Change of the Chern number at band crossings

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Abstract

Let \( H(\epsilon, x) \) be a finite dimensional hermitian matrix depending on the variable \( x \) taking its values on a 2D manifold and changing with \( \epsilon \). If at \( \epsilon = 0 \) two bands are touching, we give a formula for the change of Chern number of these bands as \( \epsilon \) passes through zero.

1 Introduction

In many problems of quantum physics, one has to compute the band spectrum of some Hamiltonian. This is what happens in solid state physics for the electronic band spectrum. This is also the case in molecular or nuclear physics with rotation bands in the high spin limit. In most of these cases, the Hamiltonian describing the dynamics can be reduced to a \( N \)-dimensional hermitian matrix-valued continuous function \( x \in M \mapsto H(x) \), where \( M \) is some manifold of parameters. For the rotation bands, \( M \) is the 2D sphere, whereas for electrons in a perfect crystal, \( M \) is a torus. Diagonalizing \( H(x) \) for all \( x \)'s gives rise to \( x \)-dependent eigenvalues \( E_1(x), \ldots, E_N(x) \) called the band functions. Moreover, each of the corresponding eigenvectors define a line in \( \mathbb{C}^N \) depending continuously on \( x \), namely a line bundle. One important question to answer is whether this bundle is trivial or not, namely if one can choose the eigenvectors for each \( x \) in such a way as to define a univalued function over \( M \). If \( H(x) \) is real valued this is always possible. However if \( H(x) \) cannot be represented in some basis by a real valued matrix depending continuously on \( x \), this is not possible in general. In physics such a situation happens whenever the dynamics is not time-reversal invariant, for instance if some magnetic field is present or if there are spin couplings. The obstruction is measured by the Chern classes of the line bundle. Such Chern classes have been related to the Quantum Hall effect for Bloch electrons in a uniform magnetic field. For rotation bands, the occurrence of Chern numbers gives rise to the quantization of a mechanical response to a torque in molecules or nuclei. In the present work, we will restrict ourself to the case for which the manifold \( M \) is two-dimensional, in view of its application to physics.

We assume now that the Hamiltonian depends upon an additional real parameter \( \epsilon \) varying in a neighbourhood of zero, say \([-1, +1]\). Since a famous result of Wigner and von Neumann, it is known that, if \( H \) depends smoothly on \((x, \epsilon)\), the set of points \((\epsilon, x)\) for which two bands of \( H(\epsilon, x) \) are touching has codimension one generically.

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From now on, we will assume that \( M \) is an oriented smooth surface, namely it has dimension 2, and that we are in this generic situation. This means that \( H \) depends smoothly on \((x, \epsilon)\), and that there is a pair \( E_-(\epsilon, x) \leq E_+ (\epsilon, x) \) of neighbouring bands and a finite set \( x_1, \ldots, x_L \) of points in \( M \) such that \( E_-(\epsilon, x) = E_+ (\epsilon, x) \) if and only if \( \epsilon = 0 \) and \( x = x_j \) for some \( j = 1, \ldots, L \). The \( x_i \)'s are called the “touching points” of the two bands. We want to compute the change of the Chern class of each of these bands while \( \epsilon \) varies from \(-1\) to \(+1\). Such a change has been observed in numerical computations \([8, 9, 10]\) related to physical models.

To give the result in a precise form, we need some notation. First of all, we will replace the \( N \times N \) Hamiltonian \( H(\epsilon, x) \) by an effective \( 2 \times 2 \) one describing the two bands under study in a neighbourhood \( \mathcal{O} \) of \( \epsilon = 0, x = x_j \). This is always possible. Using the Pauli matrices \( \vec{\sigma} = (\sigma_1, \sigma_2, \sigma_3) \), this effective Hamiltonian can be written as

\[
H_{\text{eff}}(\epsilon, x) = \frac{1}{2} (E_+(\epsilon, x) + E_-(\epsilon, x)) + \vec{\sigma} \vec{f}(\epsilon, x),
\]

