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ORIGINAL PAPER

# Rearrangement of energy bands: topological aspects

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**Abstract** Presence of energy bands in quantum energy spectra of molecules reflects the existence of "slow" and "fast" motions in corresponding classical problem. Generic qualitative modifications of energy bands under the variation of some strict or approximate integrals or motion considered as control parameters are analyzed within purely quantum description, within semi-quantum one (slow dynamical variables are classical; fast variables are quantum) and within purely classical one. In quantum approach the reorganization of bands is seen from the redistribution of energy levels between bands. In semi-quantum approach the system of bands is represented by a complex vector bundle with the base space being the classical phase space for slow variables. The topological invariants (Chern classes) of the bundle are related to the number of states in bands through Fedosov deformation quantization. In purely classical description the reorganization of energy bands is manifested through the presence of Hamiltonian monodromy.

**Keywords** Energy bands · Adiabatic approximation · Topological invariants · Hamiltonian monodromy

## 1 Introduction

It is well known that the energy spectra of a typical molecular system consists of groups of energy levels which are often called bands (electronic, vibrational, rotational, etc.). The presence of such bands is due to the natural splitting of dynamic variables into several groups in such a way that the characteristic energy excitations

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(or characteristic times) differ significantly between different types of motion. Typically, electronic excitation, $\Delta E_{\mathrm{el}}$, is much higher than typical vibrational excitation, $\Delta E_{\mathrm{vib}}$, and the rotational excitation, $\Delta E_{\mathrm{rot}}$, is still smaller. In an equivalent way we can say that electronic variables are fast, vibrational variables are slow, and rotational variables are even more slower. Such an idealized picture has obviously rather narrow range of applicability because of the modification of the relative excitations due to rovibronic interactions. At the same time very often we see that under the variation of some physical characteristics, like energy, angular momentum, polyads quantum numbers, etc., individual bands "intersect", mix in some interval of the variation of control parameters, but the band structure reappears again and the rearrangement of bands is a generic phenomenon which presents in many different molecular problems.

In what follows we introduce the mathematical formalism which is intended precisely to describe the phenomenon of rearrangement of energy bands caused by coupling of slow and fast motions (or alternatively speaking by coupling of slow and fast dynamical variables). This is in some sense a short review of one particular qualitative feature presented in families of effective Hamiltonians describing excited quantum systems and depending on some control parameters. Rearrangement of energy bands is a qualitative phenomenon which is tightly related with the adiabatic separation of variables. This is one of the approximations which is widely used in almost all quantum chemical studies. Therefore the author hope that the qualitative ideas he follows could be of interest for *ab initio* quantum chemistry community because they allow somewhat alternative interpretation of generic phenomenon of energy levels redistribution between energy bands.

For a more general reviews of qualitative theory of highly excited finite particle quantum systems (atoms and molecules) the reader is invited to see earlier publications written for differently oriented reader: for mathematicians [1–4], for physicists [5–8], for theoretical chemists and in particular for molecular spectroscopists [9,10] and references therein.

## 2 Quantum—classical correspondence. Topological and symmetry arguments

The key point of the qualitative analysis of a given quantum problem is the classical-quantum correspondence. In order to find the qualitative features of energy level system for quantum problem we construct the classical limit and study integrable approximations to it. Initial quantum Hamiltonian is supposed to be the effective Hamiltonian which describes, for example, only rotational states for one or several vibrational states, rovibrational states for one or several electronic states, etc. Several examples of different classical limits for effective quantum operators are listed in Table 1. Without going into details we just note that formal construction of limiting classical phase space for quantum problem is based on the coherent state approximation [11,12].

Topology of the limiting classical phase space and its stratification under the action of the symmetry group of the problem are responsible for the global organization of the system of classical trajectories and of the pattern of corresponding eigenvalues.

