Double and triple points in the spectra of the cubic symmetry Hamiltonian

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Abstract. Accidental degeneracy of levels is studied in the spectrum of the Hamiltonian used frequently in applications, which is a linear combination of spherical tensors of rank $n \leq 6$ invariant with respect to transformations of a cubic group. The degeneracy arises only at definite values of the Hamiltonian parameters and seems to be irrelevant with respect to increasing Hamiltonian symmetry. The basis of irreducible representations D^Γ of the cubic group is constructed in the space of irreducible representations D^J of the SO(3) group.

1. Introduction

The degeneracy of levels in the spectrum of any Hamiltonian is usually considered to be related to its symmetry with respect to some group G. However, Moshinsky and Quesne (1983), Berry and Wilkinson (1984), Dirl and Moshinsky (1985) and Siddall and Sullivan (1988) have treated a number of instances where the level degeneracy appeared to be irrelevant to the occurrence of a symmetry group for a Hamiltonian. Any consistent theory for the given type of phenomena has not been constructed yet.

Below we examine in detail the term crossing in the spectrum of the cubic-symmetry Hamiltonian of the following type used frequently in applications:

$$H = a_2 T_2 + a_4 T_4 + a_6 T_6. \tag{1}$$

The term crossing gives rise to an accidental degeneracy of eigenvalues which seems not to be associated with increasing Hamiltonian symmetry and, therefore, presents another example of 'degeneracy without symmetry'. The rank-n tensor operators T_n in (1) are invariants of one of the cubic groups (for definiteness, we shall treat the octahedral group O). They are of the form

$$T_2 = t_0^0 = J^2 = J_x^2 + J_y^2 + J_z^2$$
$$T_4 = \sqrt{\tfrac{7}{12}} t_0^4 + \sqrt{\tfrac{5}{24}} (t_4^4 + t_{-4}^4) \tag{2}$$
$$T_6 = \sqrt{\tfrac{1}{8}} t_0^6 - \tfrac{1}{4}\sqrt{7}(t_4^6 + t_{-4}^6).$$

Here we have chosen the axis of quantization to be the four-fold symmetry axis of the octahedral group. The matrices of tensor operators t_q^n on the basis of functions $|JM\rangle = Y_{JM}$ $(-J \leq M \leq J)$ labelled by angular momentum J and its projection M may be easily calculated using the Wigner-Eckart theorem

$$\langle JM| t_q^n |JM'\rangle = (-1)^{J-M} \begin{pmatrix} J & n & J \\ -M & q & M' \end{pmatrix} \langle J \| t^n \| J \rangle \tag{3}$$

where

$$\begin{pmatrix} J_1 & J_2 & J_3 \\ M_1 & M_2 & M_3 \end{pmatrix}$$

is the Wigner 3-j coefficient, and the reduced matrix elements $\langle J \| t^n \| J \rangle$ which do not depend on M or M' may be included into the phenomenological constants a_2, a_4 and a_6 of the Hamiltonian (1).

Hamiltonians of type (1) are used to describe the spectra of impurity ions in a crystal field of cubic symmetry (see, for example, Sviridov and Smirnov 1977). In this case, the ion term E_J with angular momentum J splits into a number of levels $E_{i\Gamma J}$ labelled by symbol Γ of irreducible representations (irreps) D^Γ of the group O entering the expansion

$$D^J = \sum_\Gamma \nu_\Gamma D^\Gamma \tag{4}$$

where D^J are irreps of the SU(2) group and ν_Γ are multiplicities of the irreps D^Γ. The energies $E_{i\Gamma J}$ are usually calculated by diagonalizing the matrix of the operator (1) on the basis of functions Y_{JM}.

The Hamiltonian (1) is used also to describe the rotational spectra of the non-rigid cubic-symmetry molecules (Hecht 1960, Moret-Bailly 1961, 1965). In this case the energies of rotational levels $E_{i\Gamma J}$ are calculated by diagonalizing the matrix of the Hamiltonian on the basis of the symmetrical-top eigenfunctions $|JMK\rangle = \sqrt{(2J+1)/8\pi^2}\, D_{MK}^{J*}(\alpha\beta\gamma)$. However, the matrix of effective rotational Hamiltonian (1), allowing for the effects of non-rigidity of a molecule, on the basis of the symmetrical-top eigenfunctions $|JMK\rangle$, coincides with the matrix of the Hamiltonian of an impurity ion in a crystal field on the basis of the functions Y_{JM}. Therefore, the two problems may be treated in parallel. Below we shall mainly discuss the rotational spectra of cubic-symmetry molecules, but all results may be easily reinterpreted in terms of the spectra of impurity ions in the crystal field.

Studying the rotational spectra of cubic-symmetry molecules is of particular interest because states with very high values of angular momentum ($J \sim 100$) are observed experimentally. In this case the eigenvalues of the operator (1) with a given value of J are grouped into close and almost degenerate six- and eight-fold clusters (Dorney and Watson 1972, Harter and Patterson 1977, 1979, Fox *et al* 1977, Zhilinskii 1979, Braun *et al* 1985) and, for some particular choices of the Hamiltonian parameters, 12-fold level clusters are also formed in the spectrum.

The visual geometrical explanation of the level clustering phenomenon (Harter and Patterson 1977) suggests that levels forming a cluster have an identical physical origin and correspond to rotation of a molecule about n-fold symmetry axes C_n. The equivalence of symmetry axes of the same type C_n causes degeneracy of the corresponding levels. So, the six-fold clusters, for example, are formed by degenerate levels corresponding to molecular rotations about three four-fold symmetry axes C_4 (allowing for the two feasible directions of rotation about each of the axes), while the eight-fold clusters are formed by levels corresponding to rotations about four three-fold symmetry axes C_3 and the 12-fold clusters are connected with rotations about six two-fold symmetry axes C_2.

In the classical limit $J \to \infty$, the levels forming a cluster are strictly degenerate. Nevertheless, the clusters split due to the quantum tunnel effect which causes the coupling between rotations about different equivalent symmetry axes. In this case, obviously, each of the levels may be labelled by irreps D^Γ of the group O. Thus, the

clusters have the structure $\Gamma_1 + \Gamma_2 \ldots + \Gamma_K$, i.e. they are formed by K close levels corresponding to the irreps $D^{\Gamma_1}, D^{\Gamma_2}, \ldots, D^{\Gamma_K}$ of the group O. Of course, each level pertaining to symmetry Γ is rigorously degenerate and the multiplicity of degeneration is equal to the dimension dim Γ of the irrep D^{Γ}. So, for example, six-fold clusters are either of the type $F_1 + F_2$ (two close triplets pertaining to symmetry F_1 and F_2) or $A_1 + E + F_1$ $(A_1 + E + F_2)$ (three close levels: non-degenerate pertaining to symmetry A_1 (A_2), doublet E and triplet F_1 (F_2)).

It should be borne in mind that the operator $T_2 = J^2$ entering (1) fails to give rise to the splitting of levels with the same value of J due to the effects of the non-rigidity of a molecule, and defines only the 'centre of gravity' position of the terms characterized by a certain value of the angular momentum J. Therefore, in the study of the structure of rotational spectra characterized by a given value of J, i.e. in the study of the level clustering phenomenon and of the crossing of levels comprising the above-mentioned spectra, it is of interest to examine only the $a_n T_n$-type terms with $n \geq 4$ in (1). So, we shall operate with the effective rotational Hamiltonian

$$h(\theta) = T_4 \cos \Theta + T_6 \sin \Theta \tag{5}$$

where the parameter θ defines the relative weights of the tensor operators T_4 and T_6.

Lea *et al* (1962), Harter and Patterson (1979) and Braun *et al* (1986) examined the dependence of the eigenvalues $E_{i\Gamma J}$ of the operator (5) on the parameter θ. From their numerical calculations, Lea *et al* (1962) inferred a simultaneous crossing of three terms, A_1, E, F_1 (or A_2, E, F_2), at a single point at certain values $\theta = \theta_t$. Harter and Patterson (1979) called these points the triple points and analysed them in terms of an approximate asymptotic theory. At certain values $\theta = \theta_d$, the crossing of two terms F_1 and F_2 occurs also at a definite point. We shall call points of the latter type double points.

Below, we shall examine the double and triple points in the spectrum of the Hamiltonian (5) in terms of an accurate algebraic approach. We shall demonstrate that the occurrence of double and triple points in the spectrum of the Hamiltonian (5) is quite natural and exhibits a regular behaviour. We shall rigorously prove that at definite values $\theta = \theta^i$, $i = 1, 2, \ldots$, in the general case, the spectrum of the Hamiltonian (5) contains several triple and/or double points, rather than a single point, i.e. several triplets and/or pairs of degenerate terms, rather than a single triplet or pair, are present in the spectrum at several different values of energy.

