Rearrangement of energy bands: Chern numbers in the presence of cubic symmetry

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Abstract. Formation of energy bands in the system of rotation-vibration quantum states of molecules is described within semi-quantum models under the presence of a symmetry group characterizing the equilibrium molecular configuration. Effective rotation-vibration Hamiltonians are written in two-quantum state models with rotational variables treated as classical ones. Eigen-line bundles associated with eigenvalues of 2×2 Hermitian matrix defined on rotational classical phase space which is a two-dimensional sphere are characterized by the first Chern class. Explicit procedure for the calculation of Chern numbers are suggested and realized for a family of Hamiltonians depending on extra control parameters in the presence of symmetry. Effective Hamiltonians for two vibrational states transforming according to some representations of the cubic symmetry group are studied. Chern numbers are evaluated for respective model Hamiltonians. The iso-Chern diagrams are introduced which split the parameter space into regions with fixed Chern numbers.

Keywords: energy bands, topological invariants, Chern class, molecules

1. Introduction

The energy spectra of many different quantum systems show the presence of bands, i.e. the intermittance of energy regions with high density of states (bands) and zero density of states (gaps). The well known examples are electronic bands in periodic solids, rotational multiplets in rovibrational structure of isolated molecules, Rydberg (Coulomb) shells in one-electron atomic systems etc. Very often this band structure depends on some control parameters: rotational angular momentum, external field parameters, and so on, in such a way that under variation of control parameters certain qualitative modifications of the band structure occur. These modifications are typically related to the redistribution of energy levels between bands for isolated molecules or to the discontinuity of other response quantities, like Hall conductance for solids. It is clear that the mathematical model needed for the description of such qualitative modifications should be based on topological arguments as well as the symmetry properties of the system [3, 2, 6, 7, 11, 18, 10, 20, 1].

The relevance of a topological invariant [17], namely the Chern class, to the qualitative phenomenon of the energy level redistribution between energy bands in rovibrational structure of molecules was initially suggested in [13]. The analysis was done by using a so called semi-quantum model which is based on the splitting of all dynamical variables of the problem into "slow" classical and "fast" quantum variables. In the case of rotational structure of vibrational states, classical rotational variables form a phase space which is a two-dimensional sphere and the number of quantum states taken into account corresponds to a number of analyzed vibrational states counted with their degeneracies. Further studies have shown that generically the redistribution of energy levels in the rotational band structure consists in the transfer of one energy level and is associated with the modification of Chern number by one [5, 6].

In the present paper we analyze in detail the effect of invariance properties of the system exhibiting the effect of the redistribution of energy levels between bands under the variation of control parameters. We start in Section 2 with a brief description of a two-state semi-quantum model for rotational structure of vibrational molecular states in the presence of a symmetry group of a problem. Then in Section 3 we give a construction of complex line bundles associated with the semi-quantum model and introduce the system of charts and a transition function between them which allow us to realize in Section 4 an explicit calculation of Chern numbers in terms of winding numbers. Section 5 discusses a construction of iso-Chern diagrams which describe the splitting of the space of control parameters of the model into regions associated with the same set of Chern numbers for complex line bundles. Concrete examples of Chern number calculations are studied in Section 6 by using effective rotational Hamiltonians for two vibrational states invariant with respect to the cubic symmetry group **O**. An alternative approach to the prediction of possible types of rearrangements based on a simple group theoretical arguments introduced in [19] is compared with the present analysis of Chern numbers in Section 7. Finally, Section 8 discusses directions of further applications and generalizations of our approach.

2. Semi-quantum two state models

Let us start by introducing the energy bands on a very simple purely quantum example of the coupling of two angular momenta.

Let us consider two operators **N** and **S**, acting each on irreducible finite dimensional vector space V_N and V_S whose dimensions are dim

$V_N = 2N+1$ and $\dim V_S = 2S+1$, where N, S are nonnegative integers or half integers.

The total space of the problem is the tensor product $V_N \otimes V_S$. This total space generally could be reducible. The operators acting on that space can be constructed in terms of $\mathbf{S} \otimes \mathbf{1}$ and $\mathbf{1} \otimes \mathbf{N}$ operators.

Instead of looking at the total problem we can try to introduce an additional classifying operator which splits the total space into irreducible subspaces. If the classifying operator commutes with the Hamiltonian of the dynamical system under study, it plays the role of an integral of motion and enables us to split rigorously the total space into subspaces, according to different eigenvalues of the classifying operator.

Taking into account the commutativity of the classifying operator and the Hamiltonian, the whole number of eigenstates of the Hamiltonian can be split into irreducible subspaces which are the invariant subspaces of the classifying operator. From the physical point of view such splitting is often named a band structure. The origin of such terminology becomes especially clear in a limiting situation when all the eigenvalues of the Hamiltonian corresponding to the same eigenvalue of the classifying operator are very close in value (their energy) being at the same time quite distant from energy eigenvalues corresponding to another eigenvalue of classifying operator.

Energy eigenstates corresponding to each irreducible subspace of classifying operator form an "energy band".

From the physical point of view there is a quite important and interesting question: Is it possible to generalize the notion of bands to slightly perturbed (deformed) systems, when the classifying operator does not commute exactly with the Hamiltonian? And even more interesting: Is it possible to describe and to characterize the reorganization of bands which can be easily imagined by constructing a parameter dependent family of Hamiltonians having at different limits the Hamiltonians commuting with different classifying operators and giving the decomposition into different systems of bands?

One of the possibility to realize such a construction is based on the adiabatic separation of variables responsible for an intra-band structure (so called slow motion) and inter-band structure (fast motion). After using classical variables for slow motion and quantum description for fast variables, we obtain so called semi-quantum models [15, 16, 6, 18], where the classical phase space for slow variables can be considered as a base space for a vector bundle, whose fibers are quantum eigenspaces associated to each point of the classical phase space. The Hamiltonian in this model is a matrix valued function defined over the classical limit manifold, the classical phase space for "slow" classical variables. The

rank of the vector bundle is the number of quantum states taken into account in the model.

The situation becomes simple in the case of a fiber bundle over a base space being classical phase space for a one-degree-of-freedom system. If the energy surface associated with each quantum eigenfunction and considered as a function over the classical phase space is isolated as a whole, i.e. possesses no degeneracy points with another energy surface, the fiber bundle can be decomposed into line bundles. The topology of each bundle with complex line fibers can be characterized by a topological invariant, namely the first Chern class.

Restricting ourselves to two quantum state approximation and to the two-dimensional sphere as a classical phase space, we obtain an effective rotation-vibration Hamiltonian written in the form of a 2×2 Hermitian matrix

$$\begin{pmatrix} H_{11} & H_{12} + iG_{12} \\ H_{12} - iG_{12} & H_{22} \end{pmatrix}, \tag{1}$$

where all matrix elements are functions of rotational variables J_x, J_y, J_z and probably on some control parameters $(a_i, b_i, ...)$. Taking into account the conservation of the square of the rotational angular momentum, $\mathbf{J}^2 = \text{const}$, all matrix elements are functions defined on the two-dimensional sphere (the classical phase space of the rotational problem). We can always add a diagonal matrix with $(-H_{11} - H_{22})/2$ factor to get a matrix with zero trace. In order to simplify notation we will use below the simple (x, y, z) notation instead of J_x, J_y, J_z and reparametrize matrix for fixed $\mathbf{J}^2$ value by imposing restriction $x^2 + y^2 + z^2 = 1$.