We are mainly interested in the problems where at the beginning the whole set of dynamic variables can be split into "slow" and "fast" parts (for simplicity we restrict

**Table 1** Classical limiting phase space for different quantum problems

| Effective operator | Corresponding classical phase space |
|---|---|
| Rotational | $S_2$ Two-dimensional sphere |
| Vibrational polyads formed by $n$ degenerate modes | $CP_n$ Complex projective space |
| Vibrational polyads formed by modes in $n_1 : \ldots : n_k$ resonance | $CP_{n_1,\ldots,n_k}$ Weighted projective space |
| Rydberg multiplets | $S_2 \times S_2$ |

ourselves with only two groups of variables). Whereas the complete problem is naturally quantum, in order to understand better the qualitative features of its energy spectrum we can construct the simplified models by going to classical limit either completely, or partially. There are two kinds of models.

(i) Both "fast" and "slow" variables are treated as classical. Classical limiting phase space in such a case is a product of classical phase spaces for "slow" and for "fast" variables. As an example we can take an effective Hamiltonian which describes the rotational structure of vibrational polyads formed by doubly degenerate vibrational mode. In the complete classical limit this quantum Hamiltonian corresponds to classical function with two degrees of freedom defined on the classical phase space $S_2 \times S_2$ where one $S_2$ factor corresponds to rotational phase space, and another $S_2$ factor corresponds to polyad phase space which for two degenerate modes is a $CP_1$ complex projective space which is equivalent to $S_2$.
(ii) Only "slow" variables become classical whereas "fast" variables remain quantum. Such approach is extremely useful when only a small number of quantum states over fast variables are relevant. We name such model a "semi-quantum" model. As an example of application, let consider the quantum effective rotational Hamiltonian for doubly degenerate fundamental vibrational state. Using classical limit for rotational "slow" variables we keep quantum description for vibrational states. The resulting semi-quantum model corresponds to $2 \times 2$ matrix quantum Hamiltonian defined over classical phase space $S_2$, which is the classical limiting phase space for rotational motion.

## 3 Semi-quantum model

Slightly more formal description of the semi-quantum model can be done as follows. Let us suppose that the limiting classical phase space for slow variables is a compact manifold $M$, and there are $k$ quantum states associated with the fast variables. The Hamiltonian is such a case becomes a $k \times k$ matrix symbol defined over manifold $M$. Its eigenvalues play the role of classical energy surfaces for $k$ quantum states.

Each point of the classical phase space is associated with $k$ quantum states. This means that we have a vector bundle of rank $k$ defined over the manifold $M$ which is the base space of this bundle. As soon as quantum states are described by complex numbers we have a complex vector bundle. It is known that complex vector bundles

can be topologically non-trivial. Their non-triviality is characterized by the so called Chern classes [13,14].

If there is no overlap between internal structures of different quantum states we can treat internal structure of each quantum state independently and the so obtained vector bundle can be decomposed into $k$ line bundles. In the simplest situation all these line bundles are trivial. Depending on the dimension of the base space only first of higher Chern classes are needed to characterize the topology of the bundle. All information about Chern classes can be summarized in a formal way in a Chern polynomial

$$1 + c_1 x + c_2 x^2 + \cdots , \tag{1}$$

where $x$ is an auxiliary variable and $c_i$ are $i$-th Chern class. The degree of the Chern polynomial cannot be higher than the complex dimension of the base space or the rank of the vector bundle. In order to study the reorganization of band structure in semi-quantum models we need to define the operation of "direct sum" of bundles which corresponds to "mixing" of isolated bands. More formally such operation is known as Whitney sum of vector bundles. When we form the more complicated vector bundle which describes two coupled bands from two bundles with the same base space (corresponding to energy bands for two isolated quantum states) the Chern polynomials of individual bundles should be multiplied and the rank of the sum is the sum of ranks.

