

Qualitative features of the rearrangement of molecular energy spectra from a “wall-crossing” perspective.

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Abstract

Qualitatively different systems of molecular energy bands are studied on example of a parametric family of effective Hamiltonians describing rotational structure of triply degenerate vibrational state of a cubic symmetry molecule. The modification of band structure under variation of control parameters is associated with a topological invariant “delta-Chern”. This invariant is evaluated by using a local Hamiltonian for the control parameter values assigned at the boundary between adjacent parameter domains which correspond to qualitatively different band structures.

Keywords: energy band, Chern number, wall-crossing, rotation-vibration

1. Introduction

The purpose of the present article is to discuss qualitative models describing small quantum systems of a finite number of particles and their modifications under a variation of control parameters on the basis of effective phenomenological Hamiltonians. The qualitative analysis of models along a change in parameters is based on the classical-quantum correspondence and it is to be stressed that the transition from one qualitative regime to another is similar, in the sense of basic idea, to much more general mathematical “wall crossing” formalism [17, 10] developed essentially in relation to physical models suggested in string theory.

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The general idea of qualitative description of simple quantum systems consists in studying a family of objects (or models) depending on a number of control parameters (external ones like characteristics of external potentials or internal ones characterizing through approximate dynamical parameters the effective behavior of the model).

A realization of the qualitative approach consists in finding characteristics which are defined almost everywhere (*i.e.*, for almost all values of control parameters) and are piece-wise constant on the space of control parameters. In other words, the qualitative description assumes the splitting of the space of control parameters into disjoint regions by a codimension one boundary and assumes equally the existence of boundaries of higher codimension. One of such qualitative characteristics of molecular systems to be studied in the present paper is the energy band structure which exists for some regions in the control parameter space and changes discontinuously when crossing the boundary of the region [22, 24, 6, 13]. Another example of a qualitative characteristic is the number of non-linear normal modes [21, 26], or the number of stationary points of an effective Hamiltonian in the classical limit, whose modification is associated with quantum bifurcations [28].

The concept of energy bands is most frequently associated with solid state problems and with the existence of periodic symmetry and gaps in the distribution of energy states [16, 4]. The present paper deals mainly with finite particle systems which exhibit the presence of energy bands due to the splitting of relevant dynamical variables into two qualitatively different types in association with low- and high-energy excitations [7]. On using the well known Born-Oppenheimer (or adiabatic) approximation, this splitting can be classically interpreted as a splitting into “slow” and “fast” variables. “Slow” variables describe internal structure of bands associated with low-energy excitations, while “fast” variables are related to high-energy excitations and correspond to passage from one band to another, *i.e.*, they are responsible for inter-band structure. To simplify the analysis and discussions, we suppose that in the partial classical limit with respect to the slow variables the quantum system under study is described on the compact classical phase space and consequently the resultant semi-quantum system possesses discrete quantum spectrum consisting of a finite number of energy levels distributed among a finite number of bands. In this simple situation, the modification of the band structure can be associated with the redistribution of energy levels between bands and consequently with the modification of the number of energy levels within bands. As an example of such phenomenon, Figure 1

