Generating Functions for Effective Hamiltonians.
Symmetry, Topology, Combinatorics*

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Abstract—Recent developments associated with old technique of generating functions and invariant theory which I have started to apply to molecular problems due to my collaboration with Yu.F. Smirnov about 25 years ago are discussed. Three aspects are presented: the construction of diagonal in polyad quantum number effective resonant vibrational Hamiltonians using the symmetrized Hadamard product; the decomposition of the number of state generating function into regular and oscillatory contributions and its relation with Todd polynomials and topological characterization of energy bands; qualitative aspects of resonant oscillators and fractional monodromy as one of new generalizations of Hamiltonian monodromy.

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1. HISTORICAL INTRODUCTION

At the end of 1980s I began my collaboration with Yuri Fedorovich Smirnov. We both worked at that time in Moscow State University. He worked at Physics Department (Nuclear Physics Research Institute), myself—at Chemistry Department. The reason of our collaboration was our mutual interest in applications of invariant theory, in particular of the Molien generating function technique, to construction of effective Hamiltonians for nuclear models (main field interest of Yu.F. Smirnov) and to molecular systems (my proper field of research)[1, 2]. Yu.F. Smirnov guided me through mathematical ideas of invariant theory in a way most directly related to natural questions arising in my study of qualitative theory of highly-excited finite particle quantum systems. We also started to work on new possible applications of another modern technique, quantum algebra, to molecular and nuclear systems [3], but at the beginning of 1990s I left Moscow and settled in France, whereas Yu.F. Smirnov moved to Mexico. We continued to meet and to discuss scientific problems but had no occasion to publish something together. Nevertheless, the subject that we have started together with Yu.F. Smirnov becomes one of the powerful tools which I used during last 20 years in relation to different problems of qualitative theory of highly-excited quantum molecular systems [4–9]. Some of these problems I present in the current paper which I devote to the memory of Yuri Fedorovich Smirnov.

2. HADAMARD PRODUCT
OF GENERATING FUNCTIONS

I start with simple molecular example which nevertheless has many common points with general effective vibrational Hamiltonians in molecular or nuclear physics. Let us consider vibrations of methane molecule CH\(_4\), which has equilibrium configuration of \(T_\text{d} \) symmetry. There are one nondegenerate \(\nu_1^\text{A1} \), one doubly degenerate \(\nu_2^\text{E} \), and two triply degenerate \(\nu_i^\text{F2}, i = 3, 4, \) vibrations, which moreover satisfy special resonance condition \(\nu_1 : \nu_2 : \nu_3 : \nu_4 = 2 : 2 : 1 : 1 \). Assuming slight anharmonicity, the excited vibrational states arrange into so-called vibrational polyads formed by groups of nearly degenerate vibrational states (polyads) characterized by the same effective number of quanta \(N = 2n_1 + n_2 + 2n_3 + n_4 \). In order to construct effective vibrational Hamiltonian describing inter-polyad structure, we need to take into account all properly symmetrized operators formed from harmonic oscillator creation and annihilation operators

\[
\left\{ \left[ (a_1^+)^{s_1} \times (a_2^+)^{s_2} \times (a_3^+)^{s_3} \times (a_4^+)^{s_4} \right]_\Gamma \right. \\
\left. \times \left[ (a_1)^{t_1} \times (a_2)^{t_2} \times (a_3)^{t_3} \times (a_4)^{t_4} \right]_\Gamma \right\}^{\text{A1}}
\]
satisfying additional restriction $2s_1 + s_2 + 2s_3 + s_4 = 2t_1 + t_2 + 2t_3 + t_4$ which follows directly from the resonance conditions. Along with $I_d$ geometrical invariance imposed on the Hamiltonian by physical requirements, the invariance with respect to time reversal should typically be imposed as well. The difference between spatial symmetry and time-reversal invariance is technically important because elementary creation (annihilation) operators in most cases could be chosen as transforming according to irreducible representations of the symmetry group, whereas time-reversal operation transforms creation operators into annihilation and vice versa.