### 3.1 One slow degree of freedom

The simplest situation takes place for problems with one-dimensional space of "slow" (classical) variables. In such a case two initially isolated bands are represented as line bundles with respective Chern polynomials $(1 + c_1^a x)$ and $(1 + c_1^b x)$ (see Fig. 1). The total vector bundle has rank two and it is in fact just a sum of two individual line bundles. Under the variation of some control parameter two eigenvalues of $2 \times 2$ symbol Hamiltonian over classical phase space generically pass through degeneracy points. If the degeneracy of two eigenvalues takes place the vector bundle becomes undecomposable due to the presence of degeneracy. But the degeneracy generically lifts away under further variation of control parameter. Two bands again become isolated but their first Chern classes can change. The only restriction is the conservation of the sum of first Chern classes for two bands, i.e. the conservation of the topological invariants of the total bundle.

Figure 1 shows this modification schematically. The modification of the first Chern class depends on the type of singularity which takes place at the degeneration. If there

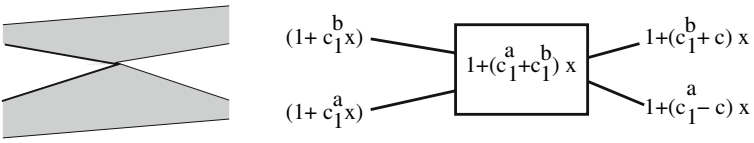


**Fig. 1** Rearrangement of two topologically non-trivial bands. Chern polynomials for each band are shown schematically on the right

are no additional symmetry requirements the modification of the first Chern class is typically $\pm 1$.

It is easy to verify by a simple manipulation with Chern polynomials that in the case of problems with one degree of freedom for slow dynamical variables the rearrangement of two trivial (or even non-trivial) bands is possible. Such rearrangement is associated with the modification of the first Chern classes of two bands. For purely quantum problem such rearrangement is manifested by the redistribution of the energy levels between bands. The fact, that the redistribution of energy levels between energy bands under the variation of control parameter is a generic qualitative phenomenon was initially stated in 1988 [15] on the example of coupling of two angular momenta and on the analysis of the rotational structure of several vibrational states. In the same paper [15] the relation between the redistribution and such topological invariant as Chern class was suggested. But only about 10 years later that the precise statement relating the number of energy levels going from one band to another and the modification of Chern numbers in the associated semi-quantum model was stated and proved [16,17]. This interpretation enables one to associate with energy bands in molecules the topological quantum numbers in a way similar to topological quantum numbers used previously in quantum Hall effect and in other domains [18].

### 3.2 Two slow degrees of freedom

The description of the rearrangement of bands becomes significantly more complicated if the number of slow degrees of freedom is larger than one. We will discuss for simplicity one concrete case of a problem with two slow degrees of freedom which naturally appears in molecular systems when one study the vibrational polyad structure of several electronic states. Electronic variables are considered as fast ones whereas the variables associated with the internal structure of vibrational polyads are treated as slow ones. In a particular case of vibrational polyads formed by three degenerate modes, the corresponding limiting classical phase space is complex projective space $CP_2$ [19,6,8]. Intra-polyad dynamics has two degrees of freedom and the introduced earlier semi-quantum model corresponds to a bundle with the base space being $CP_2$.

Now to characterize the vector bundle associated with several quantum (electronic) states we need to use both first and the second Chern classes and in particular to write the Chern polynomial including quadratic terms. To see the new features arising for problems with two slow degrees of freedom we formulate the following simple question. Is it possible for two bands with trivial topological structure to rearrange into two bands with non trivial topology? The answer is "no". To see the origin of such firbiddance it is sufficient to write the Chern polynomial for two trivial bands. As soon as all Chern classes are trivial the corresponding polynomial is simply 1. On the other hand, if we suppose that two trivial bands can be rearranged into two nontrivial bands, each of the band should be represented by a nontrivial line bundle with non-zero first Chern class. Let suppose that these two Chern polynomials are $(1+c_1x)$ and $(1+c_1'x)$. Their multiplication should give the Chern polynomial for the whole vector bundle over the base space having two degrees of freedom. But this means that when multiplying polynomials we need to conserve all terms up to degree two. As soon as we have

$$(1 + c_1 x)(1 + c_1' x) = 1 + (c_1 + c_1')x + c_1 c_1' x^2, \tag{2}$$

the total Chen polynomial can be trivial only if both $c_1$ and $c_1'$ are zero. This means that it is impossible to realize the rearrangement of two trivial bands over $CP_2$ phase space into two nontrivial bands.

