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Topological Properties of the Born–Oppenheimer Approximation and Implications for the Exact Spectrum

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Abstract. The Born–Oppenheimer approximation can generally be applied when a quantum system is coupled with another comparatively slower system which is treated classically: for a fixed classical state, one considers a stationary quantum vector of the quantum system. Geometrically, this gives a vector bundle over the classical phase space of the slow motion. The topology of this bundle is characterized by integral Chern classes. In the case where the whole system is isolated with a discrete energy spectrum, we show that these integers have a direct manifestation in the qualitative structure of this spectrum: the spectrum is formed by groups of levels and these integers determine the precise number of levels in each group.

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1. Introduction

Many mechanical systems can be considered as a fast dynamical system coupled with a comparatively slower one. In quantum mechanics this occurs, for example, in molecular dynamics, where usually the electrons have a fast motion compared to the motion of nuclei. This is also the case, e.g., for molecules like CD_4, where the vibrational motion of the nuclei is faster than the rotation of the molecule. For these quantum systems, the Born–Oppenheimer approximation is an appropriate approach which consists first in treating the slow motion as classical, characterized by classical dynamical variables X. Then for each fixed value of X, one associates the instantaneous quantum stationary states of the fast dynamical system $|\psi_n(X)\rangle$, with energies $E_n(X)$ (the index n is usually discrete). When the classical states X belong to a two-dimensional compact phase space P (this is the case for a rotational motion which occurs on a sphere), this description gives us a discrete sequence of energy bands numbered by n, see Figure 1(a). For a fixed n, the energy

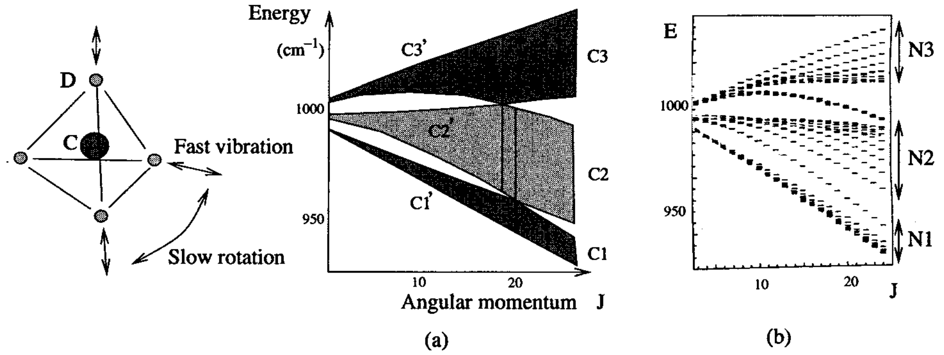

Figure 1. (a) The semi-quantal band spectrum of the CD_4 molecule (taken from [20]). The large-scale three bands structure comes from the quantization of the fast vibrational motion, while the slower rotational motion is treated classically, giving a continuous internal structure of the bands. C_n is the topological Chern index of the band n. The value of the integer C_n can change when a degeneracy occurs between consecutive bands (vertical bars).

(b) The exact quantum spectrum. The fine discrete structure of the bands comes from the quantization of the rotational motion. The number of levels N_n in band n is related to the Chern index C_n by formula (1).

varies continuously in the range of $X \to E_n(X)$, whereas the family of eigenvectors $X \to |\psi_n(X)\rangle$ describes a complex line bundle over P. This line bundle can have a nontrivial topology, characterized by an integer $C_n \in \mathbb{Z}$, the Chern index [11, 14]. This integer reveals a possible global twist of the state $|\psi_n(X)\rangle$ when X varies over P, coming from a strong enough and topologically nontrivial coupling between the slow and fast motion.

In this paper we would like to show that this somewhat abstract topological index has a precise and simple manifestation in the exact spectrum. If the total system is isolated from the outside, it is described by a total Hamiltonian $\hat{H}$ with a discrete spectrum E_i. These discrete energy levels belong to the continuous energy bands of the Born–Oppenheimer approximation. When there is no coupling, the number of levels N_n in each band n is a constant N which comes from the quantization of the classical variable X. In the case of the slow rotational motion with angular momentum j, the phase space P is the sphere S^2, and this constant is $N = 2j + 1$. When there is a coupling, we will show that the bands can have additional energy levels, in relation with the topological integer:

$$N_n = (2j + 1) - C_n. \tag{1}$$

The strategy we will use to prove this relation, is to observe that N_n and C_n can change only when a contact (a degeneracy) occurs between two consecutive bands. On the one hand, a degeneracy between two bands changes the topology in the BO approximation by ΔC_n, and on the other hand, some levels of the exact spectrum pass from one band to the other, giving a redistribution of levels ΔN_n. We will give a normal form for a generic contact and show that $\Delta N_n = -\Delta C_n$. This redistribution of levels between bands is also well observed on experimental spectra, see Figure 1(b).

In this paper we will discuss this phenomena with a model of two coupled spins, **J** and **S**. The spin **S** will be the fast variable, whereas **J** will be slower and treated in the semi-classical limit. This paper presents more details on the results which have been presented in [10], where the applications to molecular physics have been emphasized, and follows after numerous works about qualitative and global analysis of molecular spectra [5, 12, 16].

In the general case where the classical phase space P is not the two-sphere, we have to consider vector bundles of any dimension instead of only line bundles, and formula (1) has to be replaced by a more general expression, which is the Atiyah–Singer index formula. See [4] for this general formulation in deformation quantization, or [7] in geometric quantization.

2. The Classical Limit of the Angular Momentum Dynamics

In this section, we recall some well known results about the angular momentum coherent states, and their role to define the classical limit, see [15] and [21]. We would like to stress the correspondence between the quantum dynamics of an angular momentum with a fixed modulus j (integer or half integer: $2j \in \mathbb{N}$), and the classical dynamics of an angular momentum vector $\mathbf{J}_{\mathrm{cl}}$ of length 1. $\mathbf{J}_{\mathrm{cl}}$ belongs to a sphere noted S_j^2, which is the classical phase space of the angular momentum.

2.1. THE su(2) ALGEBRA AND THE COHERENT STATES

The quantum hermitian operators of the spin J_x, J_y, J_z form an irreducible representation of the su(2) algebra, in a Hilbert space $\mathcal{H}_j$ with dimension $2j+1$. A basis are the vectors $|m\rangle$, $m = -j, -j+1, \dots, +j$, eigenvectors of the J_z operator: $J_z|m\rangle = m|m\rangle$. An element of the group $g \in \mathrm{SU}(2)$ is represented by the unitary operator

$$R(\boldsymbol{\alpha}) = \exp(-i\alpha_3 J_z)\exp\big(-i\alpha_2 J_y\big)\exp(-i\alpha_1 J_z), \tag{2}$$

acting in $\mathcal{H}_j$, where $\boldsymbol{\alpha} = (\alpha_1, \alpha_2, \alpha_3)$ are the Euler angles.