The crucial initial point is the Molien theorem [4, 10–14] which in its simplest form enables one to construct the generating function for the number of irreducible representations of a given type in the decomposition of the $N$th symmetric power of one irreducible representation. More exactly, for the finite group $G$, for the initial representation $\Gamma_i$ and for the final representation $\Gamma_f$ the generating function

$$M^G(\Gamma_f \leftarrow \Gamma_i; \lambda) = |G|^{-1} \sum_{g \in G} \tilde{\chi}_f(g) \det(I_n - \lambda \Gamma_i(g))^{-1} = \sum_{N=0}^{\infty} C_N \lambda^N$$

gives the numbers $C_N$ indicating how many times the final representation $\Gamma_f$ appears in the decomposition of the $N$th symmetric power of the initial representation $\Gamma_i$. In (1) $|G|$ is the order of the finite group $G$, $\chi^G$ is the character of the irreducible representation $\Gamma$, tilde means complex conjugation. $\lambda$ is a dummy variable. This generating function typically can be written in the form of a rational function of some special form

$$\sum_k c_k \lambda^k \frac{1}{(1 - \lambda^{d_1})(1 - \lambda^{d_2})\cdots(1 - \lambda^{d_k})},$$

which has symbolic meaning specifying existence of a certain number of functionally independent denominator invariants and a number of linearly independent though algebraically dependent numerator invariants. This symbolic interpretation gives the description of the integrity basis [4] (or in other words, the homogeneous system of parameters [15]). An alternative interpretation of generating function can be done in terms of a set of generators (which are typically functionally dependent), a set of relations (syzygies) between them, a set of relations between relations, etc. [16].

Calculation of the generating functions for the number of invariants or covariants constructed from elementary tensors transforming according to a given irreducible or reducible representation of finite groups is just a relatively simple task as soon as the character table is known. A less trivial problem is the construction of generating function for operators which are diagonal within polyads. This can be achieved by extending the geometrical symmetry group with the dynamical symmetry responsible for the resonance or by constructing the needed generating function from two generating functions, one for creation operators, another for annihilation operators. The nontrivial part consists in introducing the important restriction on the numbers of creation and annihilation operators which leads to operators diagonal within polyads. Such construction was realized, for example, in [17].

More recently a slightly different approach was proposed which is based on the construction known as Hadamard product of formal power series [15, 18–20]. The advantage of this approach is due to the possibility to take into account in a simple way an additional symmetry requirements imposed simultaneously on creation and annihilation operators, like invariance with respect to time reversal, and to represent the answer again in the rational function form.

Let us remind here that the Hadamard product of two formal power series $f(z) = \sum_{n \geq 0} f_n z^n$ and $g(z) = \sum_{n \geq 0} g_n z^n$ is defined as their term-by-term product $[15, 18–20]$

$$f(z) \ast g(z) = \sum_{n \geq 0} f_n g_n z^n. \quad (2)$$

The following fact is known: the Hadamard product of two rational functions is a rational function [18]. This statement allows to convert the formal power series into a rational function form.

We start with an extremely simple example of two $A$ modes in the 1 : 1 resonance with trivial symmetry group. The generating function for creation (or equivalently for annihilation) operators takes the form depending on two dummy variables ($\lambda, k$) which count independently the degree of creation operators and the associated modifications of the polyad quantum numbers:

$$g(A \leftarrow 2A, \lambda, k) = \frac{1}{(1 - \lambda k)^2} \quad (3)$$

$$= \sum_{n=0}^{\infty} (n + 1) \lambda^n k^n.$$

Now in order to construct the generating function for diagonal operators we need to form the power series in $k$ with coefficients being squares of coefficients in (3). This operation is exactly the Hadamard product (square) of formal power series [15, 18–20]. We denote the Hadamard product by $\ast_k$ and its application to generating function (3) gives for the Hadamard square

$$\frac{1}{(1 - \lambda k)^2} \ast_k \frac{1}{(1 - \lambda k)^2} \quad (4)$$
\[
\sum_{n=0}^{\infty} (n+1)^2 \lambda^{2n} k^n = \frac{1 + \lambda^2 k}{(1 - \lambda^2 k)^3}.
\]

The degree of auxiliary variable \(\lambda\) counts now the total degree of creation and annihilation operators. At the same time the variable \(k\) counts \(\Delta n\) associated with only creation (or only annihilation) operators forming the diagonal operator.