The nontrivial rearrangement can take place if the number of bands becomes three. It is easy to see that the identity

$$1 = (1 + c_1 x)(1 - c_1 x + c_1^2 x^2) \tag{3}$$

can be interpreted as a transformation between three initial trivial bands (each is characterized by a trivial Chern polynomial 1) and two final nontrivial bands. One of two final bands corresponds to nontrivial line bundle with non zero first Chern class. Another final band corresponds to rank 2 vector bundle with both first and second Chern classes being nontrivial.

The schematic representation of such transformation is given in Fig. 2. The important feature of this transformation is the formation of only two final bands instead of three initial bands. We describe such situation as a result of a topological coupling of two bands which is possible only in the presence of the third bands. It is easy to see that the so formed topologically coupled band can not be decomposed into two bands without coupling with some extra band.

The phenomenon of formation of topologically coupled bands was first described by Faure and Zhilinskii [20]. They have studied the natural generalization of the angular momentum coupling model [15,16] based on the coupling of representations of $SU(2)$ group to the case of coupling of representations of the $SU(3)$ group. The most simple physical interpretation of the corresponding model is the rearrangement of vibrational polyads in the case of $F-f$ Jahn–Teller effect [21], i.e. in the coupling of triply degenerate electronic states and polyads formed by triply degenerate vibrations, in the presence of additional perturbation which splits slightly the electronic degeneracy.

## 4 Complete classical model. Rearrangement and monodromy

The semi-quantum model is well adapted to describe the reorganization of bands in the case when the number of bands (or equivalently the number of quantum states)

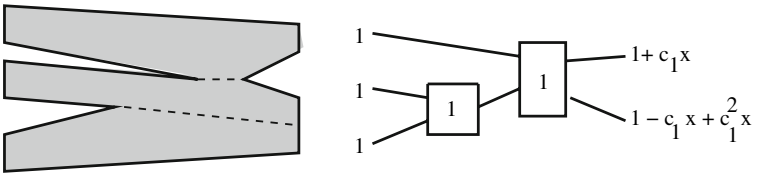


**Fig. 2** Possible rearrangement of three initially trivial bands defined over classical phase space with two degrees of freedom. Chern polynomials are schematically associated with bands on the right part of the figure

involved in the treatment is small, for example equals two or three. In contrast, if the number of bands becomes to be large, but it remains always small as compared to the number of states within each band, it is quite instructive to study the quantum problem in the classical limit with both "slow" and "fast" variables being considered as classical ones.

Such classical limit leads to the analysis of classical integrable models. One of integrals labels the bands, another characterizes the internal structure of bands. In order to relate the phenomenon of the reorganization of bands observed within the semi-quantum model with the characteristic features of the classical integrable problems we need to note that classical completely integrable problem admits the construction of local action-angle variables. These variables are related with the local toric fibration of the classical phase space by levels of constant values of classical integrals of motion. At the same time globally the action-angle variables do not generally exist. This reflects the fact that the fibering by levels of constant values of integrals of motion has singularities. The problem of existence of global action-angle variables and of obstructions to their existence was studied in papers by Nekhoroshev [22] and Duistermaat [23]. In [23] the special attention was paid to the Hamiltonian monodromy as a first obstruction to the existence of global action-angle variables.