The state $|m = -j\rangle$ corresponds to the classical vector $\mathbf{J}_{\mathrm{cl}} = (0, 0, -1)$. In order to obtain a quantum state $|\mathbf{J}_{\mathrm{cl}}\rangle$ associated to the classical vector $\mathbf{J}_{\mathrm{cl}}$ with any spherical coordinates (θ, φ) we only need to apply the rotation operator (2) on $|m = -j\rangle$, with $\boldsymbol{\alpha} = (0, \theta - \pi, \varphi)$, see Figure 2(a). Such a state $|\mathbf{J}_{\mathrm{cl}}\rangle = R(\boldsymbol{\alpha})|-j\rangle$ is called a *coherent state*. One can show that ([21]):

$$\big|\langle \mathbf{J}'_{\mathrm{cl}}|\mathbf{J}_{\mathrm{cl}}\rangle\big|^2 = \cos^{4j}\left(\frac{\Theta}{2}\right) \simeq 1 - \frac{j\Theta^2}{2} + \mathrm{o}(\Theta^2), \tag{3}$$

where Θ is the angle between $\mathbf{J}'_{\mathrm{cl}}$ and $\mathbf{J}_{\mathrm{cl}}$ on the sphere.

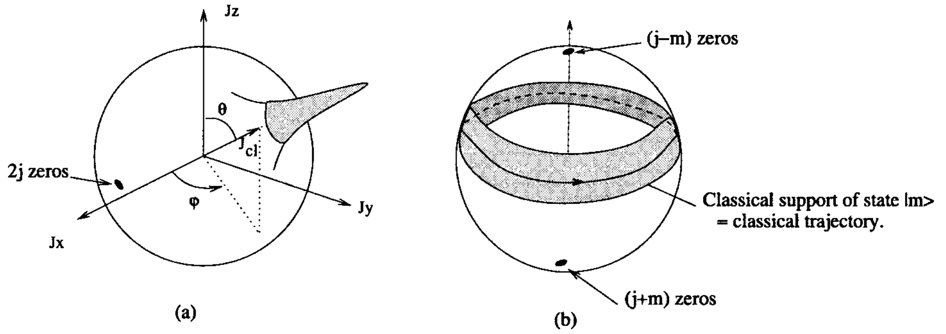

Figure 2. (a) Husimi distribution $\mathrm{Hus}_{\mathbf{J}_{\mathrm{cl}}}(\mathbf{J}'_{\mathrm{cl}}) = |\langle \mathbf{J}'_{\mathrm{cl}}|\mathbf{J}_{\mathrm{cl}}\rangle|^2$ of a coherent state $|\mathbf{J}_{\mathrm{cl}}\rangle$, with its zeros. (b) Husimi distribution $\mathrm{Hus}_{|m\rangle}(\mathbf{J}'_{\mathrm{cl}}) = | < \mathbf{J}'_{\mathrm{cl}}|m\rangle|^2$ of the state $|m\rangle$ with its zeros.

More generally, for every state $|\psi\rangle \in \mathcal{H}_j$, one can define its *Husimi distribution* [18, 19, 21]:

$$\mathrm{Hus}_\psi(\mathbf{J}_{\mathrm{cl}}) = \left|\langle \mathbf{J}_{\mathrm{cl}}|\psi\rangle\right|^2,$$

which is a positive function on the sphere.

From (3), we see that in the limit $j \to \infty$, the Husimi distribution of a coherent state $|\mathbf{J}_{\mathrm{cl}}\rangle$ becomes localized on the phase space, at point $\mathbf{J}_{\mathrm{cl}}$ with a width $\simeq 1/\sqrt{j}$. Let us also remark that if $\mathbf{J}'_{\mathrm{cl}}$ and $\mathbf{J}_{\mathrm{cl}}$ are opposite, then the function $\left|\langle \mathbf{J}'_{\mathrm{cl}}|\mathbf{J}_{\mathrm{cl}}\rangle\right|$ is zero with order $2j$.

As a second example, consider the state $|m\rangle$. One obtains that $\mathrm{Hus}_{|m\rangle}(\mathbf{J}_{\mathrm{cl}}) = |\langle \mathbf{J}_{\mathrm{cl}}|m\rangle|^2$ is maximum on the line $(\mathbf{J}_{\mathrm{cl}})_z = m/j$ as expected, with a width of order $\simeq 1/\sqrt{j}$, and $|\langle \mathbf{J}_{\mathrm{cl}}|m\rangle|$ has a zero of order $(j - m)$ at point $\mathbf{J}_{\mathrm{cl}} = (0, 0, 1)$, and a zero of order $(j + m)$ in $\mathbf{J}_{\mathrm{cl}} = (0, 0, -1)$.

2.2. EXPECTATION VALUES OF OPERATORS

One can compute [21]:

$$\langle \mathbf{J}_{\mathrm{cl}}|J_z/j|\mathbf{J}_{\mathrm{cl}}\rangle = \cos\theta = \mathbf{J}_{\mathrm{cl},z},$$
$$\langle \mathbf{J}_{\mathrm{cl}}|J_x/j|\mathbf{J}_{\mathrm{cl}}\rangle = \sin\theta\cos\varphi = \mathbf{J}_{\mathrm{cl},x},$$
$$\langle \mathbf{J}_{\mathrm{cl}}|J_z^2/j^2|\mathbf{J}_{\mathrm{cl}}\rangle = \cos^2\theta + \frac{1}{2j}\left(1 - \cos^2\theta\right) = \left(\mathbf{J}_{\mathrm{cl},z}\right)^2 + \cdots,$$

and more generally, the expectation value of an operator $\hat{O}$ over coherent states gives a function on the sphere, noted $\sigma_{\hat{O}}(\mathbf{J}_{\mathrm{cl}})$, called the *Berezin symbol of the operator* (or Normal symbol). The operators constructed from the elementary operators $\mathbf{J}/j$ as above, have a symbol which admits a formal series in power of $1/j$:

$$\sigma(\mathbf{J}_{\mathrm{cl}}) = \sigma_0(\mathbf{J}_{\mathrm{cl}}) + \frac{1}{j}\sigma_1(\mathbf{J}_{\mathrm{cl}}) + \cdots.$$

The map $\hat{O} \to \sigma_{\hat{O}}$ is injective [3], so *the symbol characterizes the operator*. The first term $\sigma_0(\mathbf{J}_{\rm cl})$ is the *principal symbol*, or *classical observable*. In the limit $j \to \infty$ the symbols are dense in the space of C^∞ functions on the sphere. See [3, 17] for the more general 'deformation quantization' framework.

3. Coupling Between Two Spins

Let us consider now two spins **J** and **S** as above, acting in separate spaces $\mathcal{H}_j$ and $\mathcal{H}_s$ with respective dimensions $2j+1$ and $2s+1$. These two spins will be coupled dynamically by an Hamiltonian operator $\hat{H}$ acting in the total quantum space $\mathcal{H}_{tot} = \mathcal{H}_j \otimes \mathcal{H}_s$ with dimension $(2j+1)(2s+1)$. We will suppose that $\hat{H}$ is constructed from the elementary operators $\mathbf{J}/j$, and **S**, because in the sequel, we will focus on the semi-classical limit $j \to \infty$. A general form of $\hat{H}$ is therefore:

$$\hat{H} = \sum_{a,\dots,f \geqslant 0} \frac{1}{j^{a+b+c}} C_{a,b,c,d,e,f} J_-^a J_0^b J_+^c S_-^d S_0^e S_+^f, \tag{4}$$

with coefficients $C_{a,b,c,d,e,f}$ such that $\hat{H}$ is self-adjoint. We will treat the following simple example:

$$\hat{H} = (1-\lambda) S_z + \lambda \frac{\mathbf{J}}{j}.\mathbf{S}, \tag{5}$$

where $\lambda \in [0, 1]$ is a fixed parameter, which allows to consider different types of dynamics: for $\lambda = 0$, there is no coupling, whereas for $\lambda = 1$, this is the well known 'spin-orbit' coupling.