The double and triple points manifest themselves in the strict degeneration of some of the six-fold clusters and/or in the strict degeneration of a pair or triplet of levels entering an eight- or 12-fold cluster. Note that the double and triple points may occur in the spectra of levels with sufficiently small values of J, when the clusters are not well formed. The level crossing associated with the double and triple points originates from the octahedral symmetry of the problem, and arises naturally for the spectra of impurity ions in the crystal field as well as for the rotational spectra of cubic-symmetry molecules.

We make use of the algebraic methods associated closely with constructing the basis of irreps D^{Γ} of the group O in the space of irreps D^J of the SO(3) group. In parallel with studying the double and triple points of the cubic Hamiltonian, we shall construct the complete set of cubic harmonics Ψ^{Γ}_{ij}. The set appears to be nearly the same as the one proposed by Cheglokov and Ulenikov (1985). Note that these authors have not given the full proof of the linear independence of the basis functions, and our study closes the problem.

The paper is organized as follows. In section 2 we discuss some properties of effective Hamiltonian (5), write down projection operators, formulate lemmas and introduce notations that are used afterwards. Section 3 treats a simple example which visualizes the physical origin of double and triple points. The algebraic treatment of double and triple points in the general case is presented in sections 4 and 5. A discussion of the results is presented in section 6.

2. Term crossing in the spectrum of the effective rotational Hamiltonian

From the explicit form (2) of the operators T_4 and T_6 it is seen that the matrix $\mathfrak{H}$ of the Hamiltonian (5) in the basis of the functions $|JMK\rangle \equiv |JK\rangle$ is tridiagonal, i.e. only the matrix elements $\mathfrak{H}_{KK'} \equiv \langle JK|h(\theta)|JK'\rangle \equiv \langle JMK|h(\theta)|JMK'\rangle$ with $K' = K, K \pm 4$ are non-vanishing. The eigenvalue problem for the Hamiltonian (5) is of the form

$$\mathfrak{H}_{K,K-4}C^\lambda_{K-4} + (\mathfrak{H}_{KK} - E_\lambda)C^\lambda_K + \mathfrak{H}_{K,K+4}C^\lambda_{K+4} = 0. \tag{6}$$

Obviously, the set of equations (6) may be broken into four independent subsets characterized by a particular value of $q = K \bmod 4$, i.e. the matrix $\mathfrak{H}$ of the Hamiltonian $h(\theta)$ may be decomposed into a direct sum of the type $\mathfrak{H} = \mathfrak{H}^0 \oplus \mathfrak{H}^1 \oplus \mathfrak{H}^2 \oplus \mathfrak{H}^3$, where the matrices $\mathfrak{H}^q$ with matrix elements $\mathfrak{H}^q_{nn'} = \langle J, 4n+q|h(\theta)|J, 4n'+q\rangle$, $q = 0, 1, 2, 3$, are tridiagonal, and the non-vanishing matrix elements $\mathfrak{H}^q_{nn}$ are the ones with $n = n'$, $n' \pm 1$. Thus, we actually meet the problem of diagonalizing four Hermitian tridiagonal matrices $\mathfrak{H}^q$.

The eigenfunctions $\mathbb{C}_\lambda \equiv \mathbb{C}^q_\lambda$ of the Hamiltonian $h(\Theta)$ are linear combinations of the basis functions $|qn\rangle \equiv |J, 4n+q\rangle$: $\mathbb{C}^q_\lambda = \Sigma_n C^\lambda_n|qn\rangle$, and the coefficients C^λ_n are components of the eigenvectors $\{C^\lambda\} = \{C^\lambda_q\}$ of the matrices $\mathfrak{H}^q$. In what follows we shall denote by n_{max} (n_{min}) the maximal (minimal) possible value of the index n of the basis functions $|qn\rangle$, and by $K^q_{max} = 4n_{max} + q$ ($K^q_{min} = 4n_{min} + q$) the maximal (minimal) possible value of the projection K of angular momentum on the internal molecular frame fixed to a rotor for given values of J and q. $N^q = n_{max} - n_{min} + 1$ is, obviously, the dimension of the Hilbert space spanned by the functions $|qn\rangle$, and the matrices $\mathfrak{H}^q$ are $N^q \times N^q$ matrices.

The eigenfunctions $\mathbb{C}_\lambda$ of the Hamiltonian (5) may be labelled by the irreps D^Γ of the group O. The discrimination of the eigenfunctions $\mathbb{C}_{\Gamma\lambda}$ belonging to the irrep D^Γ of the group O may be done using the projection operators

$$P^\Gamma = \frac{\dim \Gamma}{24} \sum_g \chi_\Gamma(g)D(g) \tag{7}$$

where g is an element (rotation) of the group O , $D(g)$ is the corresponding operator, and $\chi_\Gamma(g)$ is the character of the element g in the irrep D^Γ. Using (7) it is straightforward to obtain matrix elements $P^\Gamma_{KK'} \equiv \langle JK|P^\Gamma|JK'\rangle$ of the operators P^Γ on the $|JK\rangle$ basis:

$$P^{A_1}_{KK'} = \tfrac{1}{6}\delta_{0,K \bmod 4}[\delta_{KK'} + (-1)^J\delta_{K,-K'} + 2\mathfrak{D}_{KK'}]$$

$$P^{A_2}_{KK'} = \tfrac{1}{6}\delta_{2,K \bmod 4}[\delta_{KK'} + (-1)^J\delta_{K,-K'} - 2\mathfrak{D}_{KK'}]$$

$$P^E_{KK'} = \tfrac{1}{3}\delta_{0,K \bmod 2}[\delta_{KK'} + (-1)^J\delta_{K,-K'} - (-1)^{K/2}\mathfrak{D}_{KK'}] \tag{8}$$

$$P^{F_1}_{KK'} = \tfrac{1}{2}[\delta_{KK'}(1 - \delta_{2,K \bmod 4}) - (-1)^J\delta_{K,-K'}\delta_{0,K \bmod 4} + \delta_{1,K \bmod 2}\mathfrak{D}_{KK'}]$$

$$P^{F_2}_{KK'} = \tfrac{1}{2}[\delta_{KK'}(1 - \delta_{0,K \bmod 4}) - (-1)^J\delta_{K,-K'}\delta_{2,K \bmod 4} - \delta_{1,K \bmod 2}\mathfrak{D}_{KK'}]$$

where $\mathfrak{D}_{KK'} = 2\delta_{0,(K-K') \bmod 4}d^J_{KK'}(\pi/2)$, and $d^J_{km}(\beta)$ is the Wigner d-function.

The matrices of projection operators P^Γ are seen from (8) to be diagonal with respect to the index $q = K \bmod 4$. Thus, the eigenfunctions $\mathbb{C}_\lambda^q$ and respective eigenvalues E_λ^q, obtained by diagonalizing the matrices $\mathfrak{H}^q$, may be labelled by the index Γ of the irreps D^Γ of the group O. The set of irreps D^Γ realizable in the Hilbert space spanned by the functions $|qn\rangle$ with a given value of q may be easily determined from (8). The results are summarized in table 1.

Table 1. Irreps D^Γ of the group O compatible with a given value of $q = K \bmod 4$.

$q = K \bmod 4$	0	1	2	3
Irreps of the group O	A_1	—	—	—
	—	—	A_2	—
	E	—	E	—
	F_1	F_1	—	F_1
	—	F_2	F_2	F_2

Note, that if the irrep D^Γ is compatible with a given value of q, then among the eigenfunctions $\mathbb{C}_\lambda^q$ there should be found ν_Γ eigenfunctions $\mathbb{C}_{\Gamma\lambda}^q$ pertaining to symmetry Γ, and the dimension of the matrix $\mathfrak{H}^q$, $N^q = \Sigma_\Gamma \nu_\Gamma$, where the summation is assumed over all Γ compatible with a given value of q. The two-fold degeneracy of the eigenvalues of the matrix $\mathfrak{H}$ pertaining to symmetry E and three-fold degeneracy of the eigenvalues of the same matrix pertaining to symmetries F_1 and F_2 results from the coincidence of eigenvalues $E_{\Gamma\lambda}^q$ and $E_{\Gamma\lambda}^{q'}$ of different matrices $\mathfrak{H}^q$ and $\mathfrak{H}^{q'}$ pertaining to the same symmetry Γ $(=E, F_1$ or $F_2)$. Nevertheless, the set of eigenvalues $E_{\Gamma\lambda}^q$ pertaining to a given symmetry Γ of any matrix $\mathfrak{H}^q$ is non-degenerate. At the same time, the occurrence of double points of the type $F_1 + F_2$ and of triple points of the type $A_1 + E + F_1$ or $A_2 + E + F_2$ is associated with the degeneration of levels pertaining to different symmetries Γ and Γ', and, as seen from table 1, is associated with degeneration of a number of eigenvalues of one of the matrices $\mathfrak{H}^q$.