Generic singularity which appears in integrable classical fibration with two degrees of freedom is the so called pinched torus ("focus–focus" singularity). Pinched torus can be obtained from a regular torus by shrinking one noncontractible loop to a point. Due to presence of such singularity at some internal point in a space $\{f_1, f_2\}$ of values of integrals $F_1, F_2$ of the integrable classical problem the local action-angle variables cannot be globally defined. In particular the local variables cannot be unambiguously defined along a noncontractible loop which encircles in the $\{f_1, f_2\}$ space the critical value of integrable fibration.

The relation between classical and quantum problem enables one to associate with the classical integrable fibration the joint spectrum of mutually commuting operators $\hat{F}_1, \hat{F}_2$, corresponding to classical integrals $F_1, F_2$ in involution. In the local regions of the space $\{f_1, f_2\}$ of values of integrals where the classical local action-angle variables are defined, the joint spectrum of mutually commuting quantum operators $\hat{F}_1, \hat{F}_2$ form a regular lattice, because by simple Bohr–Sommerfeld quantization rules the quantum eigenstates correspond to integer values of action variables. The presence of singularities for classical fibration and the absence of global action-angle variables manifest themselves in the joint quantum spectrum through the absence of global quantum numbers compatible with the classical limit, or equivalently through the presence of defects in the lattice of common eigenvalues of mutually commuting operators.

The manifestation of classical Hamiltonian monodromy in the joint spectrum of mutually commuting observables for associated quantum problem was first analyzed by Cushman and Duistermaat [24] on the example of quantum spherical pendulum. More systematic description of quantum monodromy was given by Vũ Ngọc [25]. Simultaneously to this development of mathematical formalism various physical applications of quantum monodromy [27–37] and its interpretation in terms of specific defects of the lattice of quantum states [2,3,26] was suggested.

Figure 3 illustrates the notion of quantum monodromy on the example of a model system with two degrees of freedom. The chosen example [3] is the completely

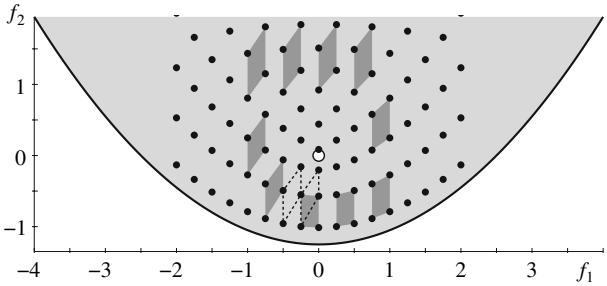


**Fig. 3** Base of the integrable fibration $F$ of the 1:(−1) resonant oscillator system and the corresponding quantum lattice (black dots). Dark gray quadrangles show the evolution of the elementary cell along the closed path $\Gamma$ which goes around the singular value (opaque circle)

integrable dynamical system defined on the four-dimensional classical phase space with $q_1$, $q_2$ coordinates and $p_1$, $p_2$ conjugated momenta by two functions in involution

$$F_1 = \frac{1}{2}(p_1^2 + q_1^2) - \frac{1}{2}(p_2^2 + q_2^2), \tag{4}$$

$$F_2 = p_1 q_2 + p_2 q_1 + \frac{1}{4}\left(p_1^2 + q_1^2 + p_2^2 + q_2^2\right)^2. \tag{5}$$

This dynamical model can be described as a dynamical system with 1:(−1) resonance. It is equivalent from the point of view of the qualitative structure of joint spectrum to problem describing the motion of single particle in a two-dimensional axially symmetric potential $V(r) = ar^4 - br^2$ often referenced as "champagne bottle" potential or "mexican hat" potential, or to vibrational motion of a quasi-linear molecule near the barrier of linearity [32]. Figure 3 shows the image of the energy–momentum map (EM) defined by two integrals $(F_1, F_2)$. The EM map establishes the correspondence between common level sets of two integrals $(F_1, F_2)$ in the four-dimensional phase space and values $(f_1, f_2)$ of these integrals in the two-dimensional space $R^2_{f_1 f_2}$. Inverse image of any regular point of EM map is a two-dimensional torus. Inverse image of the isolated critical value $(f_1 = 0, f_2 = 0)$ is a pinched torus. The presence of this singular fiber makes the fibration defined by $(F_1, F_2)$ EM map locally nontrivial and possessing the monodromy. The same Fig. 3 shows the joint spectrum of two commuting quantum observables for the corresponding quantum problem. In any local simply connected region $D \subset R^2_{f_1 f_2}$ which does not include the singular value $(f_1 = 0, f_2 = 0)$ the system of common eigenvalues form a regular lattice. Choosing an elementary cell of such lattice we can follow the evolution of the cell when transporting it along a closed path in $(f_1, f_2)$ plane which surrounds the critical value. After returning to the initial point the cell differs from the initial cell. The transformation between initial and final cell defines the quantum monodromy.

