less accurate models, known as *empirical tight-binding* approaches, where: (i) we focus only on those atomic orbitals required to describe the valence and, might be, the lowest occupied states of the system of interest; and (ii) where the Hamiltonian and Overlap matrices between them appearing in Eqs. (14a)-(14b) are parametrized in a model-building sense. Typically, the Hamiltonian matrix elements are truncated to first-neighbours, and the Overlap matrix is taken as diagonal (i. e. we assume no overlap between the localized atomic orbitals in the basis), in the so-called "orthogonal tight binding"). Since in the empirical tight-binding method the atomic orbitals are never explicitly constructed, the corresponding eigenstates of the Hamiltonian $\psi_{n\vec{k}}(\vec{r})$ are never explicitly constructed; the vector of coefficients $c_{\mu n}(\vec{k})$ in Eq. (10) plays the role of the eigenstate instead [1]. In this work, we shall follow this second strategy.

3. Our model: The two-state $s-p$ model in one dimension

The model that is going to be studied is the two state $s-p$ in one dimension. Within this model, we shall assume:

- A monoatomic infinite periodic linear chain of identical atoms.
- One atom per unit cell. The size of the unit cell will be denoted by a.
- Two basis function (of atomic-like shape) per atom. The first orbital will have a spherical even s-symmetry, while the second will display the odd symmetry characteristic of the p-orbitals.

A schematic representation of the atoms and the basis functions is shown in Fig. 2.

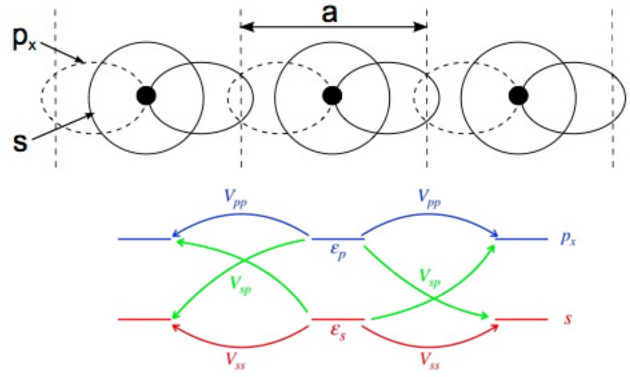

Figure 2: Schematic representation of the two-state $s-p$ model and the interactions between its orbitals, where a is the length of the unit cell.

Regarding the parameters that will be included in the model, we shall consider:

1. On-site interactions of one s- (ε_s) or p-orbital (ε_p) with itself.

2. First-neighbour interactions between two s orbitals (V_{ss}), between two p orbitals (V_{pp}) or between an s and a p orbital in neighbour atoms (V_{sp}).
3. Orthogonal orbitals: if the basis set of atomic orbitals is sufficiently localized, then they have only significant values around the atom where it is centered. To a first approximation, we can retain only the overlap of one orbital with itself, and neglect all the rest of the overlap integrals. The overlap matrix will be diagonal and, if the orbitals are normalized, the diagonal element will be the unity.
4. The orthogonality condition implies that, in a given site, the s orbital does not interact with the p orbital.

The topological transitions that we shall consider in this work will be defined by the way the eigenvectors of the Hamiltonian will change as a function of the wave vector k, that will be taken as a parameter that can be varied continuously in the first Brillouin zone. Therefore, we have to find the matrix elements of the Hamiltonian operator $H(k)$. Within our model, the dimensions of all the Hamiltonian and Overlap matrices in k-space will be (2×2). To define each matrix element, we shall make use of Eqs. (12)-(13).

The element in the position (1,1) will be the interaction between two s orbitals, H_{ss}. As only on-site and nearest neighbours interactions are going to be taken into account, then the only allowed values for the translation vector $\vec{T}$ are $\vec{T} = 0$ and $\vec{T} = \pm\vec{a}$. Summing over these translation vectors, the matrix element is

$$H_{ss}(k) = H_{ss}(\vec{T} = 0) + e^{ika} H_{ss}(\vec{a}) + e^{-ika} H_{ss}(-\vec{a}), \tag{15}$$

where $H_{ss}(\vec{T} = 0)$ is the on-site interaction, so its value is ε_s and $H_{ss}(\pm\vec{a})$ are the nearest neighbour interactions between two s orbitals, whose value is denoted as V_{ss}. Introducing these terms, and making use of the relationship $\cos x = \frac{e^{ix}+e^{-ix}}{2}$, then the matrix element reduces to

$$H_{ss}(k) = \varepsilon_s + 2V_{ss} \cos ka. \tag{16}$$

The same procedure can be used for the interaction between two p orbitals [position (2,2) of the Hamiltonian matrix in k-space], that can be written as

$$H_{pp}(k) = \varepsilon_p + 2V_{pp} \cos ka. \tag{17}$$

Now the off-diagonal terms, that account for the interactions between an s and a p orbital are going to be computed. For these matrix elements, only the interactions at $\vec{T} = \pm\vec{a}$ are needed to be taken into account, since there is no on-site interaction between these two orbitals. The matrix element (1,2) is then

$$H_{sp}(k) = e^{ika} H_{sp}(\vec{a}) + e^{-ika} H_{sp}(-\vec{a}). \tag{18}$$

Since the p orbital has a positive and a negative lobule, when the s orbital interacts with the p orbital in $\vec{T} = \vec{a}$, it is interacting with its negative part, so the interaction will have a negative sign. Using the equation $\sin x = \frac{e^{ix}-e^{-ix}}{2i}$, considering that $|H_{sp}(\pm\vec{a})| = V_{sp}$ and taking into account the polarization of the p orbital, the matrix element is given by

$$H_{sp}(k) = e^{ika}(-V_{sp}) + e^{-ika} V_{sp} = -2iV_{sp} \sin ka. \tag{19}$$

The procedure is identical for the interaction between a p and an s orbital, but this time the negative sign due to the polarization of the p orbital appears in $\vec{T}=-\vec{a}$. For this reason, the matrix element for the interaction between a p and an s orbital is

$$H_{ps}(k)=e^{ika}(V_{sp})+e^{-ika}(-V_{sp})=2iV_{sp}\sin ka. \tag{20}$$

Since all the elements are known, the Hamiltonian can be expressed in a matricial notation as

$$H(k)=\begin{pmatrix}\varepsilon_s+2V_{ss}\cos ka & -2iV_{sp}\sin ka\\ 2iV_{sp}\sin ka & \varepsilon_p+2V_{pp}\cos ka\end{pmatrix}. \tag{21}$$

Due to the polarization of the p orbital, it can be observed that when a p orbital interacts with its nearest neighbour, the interaction is always between a positive and a negative part of the orbitals. For this reason, V_{pp} will have to be negative. If the V_{pp} were taken as positive, then this polarization should be taken into account by changing the sign of the nearest neighbour interaction, and the (2,2) matrix element would be $\varepsilon_p-2V_{pp}\cos ka$.

All the (2×2) matrices can be written as a linear combination, with complex coefficients, of the three Pauli matrices, τ_i, and the identity matrix τ_0. This is due to the fact that any matrix (2×2) has only four entries, so a basis of four independent (2×2) matrices should be enough to expand them. Therefore,

$$H(k)=\sum_{i=1}^{3}h_i(k)\tau_i+h_0(k)\tau_0, \tag{22}$$

where

$$\tau_1=\begin{pmatrix}0&1\\1&0\end{pmatrix},\ \tau_2=\begin{pmatrix}0&-i\\i&0\end{pmatrix},\ \tau_3=\begin{pmatrix}1&0\\0&-1\end{pmatrix},\ \text{and}\ \tau_0=\begin{pmatrix}1&0\\0&1\end{pmatrix}. \tag{23}$$

The coefficient for the identity matrix is

$$h_0=\frac{\varepsilon_s+\varepsilon_p}{2}+(V_{ss}+V_{pp})\cos(ka). \tag{24}$$

For many purposes it can be ignored because it represents a shift in the energy that is the same for the two bands (this coefficient multiplies the diagonal unity matrix). It cannot affect the difference between the two eigenvalues or the eigenfunctions of the different bands: both of them would move upwards or downwards by the same amount and this term cannot be responsible for the closing of gap, or the exchange of character of the bands.