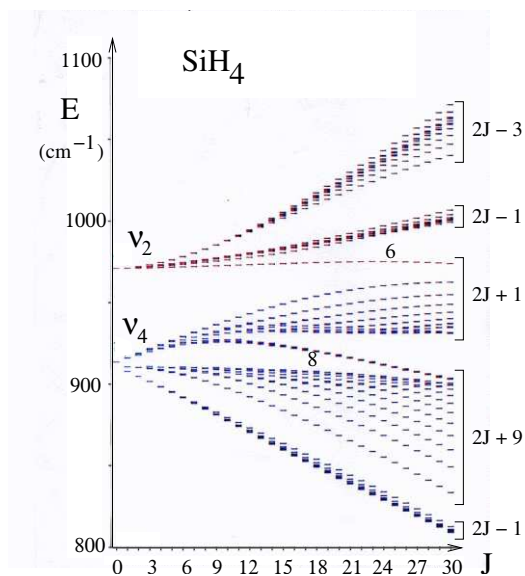


Figure 1: Reduced rovibrational energy as a function of rotational quantum number J for vibrational modes ν_4 (F_2 symmetry type) and ν_2 (E symmetry type) of SiH_4 tetrahedral molecule (T_d point symmetry group). The numbers of energy levels within clearly seen energy bands are indicated for $J \sim 30$ region. The numbers of energy levels (6 and 8) in the rotational clusters redistributed between the bands are also shown.

reproduces the rotational structure of two vibrational states (doubly degenerate ν_2 state of E symmetry and triply degenerate ν_4 state of F_2 symmetry) of the tetrahedral molecule SiH_4 , reconstructed from high resolution infrared spectroscopic data [3]. The rotational quantum number, J , serves as a control parameter. Two rearrangements of energy levels between bands are seen on this diagram. As J increases, one group of eight energy levels goes from the upper branch of ν_4 mode to the middle branch, and at slightly higher J values another group of six energy levels passes from the lower branch of ν_2 mode to the upper branch of ν_4 mode. Although the behavior of energy levels in Fig. 1 is gradual and do not show discontinuities, the transformation of the model system into a semi-quantum system through classical limit for rotational variables and the introduction of vector bundle description allow us to find an integer topological invariant, the Chern number for eigen-line bundle which exhibits piece-wise constant behavior as a function of J and characterizes the qualitative modification of band structure.

Many similar phenomena are well-known in molecular physics [23, 24, 27]

and a number of high-precision experimental data are available. The example we treat as a model below is quite close to the model [5] which describes the rearrangement of rotation-vibration bands in $\text{Mo}(\text{CO})_6$ molecule on the basis of the extensive high resolution experimental data from [2]. At the same time, a general qualitative understanding and a mathematical description of these and similar more general phenomena such as the fusion of several bands into one (see [9]) or the inverse splitting of one band into several individual ones are not yet properly formulated.

2. Conceptual setting up and a way of analysis

Recent works on quantum-classical correspondence for finite particle systems exhibiting a band structure (rotational structure of several vibrational states of an isolated molecule is a typical example of such a structure) are based on the procedure of the aforementioned partial classical limit for a particular quantum system so that the resultant semi-quantum system can be described in terms of vector bundle. The base space of this bundle is associated with classical variables describing internal structure of bands, whereas fibers are associated with quantum states forming different bands [12, 6, 8, 13].

We restrict our study in this article to vector bundles whose base space is a compact classical phase space of one degree of freedom. As a natural molecular example, the real two-dimensional sphere S^2 can serve as the phase space associated with molecular rotation. An Hermitian matrix is used to treat the complete problem in a semi-quantum model [25, 27]. Its eigenvectors assigned to all the points of S^2 form generically isolated line-bundles, which we call eigen-line bundles. This is because typically a Hermitian matrix has nondegenerate eigenvalues, since the codimension of degeneracies for a parametric family of Hermitian matrices is three (real) [1] whereas the dimension of the base space in the considered case is only 2 (real).

Consequently, an isolated semi-quantum model Hamiltonian has non-degenerate eigenvalues everywhere on S^2 , and the trivial vector bundle over S^2 can split into a direct sum of eigen-line bundles describing individual isolated bands. The topological invariant characterizing the qualitative structure of bands for such model is the system of the first Chern numbers for the set of eigen-line bundles. The relation between Chern numbers of eigen-line bundles for a semi-quantum model and the numbers of quantum levels within bands for parent purely quantum problem was demonstrated in [6, 7].