In the absence of control parameters the matrix Hamilitonian (1) depends generically on two parameters characterizing the point position on the classical phase space, S^2. Consequently this matrix has no degeneracy points of its two eigenvalues, because Hermitian matrices with degeneracy of eigenvalues have codimension 3 in the space of generic Hermitian matrices. The eigenspaces of the matrix (1) form a bundle of rank two over the base space S^2. In the absence of degeneracy points of eigenvalues this vector bundle decomposes into two complex line bundles. Each such complex line bundle is characterized by a Chern number. We can calculate explicitly the Chern numbers by analyzing eigenvectors of (1). But before going to this calculation, a short note should be made on a general method of construction of effective Hamiltonian (1) in the case of the presence of a certain symmetry group.

Let us suppose that the group G is an invariance group of the problem considered. This means that the Hamiltonian should be in-

variant with respect to G. We are mainly interested in cases when the symmetry group is a continuous or a finite point group of the equilibrium configuration extended by time reversal symmetry. Quantum states (or equivalently quantum creation and annihilation bosonic operators) should transform according to two-dimensional reducible or irreducible representation of the symmetry group G. In a similar way classical rotational variables transform according to three-dimensional representation of group G.

We write an effective Hamiltonian in terms of irreducible tensors which can be chosen in the form of tensor product of rotational and vibrational tensorial operators. Rotational tensors $R_\alpha^{\Omega(K,n\Gamma)}$ are characterized by degree Ω, rank K with respect to $SO(3)$ group, multiplicity index n, and irreducible representation Γ of group G. The index α denotes line of a multidimensional representation. The rotational tensors of even degree are invariant with respect to time reversal, whereas rotational tensors of odd degree change sign under time reversal.

If we restrict ourselves to the two state approximation for the vibrational part of the problem, there are only four quantum vibrational operators $a_1^+a_1$, $a_2^+a_2$, $a_1^+a_2 + a_2^+a_1$, $i(a_1^+a_2 - a_2^+a_1)$ which always can be chosen as belonging to irreducible (one- or two-dimensional) representations of the symmetry group G. First three of these operators are time reversal invariant. The last one changes sign under time reversal.

In the case of two vibrational states transforming according to two real one-dimensional representations Γ_1 and Γ_2 the 2×2 effective Hamiltonian has the form

$$\begin{pmatrix} R_{11}^{\Gamma_0} & R_{12,r}^{\Gamma_3} + iR_{12,im}^{\Gamma_3} \\ R_{12,r}^{\Gamma_3} - iR_{12,im}^{\Gamma_3} & R_{22}^{\Gamma_0} \end{pmatrix}, \tag{2}$$

where $\Gamma_0 = \Gamma_1^2 = \Gamma_2^2$ is a totally symmetric representation, and $\Gamma_3 = \Gamma_1 \times \Gamma_2$. Rotational tensors $R_{11}^{\Gamma_0}$, $R_{22}^{\Gamma_0}$, $R_{12,r}^{\Gamma_3}$, are of even degree in elementary rotational variables. Rotational tensor $R_{12,im}^{\Gamma_3}$ is of odd degree in elementary rotational variables.

3. Setting up a complex line bundle

Let now study an abstract 2×2 hermitian matrix

$$\begin{pmatrix} a_{11} & a_{12} + ib_{12} \\ a_{12} - ib_{12} & a_{22} \end{pmatrix}, \tag{3}$$

whose matrix elements are functions defined on the two-dimensional sphere. We want to characterize a bundle formed by normalized eigenvectors of the matrix (3).

As soon as we suppose that two eigenvalues λ_1, λ_2 are nowhere degenerate we can admit that $\lambda_1 > \lambda_2$ everywhere. Let us consider the eigenvector associated to the eigenvalue λ_1. We denote this eigenvector by

$$\begin{pmatrix} C_1 \\ C_2 \end{pmatrix}, \tag{4}$$

where C_1 and C_2 are complex numbers satisfying the normalization condition $|C_1|^2 + |C_2|^2 = 1$. Two possible alternative equations for C_1, C_2 follow from the eigenvalue equation for the matrix (3). We have from the first and the second row of the eigenvalue equation the relations

$$(a_{11} - \lambda_1)C_1^{\rm up} + (a_{12} + ib_{12})C_2^{\rm up} = 0, \tag{5}$$

and

$$(a_{12} - ib_{12})C_1^{\rm down} + (-a_{11} - \lambda_1)C_2^{\rm down} = 0, \tag{6}$$

respectively. Naturally, both relations give the same eigenvector up to phase factor but the definition domain for these two representations of the same eigenvector could be different. Each of them can be defined only in its proper domain in the base space S^2. This is why we have denoted them differently by $C_\alpha^{\rm up}$ and $C_\alpha^{\rm down}$.

The solution to (5) can be written in the form

$$\begin{pmatrix} C_1^{\rm up} \\ C_2^{\rm up} \end{pmatrix} = \frac{1}{\sqrt{(\lambda_1 - a_{11})^2 + a_{12}^2 + b_{12}^2}} \begin{pmatrix} a_{12} + ib_{12} \\ \lambda_1 - a_{11} \end{pmatrix}. \tag{7}$$

This solution is well defined everywhere on the sphere except at points where the norm of the vector goes through zero. The exceptional points occur if three conditions are satisfied:

$$a_{12} = 0; \quad b_{12} = 0, \quad a_{11} = \lambda_1. \tag{8}$$

First two conditions $a_{12} = b_{12} = 0$ generically lead to a number of isolated solutions described as isolated points on the sphere. By substituting $a_{12} = 0$ and $b_{12} = 0$ into $a_{11} = \lambda_1$ we get

$$a_{11} = \frac{1}{2}\left(a_{11} + a_{22} + |a_{11} - a_{22}|\right). \tag{9}$$

One should be reminded that λ_1 is chosen as the highest energy eigenvalue,

$$\lambda_{1,2} = \frac{1}{2}\Big(a_{11} + a_{22} \pm \sqrt{(a_{11} - a_{22})^2 + 4a_{12}^2 + 4b_{12}^2}\Big), \tag{10}$$

so that the sign plus before the square root should be chosen for the λ_1 eigenvalue.

We rewrite Eq. (9) as

$$a_{11}(\theta,\phi) - a_{22}(\theta,\phi) = |a_{11}(\theta,\phi) - a_{22}(\theta,\phi)| \tag{11}$$

to specify two parameters θ, ϕ assigning the points on the base space.

It is clear that the equation (11) is automatically satisfied in the region where $a_{11} - a_{22} \geq 0$ and it is not satisfied in the region where $a_{11} - a_{22} < 0$.

Now we define the domain $U_{\rm up}$ to be the subset of the sphere where the solution (7) is well defined. This domain includes the whole sphere with exception of a number of isolated points which can be found as a solution of the following system of equations and inequalities:

$$a_{12} = 0, \quad b_{12} = 0, \quad a_{11} - a_{22} \geq 0. \tag{12}$$

One should note that it is possible to remove the sign equality in the last relation in (12) and to consider this relation as a strict inequality. This is due to the fact that we are studying now regular points in the parameter space, which assumes that the degeneracy of eigenvalues is absent. At the same time, imposing equality in the last relation we get the system of equations corresponding to the existence of degeneracy points.

Now we can analyze the second equation (6) for the same eigenvector associated with the highest eigenvalue. The solution to (6) can be written in the form

$$\begin{pmatrix} C_1^{\rm down} \\ C_2^{\rm down} \end{pmatrix} = \frac{1}{\sqrt{(\lambda_1 - a_{22})^2 + a_{12}^2 + b_{12}^2}} \begin{pmatrix} \lambda_1 - a_{22} \\ a_{12} - i b_{12} \end{pmatrix}. \tag{13}$$

Like (8), the exceptional points occur if three conditions are satisfied:

$$a_{12} = 0, \quad b_{12} = 0, \quad a_{22} = \lambda_1. \tag{14}$$

The first two conditions $a_{12} = 0$ and $b_{12} = 0$ are exactly the same as in (8). They give on the sphere the same system of isolated points as those for "up" representation. But the third condition now rewrites as

$$a_{22} = \frac{1}{2}\left(a_{11} + a_{22} + |a_{11} - a_{22}|\right) \tag{15}$$

or equivalently as

$$a_{22} - a_{11} = |a_{11} - a_{22}|. \tag{16}$$

It is clear that condition (16) is satisfied if $a_{11} - a_{22} \leq 0$.