Now let us present two lemmas (Voevodin and Kuznetsov 1984) concerning the general properties of eigenvalues E_λ, eigenvectors $\{C^\lambda\}$ and respective eigenfunctions $\mathbb{C}_\lambda = \Sigma_n C_n^\lambda |n\rangle$ of the Hermitian tridiagonal matrices $\mathfrak{B}$. All the non-diagonal matrix elements $\mathfrak{B}_{n,n\pm1}$ are assumed to be non-zero: $\mathfrak{B}_{n,n\pm1} \neq 0$.

Lemma 1. All the eigenvalues E_λ are non-degenerate.

Lemma 2. The extreme components of any of the eigenvectors $\{C^\lambda\}$ are non-zero, i.e. $C_{n_{\max}}^\lambda \neq 0$ and $C_{n_{\min}}^\lambda \neq 0$, while all the eigenfunctions functions $\mathbb{C}_\lambda$ enter the decomposition of the extreme basis functions

$$|n_{\max(\min)}\rangle = \sum_\lambda \tilde{C}_{n_{\max(\min)}}^\lambda \mathbb{C}_\lambda \tag{9}$$

with coefficients $\tilde{C}_{n_{\max(\min)}}^\lambda \neq 0$.

From lemma 1 it follows immediately that, if all the non-diagonal matrix elements of the effective Hamiltonian $\mathfrak{H}_{K,K\pm4} = \langle JK|h(\Theta)|J, K \pm 4\rangle \neq 0$, the spectrum of the eigenvalues of any matrix $\mathfrak{H}^q$ is non-degenerate. Thus, the formation of double and triple points is associated with vanishing of non-diagonal matrix elements of the

operator (5) at certain values of the parameter $\Theta = \Theta^1, \Theta^2, \ldots$, which may be found from the equation

$$\cos \Theta^i \langle JK_i | T_4 | JK_i - 4 \rangle + \sin \Theta^i \langle JK_i | T_6 | JK_i - 4 \rangle = 0. \tag{10}$$

The solutions $\Theta^i \equiv \Theta_q^i$ for (10) are specified below by values of K_i at the fixed value of $q = K_i \bmod 4$, i.e. the index i labelling the special points $\Theta = \Theta^i \equiv \Theta_q^i$ is to be found from the equation $K_i \equiv 4n_i + q = 4(n_{\max} + 1 - i) + q$, $i = 1, 2, \ldots$. Due to the symmetry properties of the matrix $\mathfrak{H}$,

$$\mathfrak{H}_{KK'} = \mathfrak{H}_{K'K} = \mathfrak{H}_{-K,-K'} = \mathfrak{H}_{-K',-K} \tag{11}$$

which may be easily obtained from (2), (3) and (5), it is sufficient to treat only the K_i-values belonging to the interval $2 \leq K_i \leq J$. It will be shown that each of the solutions Θ^i for (10) is in correspondence with the occurrence of double and/or triple points in the spectrum.

From (10) and (11) it follows that at each special point $\Theta = \Theta_q^i$, $i = 1, 2, \ldots$, four non-diagonal matrix elements of the matrix $\mathfrak{H}$ vanish simultaneously:

$$\mathfrak{H}_{K_i,K_i-4} = \mathfrak{H}_{K_i-4,K_i} = \mathfrak{H}_{-K_i+4,-K_i} = \mathfrak{H}_{-K_i,-K_i+4} = 0 \tag{12}$$

(except for the case $K_i = 2$, when only two non-diagonal matrix elements $\mathfrak{H}_{2,-2} = \mathfrak{H}_{-2,2} = 0$). Thus, if q is even, than at the special point $\Theta = \Theta_q^i$ the matrix $\mathfrak{H}^q$ appears to be of a block-diagonal structure and may be decomposed into the direct sum of the type $\mathfrak{H}^q = H^{(1)} \oplus H^{(2)} \oplus H^{(3)}$. The matrices $H^{(j)}$ are $N^{(j)} \times N^{(j)}$ matrices, where $N^{(1)} = N^{(3)} = i$ and $N^{(2)} = N^q - 2i$, and the indices n and n' labelling the matrix elements $H_{nn'}^{(1)}$, $H_{nn'}^{(2)}$ and $H_{nn'}^{(3)}$ belong to the intervals $[n_i, n_{\max}]$, $[-n_i + 1 - q/2, n_i - 1]$ and $[n_{\min}, -n_i - q/2]$, respectively. The matrices $H^{(j)}$ are, obviously, tridiagonal. Moreover, due to (11), matrices $H^{(1)}$ and $H^{(3)}$ are identical.

If q is odd, then $\mathfrak{H}^q = H^{(1)} \oplus H^{(2)}$ at special points $\Theta = \Theta_q^i$, where $H^{(j)}$ are tridiagonal $N^{(j)} \times N^{(j)}$ matrices with $N^{(1)} = i$ and $N^{(2)} = N^q - i$. The indices n and n' labelling the matrix elements $H_{nn'}^{(1)}$ and $H_{nn'}^{(2)}$ belong to the intervals $[n_i, n_{\max}]$ and $[n_{\min}, n_i - 1]$, respectively.

In studying double and triple points we are interested only in the spectra of submatrices $\mathfrak{H}^q$ that have a block-diagonal structure due to the vanishing of non-diagonal matrix elements at special points $\Theta = \Theta_q^i$. If q is even, then $\mathfrak{H}^q$ is the only block-diagonal submatrix of the matrix $\mathfrak{H}$. If q is odd, then two submatrices $\mathfrak{H}^1$ and $\mathfrak{H}^3$ are block-diagonal but, because of (11), the submatrices $\mathfrak{H}^1$ and $\mathfrak{H}^3$ are identical. So, for any q it is sufficient to study only the spectrum of the submatrix $\mathfrak{H}^q$ at the special point $\Theta = \Theta_q^i$.

3. A simple example

In order to show the physical origin of the accidental degeneracy in the spectra of the Hamiltonian (5), let us discuss a simple example.

Suppose $J = 4$. In the case $q = 1$, $\mathfrak{H}^{q=1}$ is a 2×2 matrix. It has two eigenvalues E_{F_1} and E_{F_2} pertaining to the symmetries F_1 and F_2, respectively. For each of the symmetries F_1 and F_2 there is the unique cubic harmonic $\Psi_{q=1,J=4}^{\Gamma}$ (Sviridov and Smirnov 1977):

$$\begin{aligned} \Psi_{q=1,J=4}^{F_1} &= \sqrt{\tfrac{7}{8}} |q=1, 0\rangle + \sqrt{\tfrac{1}{8}} |q=1, -1\rangle \\ \Psi_{q=1,J=4}^{F_2} &= \sqrt{\tfrac{1}{8}} |q=1, 0\rangle - \sqrt{\tfrac{7}{8}} |q=1, -1\rangle. \end{aligned} \tag{13}$$

The functions $\Psi_{q=1,J=4}^{\Gamma}$ are, obviously, the eigenfunctions of the Hamiltonian (5) at any value of the parameter Θ. The function $|q=1, 0)$ is seen from (13) to be a linear combination of the functions $\Psi_{q=1,J=4}^{F_1}$ and $\Psi_{q=1,J=4}^{F_2}$. Nevertheless, if $\Theta = \Theta_{q=1}^{i=1}$, then the matrix $\mathfrak{H}^{q=1}$ is diagonal and the function $|q=1, 0)$ is an eigenfunction of the Hamiltonian (5). This is possible if only the terms E_{F_1} and E_{F_2} are degenerate. Thus, a double point of the type $F_1 + F_2$ occurs in the spectrum of the effective Hamiltonian (5) when Θ attains the value $\Theta_{q=1}^1$.