If now instead of an isolated model Hamiltonian we study a parametric family of Hamiltonians, the space of parameters naturally splits into regions with each of which is associated the set of constant Chern numbers for isolated bands [13]. The boundaries between different regions in the control parameter space correspond to a model Hamiltonian with degeneracy in eigenvalues [22]. Eigen-line bundles are not defined in such situation and the system of Chern numbers is a piece-wise constant function defined almost everywhere on the space of control parameters. The region where Chern numbers are defined and keep their values constant is called an iso-Chern domain [13]. The boundaries of iso-Chern domains are responsible for the modification of the band structure. Thus, a modification formula attached to the crossing of the boundary may be referred to as a wall-crossing formula.

A straightforward approach to a characterization of qualitative structure of bands within each iso-Chern domain consists naturally in calculating Chern numbers of eigen-line bundles for a suitably chosen representative Hamiltonian from each iso-Chern domain [13]. However, this procedure gets much more complicated, if the size of the matrix Hamiltonian becomes larger. On this account, it is much interesting to study only modifications in Chern numbers in association with crossing (in the control parameter space) the boundary between iso-Chern domains. The degeneracy in eigenvalues, which occurs when the parameter values fall on the boundary of the iso-Chern domain, gives rise to a local singularity for the splitting of eigen-line bundles. A topological (more exactly homotopy [15]) invariant, which we call a delta-Chern invariant or simply a delta-Chern, can be assigned to crossing each boundary of iso-Chern domains. It shows how Chern numbers of individual eigen-line bundles change (in other words, how the qualitative structure of bands changes) when passing from one iso-Chern domain into another by boundary crossing.

In what follows, we demonstrate how this approach, which is based on “delta-Chern” invariants attached to boundary crossing, works well in relatively simple molecular examples in the presence of finite symmetry groups, which are important ingredients of the formulation of a molecular problem.

With the present article, authors hope to bring attention of theoretical physicists and mathematicians working on general wall-crossing phenomena to (close in spirit) physical problem of qualitative description of finite particle systems which allows a detailed comparison of predictions of qualitative models with a rich available quantitative experimental information and suggests a natural way to pass to more general mathematical models.

3. An example of three state problem

We take here as an example an effective rotational Hamiltonian for three vibrational states of F_2 symmetry in the presence of the cubic group O (see [14] for similar effective Hamiltonians for two-dimensional vibrational representations of the O symmetry group).

In terms of tensor products of rotational and vibrational irreducible (with respect to the O symmetry group) tensor operators, this effective Hamiltonian can be written as

$$H = [V^{A_1} \otimes R^{A_1}]^{A_1} + [V^E \otimes R^E]^{A_1} + [V^{F_1} \otimes R^{F_1}]^{A_1} + [V^{F_2} \otimes R^{F_2}]^{A_1}, \quad (1)$$

where V^Γ and R^Γ are vibration and rotation tensor operators, respectively, transforming according to irreducible representations $\Gamma = A_1, A_2, E, F_1, F_2$ of the symmetry group O . Only invariant tensor operators (of A_1 symmetry type) are needed to be included in the Hamiltonian.

Taking only leading contributions (the operators of lowest degree in $\{J_x, J_y, J_z\}$ variables) for rotational tensor operators and neglecting scalar J^2 dependence, we have the following explicit form of rotational contributions in the classical limit,

$$R^{A_1} = J_x^4 + J_y^4 + J_z^4; \quad (2)$$

$$R_1^E = 2J_z^2 - J_x^2 - J_y^2; \quad R_2^E = \sqrt{3}(J_x^2 - J_y^2); \quad (3)$$

$$R_x^{F_1} = J_x; \quad R_y^{F_1} = J_y; \quad R_z^{F_1} = J_z; \quad (4)$$

$$R_x^{F_2} = J_y J_z; \quad R_y^{F_2} = J_z J_x; \quad R_z^{F_2} = J_x J_y. \quad (5)$$

Vibrational operators in their turn can be expressed, for a fundamental band of F_2 symmetry, as bilinear products of elementary annihilation and creation harmonic oscillator operators of F_2 symmetry type with respect to the symmetry group O of the problem.