For the other three coefficients required to expand the Hamiltonian matrix of Eq. (21) in the basis of Pauli matrices, h_1, h_2 and h_3, they can be expressed as a vector

$$\vec{h}(\vec{k})=\left(u, w\sin(ka), \Delta+d\cos(ka)\right), \tag{25}$$

as represented in Fig. 3, where the analytical expressions for the different terms appearing in Eq. (25) are given by

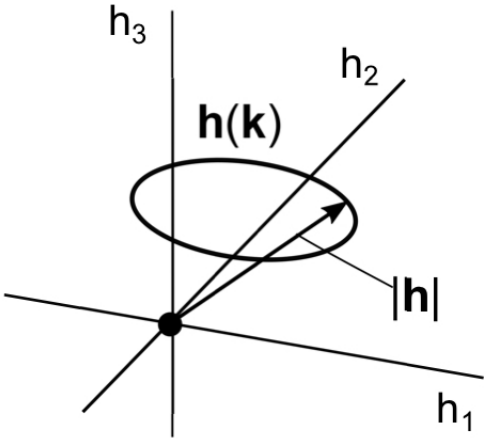

Figure 3: The three dimensional space defined by the coefficients (h_1, h_2, h_3) of the Pauli matrices are expressed as vector $\vec{h}$. The curve depicts the hamiltonian $\vec{h}(k)$ whose eigenvalues are $\pm|\vec{h}|$, where $|\vec{h}|$ is the distance to the origin. The gap vanishes if the curve passes through the origin where $\vec{h}(k) = 0$. Reproduced with permission from Ref. [3].

$$\begin{aligned} \Delta &= \frac{\varepsilon_s - \varepsilon_p}{2}, \\ d &= V_{ss} - V_{pp}, \\ w &= 2V_{sp}, \\ u &= 0. \end{aligned} \tag{26}$$

In order to obtain the eigenvalues, the Hamiltonian matrix has to be diagonalized.

As this Hamiltonian is a 2×2 matrix, it can be written as a combination of the Pauli matrices as shown in Eq. (22). In order to perform this diagonalization, the term that goes with the identity matrix (τ_0) is passed to the left-hand side, having now $H(k) - h_0\tau_0 = h_1\tau_1 + h_2\tau_2 + h_3\tau_3$. Subtracting the coefficient h_0 in the diagonal of the hamiltonian, the matrix in the left-hand side is now

$$H(k) - h_0\tau_0 = \begin{pmatrix} \frac{\varepsilon_s - \varepsilon_p}{2} + (V_{ss} - V_{pp})\cos ka & -2iV_{sp}\sin ka \\ 2iV_{sp}\sin ka & \frac{\varepsilon_p - \varepsilon_s}{2} + (V_{pp} - V_{ss})\cos ka \end{pmatrix}. \tag{27}$$

After this, both sides of the equation are squared. The right-hand side can be operated using the property that provides the value of the multiplication of any two of the Pauli matrices, excluding the identity matrix, that is

$$\tau_i\tau_j = \delta_{ij}\mathbb{1} + i\varepsilon_{ijk}\tau_k. \tag{28}$$

From this relation, it can be obtained that the product between the matrices is 0 if the matrices are different, and the identity matrix $\mathbb{1}$ if the matrices multiplied are the same matrix, meaning that the matrix is squared.

Using this property, the right-hand side of the equation is already diagonal, being $(h_1^2 + h_2^2 + h_3^3)\mathbb{1}$. In the left-hand side, the matrix still has to be squared. As the terms in the diagonal are identical with opposite sign, when obtaining the terms in the antidiagonal they cancel out each other. This means that squaring the matrix $H(k) - h_0\tau_0$ makes this matrix diagonal. As the matrix is diagonal, the terms in the diagonal are the eigenvalues of this matrix. Because of this, the eigenvalues of the Hamiltonian can be easily obtained by knowing the relation between these eigenvalues and the eigenvalues of the Hamiltonian, that is

$$\begin{pmatrix} (\varepsilon_1 - h_0)^2 & 0 \\ 0 & (\varepsilon_2 - h_0)^2 \end{pmatrix} = (h_1^2 + h_2^2 + h_3^2)\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}. \tag{29}$$

This means that given a set of parameters, and a value of the k-point, the eigenvalues will be given by $h_0 \pm |h(k)|$ and there is always an energy gap unless all three (h_1, h_2, h_3) are zero. In this particular point, both eigenvalues have the same value, h_0, and the gap closes. As explained before, the coefficient from the identity matrix h_0 only represents a shift in the energy of the eigenvalues.

It is interesting to note that the coefficient of the first Pauli matrix, $h_1 = u$, vanishes in our model. It is due to the fact that: (i) there is no interaction on the same atom between the s and the p orbital; and (ii) the "$s - p$" model has an inversion symmetry, i.e., for any atom in the chain, an identical atom exists diametrically opposite to it and at an equal distance from it.

4. SOLVING THE S-P MODEL

4.1. Case when u = 0

In this section, we shall solve a particular example of the $s - p$ model described in Sec. 3. This corresponds to the exercise 3.19 proposed in David Vanderbilt's book, "Berry phases in electronic structure theory" [1].

For this example, the values given to the interactions between orbitals are $V_{ss} = -1.40\,t$, $V_{pp} = 3.24\,t$, $V_{sp} = 1.84\,t$ and $\Delta E = \varepsilon_s - \varepsilon_p = -8.0$. Energy units in this example are arbitrary, but for the sake of completeness, and as suggested in the tables at the back of Harrison [4], we shall consider them in eV. As it can be seen, the first three values will depend on a parameter t, that can be varied in a continuous way (here it will take values ranging from 0.5 to 1.2). Therefore, k and t can be viewed as coordinates of a two dimensional space, an important fact to discuss the Berry phases (Sec. A.1).

We show in Fig. 4(a),(c) and (e) the band structure of the model along the first-Brillouin zone for three significant values of the parameter t: (i) the initial value $t = 0.5$; (ii) the final value $t = 1.2$; (iii) a critical value of t (that in this example equals $t = 0.862$) where something special happens: right at this value the gap closes. At first sight, the qualitative shape of the bands for the two extreme cases [Fig. 4(a)-(e)] looks like pretty much the same. There is a finite gap separating the two bands, and the curvature of both of them follows the same pattern. However, as we shall describe shortly, they describe different topological states.

To ellucidate their difference, in addition to the band structure, the evolution of h_2 against h_3 for these three values of t is shown in Fig. 4(b),(d) and (f). The explicit expression for h_2 and h_3 for this particular example can be derived from Eq. (25) and Eq. (26). Substituting the values of the coefficients w, Δ and d, then the coefficients of the expansions of the Hamiltonian in term of the Pauli matrices, h_2 and h_3, are

$$\begin{aligned} h_2 &= 2V_{sp}\sin ka, \\ h_3 &= \frac{\varepsilon_s - \varepsilon_p}{2} + (V_{ss} - V_{pp})\cos ka. \end{aligned} \tag{30}$$

Now, the values of the interactions between the orbitals are introduced, and the expressions for h_2 and h_3 are

$$h_2 = 3.68\, t \sin ka, \tag{31}$$

$$h_3 = -4.0 - 4.64\, t \cos ka. \tag{32}$$

From these expressions, it can be observed that both h_2 and h_3 are scalar functions of t and k. This means that for each value of t, we can still give values to k in the first Brillouin zone, from $-\pi/a$ to π/a. For this reason, we can perform a closed loop in h_2 and h_3, which is different for every different t.