Now let us discuss the case $q = 0$. For each of the symmetries A_1, E and F_1 there is also the unique cubic harmonic $\Psi_{q=1,J=4}^{\Gamma}$ (Sviridov and Smirnov 1977):

$$\Psi_{q=0,J=4}^{A_1} = \sqrt{\tfrac{5}{24}}[|q=0, 1) + |q=0, -1)] + \sqrt{\tfrac{7}{12}}|q=0, 0)$$

$$\Psi_{q=0,J=4}^{E} = \sqrt{\tfrac{7}{24}}[|q=0, 1) + |q=0, -1)] - \sqrt{\tfrac{5}{12}}|q=0, 0) \tag{14}$$

$$\Psi_{q=0,J=4}^{F_1} = \sqrt{\tfrac{1}{2}}[|q=0, 1) - |q=0, -1)].$$

The 3×3 matrix $\mathfrak{H}^{q=0}$ has three eigenvalues E_{A_1}, E_E and E_{F_1}, and at any value of the parameter Θ the corresponding eigenfunctions $C_{\Gamma}^{q=0} = \Psi_{q=0,J=4}^{\Gamma}$, $\Gamma = A_1$, E, F_1. If $\Theta = \Theta_{q=0}$, then the matrix $\mathfrak{H}^{q=0}$ appears to be diagonal, and the functions

$$|q = 0, \pm 1) = \sqrt{\tfrac{5}{24}} \Psi_{q=0,J=4}^{A_1} + \sqrt{\tfrac{7}{24}} \Psi_{q=0,J=4}^{E} \pm \sqrt{\tfrac{1}{2}} \Psi_{q=0,J=4}^{F_1}$$

$$|q = 0, 0) = \sqrt{\tfrac{7}{12}} \Psi_{q=0,J=4}^{A_1} - \sqrt{\tfrac{5}{12}} \Psi_{q=0,J=4}^{E} \tag{15}$$

are the eigenfunctions of the Hamiltonian (5), too. This is possible if only $E_{A_1} = E_E = E_{F_1}$. Thus, if $\Theta = \Theta_{q=0}^1$, then a triple point of the type $A_1 + E + F_1$ is present in the spectrum. Note that all the functions (15) correspond to the same energy.

It is seen that the occurrence of double and triple points in the spectrum at special values of the parameter $\Theta = \Theta_q^i$ is a direct consequence of two factors: (i) one of the submatrices $\mathfrak{H}^q$ is block-diagonal (in our example, diagonal) if $\Theta = \Theta_q^i$; (ii) the extreme basis function $|qn_{\max})$ is a linear combination of all cubic harmonics Ψ_{qJ}^{Γ},

$$|qn_{\max}) = \sum_{\Gamma} \alpha_{\Gamma} \Psi_{qJ}^{\Gamma} \tag{16}$$

where the summation is assumed over all Γ compatible with a given value of q. In our example, (16) has been verified using the explicit expressions for the cubic harmonics Ψ_{qJ}^{Γ} (13) and (14), which hold for any value of the parameter Θ. In the general case, the analogous expressions will be verified using the properties of eigenvalues and eigenvectors of the matrices $\mathfrak{H}^q$ at different values of the parameter Θ and lemmas 1 and 2. From (16) it follows that, for any Γ compatible with a given value of q, the functions $P^{\Gamma}|qn_{\max})$ are non-vanishing and proportional to the respective cubic harmonics Ψ_{qJ}^{Γ}. Thus, our study of the double and triple points is in close correspondence with the construction of the cubic harmonics of the type $P^{\Gamma}|qn)$.

4. Double points of the type $F_1 + F_2$

In this section we discuss the spectrum of the matrix $\mathfrak{H}^q$ at special points $\Theta = \Theta_q^i$ for the case of odd q.

First of all we shall show that (16) holds for any $J \geq 3$, when $\nu_{F_1} \geq 1$ and $\nu_{F_2} \geq 1$. The matrix $\mathfrak{H}^q$ yields ν_{F_1} eigenfunctions $C_{F_1\lambda}^q$ belonging to the irrep D^{F_1} and ν_{F_2} eigenfunctions $C_{F_2\lambda}^q$ belonging to the irrep D^{F_2}. If Θ is not equal to any solution Θ^i of (10), then by virtue of (9), the extreme basis function $|qn_{\max})$ is a linear combination

of all eigenfunctions $\mathbb{C}^q_{F_1\lambda}$ and $\mathbb{C}^q_{F_2\lambda}$. Thus, $|qn_{max}\rangle$ is a superposition of functions $\Phi^1_{F_1}$ and $\Phi^1_{F_2}$ belonging to the irreps D^{F_1} and D^{F_2}, respectively: $|qn_{max}\rangle = \Phi^1_{F_1} + \Phi^1_{F_2}$, where $\Phi^1_{F_1} = P^{F_1}|qn_{max}\rangle \neq 0$ and $\Phi^1_{F_2} = P^{F_2}|qn_{max}\rangle \neq 0$. This result surely holds for any value of Θ.

Now let $\Theta = \Theta^i_q$ and $i = 1$. In this case the submatrix $H^{(1)}$ is a 1×1 matrix. The function $|q, n_{max}\rangle$ is a single eigenfunction of this matrix and, hence, of the Hamiltonian $h(\Theta^1_q)$. The respective eigenvalue will be denoted as $E^{(1)}_1$. In complete analogy to the example in section 3, we conclude that a double point of the type $F_1 + F_2$ occurs in the spectrum at energy $E = E^{(1)}_1$ for $\Theta = \Theta^1_q$.

The submatrix $H^{(2)}$ has $N^{(2)} = \nu_{F_1} + \nu_{F_2} - 1$ non-degenerate eigenvalues $E^{(2)}_\lambda$. The eigenvalue $E^{(1)}_1$ of the matrix $\mathfrak{H}^q$ is doubly degenerate, so among eigenvalues $E^{(2)}_\lambda$ of the submatrix $H^{(2)}$ there is the one equal to $E^{(1)}_1$: $E^{(2)}_1 = E^{(1)}_1$. The respective eigenfunction $\mathbb{C}^{q(2)}_1$ is a linear combination of the functions $\Phi^1_{F_1}$ and $\Phi^1_{F_2}$ (note that the projectors P^Γ commutate with the Hamiltonian $h(\Theta)$, which is invariant with respect to transformations of the group O, so the functions $\Phi^1_{F_1} = P^{F_1}|qn_{max}\rangle$ and $\Phi^1_{F_2} = P^{F_2}|qn_{max}\rangle$ are also eigenfunctions of the Hamiltonian (5) corresponding to the same eigenenergy $E^{(1)}_1$). From the orthogonality of $\mathbb{C}^{q(2)}_1$ to $|qn_{max}\rangle$ it follows that $\mathbb{C}^{q(2)}_1 = \langle \Phi^1_{F_1}|\Phi^1_{F_1}\rangle \Phi^1_{F_2} - \langle \Phi^1_{F_2}|\Phi^1_{F_2}\rangle \Phi^1_{F_1}$.

All the remaining $\nu_{F_1} - 1$ eigenfunctions $\mathbb{C}^{q(2)}_{F_1\lambda}$ and $\nu_{F_2} - 1$ eigenfunctions $\mathbb{C}^{q(2)}_{F_2\lambda}$ of the submatrix $H^{(2)}$ pertain to the symmetries F_1 and F_2, respectively. Since $|q, n_{max} - 1\rangle$ is the extreme basis function for the submatrix $H^{(2)}$, then, according to (9), it contains in its expansion

$$|q, n_{max} - 1\rangle = b\mathbb{C}^{q(2)}_1 + \sum_{\lambda=2}^{\nu_{F_1}} b^1_\lambda \mathbb{C}^{q(2)}_{F_1\lambda} + \sum_{\lambda=2}^{\nu_{F_2}} b^2_\lambda \mathbb{C}^{q(2)}_{F_2\lambda} \qquad (17)$$

all eigenfunctions $\mathbb{C}^{q(2)}_1$, $\mathbb{C}^{q(2)}_{F_1\lambda}$ and $\mathbb{C}^{q(2)}_{F_2\lambda}$ of the submatrix $H^{(2)}$ with non-zero factors b, b^1_λ and b^2_λ. The eigenfunctions $\mathbb{C}^{q(2)}_{F_1\lambda}$, $\lambda = 2, 3, \ldots, \nu_{F_1}$ and $\Phi^1_{F_1}$ are, obviously, linearly independent. Therefore, if $\nu_{F_1} \geq 2$, the projected function

$$P^{F_1}|q, n_{max} - 1\rangle = -b\langle \Phi^1_{F_2}|\Phi^1_{F_2}\rangle \Phi^1_{F_1} + \sum_{\lambda=2}^{\nu_{F_1}} b^1_\lambda \mathbb{C}^{q(2)}_{F_1\lambda}$$

is non-vanishing and linearly independent with $P^{F_1}|qn_{max}\rangle = \Phi^1_{F_1}$. Similarly, if $\nu_{F_2} \geq 2$, then the function $P^{F_2}|q, n_{max} - 1\rangle \neq 0$ and is linearly independent with $P^{F_2}|qn_{max}\rangle$.