Now we are in a position to give explicit form to (1). To make consistent contributions from rotational operators of different degrees to a complete Hamiltonian and to keep the Hamiltonian reasonably simple, we may restrict ourselves to operators of at most second degree. This allows us to write different contributions of (1) in a matrix form with only two phenomenological parameters a, b which we consider below as control parameters of the model. For the sake of simplicity of notations, we replace below $J_\alpha = \alpha$, where

$\alpha = x, y, z$. Then, our Hamiltonian is expressed as

$$\begin{aligned} & \begin{pmatrix} 0 & iz & -iy \\ -iz & 0 & ix \\ iy & -ix & 0 \end{pmatrix} + a \begin{pmatrix} y^2 + z^2 - 2x^2 & 0 & 0 \\ 0 & z^2 + x^2 - 2y^2 & 0 \\ 0 & 0 & x^2 + y^2 - 2z^2 \end{pmatrix} \\ & + b \begin{pmatrix} 0 & xy & zx \\ xy & 0 & yz \\ zx & yz & 0 \end{pmatrix}. \end{aligned} \quad (6)$$

As we can always choose $J_x^2 + J_y^2 + J_z^2 = \text{const}$ and renormalise the model Hamiltonian by imposing this constant to be equal to 1, we may view the Hamiltonian (6) as defined on the unit sphere S^2 ; $x^2 + y^2 + z^2 = 1$. Our next step for the qualitative analysis of the Hamiltonian (6) consists in finding all values of control parameters corresponding to degeneracy of eigenvalues of the Hamiltonian (6) at some points of the classical phase space associated with rotational variables.

4. Iso-Chern domains in the control parameter space

The presence of symmetry group considerably simplifies the search for degeneracy points of eigenvalues, since the symmetry group acts also on the classical base space S^2 [19, 20]. The action of the symmetry group stratifies the phase space S^2 into orbits with different stabilizers. Criterion for degeneracy in eigenvalues (zero of the discriminant) can be formulated independently of strata. At the same time, the solution can be immediately found for each of zero-dimensional strata by restricting the Hamiltonian on each of strata.

From the discriminant of the characteristic equation for the Hamiltonian (6), we find that the set of control parameters for which the Hamiltonian possesses degenerate eigenvalues is given by the curves or lines shown in Fig. 2. For each point of the line C_i in the space of control parameters, the Hamiltonian (6) possesses degenerate eigenvalues at a finite number of points of S^2 , which form the orbit whose stabilizer is isomorphic to a cyclic group C_i . We call such an orbit a C_i orbit. There are one C_4 orbit formed by six points which belong to three axes passing through the centers of the opposite faces of the inscribed cube; one C_3 orbit formed by 8 points belonging to four axes passing through the four pairs of opposite vertices of the cube; and one C_2 orbit formed by 12 points belonging to the six axes passing through the

middle of the opposite edges of the cube. Control parameter values (for which the degeneracy points exist on respective orbits) have simple expressions given by

$$C_4 : a = \pm \frac{1}{3}; \quad C_3 : b = \pm 1; \quad C_2 : a = \frac{b^2 - 2}{3b}. \quad (7)$$

Evaluating energy eigenvalues at the degeneracy points, one obtains

$$E_{C_4}(a, b) = (a - 1, -2a, a + 1); \quad E_{C_3}(a, b) = \left(-1 - \frac{1}{3}b, 1 - \frac{1}{3}b, \frac{2}{3}b\right); \quad (8)$$

$$E_{C_2}(a, b) = \left(\frac{a-b-\sqrt{(3a+b)^2+16}}{4}, \frac{b-a}{2}, \frac{a-b+\sqrt{(3a+b)^2+16}}{4}\right). \quad (9)$$

This tells us between which bands the degeneracy occurs.