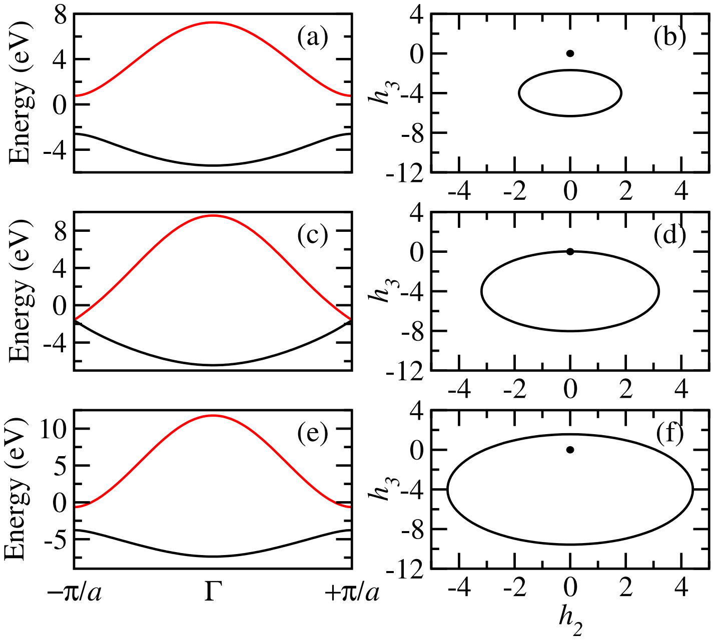

Figure 4: Bands structures (left column), and $h_2 - h_3$ coefficients of the Pauli matrices (right column) for three different values of t: $t = 0.5$ [panels (a)-(b)], $t = 0.862$ [panels (c)-(d)], and $t = 1.2$ [panels (e)-(f)]. Remember that with our symmetric model, $h_1 = 0$ in every case. The filled dot in the right panels represent the point where $h_1 = h_2 = h_3 = 0$.

In our $s - p$ model with a center of inversion [$u = 0$ in Eq. (25)], $\vec{h}$ is restricted to the $h_1 = 0$ plane and the variation of $\vec{h}(k)$ for k varying from $-\pi/a$ to $+\pi/a$ is shown as ovals in the $h_2 - h_3$ plane (right column in Fig. 4). As it can be seen in Fig. 4, the larger the value of t, the larger the area enclosed by the oval. For the smaller value of the parameter t [$t = 0.5$; Fig. 4(b)], $\vec{h}(k)$ does not wind around the origin. For the largest value of the parameter t [$t = 1.2$; Fig. 4(f)], $\vec{h}(k)$ does wind around the origin [the point $(0, 0)$ is enclosed in the oval]. Since t is changed continuously between these two cases, there is a critical value of t for which the oval touches the origin and the gap vanishes. Looking at Eqs. (31)-(32), this implies two simultaneous conditions on k and t: (*i*) $k = \pm\pi/a$ [so the sine in Eq. (31) vanishes], and (*ii*) $t = 4.0/4.64$, so h_3 cancels in Eq. (32) for the previous value of k. This is the point where the bands touch in the Brillouin zone, so they can exchange eigenvectors, i.e., a qualitative change in the electronic structure as represented in Fig. 5. There, we plot on top of the band structure the character of the different bands represented as ellipses whose size is proportional to the module of the corresponding complex coefficient in the tight-binding expansion, as given in Eq. (5).

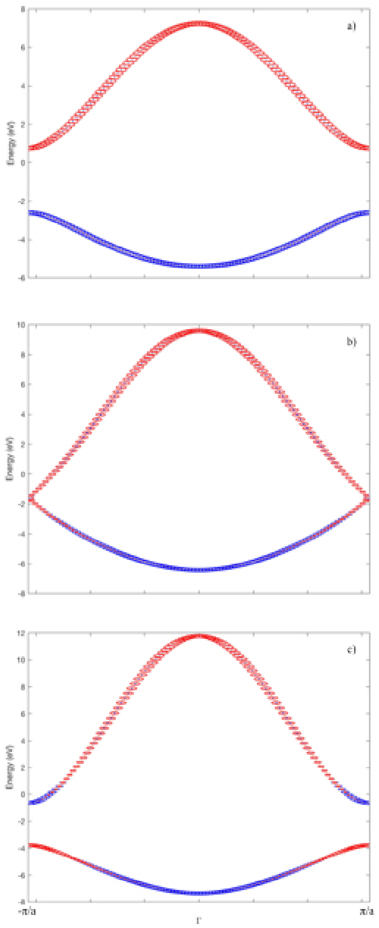

Figure 5: Character of the bands shown in Fig. 4. The circles represent the character of the band, blue for the s-like character and red for the p-like character. The size of the ellipses is proportional to the module of the corresponding complex coefficient of an eigenfunction in the tight-binding expansion, as given in Eq. (5). These characters of the band are shown for the three values of t selected before: (a) $t = 0.5$, (b) $t = 0.862$, and (c) $t = 1.2$.

As explained before, although there is not a big qualitative difference in the shape of the bands for the initial and the final values of t, however, there is a difference in the character of the bands for this set of values. The difference is more readily apparent in Fig. 6 where we plot the tight-binding coefficients of the two bands (lower band in blue, upper band in red) for the extreme values of t in our example.

Since we are going to compute the Berry phase, as will be described in Appendix A.1, we need the periodic part of the wave functions to be a smooth function of k everywhere in the loop, represented here by letting k range from $-\pi/a$ to $+\pi/a$. That implies a particular choice of the gauge. Once this is chosen in our example, the coefficient of the s orbital is always real, while the coefficient of the p orbital is purely imaginary. The wave function is normalized, so the sum of the squares of the coefficients for any given k is equal to 1.

For $t = 0.5$ the lower band is mostly s-like in character [Fig. 6(a)] while the upper band is majoritary p-type [Fig. 6(b)]. It is important to note how a gauge for the wave functions can be chosen in such a way that they are smooth functions in k, and continuous at the boundaries of the Brillouin zone.

For $t = 0.862$, where the gap closes, there is a change in the character of the bands. In the points where the gap closes, $\pm\pi/a$, the eigenstates become degenerate. For this reason, the two bands can exchange eigenvectors in these points. As seen in Fig. 5 (b), in the first band there is also an s-like character near these key points where the gap closes, while in the second band there is a p-like character close to $-\pi/a$ and $+\pi/a$.

For $t = 1.2$ the two band change the character in a continuous way: the lower band (respectively the upper band) is of p-type (respectively s-type) at $-\pi/a$, but it changes gradually when the excursion is undertaken along the Brillouin zone. At Γ the band has only s-type (respectively p-type) character and it recovers the p- (respectively s)-character at $+\pi/a$.

Since we will be interested in computing the center of the bands (the Zak phases [5], as described in the Appendix A.1), an important subtlety arises. For the Berry phase to be well defined, we need two conditions [1]: (*i*) that the periodic part of the wave function $|u_{n,k}\rangle$, has to be a smooth function of k, something already shown in Fig. 6; and (*ii*) we have also to ensure smoothness across the artificial boundary point when k crosses from $+\pi/a$ to $-\pi/a$. That is, we must insist that

$$\psi_{j,k=-\pi/a}(x) = \psi_{j,k=+\pi/a}(x). \tag{33}$$

That is, the Bloch functions at the two ends of the interval $[-\pi/a, +\pi/a]$ must be equal not just up to a phase. Due to the Bloch theorem [Eq. (3)], this condition translates into the fact that the periodic part of the wave functions are not equal at $-\pi/a$ and $+\pi/a$,

$$u_{j,k=+\pi/a}(x) = e^{-2\pi i x/a} u_{j,k=-\pi/a}(x). \tag{34}$$

In other words, $|u_{n,k=+\pi/a}\rangle$ and $|u_{n,k=-\pi/a}\rangle$ differ more than a global phase, since the phase factor depend on the position x.