Now let $\Theta = \Theta^{i=2}_q$. The 2×2 matrix $H^{(1)}$ has two non-degenerate eigenvalues, $E^{(1)}_1$ and $E^{(1)}_2$, and two linearly independent non-vanishing eigenfunctions, $\mathbb{C}^{(1)}_1$, and two linearly independent non-vanishing eigenfunctions, $\mathbb{C}^{q(1)}_1 = C^1_{n_{max}}|qn_{max}\rangle + C^1_{n_{max}-1}|q, n_{max} - 1\rangle \neq 0$ and $\mathbb{C}^{q(1)}_2 = C^2_{n_{max}}|qn_{max}\rangle + C^2_{n_{max}-1}|q, n_{max} - 1\rangle \neq 0$. Therefore, owing to the linear independence of the functions $P^\Gamma|qn_{max}\rangle$ and $P^\Gamma|q, n_{max} - 1\rangle$, the functions $P^\Gamma\mathbb{C}^{q(1)}_1$ and $P^\Gamma\mathbb{C}^{q(1)}_2$ are non-vanishing: $P^\Gamma\mathbb{C}^{q(1)}_{1,2} \neq 0$, $\Gamma = F_1, F_2$. It is clear that the functions $P^{F_1}\mathbb{C}^{q(1)}_1$ and $P^{F_2}\mathbb{C}^{q(1)}_1$ are eigenfunctions of the Hamiltonian (5) corresponding to the same eigenergy $E^{(1)}_1$. Similarly, $P^{F_1}\mathbb{C}^{q(1)}_2$ and $P^{F_2}\mathbb{C}^{q(1)}_2$ are eigenfunctions of the Hamiltonian (5) corresponding to the doubly degenerate eigenvalue $E^{(1)}_2$. So, for $\Theta = \Theta^{i=2}_q$ in the spectra of the Hamiltonian (5) there are two double points of the type $F_1 + F_2$ with energies $E^{(1)}_1$ and $E^{(1)}_2$.

Obviously, the functions $P^\Gamma\mathbb{C}^{(1)}_1$ and $P^\Gamma\mathbb{C}^{(1)}_2$ are linearly independent and, moreover, are mutually orthogonal because they correspond to different eigenvalues $E^{(1)}_1$ and $E^{(1)}_2$ of the Hamiltonian $h(\Theta^{i=2}_q)$.

The submatrix $H^{(2)}$ has $N^q - 2$ non-degenerate eigenvalues. Among them there are two eigenvalues, $E^{(2)}_1$ and $E^{(2)}_2$, degenerate with the eigenvalues $E^{(1)}_1$ and $E^{(1)}_2$ of the

submatrix $H^{(1)}$: $E_1^{(2)} = E_1^{(1)}$, $E_2^{(2)} = E_2^{(1)}$. The respective eigenfunctions are linear combinations of the functions belonging to the irreps D^{F_1} and D^{F_2}. In addition, the submatrix $H^{(2)}$ has $\nu_{F_1} - 2$ eigenvalues $E_{F_1\lambda}^{(2)}$ corresponding to the eigenfunctions $\mathbb{C}q_{F_1\lambda}^{(2)}$ belonging to the irrep D^{F_1}, and $\nu_{F_2} - 2$ eigenvalues $E_{F_2\lambda}^{(2)}$ corresponding to the eigenfunctions $\mathbb{C}q_{F_2\lambda}^{(2)}$ belonging to the irrep D^{F_2}. The eigenfunctions $\mathbb{C}q_{F_1\lambda}^{(2)}$ and $\mathbb{C}q_{F_2\lambda}^{(2)}$ are linearly independent with the functions $P^\Gamma|qn_{max})$ and $P^\Gamma|q, n_{max} - 1)$, $\Gamma = F_1, F_2$. So, using reasoning similar to the above, we conclude that if $\nu_{F_1} \geq 3$, then the function $P^{F_1}|q, n_{max} - 2)$ is non-vanishing and linearly independent with the functions $P^{F_1}|qn_{max})$ and $P^{F_1}|q, n_{max} - 1)$. Similarly, if $\nu_{F_2} \geq 3$, then the function $P^{F_2}|q, n_{max} - 2)$ is non-vanishing and linearly independent with the functions $P^{F_2}|qn_{max})$ and $P^{F_2}|q, n_{max} - 1)$.

Now, we may put $\Theta = \Theta_q^3$, $\Theta_q^4, \ldots$, and repeat the above reasoning almost word for word. As a result, the following conclusions may be drawn.

Conclusion (1a). ν_Γ functions

$$P^\Gamma|J, 4n_{max} + q\rangle, P^\Gamma|J, 4(n_{max} - 1) + q\rangle, \ldots, P^\Gamma|J, 4(n_{max} - \nu_\Gamma + 1) + q\rangle$$

(where $\Gamma = F_1$, F_2 and $q = 1, 3$) are non-vanishing and linearly independent, i.e. they form the basis of the functions belonging to the irrep D^Γ of the group O in the subspace spanned by the functions $|qn)$ with $q = 1, 3$.

Conclusion (2a). If the parameter Θ of the Hamiltonian (5) takes on the values $\Theta = \Theta_q^i$, where Θ_q^i are the roots of (10) for $K_i = 4(n_{max} - i + 1) + q$, $i = 1, 2, \ldots, \nu_{min}$ and $\nu_{min} = \min\{\nu_{F_1}, \nu_{F_2}\}$, $q = 1, 3$, then i double points of the type $F_1 + F_2$ occur in the spectrum of the Hamiltonian (5).

Note that $\nu_{F_1} + \nu_{F_2} = N^{q=1} = N^{q=3}$ and $|\nu_{F_1} - \nu_{F_2}| \leq 1$. So, if $\Theta = \Theta_q^i$ and $i > \nu_{min}$, then the dimension $N^{(2)}$ of the submatrix $H^{(2)}$ is smaller than the dimension $N^{(1)}$ of the submatrix $H^{(1)}$, and we may repeat the entire chain of rezsoning, starting from the extreme basis function $|JK_{min}^q\rangle = |qn_{min})$.

As a result, we obtain:

Conclusion (1b). ν_Γ functions

$$P^\Gamma|J, 4n_{min} + q\rangle, P^\Gamma|J, 4(n_{min} + 1) + q\rangle, \ldots, P^\Gamma|J, 4(n_{min} + \nu_\Gamma - 1) + q\rangle$$

(where $\Gamma = F_1$, F_2 and $q = 1, 3$) are non-vanishing and linearly independent, i.e. they form the basis of the functions belonging to the irrep D^Γ of the group O in the subspace spanned by the functions $|qn)$ with $q = 1, 3$.

Conclusion (2b). If the parameter θ of the Hamiltonian (5) takes on the values $\Theta = \Theta_q^i$, where Θ_q^i are the roots of (10) for $K_i = 4(n_{min} + i) + q$, $i = 1, 2, \ldots, \nu_{min}$, $q = 1, 3$, then i double points of the type $F_1 + F_2$ occur in the spectrum of the Hamiltonian (5).

5. Triple points of the type of $A_1 + E + F_1$ and $A_2 + E + F_2$

Examined below will be the spectrum of the submatrix $\mathfrak{H}^q$ at special points $\Theta = \Theta_q^i$ in the case of even q. This case may be treated by the method presented in section 4. Nevertheless, some complications arise from the more complex structure of the matrix $\mathfrak{H}^q$ in the case of even q.