In a similar manner to the previous case we can define the domain $U_{\rm down}$ of the sphere where the solution (13) is well defined. This region includes the whole sphere with exception of a number of isolated points which can be found as a solution of the following system of equations and inequalities:

$$a_{12}=0, \quad b_{12}=0, \quad a_{11}-a_{22}\leq 0. \tag{17}$$

Again, for regular points on the parameter space the last relation can be replaced by strict inequality because otherwise the degeneracy of eigenvalues occurs.

Thus we have found "exceptional" points corresponding to singularities of the norm of eigenvectors and constructed two alternative charts on the sphere, where the eigenvectors are well-defined. We have obtained two expressions, (7) and (13), of the positive eigenvector, which are defined on $U_{\rm up}$ and $U_{\rm down}$, respectively. The domain $U_{\rm up}$ consists of the whole sphere without "positive" exceptional points. The domain $U_{\rm down}$ consists of the whole sphere without "negative" exceptional points.

To get the coefficient of proportionality between (7) and (13) on the intersection $U_{\rm up}\cap U_{\rm down}$, we need to calculate the ratio of the first (or of the second) components of the same eigenvectors defined in different domains. This ratio can be rewritten by using the relation $(\lambda_1-a_{11})(\lambda_1-a_{22})=a_{12}^2+b_{12}^2$ and calculated as

$$\frac{a_{12}+ib_{12}}{\sqrt{\left(\lambda_1-a_{11}\right)^2+a_{12}^2+b_{12}^2}}\frac{\sqrt{\left(\lambda_1-a_{22}\right)^2+a_{12}^2+b_{12}^2}}{\lambda_1-a_{22}}=\varepsilon\frac{a_{12}+ib_{12}}{\sqrt{a_{12}^2+b_{12}^2}}, \tag{18}$$

where $\varepsilon=\mathrm{sgn}(\lambda_1-a_{22})$. Now we have obtained the transition rule

$$\begin{pmatrix} C_1^{\rm up}\\ C_2^{\rm up}\end{pmatrix}=\varepsilon\frac{a_{12}+ib_{12}}{\sqrt{a_{12}^2+b_{12}^2}}\begin{pmatrix} C_1^{\rm down}\\ C_2^{\rm down}\end{pmatrix} \quad \text{on} \quad U_{\rm up}\cap U_{\rm down}, \tag{19}$$

which determines the complex line bundle associated with the eigenvalue λ_1.

For notational simplicity, we describe the transition rule (19) as

$$\mathbf{u}_+=\Phi\mathbf{u}_-, \quad \Phi=\varepsilon\frac{a_{12}+ib_{12}}{\sqrt{a_{12}^2+b_{12}^2}}\in U(1), \tag{20}$$

where

$$\mathbf{u}_+=\begin{pmatrix} C_1^{\rm up}\\ C_2^{\rm up}\end{pmatrix}, \quad \mathbf{u}_-=\begin{pmatrix} C_1^{\rm down}\\ C_2^{\rm down}\end{pmatrix}, \quad \varepsilon=\mathrm{sgn}(\lambda_1-a_{22}). \tag{21}$$

Note that in the case of the initial matrix to be chosen with zero trace and $a'_{11} > 0$, we have $\varepsilon = +1$.

The following property of the transition phase factor is very useful for further analysis.

Let us take a closed path (we name it contour) on the sphere which does not pass through "exceptional" points on the sphere. Calculating the phase of the off-diagonal element $a_{12}+ib_{12}$, we can map the contour on the sphere to the complex number plane $\{\Re w, \Im w\}$. The result of this map on the w-plane is again a closed curve which can go an integer (positive or negative) number of times around the $w = 0$ point. As long as the initial contour does not go through "exceptional" points, the image of this contour cannot pass through the zero point $w = 0$. This means that even if we deform continuously the contour on the sphere (preventing it from going through "exceptional" points), the integer number (winding number) giving the number of times the image curve goes around $w = 0$ point remains invariant. Moreover, instead of using the phase of the off-diagonal element, we can equally use directly the real and the imaginary parts of the off-diagonal element without dividing by the absolute value. As long as the contour does not go through "exceptional" points, the process of dividing or multiplying by absolute value (which is strictly positive) cannot change the winding number. Only the continuity of the map is needed to guarantee the invariance of the winding number.

4. Chern number calculation through winding numbers

The local connection forms are defined on $U_{\rm up}$ and $U_{\rm down}$ to be

$$\omega_+ := \mathbf{u}_+^\dagger d\mathbf{u}_+, \quad \omega_- := \mathbf{u}_-^\dagger d\mathbf{u}_-, \tag{22}$$

respectively. Then, when differentiated, the transition equation provides the relation between ω_+ and ω_-,

$$\omega_+ = \Phi^{-1} d\Phi + \omega_- \quad \text{on} \quad U_{\rm up} \cap U_{\rm down}. \tag{23}$$

Let us put Φ in the form $\Phi = e^{i\varphi}$, where φ is determined within additive constants. Then, one obtains by differentiation $\Phi^{-1}d\Phi = id\varphi$, where $d\varphi$ is defined uniquely on $U_{\rm up} \cap U_{\rm down}$. Since $d(\Phi^{-1}d\Phi) = id(d\varphi) = 0$, the curvature form turns out to be defined globally :

$$\Omega = \begin{cases} d\omega_- & \text{on} \quad U_{\rm down} \\ d\omega_+ & \text{on} \quad U_{\rm up} \end{cases}. \tag{24}$$

The first Chern number is defined as the integral over the whole sphere

$$c_1 = \frac{i}{2\pi} \int_{S^2} \Omega. \tag{25}$$

If we are given the Hermitian matrix (1) explicitly, we can calculate the above integral to get the Chern number.

In order to calculate the Chern number according to (25), we split the whole sphere S^2 into regions S^2_+ and S^2_- in such a way that the local connection form ω_+ has no singularities in S^2_+ and the local connection form ω_- has no singularities in S^2_-. We can always do that but each region (S^2_+ or S^2_-) can consist of several connected components. The division of the whole sphere S^2 into S^2_+ and S^2_- can be done by a set of closed paths (closed curves) $C_1, C_2, \ldots, C_k$. Each closed curve C_i is always a boundary between S^2_+ and S^2_- regions. Each curve C_i should be properly oriented. An application of the Stokes theorem provides

$$\int_{S^2} \Omega = \int_{S^2_+} d\omega_+ + \int_{S^2_-} d\omega_- = \oint_{C_1+\cdots+C_k} \omega_+ + \oint_{-(C_1+\cdots+C_k)} \omega_-. \quad (26)$$

Using (23), we rewrite this expression to obtain

$$\begin{aligned} \int_{S^2} \Omega \;&=\; \oint_{C_1+\cdots+C_k} \omega_+ - \oint_{(C_1+\cdots+C_k)} \Big(\omega_+ - \Phi^{-1} d\Phi\Big) \qquad (27)\\ &= \sum_{s=1}^{k} \oint_{C_s} \Phi^{-1} d\Phi = \sum_{s=1}^{k} \oint_{C_s} d\left(\ln \Phi\right)\\ &= \sum_{s=1}^{k} 2\pi\; i\; W(C_s), \end{aligned}$$

where $W(C_s)$ denotes the winding number for C_s and where the phase of the transition phase factor between two charts is written symbolically as $\ln \Phi$. Finally, from (25) and (27), we get the expression of the first Chern number in the form of the sum of the winding numbers for appropriately chosen contours,

$$c_1 = \frac{i}{2\pi} \sum_{s=1}^{k} 2\pi\; i\; W(C_s) = -\sum_{s=1}^{k} W(C_s). \qquad (28)$$