Formula (4) follows directly from the identities (where \(t\) replaces the \(\lambda^2 k\))

\[
\frac{d}{dt} \frac{d}{dt} (1 + t + t^2 + t^3 + \ldots) = \sum_{n=0}^{\infty} (n+1)^2 t^n, \quad (5)
\]

\[
\frac{d}{dt} \frac{d}{dt} \left( \frac{1}{1-t} \right) = \frac{1 + t}{(1-t)^3}. \quad (6)
\]

In order to take into account only time-reversal invariant operators we need to use instead of simple Hadamard square the symmetrized Hadamard square \([g(\lambda) \ast_k g(\lambda) + g(\lambda^2)]/2\) which is an analog of a symmetrized square of an irreducible representation. As soon as normal Hadamard square is known, the calculation of the symmetrized square meets no difficulties. Thus, for the generating function (3) its symmetrized Hadamard square, counting the number of diagonal time-reversal invariant operators, becomes

\[
\frac{1}{2} \left[ (g \ast_k g) + g(\lambda^2) \right]
\]

\[
= \frac{1}{2} \left( \frac{1 + \lambda^2 k}{(1 - \lambda^2 k)^3} + \frac{1}{(1 - \lambda^2 k)^2} \right) = \frac{1}{(1 - \lambda^2 k)^3}.
\]

The nontrivial character of \(k\) dependence appears in the case of any \(k_1 : k_2\) resonances different form 1 : 1. We give as an example the 2 : 1 : 1 resonance between nondegenerate \(A_1\) and doubly degenerate \(E\) modes of tetrahedral molecules.

The total generating function describing all diagonal time reversal and \(T_d\)-invariant operators constructed through arbitrary intermediate representations has the following form

\[
g(A_1, TR, \Delta N = 0, \leftarrow A_1 \oplus E (2 : 1; \lambda, k) = \frac{1 + \lambda^7 k^4 + \lambda^8 k^5 - \lambda^{12} k^7 - \lambda^{13} k^8 - \lambda^{20} k^{12}}{(1 - \lambda^2 k)(1 - \lambda^2 k^2)(1 - \lambda^3 k^2)(1 - \lambda^4 k^2)(1 - \lambda^6 k^3)(1 - \lambda^9 k^6)}.\]

The generating function (7) is given in its simplest most reduced form which has six terms in the denominator and both positive and negative contributions in the numerator. Naturally, there should be only five functionally independent invariants for this problem and consequently the six terms in the denominator correspond to a system of invariants related by syzygies. We do not want to discuss here the explicit construction of a system of syzygies. This example is given in order to demonstrate that even in the case of relatively simple generating functions the structure of the associated module of invariant functions can be rather complicated.

### 3. Density of State Function and Topology of Energy Bands

The generating function for the number of states within vibrational polyads formed by resonant oscillators is an extremely interesting object from completely different points of view.

First of all, the number of states in polyads, in the case of nontrivial resonance relation between vibrational frequencies, is a quasipolynomial, i.e. this function can be split into a smooth polynomial part and an additional oscillatory contribution, whose period is related to the resonance condition \([4-6, 21]\). The generating function technique allows us to extract directly from the total generating function both regular polynomial and oscillatory contributions to the density of states.