In our tight-binding approximation, as we discussed in Sec. 2, the basis set of atomic orbitals is not explicitly constructed and we do not have access to the position dependence of the wave functions: only the coefficients of the tight-binding expansions are known at the points where the basis functions are centered. Since in our particular example, only with one atomic orbital per site, those atomic orbitals are assumed to be centered at positions $\pm na$, then the exponential in Eq. (34) is equal to one. Therefore, in our particular problem, we must impose that the coefficients of the wave functions at $-\pi/a$ and π/a are equal.

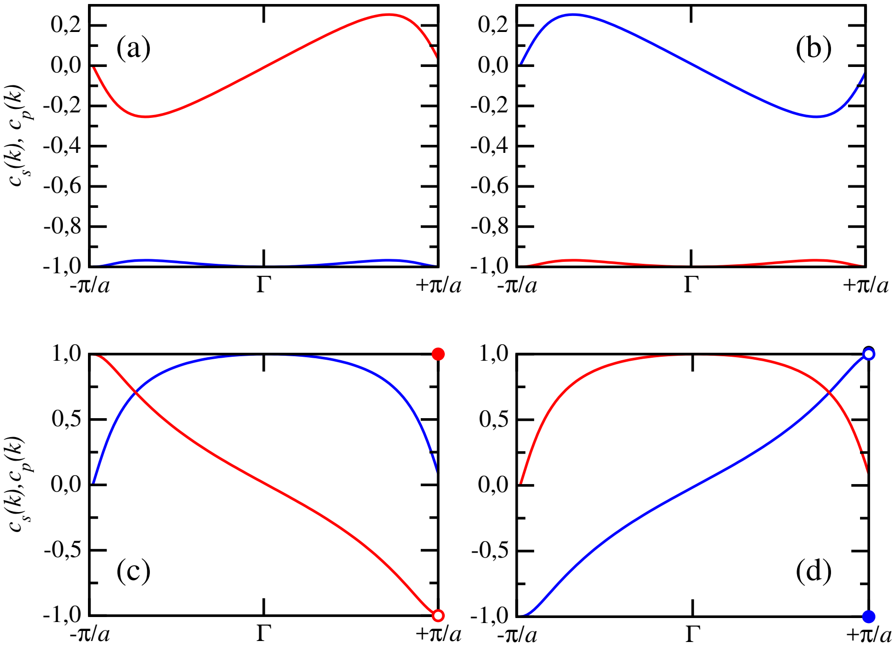

Figure 6: Coefficients of the tight-binding expansion for the lower band [panel (a) for $t = 0.5$, and panel (c) for $t = 1.2$], and for the upper band [panel (b) for $t = 0.5$, and panel (d) for $t = 1.2$]. The coefficient for the real part of the s-orbital is plotted in blue, and the coefficient for the imaginary part of the p-orbital is plotted in red.

As shown in Fig. 6 this is immediately full-filled for $t = 0.5$, a particular value before the topological phase transitions. We have checked that this condition also complies for any $t < 0.862$, point where the ellipse in Fig. 4 touches the origin, the gap closes and the topological phase transition takes place. However, as can be observed in Fig. 6(c)-(d) for $t = 1.2$, beyond the phase transition the continuity of the wave function at the Brillouin zone borders imposes a discontinuity in the tight-binding coefficients that must be used to compute the Berry phases. Instead of taking the coefficients at $+\pi/a$ marked with an empty circle, we should restore to the values at $-\pi/a$, marked with a filled circle.

This discontinuity translates into a change in the phase of the Berry phase of the band j, computed in the discrete formula as

$$\phi_j = -\Im \ln \left[\langle u_{j,k_0} | u_{j,k_1} \rangle \langle u_{j,k_1} | u_{j,k_2} \rangle \ldots \langle u_{j,k_{N-1}} | e^{-2\pi i x/a} | u_{j,k_0} \rangle \right], \tag{35}$$

In our tight-binding problem, every bracket in Eq. (35) is computed as

$$\langle u_{j,k_i} | u_{j,k_{i+1}} \rangle = c^*_{j,s}(k_i) c_{j,s}(k_{i+1}) + c^*_{j,p}(k_i) c_{j,p}(k_{i+1}). \tag{36}$$

If there is no discontinuity in the coefficients, all the products yield positive real numbers and therefore the final phase is zero. That is also the case if the discontinuity is present, with the exception of the last bracket, that becomes a negative real number. As a consequence, all the product in the square bracket of Eq. (35) is a real negative number and the phase jumps to π.

Another intuitive way of seeing this change in character in the bands is by plotting a schematic diagram of the interactions of the bands, in order to observe how the gap changes for different values of t. If there is still a gap of a substantial width, it can be considered that there is no exchange of information between the bands, meaning that there is not an important change in the character of the band. On the other hand, if the sum of these interactions is enough to overcome the width of the gap, then a change in the character of the bands would be expected.

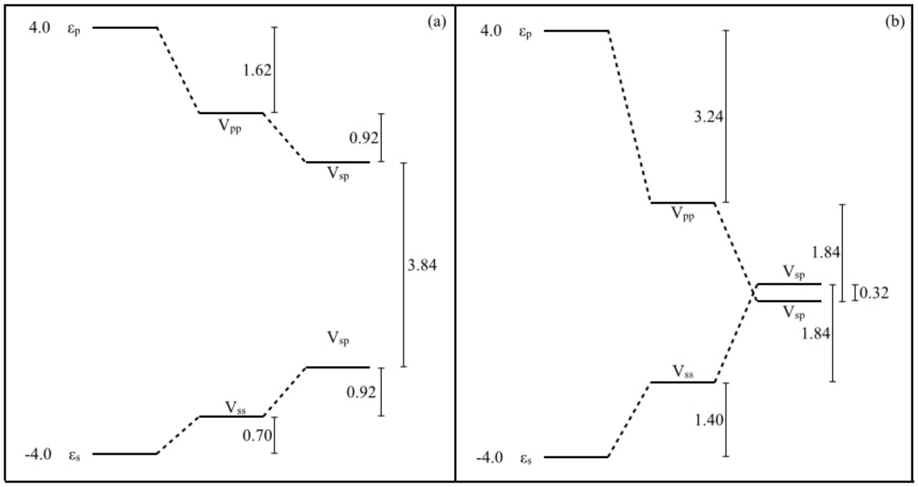

Figure 7: Schematic diagram of the interaction between the bands for (a) $t = 0.5$ and (b) $t = 1.0$.

In Fig. 7(a), which corresponds to $t = 0.5$, the values for each interaction have been obtained by introducing this value in their respective equation. The initial gap between the bands is 8.0, and it gets smaller when each interaction is applied. In the first place, each band has the interactions between neighbour orbitals of the same type (V_{ss} and V_{pp}) that bring the bands closer together. In addition to this interactions, as the orbitals interact with each other, both bands have another contribution that is V_{sp}, equal for both bands. In this case, the sum of these interactions is not enough to close the gap. For this reason, there is almost no exchange in the character of the bands, as the bands can not share any information due to the width of the gap.

In Fig. 7(b), and for the sake of simplicity, the value of t studied is 1.0. For this specific t, the topological transition has already taken place, so we would expect some change in the character of the bands. Performing the same procedure followed for $t = 0.5$ with the corresponding values for this t, it can be seen that the sum of the interactions overcome the width of the gap. However, this difference of energy is still not big enough to make the whole band have both orbital characters. Only the most energetic k points, which are the ones close to $\pm\pi/a$, would have a significant contribution from the orbital corresponding to the other band.