The answer is just the sum of winding numbers for all contours separating S^2_+ and S^2_- regions. It can be easily seen that this sum of winding numbers can be transformed into a sum over circles surrounding each exceptional point of S^2_+ region. Figure 1 shows example of such transformation of contours. The example shown in Figure 1 is artificial. Three "exceptional" points surrounded by two circular paths are chosen in order to demonstrate that the number of contours can change by continuous deformation. At a final result of deformation (shown in Figure 1, right) the winding numbers can be calculated either along two circular paths (these two paths are just the deformed versions

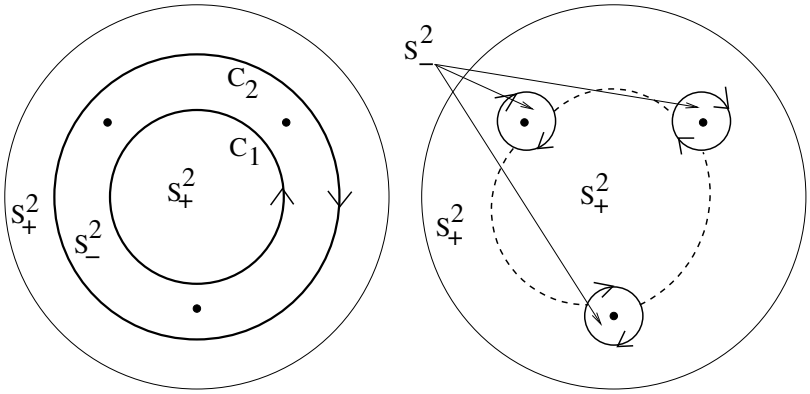

Figure 1. Example of the splitting of the sphere into S^2_+ and S^2_- regions. The part of the sphere is represented which has three "positive" zeros. These zeros are shown by three black dots. Left figure gives an example of the choice of two contours, C_1 and C_2, separating S^2_+ and S^2_- regions. The sum of integrals along C_1 and C_2 contours is equivalent to the sum of integrals along three contours surrounding "positive" zeros, as shown in the right figure. Paths shown by dashed lines in the right figure give zero contribution to the sum of contour integrals.

of initial paths) or along three new paths. Each new path surrounds one "exceptional" point.

Now we can formulate the final step in the calculation of Chern numbers for a 2×2 matrix Hamiltonian defined over the two-dimensional sphere and depending on extra control parameters.

We split the sphere into (multi-component) regions S^2_+ and S^2_- in such a way that S^2_+ includes only "negative" exceptional points and S^2_- includes only "positive" exceptional points. For each contour separating S^2_+ and S^2_-, we find the winding number for the map of this contour to the w-plane. The image of this map are components of the real and the imaginary parts of the off-diagonal matrix element of the Hamiltonian. The Chern number is expressed as an appropriate algebraic sum of winding numbers for all contours.

From the point of view of practical calculations it is useful to choose contours lying on the sphere at a constant value of one of coordinates, say z. This allows us to check easily the winding numbers by looking at the z dependence of the winding number. The winding number is not defined if the contour goes through an exceptional point. Otherwise the winding number is an integer and remains invariant under any continuous deformation of the contour if all exceptional points remain avoided under such deformation.

5. Iso-Chern diagrams

If the effective Hamiltonian depends on some control parameters, the degeneracy of eigenvalues is generically possible. All points in the control parameter space which correspond to the absence of degeneracy of eigenvalues are called regular. Parameters corresponding to the degeneracy of eigenvalues form subsets in the parameter space, which can split the parameter space into connected domains of regular values of parameters. We call those domains *iso-Chern domains*. This is because the Chern numbers assigned to each regular values of parameters are constant on such a domain.

To find the boundaries of iso-Chern domains, we need to solve the equation:

$$\det \begin{pmatrix} a_{11} & a_{12}+ib_{12} \\ a_{12}-ib_{12} & -a_{11} \end{pmatrix} = 0, \tag{29}$$

which is equivalent (assuming that a_{11}, a_{12}, and b_{12} are real) to the system of three equations

$$a_{11}=0; \quad a_{12}=0; \quad b_{12}=0. \tag{30}$$

Caution should be taken in describing iso-Chern domains in the space of control parameters. For example, trivial scaling of all terms of the Hamiltonian by the same positive factor naturally transforms regular points of the parameter space into regular points, if the Hamiltonian depends linear-homogeneously on the parameters. All such regular points should belong to the same "iso-Chern" domain of the parameter space. At the same time the simultaneous scaling of all terms of the Hamiltonian by a negative factor transforms regular points of parameter space into other regular points of the parameter space, but corresponding points are not obliged to belong to the same connected (iso-Chern) domain of the parameter space. This is due to the fact that the zero value of the scaling factor can result in a non-regular parameter value. This example in which the scaling of all terms of the Hamiltonian is performed is rather an oversimplified example. In contrast with this, it is possible that the scaling of only a part of terms of the Hamiltonian does not modify the equations defining degeneracy points for the eigenvalues. For example, the scaling of all parameters appearing in the diagonal elements of the matrix, or in the real part of the off-diagonal elements of the matrix, or in the imaginary part of the off-diagonal elements of the matrix do not change the equations (30). In such a case the simultaneous scaling by a negative factor transforms regular points into regular points, but these regular points may belong to different connected domains of the iso-Chern diagram.

6. O invariant model Hamiltonians

The choice of a symmetry group depends on which model we are interested in. Leaving the choice of $SO(2)$ and D_3 to another article [9], we here take up the cubic symmetry **O** group. According to the choice of representations of the **O** group, we here consider three types of model Hamiltonians.

6.1. A_1-A_1 VIBRATIONAL STATES FOR THE **O** GROUP

A simplest effective two-state model for totally symmetric vibrational states of a molecule with the **O** symmetry group has the following form in standard spectroscopic notations,

$$\begin{pmatrix} v + a_1 R^{4(4,A_1)} + b_1 R^{6(6,A_1)} & u + a_2 R^{4(4,A_1)} + b_2 R^{6(6,A_1)} - icR^{9(9,A_1)} \\ u + a_2 R^{4(4,A_1)} + b_2 R^{6(6,A_1)} + icR^{9(9,A_1)} & -v - a_1 R^{4(4,A_1)} - b_1 R^{6(6,A_1)} \end{pmatrix} \quad (31)$$

where the **O**-invariant rotational tensors can be taken in the following explicit form in terms of Cartesian variables $\{x, y, z\}$ (instead of writing $\{J_x, J_y, J_z\}$) [12, 11]

$$R^{4(4,A_1)} = x^4 + y^4 + z^4; \quad (32)$$

$$R^{6(6,A_1)} = x^2 y^2 z^2; \quad (33)$$

$$R^{9(9,A_1)} = xyz(x^2 - y^2)(y^2 - z^2)(z^2 - x^2). \quad (34)$$

Scalar terms are neglected in the effective Hamiltonian (31). Time reversal symmetry is included; the real part of the matrix depends on rotational variables in even degree, while the imaginary part depends on rotational variables in odd degree.

In order to find degeneracy points, we need to solve the system of four equations

$$v + a_1(x^4 + y^4 + z^4) + b_1 x^2 y^2 z^2 = 0; \quad (35)$$

$$u + a_2(x^4 + y^4 + z^4) + b_2 x^2 y^2 z^2 = 0; \quad (36)$$

$$xyz(x^2 - y^2)(y^2 - z^2)(z^2 - x^2) = 0; \quad (37)$$

$$x^2 + y^2 + z^2 = 1. \quad (38)$$

Eq. (35) corresponds to the zero of the diagonal element, and Eqs. (36) and (37) impose the real part and the imaginary part of the off-diagonal element to be zero, respectively. Eq. (38) describes the sphere.