It should be remembered that the matrix $\mathfrak{H}^q$ for $\Theta = \Theta_q^i$ is broken down into three tridiagonal submatrices: $\mathfrak{H}^q = H^{(1)} \oplus H^{(2)} \oplus H^{(3)}$. The $i \times i$ submatrices $H^{(1)}$ and $H^{(3)}$, being identical, yield identical spectra of eigenvalues $E_\lambda^{(1)}$ and $E_\lambda^{(3)}$, respectively. At a special point $\Theta = \Theta_q^i$ we thus have i crossings of, at a minimum, two terms (double points). Also, some of the eigenvalues $E_\lambda^{(2)}$ of the submatrix $H^{(2)}$ may equal the eigenvalues $E_\lambda^{(1)}$ and $E_\lambda^{(3)}$ of the submatrices $H^{(1)}$ and $H^{(3)}$. In this case, at the point $\Theta = \Theta_q^i$ we deal with the simultaneous crossing of three terms, so some (or all) of the double points turn into triple points. At the same time, if in the spectrum of the submatrix $H^{(1)}$ there are n_Γ terms $E_{\Gamma\lambda}^{q(1)}$ pertaining to symmetry Γ, then the remaining $\nu_\Gamma - n_\Gamma$ terms $E_{\Gamma\lambda}^{q(2)}$ pertaining to this symmetry being non-degenerate with the terms $E_{\Gamma\lambda}^{q(1)}$ should be sought in the spectrum of the submatrix $H^{(2)}$.

Bearing this in mind we may repeat almost word-for-word the reasoning of the previous section concerning the construction of the set of cubic harmonics. The result is the following.

Conclusion (1c). ν_Γ functions

$$P^\Gamma|J, 4n_{max} + q\rangle, P^\Gamma|J, 4(n_{max} - 1) + q\rangle, \ldots, P^\Gamma|J, 4(n_{max} - \nu_\Gamma + 1) + q\rangle$$

(where $q = 0, 2$ and $\Gamma = A_1, E, F_1$ for $q = 0$ and $\Gamma = A_2, E, F_2$ for $q = 2$) are non-vanishing and linearly independent, i.e. they form the basis of the functions belonging to the irrep D^Γ of the group O in the subspace spanned by the functions $|qn\rangle$ with $q = 0, 2$.

Conclusion (1d). ν_Γ functions

$$P^\Gamma|J, 4n_{min} + q\rangle, P^\Gamma|J, 4(n_{min} + 1) + q\rangle, \ldots, P^\Gamma|J, 4(n_{min} + \nu_\Gamma - 1) + q\rangle$$

(where $q = 0, 2$ and $\Gamma = A_1, E, F_1$ for $q = 0$ and $\Gamma = A_2, E, F_2$ for $q = 2$) are non-vanishing and linearly independent, i.e. they form the basis of the functions belonging to the irrep D^Γ of the group O in the subspace spanned by the functions $|qn\rangle$ with $q = 0, 2$.

Studying the spectrum of the matrix $\mathfrak{H}^q$ we deal only with the terms pertaining to symmetries F_1, E or A_1 in the case of $q = 0$ and with the terms pertaining to symmetries F_2, E or A_2 in the case of $q = 2$. These cases will be treated together below, using the short notation D^F and D^A for the irreps D^{F_1} and D^{A_1} in the case of $q = 0$ and for the irreps D^{F_2} and D^{A_2} in the case of $q = 2$. We shall discuss only the spectra with $J > 3$, when $\nu_A \le \nu_E \le \nu_F$.

The structure of the spectrum of the matrix $\mathfrak{H}^q$ at special points $\Theta = \Theta_q^i$ depends on the value of $i = N^{(1)}$, i.e. on the dimension of the submatrix $H^{(1)}$. We shall treat the values $i \le N^q/2 = (\nu_F + \nu_E + \nu_A)/2$, which correspond to the values $K_i \ge 2$ in (10). The values $i > N^q/2$ do not need special treatment because by virtue of symmetry properties (11) and (12) in the case of even q the spectra of the operator $h(\Theta_q^i)$ for $i = j$ and for $i = N^q - j$ are identical.

Let $i \le \nu_A$. In this case the submatrix $H^{(1)}$ yields i linearly independent eigenfunctions $\mathbb{C}_\lambda^{q(1)}$, $\lambda = 1, 2, \ldots, i$ and i eigenvalues $E_\lambda^{(1)}$. As in the previous section, we obtain that the functions $P^A \mathbb{C}_\lambda^{q(1)}$, $P^E \mathbb{C}_\lambda^{q(1)}$ and $P^F \mathbb{C}_\lambda^{q(1)}$ are non-vanishing and linearly independent. Since the operators P^Γ commute with the Hamiltonian, then each of the functions $P^\Gamma \mathbb{C}_\lambda^{q(1)}$, $\Gamma = A, E, F$ is the eigenfunction of the Hamiltonian $h(\Theta_q^i)$ corresponding to the eigenvalue $E_\lambda^{(1)}$. Thus, *each of the eigenvalues $E_\lambda^{(1)}$ of the submatrix $H^{(1)}$ turns out to be a crossing of three terms with symmetries A, E and F*, so that the

total multiplicity of degeneracy in the triple points $A+E+F$ is $1+2+3=6$. So, if the parameter θ of the Hamiltonian (5) takes on the values $\Theta = \Theta_q^i$, where Θ_q^i are the roots of (10) for $K_i = 4(n_{max}-i+1)+q$, $i = 1, 2, \ldots, \nu_A$, $q = 0, 2$, then i triple points of the type $A+E+F$ occur in the spectrum of the Hamiltonian (5).

Let $\nu_A < i \le \nu_E$. A slight modification of the above reasoning brings us to the result that, in this case, each of i eigenvalues $E_\lambda^{(1)}$, $\lambda = 1, 2, \ldots, i$, of the submatrix $H^{(1)}$ appears to be a crossing of terms of the type E and F, while only ν_A of these eigenvalues are actually triple points of the type $A+E+F$. So, if the parameter θ of the Hamiltonian (5) takes on the values $\Theta = \Theta_q^i$, where Θ_q^i are the roots of (10) for $K_i = 4(n_{max}-i+1)+q$, $i = \nu_A+1, \nu_A+2, \ldots, \nu_E$, $q = 0, 2$, then the spectrum of the Hamiltonian (5) comprises ν_A triple points of the type $A+E+F$, and $i-\nu_A$ double points of the type $E+F$.

Let $\nu_E > i$. The submatrix $H^{(1)}$ is an $N^{(1)} \times N^{(1)}$ matrix with $i = N^{(1)}$. We have $N^{(1)} \le N^q/2 = (\nu_F + \nu_E + \nu_A)/2$, while $\nu_F \ge \nu_E + \nu_A$. So, $N^{(1)} \le \nu_F$, and we are actually studying the case $\nu_E < i \le \nu_F$. Thus, if $E_\lambda^{(1)}$, $\lambda = 1, 2, \ldots, i$, are eigenvalues of the submatrix $H^{(1)}$, then each of the terms with energies $E = E_\lambda^{(1)}$, $\lambda = 1, 2, \ldots, i$, contains a component with symmetry F, but only ν_A (ν_E) of these terms contain a component with symmetry A (E). It should be remembered that each of the terms with energies $E = E_\lambda^{(1)}$, $\lambda = 1, 2, \ldots, i$ is at least two-fold degenerate due to the equivalence of the spectra of the submatrices $H^{(1)}$ and $H^{(3)}$, i.e. each of the terms is at least a double point.

Now examine the spectrum of the eigenvalues $E_\lambda^{(2)}$, $\lambda = 1, 2, \ldots, N^{(2)}$, of the $N^{(2)} \times N^{(2)}$ submatrix $H^{(2)}$. Remember that $N^{(2)} = \nu_F + \nu_E + \nu_A - 2i$. From the explicit form of the operators P^{F_1} and P^{F_2} (see (8)), it is seen that the functions $P^F|qn)$, $n \in [-n_i+1-q/2, n_i-1]$ are orthogonal to the functions $P^F|q, n)$, $n \in [n_i, n_{max}]$. Hence, among the terms with energies $E = E_\lambda^{(2)}$, $\lambda = 1, 2, \ldots, N^{(2)}$ there are only $\nu_F - i$ terms $E_{F\lambda}^{(2)}$ with symmetry F; all the terms $E_{F\lambda}^{(2)}$ do not degenerate with the eigenvalues $E_\lambda^{(1)}$ of the submatrices $H^{(1)}$ and $H^{(3)}$. The remaining $N^{(2)} - \nu_F + i = \nu_E + \nu_A - i$ terms with energies $E = E_\lambda^{(2)}$ are of symmetry A or E and degenerate with the eigenvalues $E_\lambda^{(1)}$

Table 2. Double and triple points in the spectrum of the Hamiltonian (5). (*a*) The spectrum of the matrix $\mathfrak{H}^q$ at special points $\Theta = \Theta_q^i$ for $q = 1$ or $q = 3$. (*b*) The spectrum of the matrix $\mathfrak{H}^q$ at special points $\Theta = \Theta_q^i$ for $q = 0$ (terms A_1, E, and F_1) and $Q = 2$ (terms A_2, E, and F_2).