Namely, the generating function for the number of states in polyads formed by \(d_1 : d_2 : \ldots : d_k\) resonant oscillators can be written as

\[
g_{d_1:d_2:...:d_k}(t) = \frac{1}{(1 - t^{d_1})(1 - t^{d_2}) \ldots (1 - t^{d_k})}.
\]

The coefficient \(C_N\) in the formal series

\[
g_{d_1:d_2:...:d_k}(t) = \sum_N C_N t^N,
\]

can in its turn be represented in the form

\[
C_N = a_{K-1} N^{K-1} + a_{K-1} N^{K-1} + \ldots + a_0 + \text{oscillatory part},
\]

with \(a_j\) being the polynomials of \(d_i\) exponents \([4]\)

\[
a_{K-1-i}(d_1, d_2, \ldots, d_K)
\]
The oscillatory part of the number of state function has complicated form related to the problem of counting the lattice points of rational polyhedra [22, 23], but again it can be represented with a number of the same Todd polynomials each of which now reproduces only part of values of oscillatory function for certain integer values of arguments.

Figure 1 shows an example of oscillatory contribution to the number of state function for three oscillators in the 3:5:7 resonance. It is interesting to see that a series of shifted parabolic dependencies recover all oscillatory contributions. Moreover, the quadratic polynomial turns out to be the same as the quadratic polynomial describing the regular polynomial contribution.

The appearance of Todd polynomials forces us to think about a topological interpretation and this is really the case. To see that we can use the deformation quantization approach which gives the following expression for the number of quantum states [24, 25] (the so-called general index formula):

$$\text{Tr} \hat{1} = \int \text{Ch}(V)\text{Ch}(h)\text{Todd}(M).$$  (12)

Here, Tr\(\hat{1}\) gives the number of states for the vector bundle \(V\) over manifold \(M\) characterized by its rank and Chern numbers; Todd\((M)\) is the Todd polynomial for the manifold \(M\), i.e. the Todd polynomial for the tangent fibre bundle over \(M\); Ch\((V)\) is the Chern character of the vector fibre bundle \(V\); Ch\((h)\) is the Chern character for the quantization of the trivial line bundle over \(M\).

The relation between the topology of the bands and the number of states within the band, which follows directly from the index formula (12), is supported by the description of the rearrangement of bands within the semi-quantum model [7, 26, 27].

Another interesting aspect of generating functions for the number of states within vibrational polyads can be illustrated by examining two simple and quite similar examples of vibrational resonances, namely the three-degree-of-freedom oscillators with resonance conditions 1:1:2 and 1:2:2. In both cases, the reduction of the classical problem is based on the harmonic approximation and takes into account the integral of motion corresponding to the total action of harmonic problem. From the point of view of topology, the reduced classical phase spaces are, in both cases, the weighted projective spaces \(P\{1,1,2\}\) and \(P\{1,2,2\}\), respectively. The singularity structure of these reduced spaces is naturally quite different. It is interesting to note that there is certain equivalence between \(P\{1,2,2\}\) space and a standard complex projective space \(\mathbb{C}P_2\), which is a reduced space for triply degenerate harmonic oscillator. At the same time, the \(P\{1,1,2\}\) space is essentially different [28, 29].

Working with generating functions for the number of states, it is easy to formulate an equivalent proposition. Let us start with the 1:2:2 resonance example. We can rewrite the generating function for the number of states in this case as follows

$$g_{1:2:2} = \frac{1}{(1 - t)(1 - t^2)^2} = 1 + t + 3t^2$$ (13)

$$+ 3t^3 + 6t^4 + 6t^5 + \ldots = \frac{1 + t}{(1 - t^2)^3} = \frac{1}{(1 - u)^3} + t \frac{1}{(1 - u)^3}.$$

A formal Taylor series expansion of the generating function (13) shows clearly that looking separately
on even and odd polyads we find exactly the same numbers as in the case of triply degenerate oscillator. The same effect can be seen after rearrangement of the initial generating function into a sum of two terms with denominator coinciding with the denominator of generating function for the 1:1:1 oscillator (after replacing $t^2 = u$).