Instead of analyzing the whole multi-parametric model, we are allowed to reduce the number of parameters, keeping at the same time the subdivision of the parameter space into iso-Chern domains. Two

Hamiltonians belong to the same iso-Chern domain, if their parameters can be connected by a continuous curve in the parameter space which does not cross the parameter values corresponding to the presence of degeneracy points. Thus, we need to find the description of parameters belonging to the same iso-Chern domain and of the boundary of the domain. After constructing boundaries of iso-Chern domains, we have only to take particular points in different domains to calculate Chern numbers for respective domains.

In order to make such a choice of particular (but generic) numerical values, it is useful to start by describing the space of orbits of the $\mathbf{O}_h$ group action on the sphere in terms of the basic invariant polynomials

$$\theta_4 = x^4 + y^4 + z^4, \quad \theta_6 = x^2y^2z^2. \tag{39}$$

The resulting orbit space is shown in Figure 2. This orbit space is described in details in [11], Fig. 14 and Table 6 (see also [4, 12]).

The boundary of the space of orbits corresponds exactly to the zero value of the $R^{9(9,A_1)}$ tensor. It should be noted that the orbit space described in Figure 2 is for the $\mathbf{O}_h$ group rather than for the $\mathbf{O}$ group. The orbit space for the $\mathbf{O}$ group is twice larger, because the auxiliary invariant polynomial $R^{9(9,A_1)}$ for the $\mathbf{O}$ group takes two values for each internal point of the space of $\mathbf{O}_h$ orbits characterized by two $\mathbf{O}_h$ invariant polynomials $R^{4(4,A_1)}$ and $R^{6(6,A_1)}$. But we need exactly the $\mathbf{O}_h$ orbit space to analyze in a geometrical way the solutions of the system of equations for the existence of degeneracy points. The key point is the fact that the boundary of the $\mathbf{O}_h$ orbit space is the zero of the auxiliary invariant for the $\mathbf{O}$ group, which is an index 2 subgroup of the $\mathbf{O}_h$ group.

The diagonal element and the real part of the off-diagonal element are written as linear functions of the basic invariant polynomials. Thus, graphical representations of these two equations in terms of the basic invariant polynomials are straight lines. Generically, these straight lines have one intersection point. This means that the simultaneous solution of the first, second and fourth equations is a point, which naturally in general case does not coincide with the points of the boundary of the $\mathbf{O}_h$ orbits space corresponding to zero value of the imaginary part of the off-diagonal element.

By varying the control parameters we can change the position of the intersection point of the two straight lines corresponding to the real part of the off-diagonal element and to the diagonal element. If the intersection point of these two lines takes place on the boundary of the $\mathbf{O}_h$ orbit space, the corresponding set of parameter values is associated with the effective Hamiltonian possessing degeneracy of two eigenvalues. As long as the intersection point belongs to the boundary

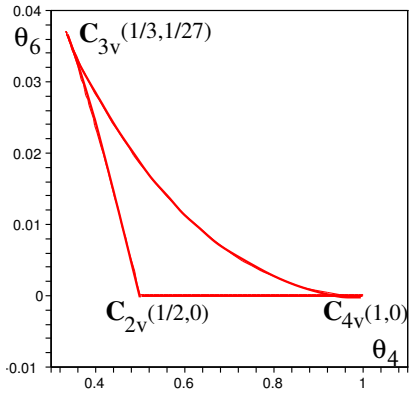

Figure 2. Space of orbits of the $\mathbf{O}_h$ group action on the sphere. The boundary of the orbit space corresponds to a zero of $R^{9(9,A_1)}$ auxiliary invariant tensor for the $\mathbf{O}$ group action, whose square is a polynomial of basic invariants θ_4, θ_6.

(but not to the apex), there are in essence 24 equivalent points. This is because the degeneracy points on the sphere form an orbit of the $\mathbf{O}$ group and the order of the $\mathbf{O}$ group is 24. In this manner, we can make effective use of the $\{\theta_4, \theta_6\}$ plane, in which the orbit space and the two straight lines corresponding to the diagonal element and the real part of the off-diagonal element are drawn, in order to figure out a geometric image of the parameter space.

An obvious consequence of this geometrical approach to Eqs. (35), (36), (37), (38) is the existence of at least two different iso-Chern domains. To each effective Hamiltonian (31) depending on seven control parameters, we put a point A on the $\{\theta_4, \theta_6\}$ plane in correspondence with the intersection point of the two straight lines representing zero of the diagonal and of the real part of the off-diagonal element. A set of parameters for which the positions of the point is outside the orbit space and a set of parameters for which the position of A is inside the orbit space cannot belong to the same iso-Chern domain, because under a continuous variation of parameters the point A should cross the boundary of the orbit space in order to pass from the outside to the inside of the orbit space and because the parameters corresponding to the moment when the point A crosses the boundary are associated with the degeneracy of the eigenvalues of the Hamiltonian.

Unfortunately, this simple analysis does not give the complete description of all iso-Chern domains existing for the Hamiltonian (31). The two intersecting straight lines on the $\{\theta_4, \theta_6\}$ plane are not unique for a given Hamiltonians. In fact, if the parameters (v, a_1, b_1) or (u, a_2, b_2)

get the opposite sign, the position of the straight line in question remains to be the same. We can distinguish those parameters by specifying the directions of the straight lines with the convention that the positive values of the associated matrix element are on the left side of the line with respect to the chosen direction. As long as the direction is specified, we cannot realize a continuous modification of parameters which results in reversing the orientation without going through some exceptional configurations of two straight lines corresponding to zero or infinite values of the diagonal element or of the real part of the off-diagonal element. Under parameter modifications two lines can also become parallel or can coincide. The conditions for the appearance of degeneracy points can become less restrictive if accidentally several coefficients goes through zero values.

It is necessary to note that each generic configuration of the two straight lines on the plane with the orbit space drawn corresponds to four different Hamiltonians. These four Hamiltonians are due to different possible choice of the sign of the diagonal element and of the real part of the off-diagonal element. Graphically we can describe these different choices by assigning the direction (arrow) to each line under the convention already mentioned. These four configurations cannot belong to the same iso-Chern domain.

The global topology of the parameter space and of the iso-Chern diagram will not be studied here. We will just analyze some simple generic modification of parameters which is represented schematically in Figure 3. The initial choice of parameter values (Figure 3, a) and the final choice of parameters (Figure 3, e) belong to the same iso-Chern domain, because the configuration of two straight lines can be evolved from that in (Figure 3, a) to that in (Figure 3, e) in such a way that the intersection point of the two lines does not either enter the orbit space nor cross the boundary. The configuration shown in Figure 3, c belongs to another iso-Chern domain.