where \( \vec{f} \) takes on values in \( \mathbb{R}^3 \) and \( |\vec{f}| = (E_+(\epsilon, x) - E_-(\epsilon, x))/2 \). From our assumptions, it follows that \( \vec{f} \) vanishes only at \((0, x_j)\) in \( \mathcal{O} \). We then set \( \vec{\omega} = \vec{f}/|\vec{f}| \) in the complement of the \((0, x_j)\)'s in \( \mathcal{O} \). Given any surface \( \Sigma_j \) in \( \mathcal{O} \) homotopic to a sphere centered at \((0, x_j)\) and not surrounding the other touching points, we set

\[
n(x_j) = \frac{1}{4\pi} \int_{\Sigma_j} \vec{\omega} \, d\omega \wedge d\omega > .
\]

This is an integer which does not depend on the choice of \( \Sigma_j \), called the degree of the map \( \vec{\omega} \). This index is actually related to Berry’s phase. In his seminal paper \([11]\), M. Berry showed that if at \( \epsilon = 0 \) the parameters \( x \) turns around \( x_j \) on a closed path \( \gamma \) close enough to \( x_j \), the eigenvector \( \psi_+ \) corresponding to the \( +\)-band experiences a phase change given by

\[
\Delta \phi = \frac{1}{2} \int_{\Sigma} \langle \vec{\omega} | d\vec{\omega} \wedge d\vec{\omega} >,
\]

where \( \Sigma \) is any oriented surface in \( \mathcal{O} \) with boundary given by \( \gamma \). For this reason, we propose to call \( n(x_j) \) the Berry index at \( x_j \). Our main result is the following:

**Theorem 1** The difference \( \Delta \text{Ch} \) between the Chern numbers of the subband corresponding to \( E_+ \) while \( \epsilon \) varies from \(-1\) to \(+1\) is given by the sum of the Berry indices at all touching points.

In Section 3 we will compute the Berry index in some cases. The generic situation corresponds to \( \vec{f} \) having a non vanishing Jacobian at the touching point and gives the following result:

**Theorem 2** If \( \vec{f} \) has a non vanishing Jacobian \( J(\vec{f}(x_j)) \) at the touching point \((0, x_j)\), the Berry index is given by \( n(x_j) = J(\vec{f}(x_j))/|J(\vec{f}(x_j))| \), namely it is the sign of the Jacobian at the touching point.

## 2 Proof of the main result

In what follows, \( M \) is an oriented smooth surface. Up to an homeomorphism, it is given by the Poincaré construction from a polygon in the Poincaré disk (see Fig. 4). Let us assume for simplicity that for \( \epsilon \neq 0 \), the spectrum of the Hamiltonian \( H(\epsilon, x) \) is simple. We then denote by \( \vec{P}(\epsilon, x) \) the eigenprojection associated to the eigenvalue \( E_i(\epsilon, x) \). It is given either by \( |\psi_i \rangle \langle \psi_i| \) where \( \psi_i \) is a corresponding normalized eigenvector, or by Cauchy’s formula as
Figure 1: The surface $M$

\[ P_l(\epsilon, x) = \frac{1}{2\pi} \oint_{\Gamma} \frac{dz}{z - H(\epsilon, x)}, \quad (4) \]

where $\Gamma$ is a small circle centered at $E_l(\epsilon, x)$ and not surrounding the rest of the spectrum. Since the spectrum is simple for $\epsilon \neq 0$, $P_l$ is smooth with respect to $(\epsilon, x)$ in the complement of the touching points in $[-1, +1] \times M$. For a given $\epsilon$ its second Chern class is given by the closed 2-form $\Omega_2$ on $M$ where

\[ \Omega_2 = \frac{1}{2\pi} \text{Tr}(P_l dP_l \wedge dP_l). \quad (5) \]

The Chern number $\text{Ch}(\epsilon)$ is obtained by integrating $\Omega_2$ over the surface $M$. That it is an integer is a standard result [12, 13, 3]. Moreover, this number does not change with $\epsilon$ as long as the $l$-th band remains isolated from the rest of the spectrum. Finally if $P_l$ is two-dimensional, namely of the form $(1 + \bar{\sigma} \bar{\omega})/2$ for some unit vector $\omega$ in $\mathbb{R}^3$, the two-form becomes $\Omega_2 = (\iota/2) \langle \bar{\omega} | d\bar{\omega} \wedge d\bar{\omega} \rangle$.