The same kind of transformation applied to the generating function for the 1:1:2 oscillator gives more complicated contributions

$$g_{1:1:2} = \frac{1}{(1-t^2)(1-t^2)}$$

We have again (after replacing $t^2 = u$) different terms with the same denominator $(1-u)^3$, which is similar to the 1:1:1 oscillator problem. At the same time, one of two terms has nontrivial numerator, $(1+u)$. The nontrivial numerator is present for bands over complex projective space in the case of quantization of topologically nontrivial vector bundles (according to general index formula). The relation between the generating function for the number of states (over
\( CP^2 \) written in the form

\[
A + Bu + Cu^2
\]

\( (1 - u)^3 \)

and the topology of the fiber bundle over \( CP^2 \) has the following form (see \([7, 26]\))

\[
r = A + B + C, \\
c_1 = -B - 2C, \\
c_2 = -B/2 - 2C + B^2/2 + 2BC + 2C^2,
\]

where \( r \) is the rank and \( c_1, c_2 \) are the first and second Chern classes of the fiber bundle.

Returning now back to the interpretation of the decomposition of generating function (14) for the \( 1 : 1 : 2 \) resonance, we can state that the internal structure of polyads formed by oscillators in the \( 1 : 1 : 2 \) resonance is equivalent to superposition of two trivial bands over \( CP^2 \) space for odd polyads and to superposition of two bands (one with trivial topology and another with nontrivial first Chern class, \( c_1 = -1 \)) for even polyads. Namely, on the basis of this concrete example it is possible to formulate a general tentative interpretation of the internal structure of polyads.

The internal structure of polyads for general resonance (over weighted projective space) can be described as formed by several polyads over standard projective space but with nontrivial topological properties (Chern classes).

4. FRACTIONAL MONODROMY AND DEFECTS OF LATTICES

In this section I want to demonstrate how the generating function formalism and, in particular, the splitting of the number of state functions into regular and oscillatory contributions turns out to be the stimulating argument for introducing a new notion of fractional monodromy. For this I need first to remind several facts about standard (integer) Hamiltonian monodromy for completely integrable classical Hamiltonian systems, and about its quantum analog and its relation to defects of regular lattices.

For classical integrable Hamiltonian systems with two degrees of freedom the image of the corresponding energy–momentum map contains regular and singular values (see Fig. 2). In order to stress that different images of energy–momentum map are quite characteristic for concrete physical problems we provide here physical examples for each of four images: (i) a particle in a “mexican hat” potential [30]; (ii) two nonlinear oscillators in the \((−2):1:1\) resonance [31]; (iii) quadratic spherical pendulum [32], or LiCN molecule [33]; (iv) three-dimensional oscillator with \( 1:1:2 \) resonance or vibrational stretching modes of CO\(_2\) like molecule [34].

Whereas inverse images of the regular values are always regular tori, the inverse images for singular values are topologically different objects (shown in Fig. 3).

The presence of isolated singular values (like in Fig. 2, left) leads to an obstruction to the existence of global action–angle variables in spite of the fact that the problem is completely integrable one. A typical generic example of an isolated critical value of the energy–momentum map for classical dynamic systems with two degrees of freedom is a so-called pinched torus (see Fig. 3). Due to its presence, the toric fibration over any closed contour surrounding critical value should be nontrivial. This nontrivial character of classical integrable (almost) toric fibration is known under the name of Hamiltonian monodromy [35, 36]. In order to see, in the simplest way, the manifestation of Hamiltonian monodromy in corresponding quantum systems we can analyze the joint spectrum of mutually commuting quantum observables. The joint spectrum is a quantum equivalent of the classical energy momentum map. For two-degree-of-freedom systems, any simply connected region of regular values of classical energy–momentum map is represented in quantum mechanics as a locally regular lattice of commun eigenvalues of two commuting integrals of motion.

Critical value manifests itself in quantum joint spectrum as a special defect of regular lattice [37]. To see the effect of a defect we can check the evolution of the elementary cell of the lattice while it makes a closed loop surrounding the critical value [38]. Figure 4 demonstrates the Hamiltonian monodromy by comparing the initial cell with the final cell. The matrix transforming initial cell into final one is the quantum monodromy matrix.