4. The Born–Oppenheimer or Semiquantal Description

In the limit $j \to \infty$, we have seen that it is convenient to consider the classical dynamics of **J**, and the 'semi-quantal' symbol of $\hat{H}$:

$$\hat{H}_s(\mathbf{J}_{\rm cl}) = \langle \mathbf{J}_{\rm cl} | \hat{H} | \mathbf{J}_{\rm cl} \rangle,$$

('semiquantal' because **S** remains an operator). This is a function on phase space S_j^2 with matrix values: for each value of $\mathbf{J}_{\rm cl}$, $\hat{H}_s(\mathbf{J}_{\rm cl})$ is a Hermitian operator acting in $\mathcal{H}_s$. Its symbol admits a formal power series in $1/j$:

$$\hat{H}_s(\mathbf{J}_{\rm cl}) = \hat{H}_0(\mathbf{J}_{\rm cl}) + \frac{1}{j} \hat{H}_1(\mathbf{J}_{\rm cl}) + \cdots.$$

We consider the spectrum of its principal symbol:

$$\hat{H}_0(\mathbf{J}_{\rm cl}) |\psi_g(\mathbf{J}_{\rm cl})\rangle = E_g(\mathbf{J}_{\rm cl}) |\psi_g(\mathbf{J}_{\rm cl})\rangle, \quad g = -s, \dots, +s.$$

The idea of Born–Oppenheimer is to stress that because **S** is a fast variable, its state should be an instantaneous stationary state at every time: $|\psi_g(\mathbf{J}_{\rm cl})\rangle$, when $\mathbf{J}_{\rm cl}(t)$ moves more slowly. Theorem 5.2 below will give a precise formulation of this idea.

Suppose that for a fixed value of g, the eigenvalue $E_g(\mathbf{J}_{\rm cl})$ *is isolated*, for every $\mathbf{J}_{\rm cl} \in S^2_j$. (We will discuss this hypothesis in the next section.) Then the range of energy levels $\{E_{g,\mathbf{J}_{\rm cl}},\ \mathbf{J}_{\rm cl} \in S^2_j\}$ for fixed g, is called the *energy band* of the level g. The associated eigenvector $|\psi_g(\mathbf{J}_{\rm cl})\rangle$ is defined up to a multiplicative constant, but the projector $P(\mathbf{J}_{\rm cl})$ on the eigenspace of $E_g(\mathbf{J}_{\rm cl})$ is well defined (globally for all $\mathbf{J}_{\rm cl} \in S^2_j$):

$$P(\mathbf{J}_{\rm cl}) = |\psi_g(\mathbf{J}_{\rm cl})\rangle\langle\psi_g(\mathbf{J}_{\rm cl})|. \tag{6}$$

4.1. DESCRIPTION OF THE FIBER BUNDLE OF THE BAND g

For more information on vector bundles and Chern classes, see, for example, [6, 11, 14].

Let us consider the map on S^2_j given by the rank 1 projectors, defined above (6);

$$P\colon \mathbf{J}_{\rm cl} \in S^2_j \to P(\mathbf{J}_{\rm cl}). \tag{7}$$

The image of the projector $P(\mathbf{J}_{\rm cl})$ associated to the point $\mathbf{J}_{\rm cl}$ is a one-dimensional complex space $L(\mathbf{J}_{\rm cl}) = \mathrm{Im}(P(\mathbf{J}_{\rm cl})) \subset \mathcal{H}_s$ (spanned by $|\psi_g(\mathbf{J}_{\rm cl})\rangle$). These spaces define a *complex line bundle* $L \to S^2_j$ where $L(\mathbf{J}_{\rm cl})$ is the fiber over the point $\mathbf{J}_{\rm cl} \in S^2_j$. See Figure 3.

Since now, we note $M = S^2_j$ the base manifold, which could be any oriented surface. It is clear that the fibers of the Moebius strip have a global nontrivial topology, a 'twist'. This is similar for the complex fibers $L(\mathbf{J}_{\rm cl})$ which can also have a nontrivial topology. This topology is characterized by the first Chern class $c_1 \in H^2(M, \mathbb{Z}) \cong \mathbb{Z}$ which can be labeled by an integer, the *Chern index* C. We explain now how to compute C [11]:

4.1.1. *Levi-Civita Connection, and Curvature*

Fibers $L(\mathbf{J}_{\rm cl})$ are continuously related as $\mathbf{J}_{\rm cl}$ varies. These fibers are subspaces of the fixed space $\mathcal{H}_s$, and the scalar product on $\mathcal{H}_s$ induces a particular connection between these fibers, the *Levi-Civita connection*. One can express it with the covariant derivative of a section. On an open set $U \subset M$, we note A^p the space of p-forms defined on U, and $A^p(L)$ the space of p-forms defined on U with values in L. *A section* $s \in A^0(L)$ is a C^∞ map: $\mathbf{J}_{\rm cl} \in U \to s(\mathbf{J}_{\rm cl}) \in L(\mathbf{J}_{\rm cl})$. The *covariant derivative* D gives information on whether the section follows or not the connection. D can be expressed explicitly with the projector P:

$$s \in A^0(L) \to Ds = P\mathrm{d}s \in A^1(L).$$

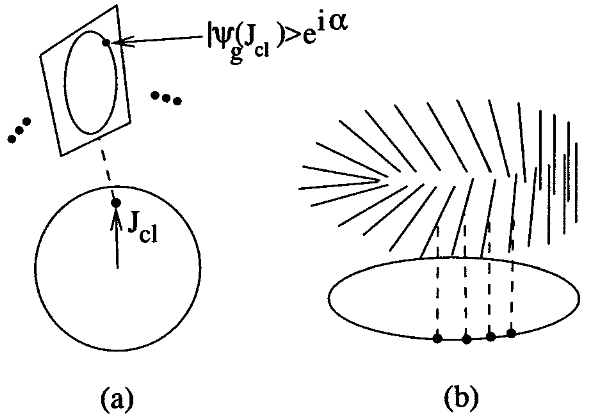

Figure 3. (a) The complex line bundle $L \to S^2_J$. A normalized eigenvector $|\psi_g(\mathbf{J}_{\rm cl})\rangle$ belongs to the fiber $L(\mathbf{J}_{\rm cl})$. Such a vector is defined up to a phase (a circle).
(b) Analogous picture for the real line bundle over the circle S^1. This is the Moebius strip, with a nontrivial global topology.

D satisfies the '*Leibnitz rule*': for $s \in A^0(L)$, $f \in C^\infty(U)$,

$$D(f.s) = \mathrm{d}f.s + f.Ds.$$

(*Proof.* $D(f.s) = P\mathrm{d}(fs) = \mathrm{d}fPs + fP\mathrm{d}s = \mathrm{d}f.s + f.Ds.$)
and '*compatibility with the metric*':

$$\mathrm{d}\langle s, s'\rangle = \langle Ds, s'\rangle + \langle s, Ds'\rangle.$$

(*Proof.* $\mathrm{d}\langle s, s'\rangle = \langle \mathrm{d}s, s'\rangle + \langle s, \mathrm{d}s'\rangle = \langle \mathrm{d}s, Ps'\rangle + \langle Ps, \mathrm{d}s'\rangle = \langle P\mathrm{d}s, s'\rangle + \langle s, P\mathrm{d}s'\rangle = \langle Ds, s'\rangle + \langle s, Ds'\rangle$.)