Since the center of the band is given by

$$\overline{x}_j = \phi_j/2\pi, \tag{37}$$

we immediately deduce how the topological phase transition has translated the center of the band from the atomic position (atomic picture) to the center of the bonding (covalent picture), as shown in Fig. 8. This change in character was already pointed out by Shockley in his milestone work [6].

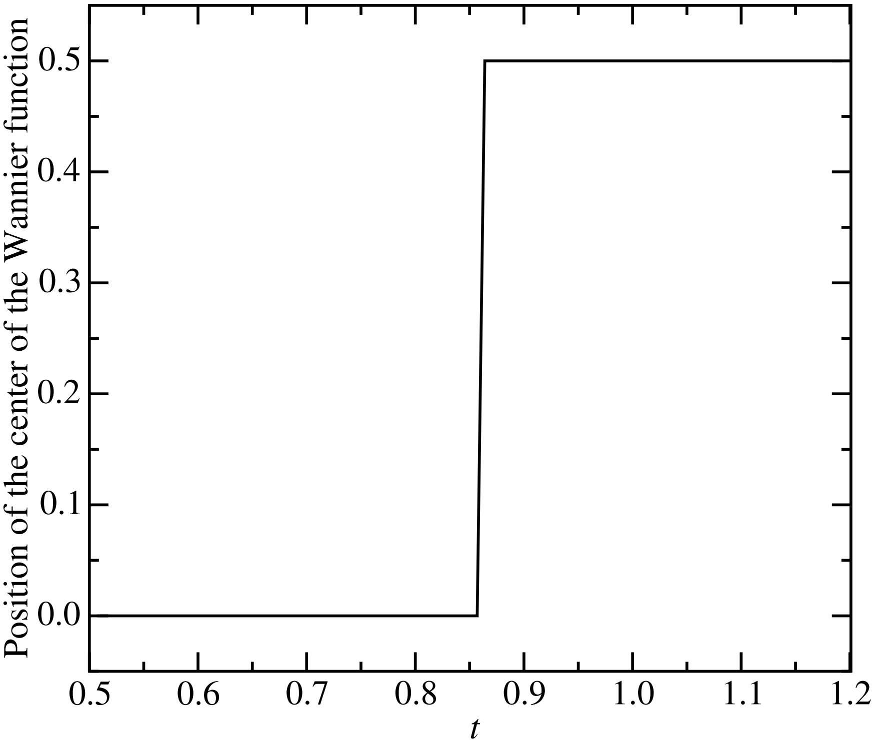

Figure 8: Position of the centers of the Wannier functions as a function of the parameter t. The centers of the two bands shown in Fig. 4 coincide. When the center of the Wannier function is 0.5 that means that is half-way between two consecutive atoms, i.e. it is a covalent-type bonding.

4.2. Case when u $\neq$ 0

Given the choice of the parameters in Sec. 4.1, the coefficient of the first Pauli matrix in Eq. (25) always vanish. Then, for any value of t, when k is varied continuously in the first Brillouin zone, the parameters h_2 and h_3 describe an oval that might or might not wind around the origin, the special point where the gap closes, the bands exchange character, and the topological phase transitions takes place (see the left panel in Fig. 9).

We might wonder if other possibilities to get this topological phase transition are possible, in particular, without the requirement of a vanishing of the gap. This alternative has been proposed by Richard Martin in his book ”Electronic Structure: Basic Theory and Practical Methods” [3].

Martin proposed to lift the constraint $h_1 = u = 0$ for the coefficient of the first Pauli matrix, in such a way that the space is expanded and we are allowed to move also in a third dimension instead of being restricted to the $h_2 - h_3$ plane (see the right panel in Fig. 9).

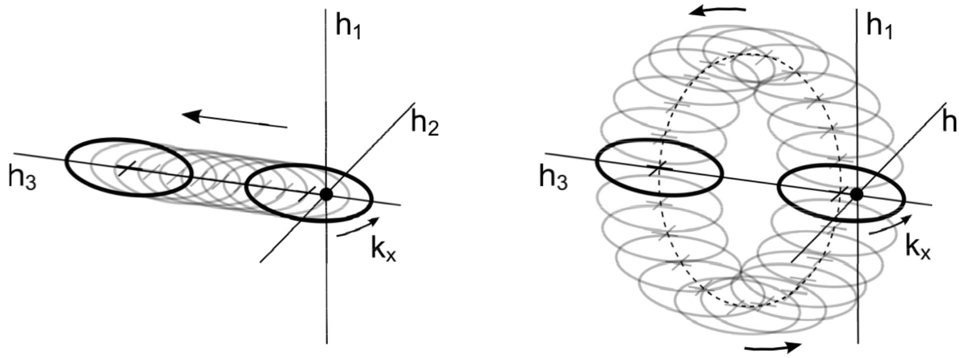

Figure 9: Schematic diagram for the possible excursions of the parameters that define the Hamiltonian in terms of the Pauli matrices [Eq. (22)]. In the left panel, h_1 is forced to be zero, as in Sec. 4.1. In the right panel, this constrained is lifted, as explained in Sec. 4.2. Reprinted with permission from Ref. [3].

If the Hamiltonian changes in a cycle in such a way that the components h_1 and h_3 vary together to form a closed loop, then the two ovals (marked in dark at the right panel of Fig. 9) should be considered at some point while the Hamiltonian returns to itself. One of them winds around the origin. The other one does not. A topological phase transition takes place but, in contrast with Sec. 4.1 the gap is never zero.

In the $s - p$ model in order to have a displacement above or below the h_1 plane, the parameter u in the expansion of the Hamiltonian in terms of Pauli matrices has to be different from zero. This corresponds to a real term in the off-diagonal matrix elements, and this can only occur if the center of inversion is broken. Then, the system is polarized either on one direction or the opposite depending on the sign of u. Here, the cycle will be directly defined in terms of the coefficients of the Pauli matrices as

$$\vec{h}(k,\lambda) = \left[D\sin\lambda, \omega\sin k, \overline{\Delta} + D\cos\lambda + d\cos k\right], \tag{38}$$

where D, ω, d and $\overline{\Delta}$ are four constants. In this work, these four constants will be set to 1. As the coefficient h_0 for the identity matrix does not change neither the shape of the bands nor their character, in this model it will be set to zero. For this reason, there will be no shift in their energy, so the gap between the bands will be centered in 0. The parameter λ, that enters h_1 under a sine and h_3 under a cosine, parametrizes the loop in the $h_1 - h_3$ plane, and can vary in a continuous way between 0 and 2π. For $\lambda = 0$, we are in the situation depicted by the left dark oval in the right panel of Fig. 9, that does not wind around the origin. For $\lambda = \pi$, we are in the situation represented by the right dark oval in the right panel of Fig. 9, that does wind around the origin. But, in contrast with Sec. 4.1, there is no value of λ for which the oval touches the origin. As it can be noticed, λ and k have comparable roles, as they appear in h_1 and h_2 inside a sine, and they both appear in h_3 inside a cosine. However, there is an important difference between them, and it is the factor i in the matrix τ_2 that does not appear in τ_1. An important difference with respect discussed in Sec. 4.1 is that the coefficients of the s and p basis functions are not in general purely real or purely imaginary, but they develop an intrinsic complex value.

Since the system is polarized, it is possible to shift the center of the Wannier functions continuously from 0 to either $+\frac{1}{2}$ or $-\frac{1}{2}$. Even, it is also possible to continue varying until the shift is by a full lattice constant, as shown in Fig. 10.