The most important for us here is the observation that the redistribution of energy levels between branches observed within the semi-quantum model with two quantum states leads to the presence of monodromy in corresponding complete classical problem. The relation between redistribution and the monodromy was observed and

formulated in [28,29]. The corresponding formal mathematical statement which consists in some generalization of the Duistermaat-Heckman theorem [38] is still lacking.

## 5 Resonances and band structure. Generating function analysis

In previous section we have shown that topological quantum numbers (essentially Chern classes) can be used to characterize energy bands. At the same time more standard way to characterize a band is to give a number of quantum states which belong to this band. In this section we will discuss the relation between the number of quantum states in the band and its topological invariants. The basic formula for such a relation is the general index formula for the deformation quantization of vector bundles over compact manifold. Several equivalent formulae were written by different authors [39,40]. We refer the Fedosov quantization formula which gives the number of quantum states for a vector bundle $V$ over a compact manifold $M$:

$$\mathrm{Tr}\hat{1} = \int \mathrm{Ch}(V)\exp(Nx)\mathrm{Todd}(M). \tag{6}$$

Here $\mathrm{Tr}\hat{1}$ is the number of states for the Vector bundle $V$ over manifold $M$. $\mathrm{Todd}(M)$ is the Todd polynomial for the tangent fiber bundle over the manifold $M$. $\mathrm{Ch}(V)$ is the Chern character of the vector bundle $V$, $N$ is the quantum number corresponding to the integral of motion associated with the subspace of slow variables (with the base of the vector bundle).

In a particular simple case of a vector bundle over $CP_2$ we have for Todd class

$$\mathrm{Todd}(CP_2) = 1 + \frac{3}{2}x + x^2, \tag{7}$$

and for the Chern character of the vector bundle $V$

$$\mathrm{Ch}(V) = r + c_1 x + (c_1^2/2 - c_2)x^2, \tag{8}$$

where $r, c_1, c_2$ are the rank and first and second Chern classes of the vector bundle $V$. To calculate the $\mathrm{Tr}\hat{1}$ we need to expand the $\exp(Nx)$ and to keep the coefficient at $x^2$ under the integral. The result is

$$\mathrm{Tr}\hat{1} = \frac{r}{2}N^2 + \frac{3r + 2c_1}{2}N + \frac{2r + c_1^2 + 3c_1 - 2c_2}{2}. \tag{9}$$

This expression gives the number of states in the band as a function of topological invariants of the vector bundle. Otherwise speaking the most general expression of the number of states in a vector bundle over $CP_2$ space can be written in the form of a generating function

$$\frac{A + Bu + Cu^2}{(1-u)^3}. \tag{10}$$

The coefficients $A$, $B$, $C$ are related to topological invariants (rank $r$, first Chern class $c_1$, and second Chern class $c_2$) of the vector bundle as

$$r = A + B + C; \tag{11}$$
$$c_1 = -B - 2C; \tag{12}$$
$$c_2 = -B/2 - 2C + B^2/2 + 2BC + 2C^2. \tag{13}$$

The so obtained relation between the coefficient of the generating function for the number of states in bands and topological invariants of bands leads to very interesting generalization. Instead of looking for bands defined over $CP_2$ phase space which is related with the polyads formed by triply degenerate vibrational mode, we can study more general polyads formed by three modes in resonance $k_1$:$k_2$:$k_3$ with integers $k_i$. Polyads with such resonance are described in the classical limit by weighted projective space $CP_{k_1k_2k_3}$ which is a natural generalization of $CP_2$.