Intersection of two, C_i and C_j , lines corresponds to control parameter values for which the Hamiltonian (6) possesses simultaneously degeneracy points at both C_i and C_j orbits. The presence of points of simultaneous intersection of three lines is due to a non-generic feature of the model Hamiltonian whose entries are restricted within the terms up to second degree of rotational contributions. For these special control parameter values, the model Hamiltonian (6) possesses a continuous set of degeneracy points on S^2 . However, a small deformation of the Hamiltonian (6) by adding higher order terms removes the triple intersection of degeneracy lines and puts the Hamiltonian in such a generic situation that a family of Hamiltonians possesses only generic (simple) intersection of degeneracy lines in the control parameter space.

Six lines C_i shown in Figure 2 split the plane of control parameters into 15 open simply-connected regions. Each region corresponds to one qualitative type of band structure formed by three energy bands. We characterize the qualitative type of the energy band by the Chern number for the eigen-line bundle associated with each of isolated eigenvalues of the model Hamiltonian. Since Chern numbers of eigen-line bundles cannot change against a change in parameters without forming degeneracy points of eigenvalues, these regions are called iso-Chern domains.

To characterize qualitatively the system of energy bands in each iso-Chern domain, one needs to calculate Chern numbers for each of eigen-line bundle for a Hamiltonian at one particular set of values of control parameters. At the same time it is clear that at the boundary of iso-Chern domain Chern numbers are not defined only for those bands which correspond to a couple

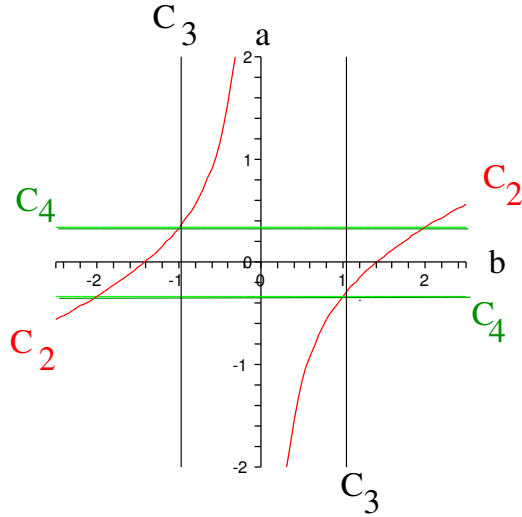


Figure 2: Degeneracy points (on C_2, C_3, C_4 orbits) in the space of control parameters (a, b) for the Hamiltonian (6).

of degenerate eigenvalues, as is observed from (8) and (9). This fact allows us to simplify significantly the study of a family of Hamiltonians near the boundary of iso-Chern domain. Only two bands are to be taken into account. The third one or in N-state problem all except two can be neglected. Moreover, as long as we are interested in qualitatively describing a modification in Chern number, which should be an integer invariant, in crossing the boundary of an iso-Chern domain, small perturbations caused by neglecting eigenvalues distant from the two degenerate ones in question cannot change the integer invariant. We call such an invariant a delta-Chern invariant or simply a delta-Chern. From the mathematical point of view, the delta-Chern is a homotopy invariant rather than simply a topological invariant [15]. It is important to note here that owing to the symmetry group action the degeneracy points appear simultaneously on all points belonging to the same orbit of the symmetry group. Taking into account the fact that degeneracy points are generically isolated for a finite group, we can restrict the calculation of the delta-Chern invariant to a small neighborhood of the degeneracy point in the space of classical variables (small neighborhood of a point on the S^2 classical phase sphere) and to a small neighborhood of a degeneracy point in the space of control parameters. This explains why we can simplify significantly

the calculation of the delta-Chern invariant by restricting to a local two-state Hamiltonian and even by making the linearization of the Hamiltonian near the degeneracy point.