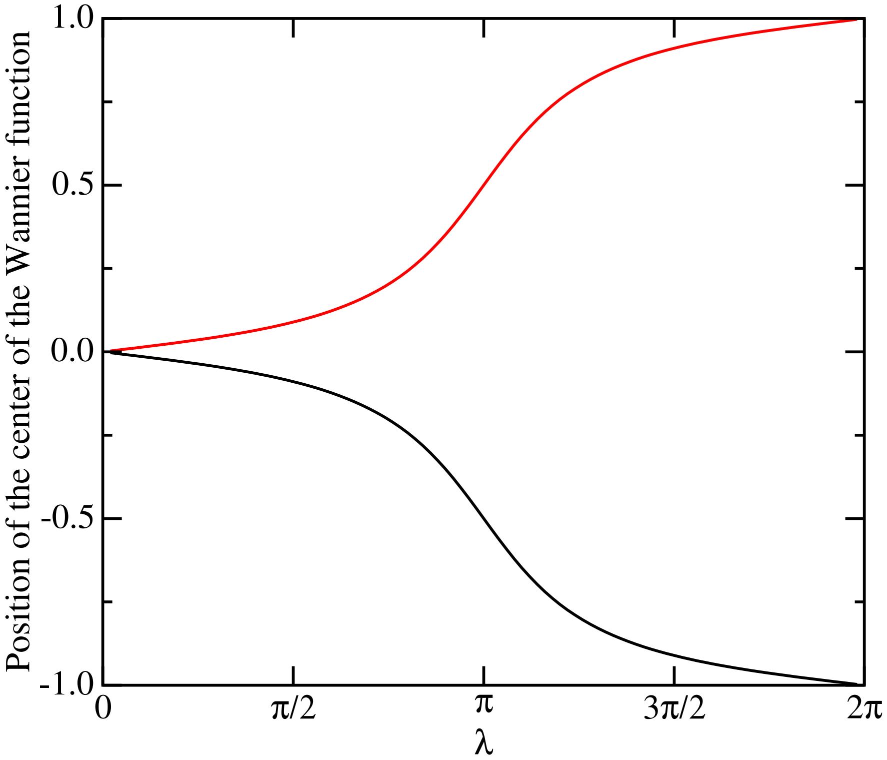

Figure 10: Center of the Wannier functions as a function of the λ parameter used to define the Hamiltonian in Eq. (38). Black (respectively red) solid line corresponds to the center of the first (respectively second) band.

5. Bulk-boundary correspondence

Topology is a global property of the electronic structure of the bulk. It is a property of the states as a function of k in an infinite periodic crystal with no surface. That is what we have analyzed up to now, where the electronic states of an infinite chain (no border) has been analyzed.

However, since the seventies, the role of the so-called “bulk-boundary” correspondence has been recognized. The principle of the “bulk-boundary” correspondence guarantees that there will be surface states in the gap in the non-trivial topological phases [7].

Let us assume a Hamiltonian that slowly interpolates between two insulating states with different topologies. That is the case, for instance, presented in Sec. 4.2 with $\lambda = 0$ and $\lambda = \pi$. At some point the energy gap has to vanish because otherwise it is impossible for the topological invariant to change. In the previous example, the center of the bands gradually changes between the atomic limit (center of the bands on the atoms) for $\lambda = 0$ to the covalent limit (center of the bands at midpoint between the atoms) for $\lambda = \pi$. Jackiw and Rebbi mapped the problem to an interface, and postulated that there might be surface states bound to the interface region, and these states form bands that propagate along the interface. For some particular value of the parameter λ, the surface states touch each other, closing the gap. In our former model, as can be seen in Fig. 11, this happens for $\lambda = \pi$.

In Fig. 11 we assume that our chain is finite, with only 19 atoms. The Hamiltonian parameters remain the same as in Sec. 4.2, for the different values of λ. Indeed, the on-site and hopping parameters can be reconstructed from the coefficient of the Pauli matrices as

$$\begin{aligned}
\varepsilon_{ss} &= \overline{\Delta} + D\cos\lambda, \\
\varepsilon_{pp} &= -\overline{\Delta} - D\cos\lambda, \\
V_{ss} &= \frac{d}{2}, \\
V_{pp} &= -\frac{d}{2}, \\
V_{sp} &= \frac{\omega}{2}, \\
V'_{sp} &= D\sin\lambda. \qquad (39)
\end{aligned}$$

In this model the parameter h_1 is not restricted to 0. Because of this, when varying this coefficient, an on-site interaction between the s and the p orbital appears, which is V'_{sp}.

Then, since we cannot apply the Bloch theorem for our finite system, a square Hamiltonian of size $(2 \times 19, 2 \times 19)$ is written considering the interaction between a given orbital and their neighbours. A particular example of the Hamiltonian for a slightly smaller chain of only for 4 atomic sites (in order to fit in one page) is written below

$$\begin{pmatrix}
\varepsilon_{ss} & V'_{sp} & V_{ss} & -V_{sp} & 0 & 0 & 0 & 0 \\
V'_{sp} & \varepsilon_{pp} & V_{sp} & -V_{pp} & 0 & 0 & 0 & 0 \\
V_{ss} & V_{sp} & \varepsilon_{ss} & V'_{sp} & V_{ss} & -V_{sp} & 0 & 0 \\
-V_{sp} & -V_{pp} & V'_{sp} & \varepsilon_{pp} & V_{sp} & -V_{pp} & 0 & 0 \\
0 & 0 & V_{ss} & V_{sp} & \varepsilon_{ss} & V'_{sp} & V_{ss} & -V_{sp} \\
0 & 0 & -V_{sp} & -V_{pp} & V'_{sp} & \varepsilon_{pp} & V_{sp} & -V_{pp} \\
0 & 0 & 0 & 0 & V_{ss} & V_{sp} & \varepsilon_{ss} & V'_{sp} \\
0 & 0 & 0 & 0 & -V_{sp} & -V_{pp} & V'_{sp} & \varepsilon_{pp}
\end{pmatrix}. \qquad (40)$$

The Hamiltonian is diagonalized for different values of λ, and the eigenvalues are plotted in Fig. 11.

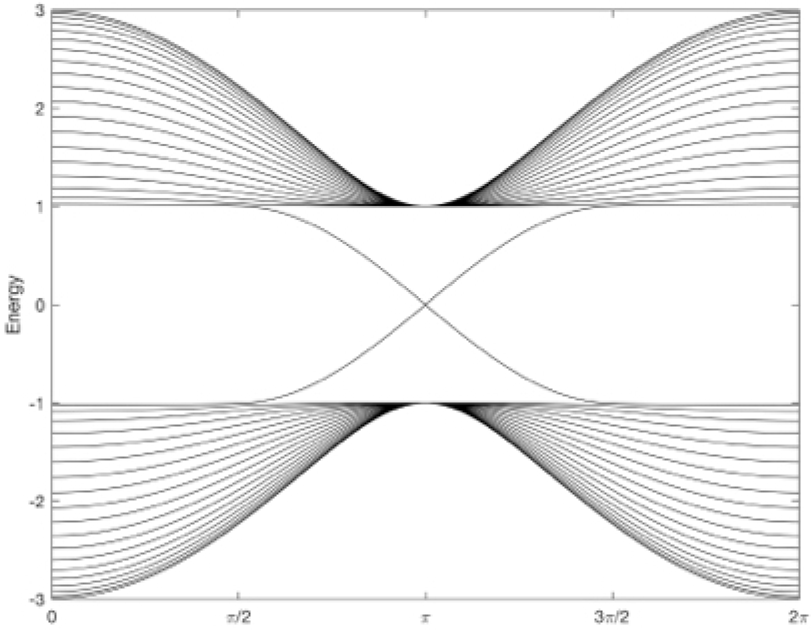

Figure 11: States of a finite chain of 19 atoms for a closed loop in the parameter λ.