The generating function [41] for the number of states in polyads formed by three vibrational modes in $k_1$:$k_2$:$k_3$ resonance has very simple form

$$g_{k_1:k_2:k_3} = \frac{1}{(1-t^{k_1})(1-t^{k_2})(1-t^{k_3})} = \sum_N C_N t_N. \tag{14}$$

Here $t$ is the auxiliary variable, $C_N$ is the number of quantum states in polyad with polyad quantum number $N$. (We remind that the quantum state with $n_i$ quanta in $i$-th mode belong to polyads with polyad quantum number $N = n_1k_1 + n_2k_2 + n_3k_3$.)

The special feature of polyads formed by vibrational modes in nontrivial resonance is the fact that the number-of-state function $C_N$ has both smooth polynomial and oscillating (periodic) contributions. More strictly speaking the number-of-state function is a quasi-polynomial [42].

Manipulations with generating functions [5,6] shows that in general case the $C_N$ function can be represented in terms of Todd polynomials and this gives the idea to try to find topological information about bands for general bands of polyads directly from generating functions.

To see what kind of information can be obtained let us consider two examples of polyad bands formed by three vibrational modes with two different resonance conditions.

### 5.1 1:2:2 resonance

The first case is 1:2:2 resonance. Physically this resonance takes place, for example, for triatomic ABA molecules like $H_2O$. The generating function for the number of states in polyads is

$$g_{1:2:2} = \frac{1}{(1-t)(1-t^2)^2} = \sum_N C_N t^N \tag{15}$$
$$= 1 + t + 3t^2 + 3t^3 + 6t^4 + 6t^5 + 10t^6 + 10t^7 + \cdots$$

Each polyad is a line bundle of quantum states over weighted projective space $P(1, 2, 2)$. The numbers of states which appear in the power series expansion (15) coincide with numbers present in the expansion for 1:1:1 resonance. Each number in (15) appears twice at neighboring places. In other words taking only even or only odd terms we get the sequence of numbers identical to sequence of numbers of states in polyads for 1:1:1 resonance. From the formal point of view this is equivalent to rewriting the generating function $g_{1:2:2}$ as

$$g_{1:2:2} = \frac{1+t}{(1-t^2)^3} = \frac{1+t}{(1-u)^3} = \sum_N C_N(t)u^N \tag{16}$$
$$= (1+t)(1+3u+6u^2+10u^3+15u^4+\cdots).$$

Here $u$ stands for $t^2$. The whole series can be interpreted as describing pairs of quantum bands over standard $CP^2$ space, i.e. trivial rank 2 vector bundle over $CP^2$.

It is tentative to say that each vibrational polyad for 1:2:2 resonance can be described as a line bundle over weighted projective space $P(1, 2, 2)$ or as a trivial line bundle (with the appropriate choice of polyad number) over standard $CP^2$ space. In a equivalent way this means that each vibrational polyad for 1:2:2 resonance with polyad quantum number $N$ can be considered as vibrational polyad for 1:1:1 resonance with effective polyad quantum number $N^\star$. For $N = \alpha \bmod 2$, $N^\star = (N-\alpha)/2$.

### 5.2 1:1:2 resonance

1:1:2 resonance appears in many molecules with doubly degenerate bending vibrations and one stretching vibration with twice higher frequency. Typical example is the $CO_2$ molecule in which only bending and symmetric stretching are taken into account. The antisymmetric stretching is not in resonance and can be averaged out.