Let us summarize now numerical results for the positions of exceptional points for the effective Hamiltonian (31) with the following parameters:

$$v = 0.4;\ u = 0.6;\ a_1 = -1;\ b_1 = 1;\ a_2 = 1.36;\ b_2 = -1;\ c = 1. \quad (40)$$

These parameters correspond to the position of the intersection point of the two straight lines inside the orbit space. There are 24 "positive" real exceptional points, 24 "negative" real exceptional points and 48 complex solutions for zeros of the off-diagonal element for this set of control parameters, where "positive" and "negative" are attached to indicate the sign of a_{11}, the diagonal element, for exceptional points in question. We are interested only in real solutions. They correspond to

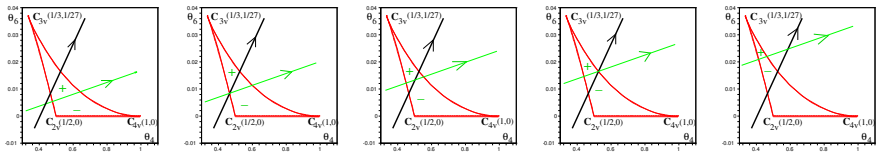

Figure 3. Parametric evolution of an **O** symmetric Hamiltonian. Thin straight (green) line represents zero value of the diagonal matrix element. Thick straight (black) line represents zero value of the real part of off-diagonal element. Boundary (red) of the orbit space corresponds to zero value of the auxiliary invariant $R^{9(9,A_1)}$. The value of v parameter varies from (a) to (e). The intersection point of two straight lines corresponds to simultaneous zero of the diagonal and the real part of the off-diagonal element. (b) and (d) correspond to the set of parameters associated with the formation of 24 degeneracy points. When the intersection point is outside of the orbit space, i.e. in (a) and (e) cases, the Chern numbers for two eigen-line bundles are zero. When the intersection point is inside the orbit space, case (c), the Chern numbers are ± 24.

two intersection points of the line corresponding to the real part of the off-diagonal element with the boundary of the orbit space. These two points lie at different sides of the straight line representing zero of the diagonal element and consequently they are associated with different sign of the diagonal element. These exceptional points form two orbits of the **O** group action on the sphere. Each orbit consists of 24 points and has a trivial stabilizer C_1 of the **O** group. With respect to a larger $\mathbf{O}_h$ group the stabilizer of each orbit is C_s. If we use the geometric representation of the $\mathbf{O}_h$ orbit space in terms of the basis invariant polynomials ($\theta_4 = x^4 + y^4 + z^4, \theta_6 = x^2y^2z^2$), these two orbits have coordinates

$$\theta_4 = 0.422181, \quad \theta_6 = 0.0258329, \quad a_{11} > 0,$$

for positive exceptional points and

$$\theta_4 = 0.428552, \quad \theta_6 = 0.0171687, \quad a_{11} < 0,$$

for negative exceptional points.

The $\{x, y, z\}$ coordinates of the real exceptional points are listed in Table I.

In order to calculate the Chern number, we split the sphere into UP and DOWN domains by $z_\alpha = \text{const}$ sections, $\alpha = 1, \ldots, 6$, subject to
$0.7594 > z_1 > 0.6777$; $\quad 0.6777 > z_2 > 0.4600$;
$0.4600 > z_3 > 0.2852$; $\quad -0.2852 > z_4 > -0.4600$;
$-0.4600 > z_5 > -0.6777$; $\quad -0.6777 > z_6 > -0.7594$.

Table I. Exceptional points for Hamiltonian (41) with parameters given in (40). Each line corresponds to four exceptional points with all possible combinations of signs of x and y coordinates.

z	y	x	a_{11}
0.75941	$\pm$0.46004	$\pm$0.46004	+
0.67772	$\pm$0.67772	$\pm$0.28527	−
0.67772	$\pm$0.28527	$\pm$0.67772	−
0.46004	$\pm$0.75941	$\pm$0.46004	+
0.46004	$\pm$0.46004	$\pm$0.75941	+
0.28527	$\pm$0.67772	$\pm$0.67772	−
−0.28527	$\pm$0.67772	$\pm$0.67772	−
−0.46004	$\pm$0.46004	$\pm$0.75941	+
−0.46004	$\pm$0.75941	$\pm$0.46004	+
−0.67772	$\pm$0.28527	$\pm$0.67772	−
−0.67772	$\pm$0.67772	$\pm$0.28527	−
−0.75941	$\pm$0.46004	$\pm$0.46004	+

These $z_\alpha = \text{const}$ sections separate regions with positive and negative exceptional points.

Both the real and the imaginary parts of the off-diagonal element are **O**-invariant function in the studied case of two totally symmetric states. As soon as the z axis coincides with the order four symmetry axis, the winding number can be calculated as four times the winding number corresponding to the closed contour associated to the range of ϕ angle between 0 and $\pi/2$. This sub-contour is closed on the w-plane owing to the C_4 symmetry.

Figure 4 shows winding numbers for three contours with positive z_α values. Each contour gives contribution ± 4 to the Chern numbers. After summing winding numbers with appropriate signs, the Chern numbers for two eigen-line bundles are found to be ± 24.

When the parameters are such that the intersection point of two lines shown in Figure 3 is located outside the orbit space, all exceptional points have the same sign. Both intersection points of the straight line corresponding to zero of the off-diagonal element with the boundary of the orbit space are located in the same half-plane with respect to the line corresponding to zero of the diagonal element. The immediate consequence of this fact is the zero Chern numbers for both components.

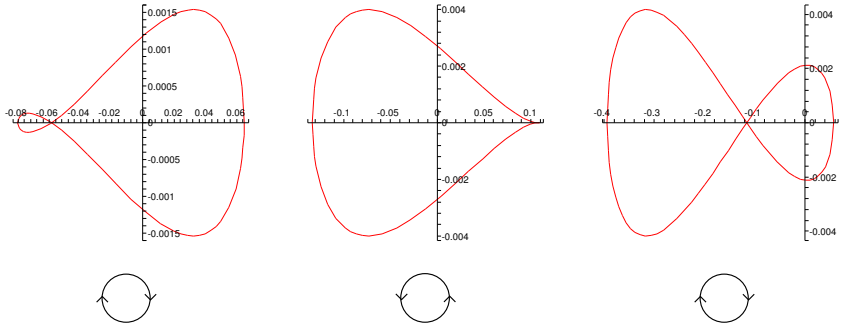

Figure 4. Winding number calculation for contours corresponding to $z = 0.7$, $z = 0.6$, $z = 0.4$. Due to C_4^z symmetry of the imaginary part of off-diagonal element the plot is done for $0 \leq \phi \leq \pi/2$. The winding number for the whole contour corresponding to $0 \leq \phi \leq 2\pi$ is four times larger. The absolute value of total winding number for each $z = const$ section is four. The sign of winding numbers is shown by a diagram below the contour in the complex plane.

6.2. A_1-A_2 VIBRATIONAL STATES FOR THE **O** GROUP

If we take into account rotational tensors up to degree six, an effective rotational Hamiltonian for two vibrational states with A_1, A_2 type representations of the **O** symmetry group has the form

$$\begin{pmatrix} v + a_1 R^{4(4,A_1)} + b_1 R^{6(6,A_1)} & a_2 R^{6(6,A_2)} - icR^{3(3,A_2)} \\ a_2 R^{6(6,A_2)} + icR^{3(3,A_2)} & -v - a_1 R^{4(4,A_1)} - b_1 R^{6(6,A_1)} \end{pmatrix} \quad (41)$$

The A_2 tensors can be chosen to take the form

$$R^{3(3,A_2)} = xyz; \quad (42)$$

$$R^{6(6,A_2)} = (x^2 - y^2)(y^2 - z^2)(z^2 - x^2). \quad (43)$$

In order to represent degeneracy points on the orbit space, we need to find expressions for the square of $R^{3(3,A_2)}$ and of $R^{6(6,A_2)}$ in terms of basic invariants used in the preceding subsection;

$$\left(R^{3(3,A_2)}\right)^2 = R^{6(6,A_1)}; \quad (44)$$

$$\left(R^{6(6,A_2)}\right)^2 = \frac{1}{2}\left(R^{4(4,A_1)}\right)^3 - 27\left(R^{6(6,A_1)}\right)^2 - 9R^{4(4,A_1)}R^{6(6,A_1)} - \frac{5}{4}\left(R^{4(4,A_1)}\right)^2 + 5R^{6(6,A_1)} + R^{4(4,A_1)} - \frac{1}{4}. \quad (45)$$

In fact, the answer is trivially related to the syzygy used earlier for the $\mathbf{O}_h$ group (see [11], Eq. (116)). The auxiliary invariant $R^{9(9,A_1)}$ is

simply a product of two A_2 covariants:

$$R^{9(9,A_1)} = R^{3(3,A_2)} R^{6(6,A_2)}.$$

Thus, the imaginary part of the off-diagonal element becomes zero, $R^{3(3,A_2)} = 0$, only at the boundary of the $\mathbf{O}_h$ orbit space, corresponding to $R^{6(6,A_1)} = 0$ (i.e. on the closure of C_h stratum of the $\mathbf{O}_h$ group, where C_h class includes three reflections in planes orthogonal to three C_4 axes). The real part of the off-diagonal element takes zero value at two other sides of the O_h orbit space (on the closure of C_s stratum of the $\mathbf{O}_h$ group, where C_s class includes six reflections in planes orthogonal to six $C_2^{(d)}$ axes). Common zero of the real and the imaginary parts of the off-diagonal elements occurs always [for any non-zero choice of parameters of the Hamiltonian written in the form (41)] at C_{4v} and C_{2v} isolated orbits of the $\mathbf{O}_h$ group.