In Fig. 12 we plot the square of the coefficients of the wave functions for the states that close the gap at $\lambda = \pi$. Clearly, they are peaked at the two surfaces and the weight decreases in the interior atoms, indicating that we are dealing with surface states.

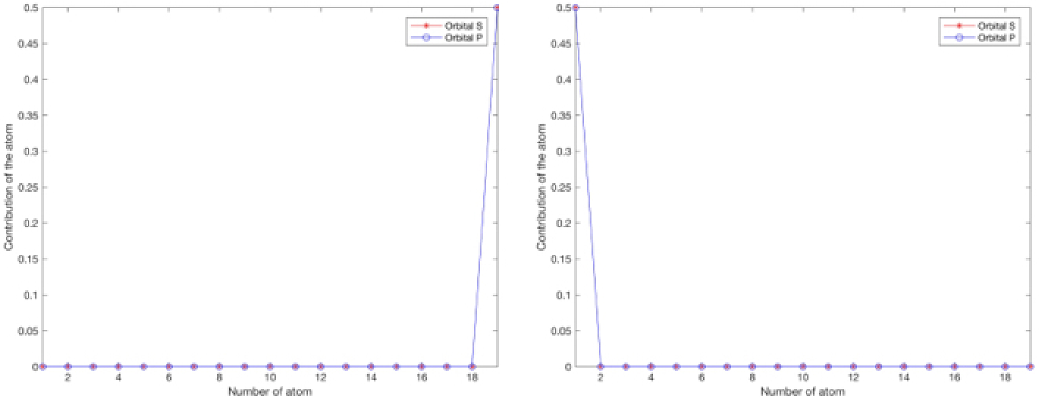

Figure 12: Square of the coefficients of the s and p orbitals in the chain for the two states that cross at the center of the gap at $\lambda = \pi$.

6. CONCLUSIONS

In this work, we have solved the one dimensional $s-p$ model, which has one atom and an s and a p orbital per unit cell, and we have studied the topological phase transitions that take place in this model in two different ways.

In the first way, we solved the exercise 3.19 proposed in David Vanderbilt's book "Berry phases in electronic structure theory" [1]. In this particular example, the interactions between the orbitals will depend on a parameter that will be varied continuously in order to study the topological transition. When varying the interaction values, which directly varies the Hamiltonian, there is a critical value for which the gap closes. This is the specific point in which the topological transition occurs. In this point, the center of the bands are translated from being centered in the position of the atoms to being centered in the bonding between them. This is a quantum transition, as there is a well-defined jump between the two situations.

The second way studied in this work to get this topological phase transitions follows the method proposed in Richard Martin's book "Electronic Structure: Basic Theory and Practical Methods" [3]. As every 2×2 matrix can be described by the Pauli matrices, in this method the parameter introduced does not directly vary the interactions between the orbitals, but instead it varies the coefficients from the Pauli matrices that describe the Hamiltonian. The main difference between these two methods is that in this one the gap is never closed. Here, the topological phase takes place in a soft way. The center of the Wannier functions is shifted continuously, rather than in a sudden way as in the first method.

Finally, we studied what is known as "bulk-boundary" correspondence. In this last model, the Hamiltonian slowly interpolates between two insulating states with different topologies, found in $\lambda = 0$ and $\lambda = \pi$. If the gap did not close, it would be impossible for the topological invariant to change. It was found that this problem can be mapped to an interface, and that there are surface states bound to the interface region which form bands that propagate along the interface. We found that for the particular value of $\lambda = \pi$, these surface states touch each other, closing the gap and performing the topological phase transition.

A. APPENDIX

A.1. Berry phase, Zak phase and the centers of the bands

Let's define $\hat{H}$ as a Hamiltonian which depends on a set of parameters $\vec{\lambda}$. Some examples of parameters on which the Hamiltonian may depend are the atomic coordinates of the atoms, a $\vec{k}$ point, or the direction of a magnetic field. In our case the parameters will be: (*i*) the parameters t (in Sec. 4.1), or λ (in Sec. 4.2) that controls the interatomic tight-binding terms; and (*ii*) the k point in the first-Brillouin zone.

For any values of the parameters, the natural basis of the Hamiltonian is assumed to be discrete, so for any possible value of these parameters, the Hamiltonian can be diagonalized as

$$\hat{H}(\vec{\lambda})\,|u_n(\vec{\lambda})\rangle = E_n(\vec{\lambda})\,|u_n(\vec{\lambda})\rangle\,. \tag{41}$$

With this diagonalization, all the eigenvalues and eigenvectors of the Hamiltonian are known for any possible value of $\vec{\lambda}$. It is important to notice the fact that this equation does not imply any relation between the phases of the eigenstates $|u_n(\vec{\lambda})\rangle$ at different $\vec{\lambda}$, so an arbitrary phase can be chosen for each point.

Let's now assume that the system is prepared so that at $t = 0$ it is in one of the eigenstates n

$$|\psi_n(t=0)\rangle = |u_n(\vec{\lambda}(t=0))\rangle\,. \tag{42}$$

Now, the eigenstate takes an excursion between times $t = 0$ and t. This excursion can be seen as a trajectory in the $\vec{\lambda}$ space phase, as shown in Figure (13). It is also assumed that the levels do not cross along the $\vec{\lambda}$ path, so the $n = 1$ level will always remain the first level and so on.

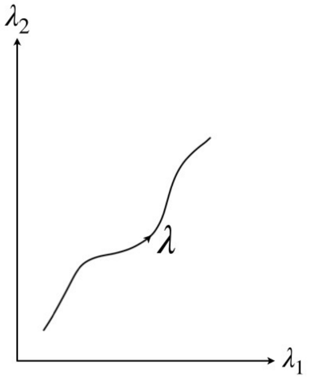

Figure 13: Schematic representation of a trajectory in the $\vec{\lambda}$ space, dependent on two parameters λ_1 and λ_2.

At time t, the system is at the point of the trajectory $\vec{\lambda}(t)$. In this moment, the state of the system at time t can be described from the natural basis for the corresponding $\vec{\lambda}(t)$. Adiabatically, a system as this one which was prepared in one of the eigenstates, will evolve with the Hamiltonian as

$$|\psi_n(t)\rangle = \exp\left[-\frac{i}{\hbar}\int_0^t E_n(\vec{\lambda}(t'))dt'\right]\exp(i\phi_n(t))\,|u_n(\vec{\lambda})\rangle\,. \tag{43}$$

In the right-hand side of the equation, the following two phases are found:

- The first phase, $\exp\left[-\frac{i}{\hbar}\int_0^t E_n(\vec{\lambda}(t'))dt'\right]$, is the usual dynamical phase
- The second phase, $\exp(i\phi_n(t))$, is an extra phase factor that may include, for example, whether there is a phase dependent on the trajectory chosen between the initial and the final state, or the differences in phases chosen at the time of computing the natural basis

This extra phase ϕ can be computed by introducing this state in the time dependent Schrödinger equation, $i\hbar\frac{d|\psi_n\rangle}{dt} = \hat{H}\,|\psi_n\rangle$.