In practice, one chooses a local section r which never vanishes on an open set $U \subset M$. So r gives a *local trivialization* of L, and we write:

$$Dr = \theta_r r, \quad \theta_r \in A^1, \quad \text{1-form}.$$

The 1-form θ_r characterizes the connection on U, but depends on the choice of r. If r is normalized, ($|r|^2 = 1$), then θ_r takes values in $i\mathbb{R}$, because

$$0 = d\langle r, \quad r\rangle = \langle Dr, \quad r\rangle + \langle r, \quad Dr\rangle = \theta_r + \overline{\theta_r}.$$

The connection D can be extended to $A^p(L) \to A^{p+1}(L)$ by setting for $\psi \in A^p$, $s \in A^0(L)$,

$$D(\psi \otimes s) = \mathrm{d}\psi \otimes s + (-1)^p \psi \wedge Ds,$$

then for $\eta \in A^q(L)$, we have

$$D(\psi \wedge \eta) = \mathrm{d}\psi \wedge \eta + (-1)^p \psi \wedge D\eta.$$

Remark that for $s \in A^0(L)$, $f \in C^\infty(U)$, we have

$$D^2(f.s) = D(\mathrm{d}f \otimes s + fDs) = -\mathrm{d}f \wedge Ds + \mathrm{d}f \wedge Ds + f \wedge D^2 s = f.D^2 s \in A^2(L).$$

So D^2 is a tensor, and at point $\mathbf{J}_{\mathrm{cl}}$, one has

$$\left(D^2\right)_{\mathbf{J}_{\mathrm{cl}}} \in A^2_{(\mathbf{J}_{\mathrm{cl}})} \otimes \mathrm{Hom}(L(\mathbf{J}_{\mathrm{cl}}), L(\mathbf{J}_{\mathrm{cl}})) \equiv A^2_{(\mathbf{J}_{\mathrm{cl}})}.$$

One can write $D^2 s = \Theta s$, $\Theta \in A^2$. If r is a never vanishing section on U, then

$$D^2 r = D(\theta_r r) = \mathrm{d}\theta_r r - \theta_r \wedge Dr = \mathrm{d}\theta_r r - \theta_r \wedge \theta_r = \mathrm{d}\theta_r r,$$

so $\Theta = \mathrm{d}\theta_r$, where Θ takes values in $i\mathbb{R}$, and does not depend on the choice of r.
One can also show that $\Theta = P\mathrm{d}P \wedge \mathrm{d}P$.

4.1.2. *Parallel Transport and Holonomy*
The section s is said to be parallel transported in the direction $X \in T_{\mathbf{J}_{\mathrm{cl}}}M$, at point $\mathbf{J}_{\mathrm{cl}} \in M$, if $D_X s = 0$.

If $\gamma(t) \in M$, $t \in [0, 1]$ is a path, and r a section which never vanishes on γ, then for any section s, one can write $s(\gamma(t)) = f(\gamma(t))r(\gamma(t))$ with $f(t) \in C^\infty[0, 1]$. If s is parallel transported along γ, then

$$0 = D_{\gamma'(t)} s = \frac{\mathrm{d}f(\gamma(t)}{\mathrm{d}} t + \theta_r(\gamma'(t)).f(t).$$

So there is a unique solution $f(1) = f(0).\mathrm{e}^{-\int_\gamma \theta_r}$. If, moreover, γ is a closed path, one sets:

$$\mathrm{e}^{i\varphi_\gamma} = \frac{f(1)}{f(0)} = \mathrm{e}^{-\oint_\gamma \theta_r},$$

which does not depend on the parameterization of the path γ. The holonomy of the connection, or Berry's phase [2] along γ is $\varphi_\gamma = i\oint_\gamma \theta_r$.

4.1.3. *Chern Index and Topology of the Fiber Bundle*
The first Chern class *is:*

$$c_1(L) = \frac{i}{2\pi}[\Theta] \in H^2_{DR}(M, \mathbb{Z}).$$

This is an integer class, which means that

$$C = \int_M c_1(L) \in \mathbb{Z} \tag{8}$$

is an integer, the Chern index. *C characterizes the topology of L, and does not depend on the connection.*

Proof. If $M = S^2$, and if $\gamma \subset M$ is a closed curve, which separates M in two simply connected parts: $M = M_1 \cup M_2$, and $\gamma = \partial M_1 = -\partial M_2$. One chooses sections which not vanish on M_1 and M_2, and with Stokes theorem, the holonomy along γ, is

$\varphi = i \oint_\gamma \theta_e = i \int_{M_1} \Theta = -i \int_{M_2} \Theta\ [2\pi]$. So $i/2\pi \int_M \Theta \in \mathbb{Z}$. (If M is any surface, M can be represented by a disk $\mathcal{D}$ with appropriate identifications of its boundary $\partial\mathcal{D}$, and we take $\gamma = \partial\mathcal{D}$.)

4.1.4. *Expression of the Index C from the Zeros of a Section*
If s is a global section of the fiber L with generic zeros, then one can associate a sign $\iota_p = \pm 1$ *at each zero p, which is the degree of the map* $\mathbf{J}_{\rm cl} \in S_j^2 \to s(\mathbf{J}_{\rm cl}) \in L$ *in a neighborhood of the zero. Then the sum, which does not depend on the section s, is the Chern index:*

$$C = \sum_p \iota_p. \tag{9}$$

If the zeros are not generic, they can overlap, and $\iota_p \in \mathbb{Z}$.

Proof. One can choose a particular section with zero curvature outside the disks D_p surrounding each isolated zero p: the domain is $U = M \setminus \left(\cup_p D_p\right)$, and one has to set $\theta_s = 0$ on U. On every disk D_p, with a local trivialization r, one has $s = f.r$, $Ds = (\mathrm{d}f + \theta_r f)r$. Using Stokes' theorem:

$$C = \frac{i}{2\pi}\int_M \Theta = \frac{i}{2\pi}\sum_p \int_{D_p} \mathrm{d}\theta_r = \frac{i}{2\pi}\sum_p \oint_{\partial D_p} \theta_r = \frac{i}{2\pi}\sum_p \oint_{\partial D_p} \frac{-\mathrm{d}f}{f},$$

and if on ∂D_p, α is a polar coordinate, and $f(\alpha) = \mathrm{e}^{i\varphi(\alpha)}$, then $\mathrm{d}f/f = i\mathrm{d}\varphi$, so

$$C = \frac{1}{2\pi}\sum_p (\varphi(2\pi) - \varphi(0)) = \sum_p \iota_p$$

There is another equivalent expression of the Chern index:

4.1.5. *Expression of the Index C from the Intersection of* Im (P) *with a Hyperplane*
Let us consider Im(P)*, the image of* S_j^2 *in the projective space* $\mathbb{P}(\mathcal{H}_s)$ *by the map (7). If* H *is an hyperplane of* $\mathbb{P}(\mathcal{H}_s)$ *(i.e. hyperplane of* $\mathcal{H}_s$*), then the intersection* $I = H \cap \mathrm{Im}(P)$ *consists of isolated points p (generically), and one can associate to each point p, an orientation* $\iota_p = \pm 1$*, depending on the relative orientations of* H *and* Im(P)*. Then*

$$C = \sum_p \iota_p. \tag{10}$$

If the points p overlap, one must count the multiplicities, and $\iota_p \in \mathbb{Z}$.