For the Hamiltonian of the form (41), the representation of the zeros of diagonal elements is a straight line on the $\{\theta_4, \theta_6\}$ plane. In order to describe the situations corresponding to the formation of degeneracy points (simultaneous zero of the diagonal and the off-diagonal elements), we first note that varying coefficients in the off-diagonal element (one coefficient for the real part and another coefficient for the imaginary part) does not alter the position of zeros of the off-diagonal element, which are fixed at C_2 and C_4 axis positions except for cases when a_2 or c coefficients become zero. Varying coefficients of the diagonal part changes the position of the straight line representing zeros of the diagonal elements on the $\{\theta_4, \theta_6\}$ plane.

Let us say that the straight line is regular if it does not pass through C_{2v} or C_{4v} orbit and singular if it passes through at least one of these orbits. There are two different equivalence classes of regular straight lines, which can be continuously transformed one into another without passing through one singular line. One such class consists of all lines which cross the line segment $((1/2, 0), (1, 0))$. Another class consists of all lines which do not cross the line segment $((1/2, 0), (1, 0))$. This gives rise to the splitting of the parameter space of the effective Hamiltonians into different iso-Chern domains.

For the more accurate description of different iso-Chern domains, one should take into account the location of positive and negative values of the diagonal matrix elements, which can be done by specifying the direction of the line. With such directions taken into account, there are two different iso-Chern domains associated with lines crossing the C_h stratum and two different iso-Chern domains associated with lines which do not cross the C_h stratum.

One class of singular lines passes through C_{2v} orbit. It corresponds to the formation of 12 equivalent degeneracy points. Another class of

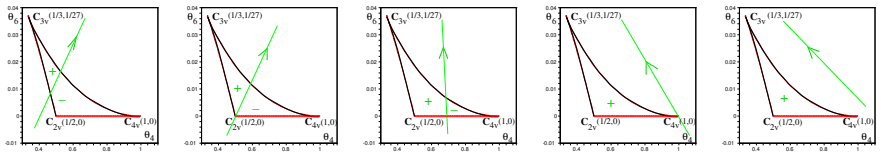

Figure 5. Parametric evolution of rotational structure for effective Hamiltonian for two vibrational states of A_1 and A_2 symmetry types in the presence of **O** symmetry. The representation is done in basic invariants of $\mathbf{O}_h$ group. Straight (green) lines correspond to zero of diagonal element. $\theta_6 = 0$ part (red) of the boundary corresponds to zero of the imaginary part of the off-diagonal element. $\theta_6 \neq 0$ part (black) of the boundary corresponds to zeros of the real part of the off-diagonal element. All figures correspond to the existence of 12 equivalent C_2 zeros and 6 equivalent C_4 zeros of the off-diagonal element. (a), (c), (e) figures represent regular cases with the absence of degeneracy points. (b) corresponds to the existence of 12 degeneracy points at C_2 positions. (d) corresponds to the existence of 6 degeneracy points at C_4 positions.

singular lines passing through C_{4v} orbit corresponds to the formation of 6 equivalent degeneracy points. It should be noted here that the degeneracy points at C_{2v} and C_{4v} orbits differ by their multiplicity. While the degeneracy point belonging to C_{2v} orbit has multiplicity one, the degeneracy point at C_{4v} orbit has multiplicity two. This explains the same amount of change in Chern numbers when the parametric evolution of the effective Hamiltonian in the parameter space crosses the boundary of iso-Chern domains at C_{2v} or C_{4v} orbits.

The same situation occurs in the multiplicity of zeros of the off-diagonal elements. For any regular Hamiltonian there are 12 equivalent zeros at C_{2v} orbit and 6 equivalent zeros at C_{4v} orbit. The winding number for each zero on C_{4v} orbit is twice the winding number for any zero on C_{2v} orbit.

Finally the answer about possible values of Chern numbers can be formulated for the effective Hamiltonian (41) in a rather simple way. There are two possible sets of Chern numbers for two eigen-line bundles for the effective Hamiltonian (41) in the absence of degeneracy points.

(i) Chern numbers are zero for two eigen-line bundles for the effective Hamiltonians corresponding to figures where the line of zeros of the diagonal element does not cross C_h stratum.

(ii) Chern numbers are ± 12 for two eigen-line bundles for the effective Hamiltonians corresponding to figures with the line of zeros of the diagonal element crossing C_h stratum.

Such a simple geometric representation is a consequence of a relatively simple form of the effective Hamiltonian which includes a small

number of tensor contributions for the real and the imaginary parts of the off-diagonal matrix elements (in fact, only one contribution for the real and one for the imaginary part of the off-diagonal element). Another simplifying factor is the small number of auxiliary invariants needed to construct all invariant and covariant tensors.

6.3. E VIBRATIONAL STATE FOR THE $\mathbf{O}$ GROUP.

Let us now consider a simple effective Hamiltonian for a doubly degenerate E vibrational state in the presence of the $\mathbf{O}$ symmetry group, by taking into account terms up to third degree in elementary rotational operators;

$$\begin{pmatrix} aR_1^{2(2,E)} & aR_2^{2(2,E)} - ibR^{3(3,A_2)} \\ aR_2^{2(2,E)} + ibR^{3(3,A_2)} & -aR_1^{2(2,E)} \end{pmatrix}. \tag{46}$$

Here we follow the choice of effective Hamiltonian done in [14] with simplifying notation $\{J_x, J_y, J_z\} \sim \{x, y, z\}$;

$$R_1^{2(2,E)} = 2z^2 - x^2 - y^2; \tag{47}$$

$$R_2^{2(2,E)} = \sqrt{3}(x^2 - y^2); \tag{48}$$

$$R^{3(3,A_2)} = xyz. \tag{49}$$

There are only two control parameters a, b in the Hamiltonian (46). In spite of the fact that the diagonal element and the real and the imaginary parts of the off-diagonal elements are not invariant functions, it is still possible to express the condition for the appearance of degeneracy points in terms of the basic invariant polynomials. The condition for zero value of the imaginary part of the off-diagonal element reads

$$\left(bR^{3(3,A_2)}\right)^2 = 0 \quad \Leftrightarrow \quad b^2 R^{6(6,A_1)} = 0. \tag{50}$$

The condition for zero value of the real part of the off-diagonal element and of the diagonal element can be written as

$$a^2 \left[\left(R_1^{2(2,E)}\right)^2 + \left(R_2^{2(2,E)}\right)^2\right] = 0 \quad \Leftrightarrow \quad a^2 \left(3R^{4(4,A_1)} - 1\right) = 0. \tag{51}$$

This means that for the effective Hamiltonian (46) the degeneracy points can appear only when one of the control parameters a, b is zero. If both a and b parameters are non-zero, there is no degeneracy points. If $b = 0$, the degeneracy points always exist on C_{3v} orbit defined on the space of orbits by the equality $R^{4(4,A_1)} = 1/3$. When $a = 0$ the Hamiltonian is highly degenerate. There are three circles on the sphere $x = 0, y = 0, z = 0$ consisting of degeneracy points.