(*a*)

i	Number of double points $F_1 + F_2$	Number of non-crossing terms	
		F_1	F_2
$i \le \min(\nu_{F_1}, \nu_{F_2})$	i	$\nu_{F_1} - i$	$\nu_{F_2} - i$

(*b*)

i	Number of triple points $A+E+F$	Number of double points		Number of non-crossing terms		
		$A+F$	$E+F$	A	E	F
$i \le \nu_A$	i	—	—	$\nu_A - i$	$\nu_E - i$	$\nu_F - i$
$\nu_A - i \le \nu_A$	ν_A	—	$i - \nu_A$	—	$\nu_E - i$	$\nu_F - i$
$\nu_E < i \le \nu_F$	$\nu_E + \nu_A - i$	$i - \nu_E$	$i - \nu_A$	—	—	$\nu_F - i$

of the submatrices $H^{(1)}$ and $H^{(3)}$. Therefore, $\nu_E + \nu_A - i$ eigenvalues of each of the submatrices $H^{(1)}$, $H^{(2)}$ and $H^{(3)}$ are the same, i.e. $\nu_E + \nu_A - i$ eigenvalues of the initial matrix $\mathfrak{H}^q$ are triply degenerate. This means that the spectrum of the Hamiltonian $h(\Theta_q^i)$ comprises $\nu_E + \nu_A - i$ triple points of the only possible type $A + E + F$. Besides, $i - (\nu_E + \nu_A - i) = 2i - \nu_E - \nu_A$ terms with energies $E = E_\lambda^{(1)}$ are double points of the type of $F + A$ or $F + E$. Since $\nu_E + \nu_A - i$ terms with symmetry A are included in the triple points, the spectrum comprises $\nu_A - (\nu_E + \nu_A - i) = i - \nu_E$ double points of the type $F + A$ and $i - \nu_A$ double points of the type $F + E$.

So, if the parameter Θ of the Hamiltonian (5) takes on the values $\Theta = \Theta_q^i$, where Θ_q^i are the roots of (10) for $K_i = 4(n_{max} - i + 1) + q$, $i = \nu_E + 1, \nu_E + 2, \ldots, \nu_F$, $q = 0, 2$, then the spectrum of the Hamiltonian (5) comprises $\nu_E + \nu_A - i$ triple points of the type $A + E + F$, $i - \nu_E$ double points of the type $A + F$, and $i - \nu_A$ double points of the type $E + F$.
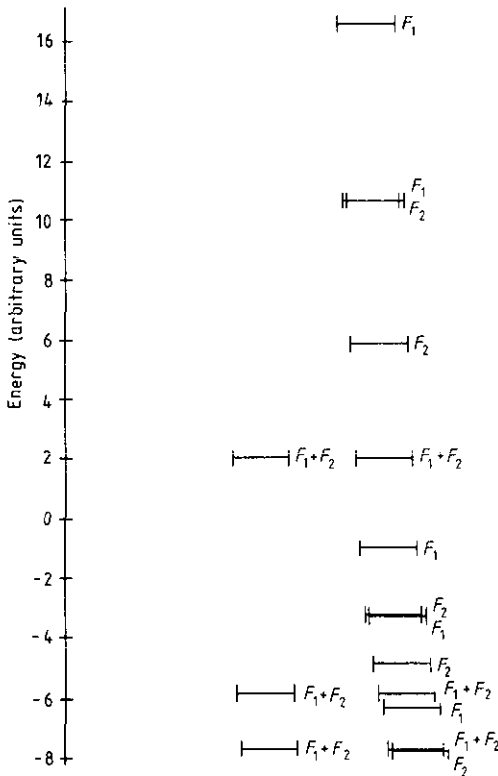

Figure 1. The spectrum of the levels of the matrix $\mathfrak{H}^q$ at $q = 1$, $J = 32$ at the special point $\Theta = \Theta_q^i$, $i = 3$, which corresponds to $K_i = 21$. To the left is the energy spectrum of the submatrix $H^{(1)}$; to the right is the energy spectrum of the submatrix $H^{(2)}$. Each of the levels is labelled with its symmetry. Since some of the levels of a given submatrix are close to each other, by virtue of the cluster structure of the spectrum, each of the levels presented is shifted slightly to the right with respect to the nearest-neighbouring high-lying level to avoid their merging.
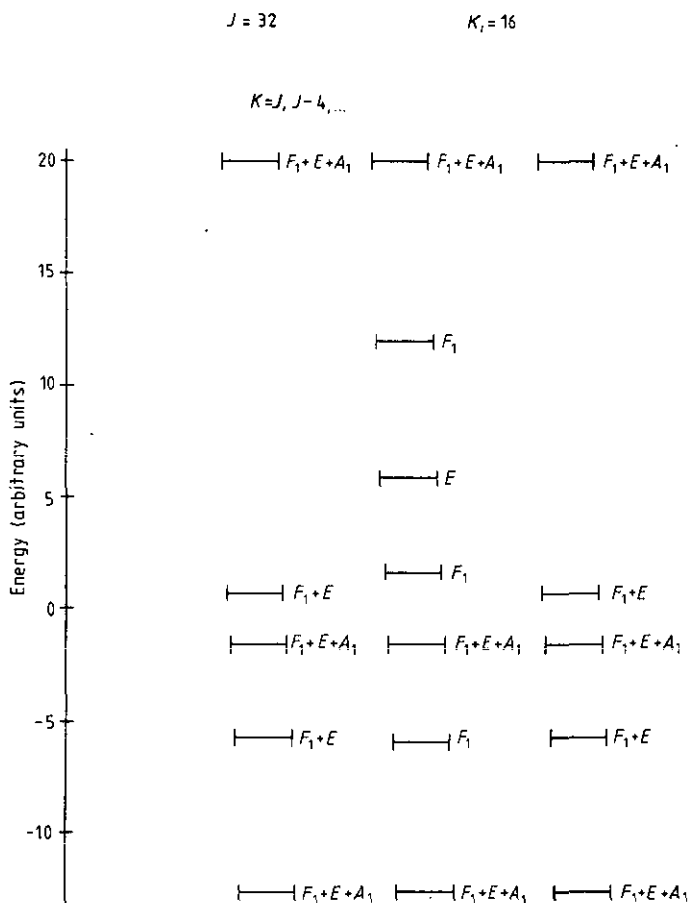
Figure 2. The spectrum of the levels of the matrix $\mathfrak{H}^q$ at $q = 0$, $J = 32$ at the special point $\Theta = \Theta_q^i$, $i = 5$, which corresponds to $K_i = 16$. To the left, middle and right are the energy spectra of the submatrices $H^{(1)}$, $H^{(2)}$ and $H^{(3)}$, respectively. The remaining designations are the same as in figure 1. At $J = 32$ we have $\nu_{A_1} = 3$, $\nu_{F_1} = 8$, $\nu_E = 6$, i.e. $\nu_{A_1} < i < \nu_E$ and the spectrum comprises three triple points of the type $A_1 + E + F_1$ and two double points of the type $E + F_1$.

Table 2 summarizes the results of our analysis of the double and triple points of the Hamiltonian (5). Note that the total multiplicity of degeneration of levels is six at the triple points $A + E + F$, six at the double points $F_1 + F_2$, five at the double points $E + F$, and four at the double points $A + F$. Figures 1 and 2 show some examples of the spectra of eigenvalues of the matrices $\mathfrak{H}^q$ at the special values of the parameter $\Theta = \Theta_q^i$.

6. Discussion

We have established that simultaneous crossings of terms occur at several different energies at the special points $\Theta = \Theta^i$ in the spectrum of the Hamiltonian (5). The degeneration of terms belonging to different irreps $D^{\Gamma_1}, D^{\Gamma_2}, \ldots, D^{\Gamma_s}$ of the symmetry group G of a quantum system is usually accounted for by the actual higher symmetry

$\mathcal{G} \supset G$ of the Hamiltonian H, so that the space of representations $D^{\Gamma_1} + D^{\Gamma_2} + \ldots + D^{\Gamma_s}$ reducible with respect to the group G proves to be irreducible with respect to the group $\mathcal{G}$.