In the first place, the derivative at the left-hand side is taken

$$\begin{aligned} E_n(\vec{\lambda}(t))\exp\left[\int_0^t E_n(\vec{\lambda}(t'))\right]&\exp(i\phi_n(t))\,|u_n(\vec{\lambda}(t))\rangle \\ +i\hbar\left[\int_0^t E_n(\vec{\lambda}(t'))\right] i\frac{d\phi_n}{dt}&\exp(i\phi_n(t))\,|u_n(\vec{\lambda}(t))\rangle \\ +i\hbar\left[\int_0^t E_n(\vec{\lambda}(t'))\right]\exp(i\phi_n(t))&\frac{d\,|u_n(\vec{\lambda}(t))\rangle}{d\vec{\lambda}}\frac{d\vec{\lambda}}{dt}. \end{aligned} \tag{44}$$

Now, the right-hand side is computed

$$\hat{H}\,|\psi_n(\vec{\lambda}(t))\rangle = E_n(\vec{\lambda}(t))\,|\psi_n(\vec{\lambda}(t))\rangle = E_n(\vec{\lambda}(t))\exp\left[\int_0^t E_n(\vec{\lambda}(t'))dt'\right]\exp(i\phi_n(t))\,|u_n(\vec{\lambda}(t))\rangle\,. \tag{45}$$

This term cancels out with the first term of the left-hand side, so operating the equation

$$-\hbar\exp\left[\int_0^t E_n(\vec{\lambda}(t'))dt'\right]\frac{d\phi_n}{dt}\exp(i\phi_n(t))\,|u_n(\vec{\lambda}(t))\rangle + i\hbar\exp\left[\int_0^t E_n(\vec{\lambda}(t'))dt'\right]\exp(i\phi_n(t))\frac{d\,|u_n(\vec{\lambda}(t))\rangle}{d\vec{\lambda}}\frac{d\vec{\lambda}}{dt} = 0. \tag{46}$$

The common terms in both addends can be taken away and the equation reorganized as

$$i\frac{d\phi_n}{dt}\,|u_n(\vec{\lambda}(t))\rangle = -\frac{d\,|u_n(\vec{\lambda}(t))\rangle}{d\vec{\lambda}}\frac{d\vec{\lambda}}{dt}. \tag{47}$$

Now, both sides are multiplied by the bra $\langle u_n(\vec{\lambda}(t))|$

$$\frac{d\phi_n}{dt} = i\frac{d\vec{\lambda}}{dt}\,\langle u_n(\vec{\lambda}(t))|\,\frac{d}{d\vec{\lambda}}\,|u_n(\vec{\lambda}(t))\rangle = \vec{A}_n(\vec{\lambda})\frac{d\vec{\lambda}}{dt}, \tag{48}$$

where $\vec{A}_n(\vec{\lambda}) = i\,\langle u_n(\vec{\lambda}(t))|\,\frac{d}{d\vec{\lambda}}\,|u_n(\vec{\lambda}(t))\rangle$ is known as the Berry connection. Now, the change in the geometrical phase can be integrated between an initial and a final time

$$\begin{aligned} \phi_n(t_f) &= \int_{t_i}^{t_f}\vec{A}_n(\vec{\lambda})\frac{d\vec{\lambda}}{dt}dt \\ \phi_n(\Gamma) &= \int_{\vec{\lambda}_i}^{\vec{\lambda}_f}\vec{A}_n(\vec{\lambda})d\vec{\lambda}. \end{aligned} \tag{49}$$

This quantity depends only on the path taken between the initial and final points, so it is a geometric phase. As the Berry connection is real, this geometric phase is also real. The eigenstates are only defined up to a phase. This means that if $|u_n(\vec{\lambda})\rangle$ is an eigenstate of the Hamiltonian, then $\exp^{-i\beta_n(\vec{\lambda})}|u_n(\vec{\lambda})\rangle$ is also a valid eigenstate. $\beta_n(\vec{\lambda})$ is assumed to be real and smooth in $\vec{\lambda}$, meaning that there is no level crossing.

When there is a change in the gauge, the Berry connection changes as

$$\tilde{\vec{A}}_n = \vec{A}_n + \frac{d\beta_n}{d\vec{\lambda}}, \tag{50}$$

and the corresponding phase changes as

$$\widetilde{\phi}_n = \phi_n + \beta_n(\vec{\lambda}_f) - \beta_n(\vec{\lambda}_i). \tag{51}$$

Because of this, a gauge can always be chosen where the geometric phase of the path disappears, and only the dynamical phase remains. However, let's now consider a closed path. The circuit is parametrized by a scalar λ, which takes values between 0 and 1. As both $\lambda = 0$ and $\lambda = 1$ label the same state, it is required that in both gauges $|u_n(\lambda = 1)\rangle = |u_n(\lambda = 0)\rangle$ and $|\widetilde{u}_n(\lambda = 1)\rangle = |\widetilde{u}_n(\lambda = 0)\rangle$. According to Eq. ((51)), this implies that

$$\beta_n(\lambda = 1) = \beta_n(\lambda = 0) + 2\pi l, \tag{52}$$

where l is the "winding number" of the gauge transformation. Then, the geometrical phase $\widetilde{\phi}_n$ changes by

$$\widetilde{\phi}_n = \phi_n + 2\pi l. \tag{53}$$

The Berry phase is defined as

$$\phi_n(\Gamma) = \oint \vec{A}_n(\vec{\lambda})d\vec{\lambda}. \tag{54}$$

For closed paths, the geometrical phase $\exp^{i\phi_n}$ is gauge invariant, so it can not be removed by performing a gauge transformation. In addition to this, being a gauge invariant means that the Berry phase is potentially a physical observable.

Let's now focus on the two state s-p model in one dimension explained before. The hamiltonian must depend in at least two λ parameters, due to the fact that if it only depended in one parameter, a closed loop could not be performed, as it would come and go by the same path following a straight line.

The first λ parameter will be $\vec{k}$, which is the position in the reciprocal space. As stated before, because of the periodicity of the potential, the Bloch theorem can be applied, meaning that $|\psi_{n,\vec{k}+\vec{G}}\rangle = |\psi_{n,\vec{k}}\rangle$. The vector in k will be removed from now on, as there is only one dimension. Since $veck$ and $\vec{k} + \vec{G}$ are just two labels for the same state, this implies that only a zone in the reciprocal space with the length of the unit cell is sufficient to describe all the states one and only once. This zone is known as the Brillouin zone. The length is $2\pi/a$, being a the length of the unit cell, and it goes from $-\pi/a$

to π/a. The Brillouin zone will be key to find the Berry phase for this model, as its periodicity allows to perform a closed loop in the space of $\vec{\lambda}$.

The path along which the Berry phase will be calculated can be discretized in N steps, as shown in Figure (14). For each point of the path, the $\vec{\lambda}$ parameters are different, so the wavefunctions are different in every step. As it is a closed loop, $|u_N\rangle$ must be equal to the initial wavefunction $|u_0\rangle$.

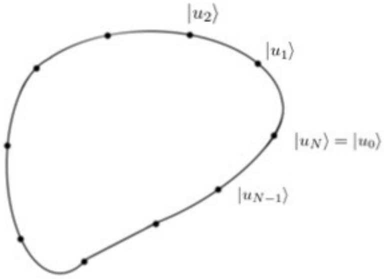

Figure 14: Schematic illustration of a closed loop in the $\vec{\lambda}$ space, with a discrete set of steps along the path.

At any two adjacent points of these discrete steps, the relative phases of the wavefunctions at those points can be expressed as

$$\Delta\phi_{j,j+1} = \Im \ln\left[\langle u_j|u_{j+1}\rangle\right], \tag{55}$$

using the relation that provides the phase α of $z = |z|e^{i\alpha}$, $\alpha = \Im \ln z$. With this discretization, the Berry phase can be obtained as

$$\phi = -\Im \ln\left[\langle u_0|u_1\rangle \langle u_1|u_2\rangle \langle u_2|...|u_{N-1}\rangle \langle u_{N-1}|u_0\rangle\right]. \tag{56}$$

Finally, it can be proved that in one-dimensional systems with isolated bands, as the ones we are dealing with in this work, the centers of the Wannier functions can be identified with the Berry phases computed as in Eq. (56) as

$$\overline{x}_n = \frac{\phi_n}{2\pi} a, \tag{57}$$

an idea already introduced by Zak [5]. This is used in Sec. 4.1 and 4.2 to compute the centers of the bands.

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