To justify this formula from the previous one, consider the hyperplane orthogonal to a fixed vector $|\psi_0\rangle$:

$$H = \left\{|\psi\rangle \in \mathcal{H}_s, \quad \text{s.t. } \langle\psi|\psi_0\rangle = 0\right\}.$$

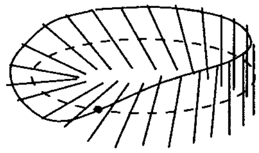

Figure 4. In this example, one can observe that a global section (full line) of the Moebius strip, vanishes an odd number of times: the zeros of a global section reveal a nontrivial topology of the bundle.

In this case, $s(\mathbf{J}_{\rm cl}) = P(\mathbf{J}_{\rm cl})|\psi_0\rangle \in L(\mathbf{J}_{\rm cl})$ is a global section of L, and formula (9) is Equation (10).

Below we will calculate ι_p by choosing a local section $|\psi(\mathbf{J}_{\rm cl})\rangle$ which does not vanish near p, and calculate the degree of the map: $\mathbf{J}_{\rm cl} \to \langle\psi(\mathbf{J}_{\rm cl})|\psi_0\rangle \in \mathbb{C}$.

4.1.6. *Additivity of the Indices*

From the additivity of the first Chern class [6], and because of the triviality of the total bundle $\mathcal{H}_s \to M$, one has $\sum_g c_1(L_g) = c_1(\oplus_g L_g) = c_1(\mathcal{H}_s) = 0$. So $\sum_{g=-s}^{+s} C_g = 0$.

4.2. COMPUTATION OF THE INDICES IN THE SPIN-ORBIT MODEL

We now compute the topological indices of the bands of model Equation (5).

For $\lambda = 0$, $\hat{H}_s = S_z$ does not depend of $\mathbf{J}_{\rm cl}$. The eigenvalues $E_g = g$ are isolated ($g = -s \cdots +s$), and the eigenvectors are independent of $\mathbf{J}_{\rm cl}$, so the bundles L_g are trivial, and $C_g^{(0)} = 0$.

For $\lambda = 1$, we have $\hat{H}_s(\mathbf{J}_{\rm cl}) = (\mathbf{J}_{\rm cl}.\mathbf{S})$ with operators $\mathbf{S}$ acting in $\mathcal{H}_s$, and with $\mathbf{J}_{\rm cl}$ a fixed classical parameter. This Hamiltonian generates the rotations of spin $\mathbf{S}$ around the axis $\mathbf{J}_{\rm cl}$. The eigenvalues are then $E_g = g$ with ($g = -s \cdots +s$), and the eigenvectors $|\psi_g(\mathbf{J}_{\rm cl})\rangle$ are obtained from the state $|m_s = g\rangle$ by a rotation which transforms the axis z into the axis $\mathbf{J}_{\rm cl}$. See Figure 5.

In order to calculate C_g, by the algebraic method explained above, we choose as reference state a coherent state $|\psi_0\rangle = |\mathbf{S}_0\rangle$, and we count the degrees of the zeros of the map $\mathbf{J}_{\rm cl} \to \langle\psi_g(\mathbf{J}_{\rm cl})|\mathbf{S}_0\rangle$. From the Figure (5), obtained from Figure (2), we see that when the axis $\mathbf{J}_{\rm cl}$ moves with direct orientation on the whole sphere, the $(s-g)$ zeros pass with a positive orientation over the fixed point $\mathbf{S}_0$, whereas the $(s+g)$ zeros pass with negative orientation. We deduce that

$$C_g^{(1)} = (s-g) - (s+g) = -2g. \qquad (11)$$

Remark. one can obtain the same result with a curvature integral, but this is less simple, see [1] p. 599.

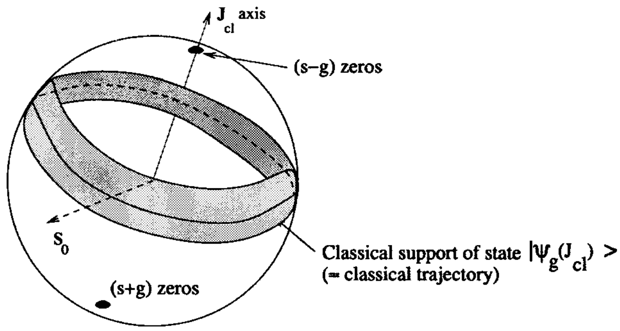

Figure 5. The Husimi distribution $|\langle \mathbf{S}_0|\psi_g(\mathbf{J}_{cl})\rangle|^2$ with its zeros, showing that $C_g^{(1)} = (s-g) - (s+g) = -2g$.

4.3. GENERIC MODIFICATION OF OPERATORS

4.3.1. *Codimension of Generic Degeneracies between Bands*

We have supposed that the level $E_g(\mathbf{J}_{cl})$ has no degeneracies for $\mathbf{J}_{cl} \in S_j^2$. This hypothesis is justified, because in a generic family of Hermitian matrices, degeneracies have codimension three; this means that we need to vary three independent parameters to find a degeneracy between two levels. To explain that, consider two consecutive levels, and the restriction of the Hermitian matrix to these two levels. This gives a (2×2) matrix A. One can subtract a multiple of Identity (i.e. change the reference of energy) so that A has zero trace. But a general (2×2) matrix with zero trace can be written as

$$A = \begin{pmatrix} -z & x - iy \\ x + iy & +z \end{pmatrix}, \tag{12}$$

with three parameters $(x, y, z) \in \mathbb{R}^3$, and only the point $(x = y = z = 0)$ gives a degeneracy. This shows that degeneracies have codimension three.

The eigenvalues of A are

$$E_\pm = \pm\sqrt{x^2 + y^2 + z^2},$$

The functions $E_\pm(x, y, z)$ form two cones, with a contact *conical point* at $(0, 0, 0)$.

4.3.2. *Variation of the Indices*

In our problem, the space of parameters $\mathbf{J}_{cl}$ has dimension $\dim(S_j^2) = 2$. We need then an extra parameter $\lambda \in \mathbb{R}$, to obtain degeneracies between two bands. (This is the role of parameter λ in Equation (5).) In the space $(\mathbf{J}_{cl}, \lambda)$, one can observe degeneracies, see Figure 6. We want to show now that a degeneracy will change the values of Chern indices.

From the additivity of the first Chern class, and because the rank 2 vector bundle of the two bands is well defined: $C_1 + C_2 = c_1(L_1 \oplus L_2) = c_1(L_1' \oplus L_2') = C_1' + C_2'$.

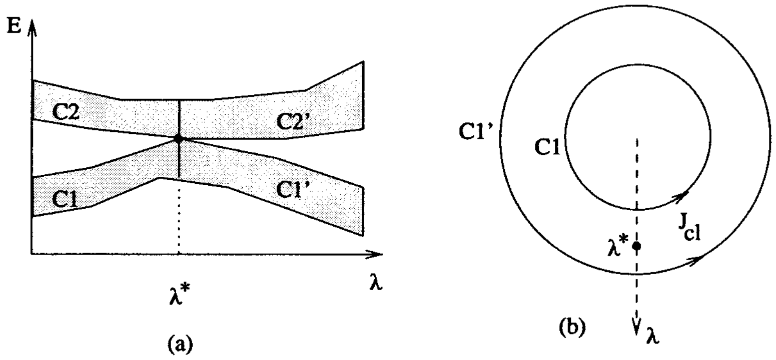

Figure 6. (a) Two consecutive bands (1 and 2) in the space (E, λ), with a degeneracy at $(\mathbf{J}^*_{\mathrm{cl}}, \lambda^*)$. The indices of the bands are C_1, C_2, C'_1, C'_2.
(b) Same picture in the space $(\mathbf{J}_{\mathrm{cl}}, \lambda)$.