Judd (1957) has demonstrated that a linear combination of the rank-six invariants of the cubic group may possess icosahedral symmetry Y. However, the group Y possesses irreps of dimensions one, three, three, four and five, and cannot be responsible for the six-fold degeneration of levels forming triple or double points. The Hamiltonian $h(\Theta)$ at special values of the parameter $\Theta = \Theta^i$ may have been expected to be symmetric with respect to some point group $\mathcal{G}$ in the four-dimensional space or in a space of a higher dimension, for example with respect to the symmetry group of a four-dimensional cube. However, the symmetry with respect to the multidimensional point group $\mathcal{G} \supset O$ should give rise to degeneration of not only one or several terms of the type $\tau = A_1 + E + F_1$ belonging to the irrep D^τ of the group $\mathcal{G}$, but also to a simultaneous degeneration of all the triplets of terms A_1, E and F_1 forming other levels with symmetry τ of the Hamiltonian $h(\Theta^i)$. Besides, degeneration of terms forming other irreps $D^{\tau'}$, $D^{\tau''}, \ldots$ of the group $\mathcal{G}$ should be also expected at the same value of $\Theta = \Theta^i$. Indeed, the degeneration of terms of the types $\tau' = A_2 + E + F_2$ and $\tau'' = F_1 + F_2$ are observed in the spectrum, but at other values of the parameter $\Theta = \Theta^{i'}$ and $\Theta = \Theta^{i''}$.

It should be noted that the number N of the values of the parameter $\Theta = \Theta^1$, $\Theta^2, \ldots, \Theta^N$ at which the spectrum of the operator $h(\Theta^i)$ comprises triple or double points is sufficiently large ($N \sim J$). Had the double and triple points been relevant to the existence of a multidimensional symmetry group $\mathcal{G}^i$ of the Hamiltonian $h(\Theta)$ for $\Theta = \Theta^i$, $i = 1, 2, \ldots, N$, the symmetry group $\mathcal{G}^i$ should have been replaced consecutively by groups $\mathcal{G}^{i+1}$, $\mathcal{G}^{i+2}, \ldots$ for $\Theta = \Theta^{i+1}$, $\Theta^{i+2}, \ldots$. Such a number of high-symmetry groups for the Hamiltonian $h(\Theta)$ seems unlikely. Therefore, the accidental degeneracy of the spectrum of the Hamiltonian (5) in the form of double and triple points is most probably irrelevant to increasing symmetry of the Hamiltonian.

If $J \to \infty$, then for sufficiently large values of $|K|$ we have $|\mathfrak{H}_{KK}/\mathfrak{H}_{K,K\pm4}| \to 0$ (see Harter and Patterson 1977, 1979, Zhilinskii 1979). So, in the classical limit $J \to \infty$, we may neglect non-diagonal matrix elements $\mathfrak{H}_{K,K\pm4}$ with sufficiently large values of $|K|$ in (6) and interpret the degeneration of the six-fold clusters in the limit as the formation of the double and triple points of the type $F_1 + F_2$ and $A + E + F$, respectively. In the general quantum case, the six-fold clusters are non-degenerate, but as a reflection of the classical degeneration the exact accidental degeneracy occurs at special values of the parameter $\Theta = \Theta^i$. The larger is the value of J the more often the accidental degeneracy occurs and, in the classical limit $J \to \infty$, all the values of the parameter Θ give rise to the occurrence of double and triple points.

Note, that the 'number-theoretic' accidental degeneracy discussed by Berry and Wilkinson (1984) and by Dirl and Moshinsky (1985) exhibits the same tendency in the classical limit.

In experimental studies of rotational spectra of cubic-symmetry molecules, double and triple points should manifest themselves as an anomalously low splitting of some of the six-fold clusters at the values of Θ close to one of the special points Θ^i prescribed by (10) and, also, as an anomalously low splitting between a pair or a triplet of levels forming some of the eight- or 12-fold clusters if the value of Θ^i is sufficiently large. Obviously, the parameter Θ is a constant characterizing a given particular molecule and does not depend (or depends little) on the total angular momentum J. At the same time, for sufficiently large values of J, $\langle J \| t^6 \| J \rangle / \langle J \| t^4 \| J \rangle \sim J(J+1)$, thus, from (10) we obtain $\tan \Theta^i \sim [J(J+1)]^{-1}$, i.e. the positions of the special points Θ^i are different for

different values of *J*. Therefore, the anomalously low splitting of levels due to the occurrence of double or triple points in the spectrum should be observed only at some values of *J*, rather than at any value of *J*. So, by increasing the angular momentum *J*, we may attain the situation where the value of the parameter Θ will successively approach the special points Θ^i, Θ^{i+1}, Θ^{i+2}, ..., so that the number of double and/or triple points in the spectrum will be different at each new value J_i, J_{i+1}, J_{i+2}, ... From the quasiclassical estimates (Harter and Patterson 1977, 1979, Braun *et al* 1985) it follows that the splitting of the levels in a cluster decrease smoothly with increasing of *J*. The occurrence of double and triple points in the spectrum will result in a sudden pronounced decrease of the splitting of N_1 triplets of levels F_1, A_1 and E at a certain value of $J = J_1$, of N_1 pairs of levels F_1 and F_2 at $J = J_2 > J_1$, of N_1 triplets of levels F_2, A_2 and E at $J = J_3 > J_2$, of N_1 pairs of levels F_1 and F_2 at $J_4 > J_3$, of $N_1 + 1$ triplets of levels F_1, A_1 and E at $J = J_5 > J_4$, etc.

It should be pointed out that the accidental degeneracy is the general property essential to any system pertaining to cubic symmetry, and the double and triple points should be observed not only in the rotational spectra of cubic-symmetry molecules, but in the spectra of an impurity ion in a crystal field as well. In studying the spectra of an impurity ion, half-integer values of *J* are actual, too. All the above treatment may be generalized to the case of the half-integer *J*. As the result we obtain that the double points of the type $E' + G$ or $E'' + G$ with the total six-fold degeneracy occur in the spectrum at special points $\Theta = \Theta^i$. For details see the paper of Sviridov *et al* (1991).

In parallel with studying the double and triple points in the spectrum of the cubic-symmetry Hamiltonian (5), we constructed the basis of irreps D^Γ ($\Gamma = A_1$, A_2, E, F_1, F_2) of the group O in the subspace of irrep D^J of the SO(3) group. Summarizing conclusions (1a), (1b), (1c) and (1d) we may formulate:

Theorem 1. All the functions $P^\Gamma | q, n_{max} + 1 - i)$, where $i = 1, 2, \ldots, \nu_\Gamma$, $\Gamma = A_1$, A_2, E, F_1, F_2, and *q* takes on any value compatible with a given symmetry Γ, are non-vanishing and linearly independent, i.e. they form the basis of irreps D^Γ of the group O in the space of irreps D^J of the SO(3) group.

Theorem 2. All the functions $P^\Gamma | q, n_{min} - 1 + i)$, where $i = 1, 2, \ldots, \nu_\Gamma$, $\Gamma = A_1$, A_2, E, F_1, F_2, and *q* takes on any value compatible with a given symmetry Γ, are non-vanishing and linearly independent, i.e. they form the basis of irreps D^Γ of the group O in the space of irreps D^J of the SO(3) group.

Nearly the same basis has been proposed by Cheglokov and Ulenikov (1985), but they have not proved the linear independence of the basis functions. Theorems 1 and 2 may be generalized for the case of the double cubic group O' and half-integer values of *J* (Sviridov *et al* 1991).

From the explicit form of the projection operators (8) and with relation $P^\Gamma P^\Gamma = P^\Gamma$ it is seen that the basis functions $P^\Gamma | q, n)$ with $n = n_{max}, n_{max} - 1, \ldots, n_{max} - \nu_\Gamma + 1$ ($n = n_{min}, n_{min} + 1, \ldots, n_{min} + \nu_\Gamma - 1$) and $\Gamma = F_1$ or $\Gamma = F_2$ for $q = 0$, 2 are mutually orthogonal. Nevertheless, all the other basis functions of the type $P^\Gamma | q, n)$ are not orthogonal. The most natural orthogonalization procedure seems to be the diagonalization of the operator T_4 in the given basis with a view to using its eigenfunctions as an orthogonal basis. The commutativity of the operators P^Γ and T_4 may readily be used to reduce the orthogonalization of the basis to the diagonalization of tridiagonal $\nu_\Gamma \times \nu_\Gamma$ matrices.

In conclusion, it should be noted that the methods based on the properties of eigenvalues and eigenfunctions at different values of the parameter Θ of the operator invariant with respect to a given group were probably not used earlier to construct the bases of irreps of the groups. Nevertheless, the method may prove to be useful in some problems, for example in the problem of constructing the basis for the SU(3) group in the Elliot scheme, if the operators T_4 and T_6 are replaced by the operators Ω (Bargman and Moshinsky 1961) and Ω' (Judd *et al* 1974).

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