5. Local Hamiltonians near degeneracy point and associated delta-Chern invariant

The importance of the analysis of local behavior of eigenvalues and eigenvectors near the degeneracy point for the description of the qualitative phenomenon of redistribution of energy levels between bands was noticed in initial works on the redistribution phenomenon [22, 23, 6]. The systematic procedure for the calculation of Chern numbers for isolated bands in the absence of degeneracy points was suggested in [13]. It is performed by calculating all contributions from so-called exceptional points which are associated with singularities of eigenvectors defined open-densely on S^2 . Though the method to be applied in the case of the absence of degeneracy points cannot be applied if degeneracy appears, a modified approach can be made so as to be applicable in the case of the presence of degeneracy points of eigenvalues. The application of the modified approach to delta-Chern calculation relies on the appropriate choice of the basis for the matrix Hamiltonian and of the basis of the tangent plane to the S^2 base space. If such a set-up is well made, the modification of a system of exceptional points (at which eigenvectors are not defined) against a change in the control parameters may be observed in a small neighborhood of the degeneracy point in question, and hence the delta-Chern invariant can be calculated explicitly within the local approach.

In general, if a symmetry group G and its action on the classical phase space (the base space of the fiber bundle in the semi-quantum model) is known, the possible local symmetry is also known at points of the classical phase space. If the local symmetry (stabilizer) at a given point is a subgroup $G_i \subset G$, the number of point in the orbit is $[G]/[G_i]$, where $[G_i]$ is the order of group G_i . In the present case, G is the O group and G_i is a cyclic group C_i . Taking into account the above-mentioned fact that the degeneracy points appear simultaneously at all points of the orbit and the delta-Chern contributions from different points of the same orbit are identical, we get immediately certain restrictions on possible modifications of the band structure for a given symmetry group.

Figure 3 illustrates a typical modification in exceptional points for a family of local Hamiltonians defined in a neighborhood of a degeneracy point.

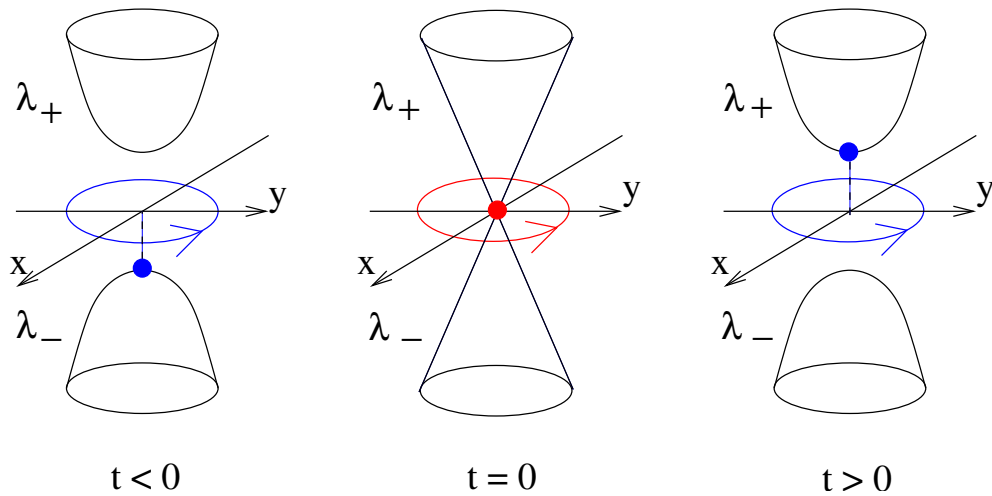


Figure 3: Schematic representation of the evolution of eigenvalues of a local linearized model Hamiltonian in a two-level approximation along with variation of a control parameter t crossing the boundary of the iso-Chern domain. Exceptional points (blue points) in the chosen representation are shown for λ_+ and λ_- components.