The construction of the “monodromy defect” of a regular lattice (as it is shown in Fig. 5) is based essentially on the “cutting and glue” procedure widely
used in solid state physics in order to explain the structure of dislocations and disclinations [39]. The main feature of the construction consists of removing a slice from the regular lattice in such a way that the number of removed points with a given value of one of the integrals of motion varies linearly with the value of that integral. The mathematical origin of such construction is the Duistermaat–Heckman theorem [40] which formulates, in particular, that the volume of reduced phase space for integrable system with two degrees of freedom is a piece-wise linear function of the integral value. In quantum mechanics the volume of the reduced phase space should be replaced by the number of quantum states for the reduced problem. It is interesting to note, that so constructed “elementary monodromy defect” is quite different from standard dislocations, disclinations, and other defects suggested and studied in solid state physics. The natural question, which appears together with an interpretation of Hamiltonian monodromy as a defect of regular lattice, is: how can we generalize the “elementary monodromy defect” and the notion of Hamiltonian monodromy itself just by trying to generalize the concept of lattice defects and at the same time keeping in mind the realization of lattice as a joint spectrum of several commuting operators? Here it is just the time to remind the typical for molecular problem oscillatory behavior of the density of state function. Instead of removing a wedge from the regular lattice with the number of removed states being the linear function of the integral of motion, we can remove more complicated wedge with the number of removed states being the quasi-polynomial function (having oscillatory contribution) of the integral of motion. The simplest situation of such kind corresponds to oscillatory contribution with period 2. Naturally, in this case the gluing of the cut after removing the wedge should lead to linear rather than point defect (in the case of two-dimensional lattices).

The construction of the rational 1:2 defect is shown in Fig. 6. It is clear, that in the presence of such fractional defect the elementary cell cannot unambiguously cross the defect line. In the case of 1:2 fractional defect the elementary cell can take two different forms after crossing the defect line depending on the place of crossing point. At the same time, looking at the evolution of the double cell during
crossing the defect line, one can see that the result is completely independent of the crossing point.

A formal interpretation of the monodromy matrix in terms of elementary cell transformation leads in such a case to monodromy matrix with fractional entries. Nevertheless, one should not forget that the elementary cell itself is not passable through the fractional cut. Only multiple cells are passable and writing monodromy matrix in terms of multiple cells (or, in more mathematical terms, in terms of a subgroup of the homology group) leads naturally to a monodromy matrix with integer entries. This allows us to give another description of the fractional defect, namely, the fractional defect (which has codimension one) can be removed by going to the sublattice with bigger “elementary” cells. These “bigger” cells are, in fact, multiple cells of the original lattice, and these multiple cells are passable from the point of view of fractional defect under study.

From the classical dynamics point of view the topological structure of critical fibers associated with fractional defect line is the curled torus, shown in Fig. 3. The appearence of corresponding singularity in integrable fibration is due to nonlinear resonance between two modes. The simplest mathematical model of fractional defect is related to two nonlinear oscillators with $1 : (-2)$ resonance [31]. Similar singularity can equally appear in models of coupling of two angular momenta (see Fig. 7). Detailed analysis of such model problem with interaction of two angular momenta leading to fractional monodromy defect was done in [41] by using the effective Hamiltonian

$$H = \frac{1 - \lambda}{|S|} S_z$$

$$+ \lambda \left( \frac{1}{|S||N|} S_z N_z + \frac{1}{2|S||N|^2} (N^2 S_+ + N^2 S_-) \right),$$

written in terms of two angular momenta $N = (N_x, N_y, N_z)$ and $S = (S_x, S_y, S_z)$. As a more realistic example, we can cite such simple and in the same time fundamental physical system as hydrogen atom in presence of static electric and magnetic fields which was recently shown to possess many different qualitative effects [42] including fractional monodromy and a new, recently introduced notion of bidromy [43].

5. CONCLUSION

I would like to note in the conclusion that the generating function technique, being rather old mathematical tool, remains unfortunately until now a relatively exotic method which has a few applications in molecular and atomic physics. At the same time the generating functions are at the intersection of a number of quite different mathematical fields. We have mentioned combinatorics, topology, symmetry, dynamical systems. We hope that this multidisciplinary aspect of generating function will stimulate various application in molecular physics and in natural science in general.

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