So $\Delta C_1 = -\Delta C_2$. Figure 7 shows that the variation ΔC_2 is the *'topological charge of the degeneracy'.*

We have now to calculate ΔC_2. Consider the restriction of the operator $\hat{H}_s$ to two bands, represented by matrix (12). This defines locally a map $D: (\mathbf{J}_{\mathrm{cl}}, \lambda) \to (x, y, z)$, which takes $(\mathbf{J}^*_{\mathrm{cl}}, \lambda^*)$ to $(0, 0, 0)$. One can choose the axis of $\mathbf{J}_{\mathrm{cl}}$, and the origin of λ such that the degeneracy is at $\mathbf{J}_{\mathrm{cl}} = (0, 0, -1)$ and $\lambda = 0$. One can then make a homotopic deformation of this map, such that in a neighborhood of the degeneracy, one has $x = J_x$, $y = J_y$, $z = \pm\lambda$ (the sign $\pm$ depends if the map D conserves orientation or not). The local model is then

$$A_{\pm} = \begin{pmatrix} \mp\lambda & J_{\mathrm{cl},x} - iJ_{\mathrm{cl},y} \\ J_{\mathrm{cl},x} + iJ_{\mathrm{cl},y} & \pm\lambda \end{pmatrix}, \tag{13}$$

(on Figure 7, a direct frame is $(J_x, J_y, -\lambda)$!)

The calculation of the topological charge can be made with the algebraic method. (See also [2] for a computation using the curvature integral.) One can write $A_{\pm} = \mathbf{B}.\mathbf{S}$ with $\mathbf{B} = (J_x, J_y, \mp\lambda)$. The Chern index of the bundle for the highest eigenvalue has been computed in Equation (11) for $g = 1/2$ (with a change of orientation) and gives:

$$\Delta C_2 = \mp 1. \tag{14}$$

5. Manifestation of the Topological Indices in the Exact Spectrum

The natural question is: we have just calculated the topological indices C_g, $g = -s, \ldots, +s$ of the bands in the Born–Oppenheimer approximation. What is the physical meaning of C_g? What is their manifestation in the exact approach

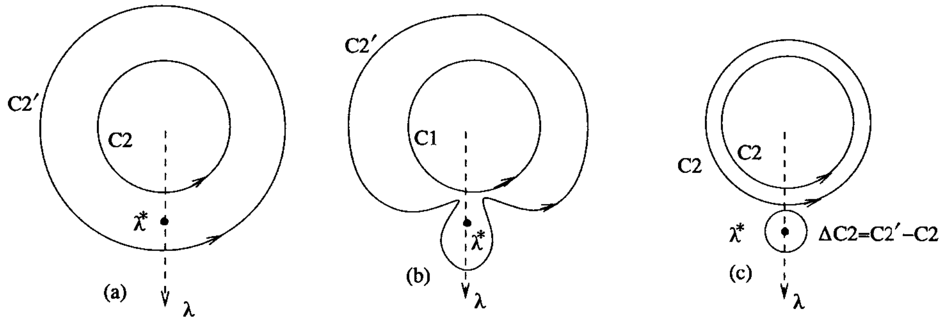

Figure 7. If we deform continuously the external sphere in the space $(\lambda, \mathbf{J}_{cl})$, we deduce that $\Delta C_2 = C_2' - C_2$ is the topological charge of the degeneracy, i.e. the Chern index of the fiber bundle associated to the highest eigenvalue, over a small sphere surrounding the degeneracy.

of the problem? In order to guess the answer, let us study first the quantum 'spin-orbit' model (5). Now $\mathbf{J}$ is an operator, and no more a classical variable.

5.1. SPECTRUM OF THE SPIN-ORBIT MODEL

For $\lambda = 0$, one has $\hat{H} = S_z$. The spectrum has $(2s+1)$ energy levels $E_g = g$, with $g = -s, \ldots, +s$, but each level has multiplicity $2j+1$, because $\hat{H}$ does not depend on $\mathbf{J}$. There is thus $(2s+1)$ groups of levels, in correspondence to each band, and each group contains

$$N_g^{(0)} = 2j + 1 = \dim(\mathcal{H}_j),$$

sub-levels.

For $\lambda = 1$, one has $\hat{H} = 1/j\mathbf{J}.\mathbf{S}$. One can find the spectrum of $\hat{H}$ by introducing the total angular momentum $\mathbf{N} = \mathbf{J} + \mathbf{S}$. Then $\hat{H} = 1/2j(\mathbf{N}^2 - \mathbf{J}^2 - \mathbf{S}^2)$. The eigenvalues of $\mathbf{N}^2$ are $n(n+1)$ with $n = (j-s), \ldots, (j+s)$ (as soon as j), with multiplicity $2n+1$. We deduce that the eigenvalues of $\hat{H}$ are

$$E_g = \frac{1}{2j}(n(n+1) - j(j+1) - s(s+1))$$

(with $g = n - j = -s, \ldots, +s$), with multiplicity

$$N_g^{(1)} = (2j+1) + 2g = \dim(\mathcal{H}_j) + 2g.$$

See Figure 8, which shows the total spectrum. From this computation, two results appear for this simple model:

(1) The exact energy levels of $\hat{H}$ come in groups; each group corresponds to an isolated band in the Born–Oppenheimer approximation.

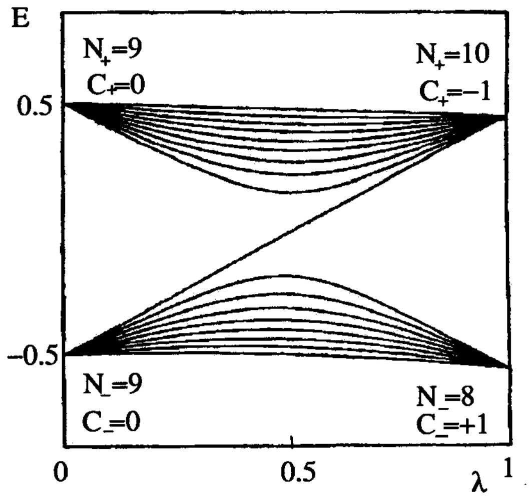

Figure 8. The exact spectrum of the spin-orbit model (5), for $s = 1/2$ and $j = 4$. The values of C_g and N_g are related by Equation (15).

(2) The number of levels N_g of the isolated band g is in accordance with 1:

$$N_g = \dim(\mathcal{H}_j) - C_g. \tag{15}$$

In the next sections, we will justify these two results for a general Hamiltonian such as Equation (7).