The details of the mathematical analysis through this typical modification will be given in [15], where particular attention is paid to the sign of the local contribution to the delta-Chern. The global value of the delta-Chern follows directly from local contribution by multiplying local contribution by the order of the orbit of the degeneracy point. For our Hamiltonian (6), the delta-Cherns in crossing the boundaries are shown in Fig. 4.

We are now in a position to make a qualitative description of band rearrangement. So far we have associated with each boundary the corresponding delta-Chern invariant (see Figure 4), it is sufficient for us to calculate the Chern numbers for just one point in the control parameter space which can be chosen to assure the simplest possible form of the effective Hamiltonian.

Combining this single point calculation of Chern numbers with all known delta-Chern invariants, we can easily reconstruct the complete Chern diagram to give Chern indices for all bands in all iso-Chern domains. Note that the sum of Chern numbers for isolated line bundles remains invariant when the control parameter value passes a degeneracy point. In particular, the sum of the whole set of Chern numbers for the set of associated line bundles in this paper is zero, and further, the symmetry restrictions do not allow the trivial vector bundle to decompose generically into a sum of trivial line bundles.

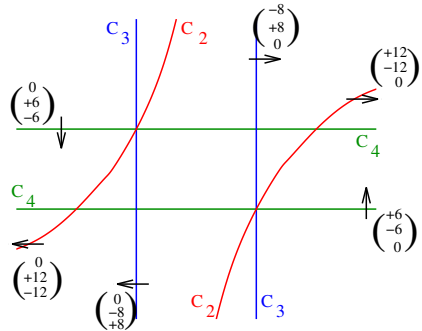


Figure 4: Delta-Chern diagram for three state model (6) represented in the space of control parameters (a, b) . Each degeneracy line (the boundary of the iso-Chern domain) is associated with a three component column giving delta-Chern for each of three bands and with an arrow indicating the direction of the path in the control parameter space associated with the shown modifications of Chern numbers.

The Figure 5 is obtained in this manner and gives a complete information on possible band rearrangements under the variation in control parameters of the initial Hamiltonian (6).

So far we have treated mainly a three-level Hamiltonian from the view point of delta-Chern. The concept of delta-Chern is valid also for N -level models. Returning now to the example represented in Fig. 1, we illustrate qualitative description of band rearrangements occurring in Fig. 1 using the correspondence between the number of quantum states in bands and the associated Chern numbers as given in Table 1 for low $J \sim 8$ and high $J \sim 30$ values. Though the correspondence has not been given a rigorous proof, it is supported by a number of examples.

Without forming an explicit semi-quantum model, we assume that there is an appropriate five-level model semi-quantum Hamiltonian and the delta-Chern formula applies to this model. Then, from Fig. 1 it turns out that the formation of at least two types (C_3 and C_4) of degeneracy points is needed to pass from the low- J to the high- J band structure. The corresponding systems of delta-Chern together with values of Chern numbers are shown in Fig. 6. They are consistent with the well-known decomposition of doubly and triply degenerate bands for tetrahedral molecules at low J values.

Another interesting and important conclusion from the viewpoint of applications is that possible rearrangements of the band structure can be formulated for problems with certain symmetry. We have already found a possible

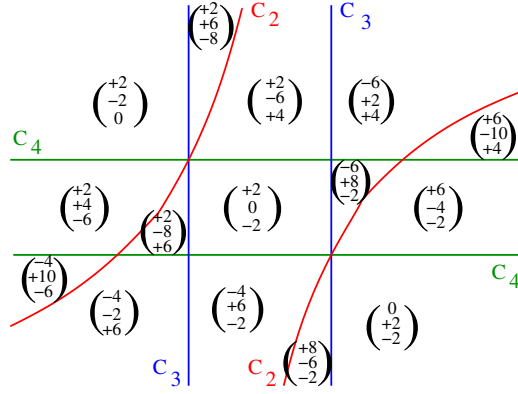


Figure 5: Iso-Chern diagram for three state model. Vertical (blue) lines represent boundaries with degeneracy points at C_3 positions. Horizontal (green) lines represent boundaries with degeneracy points at C_4 positions. Curved (red) lines represent boundaries with degeneracy points at C_2 positions. Each open iso-Chern domain is characterized by three Chern numbers associated with three bands arranged according to their energy. Upper, middle and lower numbers in each symbol give respectively Chern numbers for the band with higher, middle and lower energy.