Now, we assume that, at $\epsilon = 0$, the band $E_+ = E_l$ touch $E_- = E_{l-1}$ at one point $x_0 \in M$ only. The general case can be obtained in a similar way. Let $D$ be a small open neighbourhood of $x_0$ in $M$ diffeomorphic to the unit disk in $\mathbb{R}^2$. Let then $\gamma$ be the oriented boundary of $D$ and $M_D$ be the complement of $D$ in $M$ endowed with the same orientation as $M$. Therefore, as an oriented path $\partial M_D = -\gamma$. For $0 \leq \eta \leq 1$, we construct a new surface $\hat{M}_D(\eta)$ by gluing together $\{+\eta\} \times (-M_D)$, $[-\eta, +\eta] \times \gamma$ and $\{-\eta\} \times (M_D)$, where $-M'$ denotes the manifold $M'$ with opposite orientation (see Fig. 3).

We give $\hat{M}_D(\eta)$ the natural orientation to make it closed. As $\eta \to 0$ this surface is homotopic to itself and becomes two copies of $M_D$ with opposite orientations glued along $\gamma$. Moreover, for every $\eta$, this surface contains no point on which the spectrum of $H$ is degenerate. Therefore $P_l$ defines a line bundle on it. Its Chern class is given by integrating $\Omega_2$ on $\hat{M}_D(\eta)$. Owing to the homotopy invariance of this Chern number, it is enough to compute it for $\eta = 0$ and gives the obvious result
On the other hand, \( \hat{M}_D(\eta) \) can be decomposed into three closed surfaces (see Fig. 2), namely it is homologous to the sum of the following three cycles \( M_+ = \{+\eta\} \times (-M) \), \( M_- = \{-\eta\} \times (M) \) and \( C \) which is obtained by gluing together \( \{+\eta\} \times (D), \{-\eta\} \times (-D) \) and \( [-\eta, +\eta] \times \gamma \) with the corresponding orientation. Integrating \( \Omega_2 \) over \( M_+ \) gives \(-\text{Ch}(+1)\), namely the opposite of the Chern number of the \( l \)-th band for \( \epsilon > 0 \). Integrating it over \( M_- \) gives \( \text{Ch}(-1) \), namely the Chern number of the \( l \)-th band for \( \epsilon < 0 \). Finally the contribution of \( C \) is precisely the Berry index defined by eq. (2) in the introduction, because \( C \) is homotopic to a sphere surrounding the touching point once.

3 Computation of the Berry index

Generic touchings - In the generic case, the function \( \vec{f} \), in eq. (3), expressed in a suitable local chart, admits a Taylor expansion about the touching point \( x_0 \) given by

\[
\vec{f}(\epsilon, x_0 + \xi) = \epsilon \vec{f}_0 + \xi_1 \vec{f}_1 + \xi_2 \vec{f}_2 + \mathcal{O}(\epsilon^2 + \xi_1^2 + \xi_2^2),
\]