The generating function for the number of states in polyads is

$$g_{1:1:2} = \frac{1}{(1-t)^2(1-t^2)} = \sum_N C_N t^N \tag{17}$$
$$= 1+2t+4t^2+6t^3+9t^4+12t^5+16t^6+20t^7+\cdots.$$

Each polyad is a line bundle of quantum states over weighted projective space $P(1, 1, 2)$. The numbers of states which appear in the power series expansion (17) differ significantly from numbers in the expansion for 1:1:1 resonance. In order to compare numbers in (17) with numbers for 1:1:1 resonance model we rewrite again the generating function (17):

$$g_{1:1:2} = \frac{1+2t+t^2}{(1-t^2)^3} = \frac{2t}{(1-u)^3} + \frac{1+u}{(1-u)^3}. \tag{18}$$

Each of two contributions in (18) gives the coefficients in the series which coincide with coefficients in expansion (17) if one takes only even or only odd terms.

$$\frac{2t}{(1-u)^3} = t(2 + 6u + 12u^2 + 20u^3 + 30u^4 + \cdots), \tag{19}$$

$$\frac{1+u}{(1-u)^3} = 1 + 4u + 9u^2 + 16u^3 + 25u^4 + \cdots . \tag{20}$$

The interpretation of such decomposition can be as follows. Polyads for 1:1:2 resonance problem with odd polyad quantum number $N$ can be considered as a trivial rank 2 vector bundle over standard $CP^2$ space with effective polyad quantum number $N^\star = (N-1)/2$. In other words, the internal structure for odd polyads for 1:1:2 model with quantum number $N$ can be represented as a simple superposition of two polyads for 1:1:1 resonance with effective polyad number $N^\star = (N-1)/2$. Each such effective polyad gives a half of states of the initial $N$ polyad for 1:1:2 problem.

If we look for the internal structure of 1:1:2 polyads for swing spring problem [35,36] it is clearly seen that odd polyads split into "identical" $l < 0$ and $l > 0$ parts which in its turn strongly resemble generic lattice of quantum states for the internal structure of 1:1:1 resonance problem with effective polyad quantum number $N^\star = (N-1)/2$.

The generating function for even polyads has the form

$$\frac{1+u}{(1-u)^3}$$

and can be interpreted as a generating function for the number of states of rank $r = 2$ vector bundle (with nontrivial topology) over $CP^2$ space. To characterize the topology of vector bundle over $CP^2$ two Chern numbers, $c_1, c_2$, are needed. Together with the rank, $r$ of the vector bundle we have three integers, $c_1, c_2, r$ which from the point of view of numbers of states in polyads are equivalent to three coefficients in the numerator of the generating function. In this particular case the rank of vector bundle is $r = 2$, and the Chern numbers are $c_1 = -1, c_2 = 0$. The effective polyad quantum number $N^\star$ for rank 2 model over $CP_2$ is naturally $N^\star = N/2$.

On the basis of these examples we suggest that the internal structure of polyads in the case of general resonance can be put in equivalence with the internal structure of a finite set of topologically nontrivial bands over standard complex projective space. The needed numbers of bands and their topological invariants can be deduced from the analysis of generating functions.

## 6 Conclusions

In this paper we have put in evidence the relation between the structure of bands and the topological invariants introduced in completely classical or semi-quantum models. The rearrangement of bands through the redistribution of energy levels between bands under the variation of some control parameters is a generic phenomenon which

is characterized by the modification of such topological invariants as Chern classes. The simplest rearrangement of bands takes place for problems with only one degree of freedom responsible for the internal structure of bands. In this case the rearrangement consists generically in a redistribution of energy levels between two branches while the number of bands remains fixed. When the internal structure of bands is due to several degrees of freedom the rearrangement of bands can involve the modification of the number of bands. The formation of topologically coupled bands is a new characteristic feature which was up to now analyzed in details only for model problem with slow variables being defined over the phase space with two degrees of freedom. The classification of generic rearrangements of bands for problems with arbitrary dimension and topology of the classical phase space of slow variables remains to be an interesting open problem.

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