Table 1: Energy bands and corresponding Chern numbers for example shown in figure 1.

Band	$J \sim 8$	$J \sim 8$	$J \sim 30$	$J \sim 30$
	Numb. lev.	Chern numb.	Numb. lev.	Chern numb.
ν_2 (upper)	$2J - 3$	-4	$2J - 3$	-4
ν_2 (lower)	$2J + 5$	$+4$	$2J - 1$	-2
ν_4 (upper)	$2J + 3$	$+2$	$2J + 1$	0
ν_4 (middle)	$2J + 1$	0	$2J + 9$	$+8$
ν_4 (lower)	$2J - 1$	-2	$2J - 1$	-2

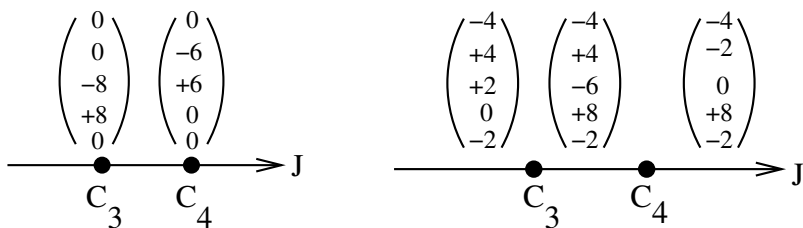


Figure 6: Schematic representation of the evolution of the band structure represented in Figure 1 as a function of one control parameter, the rotational quantum number J . Left - delta Chern associated with two, C_4 and C_3 , orbits of degeneracy points. Right - Chern numbers for isolated line bundles vs control parameter J .

rearrangement in the name of delta-Chern in the case where the symmetry group is the O group. Interesting implication in generic situation is the existence of selection rules for possible values of Chern numbers for bands in the presence of symmetry, if we are looking for possible modifications of several bands forming initially trivial vector bundle with zero Chern numbers. Several examples of such selection rules for Chern numbers of individual bands in the presence of symmetry was formulated in [14]. The so-obtained selection rules for Chern numbers reproduce similar selection rules for possible types of vibrational components in molecular systems in the presence of symmetry [29], which are based on reduction induction of representations in elementary group theory. Possible relation with McKay correspondence [18, 11] remains an interesting point to study.

6. Possible generalizations

The above-studied particular example of model Hamiltonian (6) is rather a simple example in several factors. It should be modified so as to allow application to a larger class of molecular examples.

Rather serious restriction is the dimension of the space of classical variables. Physical examples where “slow” variables are rotational variables describing molecular rotation lead to a classical phase space of dimension two (one degree of freedom). A number of other molecular effective Hamiltonians describing band structure are possible, where the number of degrees of freedom for slow variables is larger than one. Rather general model describes, for example, vibrational polyads (formed by excited states of a multidimensional isotropic oscillator) for a molecule possessing several close lying electronic

states [9]. Depending on the number N of vibrational degrees of freedom, the internal structure of vibrational polyads is described in the classical limit by a model with compact phase space diffeomorphic to $\mathbb{C}P^{N-1}$ [26]. If, as it often occurs in molecular problems, the frequencies of vibrations are in resonance relation $n_1\nu_1 = n_2\nu_2 = \dots$, the corresponding classical phase space for slow vibrational motion is a weighted projective space. Although molecular systems which can be described within such direction of generalization certainly exist, the preliminary construction of mathematical formalism adapted to qualitative study of such molecular models should be done in order to understand how one can work with such more complex systems within the qualitative approach.

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