5.2. GROUP OF LEVELS OF THE BAND g

This is a result of C. Emmrich and A. Weinstein ([8], theorem 2.1):

5.2.1. *Theorem for 'Born–Oppenheimer'*
We note

$$H_s(\mathbf{J}_{cl}) = H_0(\mathbf{J}_{cl}) + 1/jH_1(\mathbf{J}_{cl}) + \cdots,$$

the symbol of $\hat{H}$ *(which characterizes it). Suppose that* $E_{0,g}(\mathbf{J}_{cl})$ *is an isolated eigenvalue of* $H_0(\mathbf{J}_{cl})$ *for every* $\mathbf{J}_{cl} \in S_j^2$*. We note* $P_0(\mathbf{J}_{cl}) = |\psi_{0,g}(\mathbf{J}_{cl})\rangle\langle\psi_{0,g}(\mathbf{J}_{cl})|$ *the projector on the associated eigenspace. Then for every* $k \in \mathbb{N}$*, there exists a symbol*

$$P(\mathbf{J}_{cl}) = P_0(\mathbf{J}_{cl}) + \frac{1}{j}P_1(\mathbf{J}_{cl}) + \cdots + \frac{1}{j^k}P_k(\mathbf{J}_{cl}),$$

which defines a self-adjoint operator $\hat{P}$ such that

$$\hat{P}^2 = \hat{P} + \mathcal{O}\left(\frac{1}{j^{k+1}}\right), \qquad \textit{quasi-projector,} \tag{16}$$

$$\left[\hat{H}, \hat{P}\right] = \mathcal{O}\left(\frac{1}{j^{k+1}}\right) \qquad \textit{almost commute.} \tag{17}$$

Remarks

- In [8], the hypothesis are more general: the phase space is any symplectic manifold, and the operators need not to be self-adjoint, nor the projector P_0 need to have rank one.
- How can one define the rank of the 'quasi-projector' $\hat{P}$? A consequence of equality (16), is that the eigenvalues of $\hat{P}$ are either close to 1 or to 0 within a range of order $\mathcal{O}(1/j^{k+1})$: if one diagonalizes $\hat{P} = UDU^+$, with $D = (d_1, d_2, \ldots, d_{2s+1})$ eigenvalues of $\hat{P}$, one obtains

  $$\|D^2 - D\| = \varepsilon = \mathcal{O}\left(\frac{1}{j^{k+1}}\right),$$

  so $\max_i |d_i^2 - d_i| = \varepsilon$, so $|d_i| \leqslant \varepsilon$ or $|1 - d_i| \leqslant \varepsilon$. One can thus modify $\hat{P}$ (move slightly the eigenvalues towards 1 or 0, without moving the eigenspaces) to obtain a true projector $\hat{P}'$ whose image is a space $L_g \subset \mathcal{H}_{\text{tot}}$. The rank of this projector is

  $$N_g = \text{Rank}(\hat{P}') = \dim L_g,$$

Remark. N_g is already the number of eigenvalues close to 1 of the principal symbol $P_0(\mathbf{J}_{\text{cl}})$ for band g, (because the error is $\varepsilon = \mathcal{O}(1/j) \ll 1$).

- What can we say about the eigenvectors or eigenvalues of $\hat{H}$ defined by $\hat{H}|\phi_i\rangle = E_i|\phi_i\rangle$? From equality (17), one can almost diagonalizes $\hat{H}$ in the eigenspaces L_g. To be more precise, remark that if one diagonalizes the restriction of $\hat{H}$ in L_g: $\hat{H}' = \hat{P}'\hat{H}\hat{P}'$, the obtained eigenvalues E_i' are close to the real eigenvalues E_i within a distance $\delta E = \mathcal{O}(1/j^{k+1})$. But from the Weyl formula, one expects that generically, every eigenvalue E_i is apart from the other eigenvalues by a distance $\Delta E = \mathcal{O}(1/\dim \mathcal{H}_{\text{tot}}) = \mathcal{O}(1/j)$ for $j \to \infty$. If $k \geqslant 1$, then $\delta E \ll \Delta E$, and a result on quasi-modes ([13], p. 235) states that the eigenvector of $\hat{H}$ associated to the eigenvalue E_i, belongs to the space L_g with an error $(\delta E/\Delta E) \ll 1$. Stated in another way: in the generic case, in the spectrum of $\hat{H}$ one can identify a group of N_g levels associated to the band g. For each eigenvalue E_i and eigenvector $|\phi_i\rangle$, $i \in [1, \ldots (2s+1)(2j+1)]$, one can associate a precise band number $g \in [-s, \ldots, +s]$.

- The ranges of energy for different bands can overlap, and so the levels E_i of different bands can be mixed. But their identification is still possible.
- Discussion of the non generic case: if two levels E_i, E_j of two different bands g, g' are close enough, it is possible that each eigenvector has components on different bands, as it occurs usually in the tunneling effect.
- Equality 20 reflects the idea of Born–Oppenheimer: a consequence is that a quantum state which initially belongs to the space L_g (i.e. band g), will stay in this space forever during its evolution, with a good approximation (if k high).

Indications for the proof. For the proof of the theorem, see [8].The proof is by induction. Check that the result is true for $k = 0$, then suppose it true for $k \in \mathbb{N}$, and write

$$\hat{P}^2 - \hat{P} = \frac{1}{j^{k+1}} \hat{A} + \mathcal{O}\left(\frac{1}{j^{k+1}}\right)$$

and

$$[\hat{P}, \hat{H}] = \frac{1}{j^{k+1}} \hat{F} + \mathcal{O}\left(\frac{1}{j^{k+1}}\right).$$

We look for the symbol $\hat{K}$ such that $\hat{P}' = \hat{P} + 1/(j^{k+1})\hat{K}$ verifies (16), (17), at order $k+1$. Writing these conditions, one obtains that $\hat{K}$ exists and is uniquely determined by $\hat{A}$ and $\hat{F}$ (choose a basis of $\mathcal{H}_s$ where $\hat{H}_0$ and $\hat{P}_0$ are diagonal).

5.3. RELATION BETWEEN C_g AND N_g

We will justify the formula (15), in the general case, by studying specifically the degeneracies between bands. This is because far from degeneracies, C_g is constant, and the number N_g is well defined and constant from theorem in Section 5.2. It is sufficient then to check the relation (15) in a neighborhood of a degeneracy.

5.3.1. *A Normal Form Near a Degeneracy*

In order to understand the phenomenon, we take again the spin-orbit model (5). We have observed that for $\lambda < 1/2$, $C_g = 0$, and for $1 \geqslant \lambda > \frac{1}{2}$, $C_g = -2g$. The change in C_g occurs at $\lambda = \frac{1}{2}$, with a degeneracy between bands located at $\lambda = \frac{1}{2}$, $\mathbf{J}_{\mathrm{cl}} = (0, 0, -1)$, giving $\hat{H}_s(\mathbf{J}_{\mathrm{cl}}) = 0$ (a collective degeneracy). This collective degeneracy is not generic from the above study, except for two bands (if $s = \frac{1}{2}$). Consider then the case $s = \frac{1}{2}$ with two bands numbered by $g = \pm\frac{1}{2}$, and in the neighborhood of the conical degeneracy point $\mathbf{J}_{\mathrm{cl}} = (0, 0, -1)$. In the basis $|\pm\rangle = |m_s = \pm\frac{1}{2}\rangle$ of $\mathcal{H}_s$, where S_x,S_y,S_z are represented by the Pauli 2×2 matrices, we write:

$$\hat{H} = (1-\lambda)S_z + \lambda \frac{\mathbf{J}}{j}.\mathbf{S} \tag{18}$$

$$= \frac{1}{2}\begin{pmatrix} (1-\lambda) + \lambda \dfrac{J_z}{j} & \dfrac{\lambda}{j}(J_x - iJ_y) \\ \dfrac{\lambda}{j}(J_x + iJ_y) & -(1-\lambda) - \lambda \dfrac{J_z}{j} \end{pmatrix}. \tag{19}$$