In order to calculate the Chern numbers for the Hamiltonian with $a \neq 0, b \neq 0$, we need to find a system of "exceptional" points. It is important to note that exceptional points do not form orbits of the symmetry group, because the real part of the off-diagonal element belongs to a two-dimensional representation of the **O** group. Nevertheless we can consider it as an invariant of D_2 subgroup. The calculation of exceptional points in this simple example is carried out straightforwardly. In fact, the solutions of the two equations

$$xyz = 0, \quad x^2 - y^2 = 0; \tag{52}$$

are

$$(x = 0, y = 0, z = \pm 1); (x = \frac{1}{\sqrt{2}}, y = \pm\frac{1}{\sqrt{2}}, z = 0); (x = -\frac{1}{\sqrt{2}}, y = \pm\frac{1}{\sqrt{2}}, z = 0).$$

Among these six exceptional points there are two lying on the z axis and four lying in the xy plane. Their signs are opposite. We can calculate winding numbers either around positive or around negative exceptional points. The off-diagonal element has C_2 symmetry with respect to the two exceptional points on the z axis. That is why the winding numbers for these points are ± 2, depending on the sign of parameters. At the same time the winding number for the exceptional point lying in the equatorial plane is ± 1. But the number of equatorial points is four. So in any case the Chern numbers for two eigen-line bundles for the effective Hamiltonian (46) with $a \neq 0$ and $b \neq 0$ are ± 4.

7. Symmetry analysis of rearrangements

We can look at the problem of band formation and their rearrangements from the point of view of symmetry effects by using completely different approach based on the analysis of purely quantum problem.

In order to make the suggested below construction more physically meaningful, let us suppose first that for a molecule with a given symmetry group G we have a system of rotational multiplets associated with isolated vibrational states having certain symmetry types $\Gamma_{\mathrm{vib},i}$. Then for totally symmetric vibrational state there are $2J + 1$ rotational levels for each value of the rotational quantum number J whose purely rotational symmetry can be found by decomposing the irreducible representation (J) of rotational dynamic symmetry group $SO(3)$ (or $SU(2)$ if half integers values of J are allowed) into irreducible representations of the invariance symmetry group G. (For simplicity we assume that the symmetry group is a purely rotational group without improper (reflection) symmetry operations.)

The total set of rotation-vibration states in the case of a system of vibrational states of different symmetry types, $\Gamma_{\mathrm{vib},i},\ i = 1\ldots, k$ spans the representation

$$\left(\sum_{i=1}^{k} \Gamma_{\mathrm{vib},i}\right) \otimes (J),$$

where (J) denotes the decomposition of a rotational multiplet of weight J into irreducible representations of the symmetry group G. The sum over index

i is the sum over all vibrational states, or equivalently over all irreducible representations (with their multiplicity taken into account) span by the set of vibrational states.

Such presentation should be valid globally for all J values, if the rotational multiplets for different vibrational states remain isolated and do not change. The sequence of rotational multiplets with different J values forms a band. We say that the redistribution of energy levels between bands takes place [19, 18] if we can rewrite the above expression in an alternative form

$$\Big(\sum \Gamma_{\mathrm{vib},i}\Big) \otimes (J) = \sum \Big(\Gamma_{\mathrm{vib},j} \otimes (J + \Delta_j)\Big) \tag{53}$$

with $\Delta_j \neq 0$ for at least some j. The sum over index i in the left-hand side and the sum over the index j in the right-hand side of (53) could be over a different set of representations but the total dimension of the whole set of vibrational states should be naturally the same.

This is in some way a generalization of the relation in the decomposition of the product of two representations of $SU(2)$ group with weights $(\frac{1}{2})$ and (J)

$$\left(\frac{1}{2}\right) \otimes (J) = \left(J + \frac{1}{2}\right) \oplus \left(J - \frac{1}{2}\right)$$

corresponding to the rearrangement of two rotational bands described by the simplest model with $S_z + t(\mathbf{J} \cdot \mathbf{S})$ Hamiltonian [13, 16, 5].

For the symmetry group $\mathbf{O}$, formally imaginable redistributions of states between two rotational multiplets associated with totally symmetrical quantum states are

$$(J)_{A_1} + (J)_{A_1} \to (J + \Delta)_{A_1} + (J - \Delta)_{A_1}, \tag{54}$$

among which the only possibilities are those corresponding to $\Delta = 12k$, where $(J)_{A_1}$ denotes a tensor product representation of the (J) representation of $SO(3)$ group considered as a reducible representation of the cubic symmetry group $\mathbf{O}$ by the A_1 irrep of the $\mathbf{O}$ group, and the other similar notations are defined likewise.

In a similar way we can analyze the situation with two different one-dimensional representations and rotational part in the case of $\mathbf{O}$ symmetry.

Verifying the decompositions for the rearrangements of type

$$(J)_{A_1} + (J)_{A_2} \to (J + \Delta)_{A_1} + (J - \Delta)_{A_2}, \tag{55}$$

we find that only $\Delta = 6k$ with k any integer is possible.

An important fact is that the smaller value for Δ is possible in the case of two different representations as compared to the case of two identical representations for quantum states.

Let us consider finally the case of doubly degenerate vibrational representation of the symmetry group $\mathbf{O}$ and corresponding rotational structure. It is easy to see that the E band cannot be decomposed into two bands with both bands having the same number of states and keeping the appropriate set of irreducible representations of the $\mathbf{O}$ group. It follows just from the fact that

for $J = 0$ the E representation cannot be reduced. More generally, at any J the number of E representations is the same for A_1 band and for A_2 band. At the same time for E band the number of E representations for some J values is even but for some is odd.

In contrast, the rearrangement of type

$$(J)_E \leftrightarrow (J+\Delta)_{A_1} + (J-\Delta)_{A_2} \tag{56}$$

is possible, for example, for $\Delta = \pm 2, \pm 4$. At the same time the rearrangement is not possible for $\Delta = \pm 3$ nor for $\Delta = 0$.

General analysis shows [19] :

For the **O** group with doubly degenerate vibrational representation, the decomposition into individual bands according to (56) is possible for values of Δ being any even non-zero integer except those multiple to 6: $\Delta \neq 2k+1$, $\Delta \neq 6k$, $k = 0, 1, 2 \ldots$. More formally $\Delta = \pm 2 \bmod 6$.

One of the goal of the present paper is to demonstrate that such a simple group theoretical analysis gives the same results as the topological analysis which in the presence of symmetry restricts the possible values of topological invariants (Chern numbers) for individual bands. To correlate the results, one needs to remember that changing J by Δ is associated with the modification of the energy levels within the band by 2Δ and the modification of a Chern number of an isolated band by δ is associated with the modification of the energy levels within the band by δ. In view of this, it turns out that the agreement between analysis of Chern numbers and symmetry decomposition done in this paper is exact.

8. Conclusion

We have studied rather particular problems of rearrangement of energy levels between bands under a variation of control parameters of the model in the presence of a point symmetry group. Our results show that possible values of Chern numbers characterizing individual energy bands is strongly influenced by the symmetry. Direct calculation of Chern numbers for a semi-quantum model allows us to find possible values of Chern numbers and their modifications, but the formulation of general result similar to that obtained by completely different arguments within group theoretical analysis of purely quantum problem is still lacking. Another big step to realize consists in a generalization of this analysis to fiber bundles defined over higher dimensional base space. First attempts in that direction was done in [8]. Authors hope that the present analysis will be of help for advance in that direction.

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