where \( \xi = (\xi_1, \xi_2) \) is a small vector in \( \mathbb{R}^2 \) and the three vectors \( \vec{f}_j \) are linearly independent. We do not change the homology class of the closed two-form \( \Omega_2 \) in eq. (3) by modifying \( \vec{f} \) homotopically. We can therefore ignore the remainder and deform continuously the basis \( \vec{f}_j \) to make it coincide with the canonical one up to orientation. The orientation is given by the sign \( \epsilon \) of \( \langle \vec{f}_0 | \vec{f}_1 \times \vec{f}_2 \rangle \), namely the sign of the Jacobian of \( \vec{f} \) at the touching point \( \epsilon = 0, x = x_0 \). Therefore, up to homotopy, we can assume \( \vec{f}(\epsilon, x_0 + \xi) = \epsilon(\epsilon, \xi) \). Using polar coordinates \( (\theta, \phi) \) in \( \mathbb{R}^3 \), this gives \( \vec{\omega} = \vec{f}/|\vec{f}| = \epsilon(\cos(\theta), \sin(\theta) \cos(\phi), \sin(\theta) \sin(\phi)) \), and thus
\[ \Omega_2 = \varepsilon \sin(\theta)d\theta \wedge d\phi. \] Since \( C \) is homotopic to a sphere, it follows that the Berry index in this case is

\[ n(x_0) = \varepsilon = \text{sgn} \det \left( \frac{\partial \vec{f}}{\partial (\epsilon, x)} \right)_{\epsilon=0, x=x_0} = \frac{J \vec{f}(x_0)}{|J \vec{f}(x_0)|}. \]

\[ \square \]

**Parabolic touchings** - Parabolic touching may occur non generically. Such examples have been encountered in the literature \[9, 10, 14\] in connection with either quantum chaos or Bloch electrons in magnetic fields. By redefining the parameter \( \epsilon \) if necessary, we may assume that \( \vec{f} \) vanishes linearly in \( \epsilon \) at \( x = x_0 \). We will say that the touching is “parabolic non degenerate” whenever

\[ \vec{f}(\epsilon, x_0 + \xi) = \epsilon \vec{f}_0 + \xi_1 \vec{f}_{11} + \xi_2 \vec{f}_{22} + 2\xi_1 \xi_2 \vec{f}_{12} + O(\epsilon^2, |\xi|^3), \]

where the three vectors \( \{\vec{f}_{11}, \vec{f}_{22}, \vec{f}_{12}\} \) are linearly independent. Let \( \varepsilon = \pm 1 \) be the orientation of this basis. Again by homotopy, we can neglect the remainder and replace these three vectors by the canonical basis of \( \mathbb{R}^3 \), up to the sign \( \varepsilon \). Thus \( \vec{f} = \epsilon \vec{f}_0 + \varepsilon \vec{g}(\xi) \) where

\[ \vec{g}(\xi) = (\xi_1^2, \xi_2^2, 2\xi_1 \xi_2). \]

Whenever \( \xi \) varies in \( \mathbb{R}^2 \), \( \vec{g}(\xi) \) describes the cone \( \mathcal{K} = \{(x, y, z) \in \mathbb{R}^3; x \geq 0, y \geq 0, (x + y)^2 = (x - y)^2 + z^2 \} \). This is a cone with vertex at the origin, with axis parallel to (1, 1, 0) and with basis given by the ellipse perpendicular to the axis. If moreover, \( \xi \) describes a small circle \( \gamma \) in \( \mathbb{R}^2 \), \( \vec{g}(\xi) \) describes an ellipse similar to the basis of the cone and approaching the cone vertex as the radius of \( \gamma \) decreases to zero. In addition, this ellipse is described twice as \( \gamma \) is described once. Therefore we find two situations compatible with our hypothesis. Either \( \pm \vec{f}_0 \) belongs to the interior of this cone, and then the surface \( \vec{f}(C) \) surrounds the origin twice, with the orientation given by \( \varepsilon \), or it does not and \( \vec{f}(C) \) does not surround the origin at all. In the former case the Berry index is \( n(x_0) = 2\varepsilon \) in the latter \( n(x_0) = 0 \).

If the touching is “parabolic degenerate”, namely if the three vectors \( \{\vec{f}_{11}, \vec{f}_{22}, \vec{f}_{12}\} \) are linearly dependent, the same argument shows that the cone \( \mathcal{K} \) is flat so that the Berry index vanishes. This is the case if for instance \( \vec{f}_{12} = 0 \) \[14\].
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