Take $\tilde{\lambda} = (2\lambda - 1)\sqrt{2j}$. Then for $j \to \infty$, and $\mathbf{J}_{\rm cl} \simeq (0, 0, -1)$, we have $[J_-, J_+] = -2J_z \simeq 2j$, so

$$a = \frac{1}{\sqrt{2j}} J_- = \frac{1}{\sqrt{2j}}\big(J_x - iJ_y\big), \qquad a^+ = \frac{1}{\sqrt{2j}} J_+ = \frac{1}{\sqrt{2j}}\big(J_x + iJ_y\big),$$

fulfill the commutation relations $[a, a^+] \simeq 1$ of the harmonic oscillator. This allows us to write:

$$\hat{H} \simeq \frac{1}{2\sqrt{2j}}\begin{pmatrix} -\tilde{\lambda} & a \\ a^+ & +\tilde{\lambda} \end{pmatrix}. \tag{20}$$

In the sequel, we call Equation (20) the conical model.

Write $\tilde{E} = E\,2\sqrt{2j}$. The spectrum of $\hat{H}$ is obtained by solving $\hat{H}|\phi\rangle = E|\phi\rangle$, with $|\phi\rangle = |\varphi_+\rangle|+\rangle + |\varphi_-\rangle|-\rangle$. This gives

(1) For $n > 0$

$$\tilde{E}_n^{\pm} = \pm\sqrt{n + \tilde{\lambda}^2},$$
$$|\phi_n^{\pm}\rangle = \frac{\sqrt{n}}{\tilde{E}_n^{\pm} + \tilde{\lambda}}|n-1\rangle|+\rangle + |n\rangle|-\rangle,$$

(2) For $n = 0$

$$\tilde{E}_0 = \tilde{\lambda}, \qquad |\phi_0\rangle = |0\rangle|-\rangle.$$

5.3.2. *Asymptotic Behavior of the Spectrum*

The lowest states of the upper band for $\tilde{t} < 0$ are

$$|\phi_n^{+}\rangle = \frac{1}{\tilde{E}_n^{+} + \tilde{\lambda}}|n-1\rangle|+\rangle + |n\rangle|-\rangle, \quad n \geqslant 1,$$

which converge towards $|n-1\rangle|+\rangle$for $\tilde{t} \to -\infty$. (because $1/(\tilde{E}_n^+ + \tilde{\lambda}) \simeq -2\tilde{\lambda}/n$). Similarly, one calculates the three other asymptotics.

The result is sketched in Figure 9.

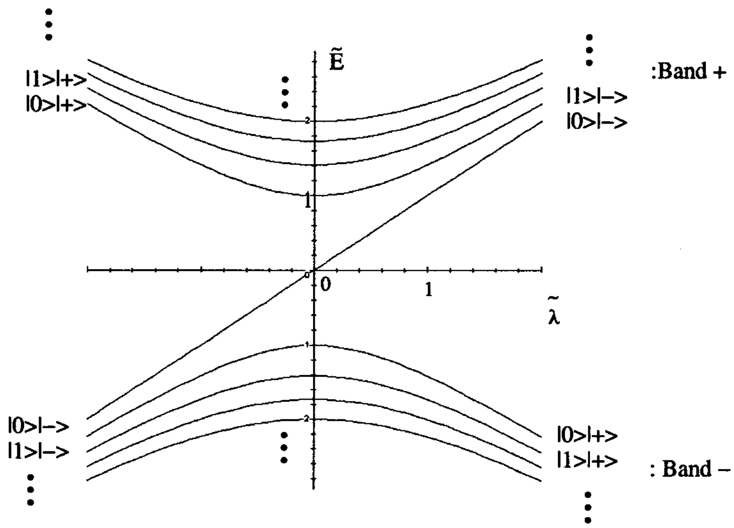

Figure 9. Spectrum of the conical model (20).

The figure shows clearly the exchange of one state between the two bands ($\pm$) giving a variation of number of states:

$$\Delta N_{\pm} = \pm 1.$$

5.3.2. *Topological Charge of the Degeneracy, and Conservation Law*

On can consider the model Equation (20) at the semi-quantal level with classical variables $\mathbf{J}_{\rm cl}$. Write $a_{\rm cl} = (x + ip)$. We have a 2×2 matrix which depends on $(\tilde{\lambda}, x, p) \in \mathbb{R}^3$:

$$\hat{H}_s = \frac{1}{\sqrt{2j}} \begin{pmatrix} -\tilde{\lambda} & x - ip \\ x + ip & \tilde{\lambda} \end{pmatrix}.$$

As studied with Equation (14), in space $(x, p, -\tilde{\lambda}) \in \mathbb{R}^3$, this matrix has a conical degeneracy at $(0, 0, 0)$, with a topological charge $\Delta C_{\pm} = \mp 1$. We therefore obtain $\Delta(C_g + N_g) = 0$ or, said in another way, $C_g + N_g$ is a conserved quantity for each band, even when a degeneracy occurs. The formula (15) in the case $g = 1/2$ can be deduced directly.

Sketch of a proof in the general case. The previous study suggests a proof of formula (15) for a general Hamiltonian $\hat{H}$ as Equation (4). Consider a continuous generic deformation $\hat{H}_\lambda$ from $\hat{H}_{\lambda=1} = \hat{H}$ to $\hat{H}_{\lambda=0} = S_z$ (which is the trivial case). This is a path Γ in the space of Hamiltonian operators from $\hat{H}_0 = S_z$ to $\hat{H}_1 = \hat{H}$. Each operator $\hat{H}_\lambda$ is characterized by its symbol $H_s(\lambda, \mathbf{J}_{\rm cl})$. Along the path Γ, degeneracies between bands of $H_s(\lambda, \mathbf{J}_{\rm cl})$ can occur at isolated points λ^*, and as we saw, after a suitable choice of local coordinates, $H_s(\lambda, \mathbf{J}_{cl})$ is described in the neighborhood of degeneracy point λ^* by the model (13). We have studied this model, and obtained that for each band $(C_g + N_g)$ is a conserved quantity even when the path crosses a degeneracy point. So $(C_g + N_g)$ is constant along the path Γ, and its value for $\lambda = 0$ has been calculated:

$$C_g + N_g = 2j + 1 = \dim \mathcal{H}_j.$$

This gives formula (15).

6. Perspectives

Our study was only for a slow dynamical variable $\mathbf{J}_{cl}$ which belongs to a two-dimensional phase space $M = S_j^2$. To generalize it for phase spaces with higher dimensions, we must remark first that the theorem (5.2) is still valid on the quantum side, and that N_g is still well defined for isolated bands. On the semiquantal side, the topology of an isolated band is characterized by its first Chern class $c_1(L) \in H^2(M, \mathbb{Z})$, characterized by b_2 integers (second Betty number) plus torsion numbers. These two informations should be related by a formula similar to the Riemann–Roch–Hirzebruch formula (or Atiyah–Singer index formula). See [4, 7]. This generalization could find interesting applications in molecular physics.

We must also remark that for $\dim M > 2$, it is no more possible to separate the bands by an argument of genericity as above. We must therefore consider vector bundles of higher dimensions, and topological obstructions play a major role. It should also be possible to develop semiclassical rules for the computation of the indices C_g with a similar approach as in [9].

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