Symmetry breaking and symmetry defects. Invariant theory applications

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“The great book of the universe stays open before our eyes; but to understand it, we have first to learn the language in which it is written, the mathematics.”

Galileo Galilei, 1623

“ La filosofia è scritta in questo grandissimo libro, che continuamente ci sta aperto innanzi agli occhi (io dico l’universo), ma non si può intendere sa prima non s’impara a intender la lingua, a conoscer i caratteri, ne quali è scritto. Egli è scritto in lingua mathematica...”

Formal initial construction

$\{q_i\}$ - set of initial variables.

G - symmetry group of the problem.

$\Gamma_{\rm in}$ - representation of G, span by variables $\{q_i\}$.

We are interested in

General polynomial expression for tensors $T^{\Gamma_{\rm fin}}$ transforming according to a given irreducible representation $\Gamma_{\rm fin}$.

Trivial example : x - variable, Z_2 reflection group $x \to -x$;

General polynomial invariant: $P(x^2)$;

General polynomial covariant: $xQ(x^2)$.

Group action on variables.

Group orbit - the set of transforms of a given point m by G.

Stabilizer - set of elements of G which leave m fixed.

Space of orbits - “orbifold“. Each orbit is represented by one point.

Type of orbits - orbits with the same conjugacy class of stabilizers are of the same type.

Stratum - union of orbits of the same type.

Critical orbits - orbits isolated in their strata.

Generating function

$$M^G(\Gamma_{\rm fin} \leftarrow \Gamma_{\rm in}; t) = \sum_{n=0}^{\infty} C_n t^n$$

G - symmetry group;

$\Gamma_{\rm in}$ - initial representation;

$\Gamma_{\rm fin}$ - final representation;

t - auxiliary variable.

gives the number C_n of linearly independent tensors of degree n and of symmetry type $\Gamma_{\rm fin}$ constructed from variables transforming according to $\Gamma_{\rm in}$.

Molien theorem for finite groups

$$M^G(\Gamma_{\rm fin} \leftarrow \Gamma_{\rm in}; t) = \frac{1}{[G]} \sum_{g \in G} \frac{\chi_g^{(\Gamma_{\rm fin})*}}{\det\left(E - t\Gamma_{\rm in}(g)\right)}$$

$[G]$ - the order of group G;

$\chi_g^{(\Gamma_{\rm fin})}$ - character of $g \in G$ in the final representation;

$\Gamma_{\rm in}(g)$ - matrix representation of $g \in G$ in the initial representation.

Practical simplifications / alternative forms

Sum over group elements can be replaced by sum over classes of conjugate elements.

$$\sum_{g\in G}(...) \;=\; \sum_{p\in G} n_p(...)$$

n_p - number of elements in the class p of conjugate elements.

Characteristic polynomial can be expressed as a product of polynomials for irreducible components or as a product of factors depending on eigenvalues of representation matrices.

$$\det\left(E - t\Gamma_{\mathrm{in}}(g)\right) = (1 - t\lambda_1)\cdots(1 - t\lambda_k).$$

Characteristic polynomial can be expressed in terms of characters only.

$$\det\left(E - t\Gamma_{\text{in}}(g)\right) = 1 - \chi_g^{(A_1)}t + \chi_g^{(A_2)}t^2 - \ldots + (-1)^k\chi_g^{(A_k)}t^k + \ldots$$

$$A_1 = \Gamma_{\text{in}};$$

$$A_2 = \{\Gamma_{\text{in}} \times \Gamma_{\text{in}}\}^{As} \equiv \Gamma_{\text{in}} \otimes [1^2];$$

$$A_3 = \{\Gamma_{\text{in}} \times \Gamma_{\text{in}} \times \Gamma_{\text{in}}\}^{As} \equiv \Gamma_{\text{in}} \otimes [1^3];$$

$$\ldots$$

Rational form of Molien function for finite groups suitable for symbolic interpretation (is not unique).

$$\frac{N(t)}{D(t)} = \frac{\sum_{i=0}^{K} m_i t^{n_i}}{(1-t^{d_1})(1-t^{d_2})\cdots(1-t^{d_s})}$$

All m_i are positive. For invariants $m_0 = 1$. For covariants $m_0 = 0$.

d_j - degrees of algebraically independent invariants. $s = [\Gamma_{\rm in}]$.

n_i - degree of linearly independent but algebraically dependent invariants/covariants.

In the case of a generating function for invariant of a group generated by reflections $N(\lambda) = 1$, and $d_1 d_2 \cdots d_s = [G]$.

Integrity basis for invariants.

There are s algebraically independent invariants of degree $d_1, d_2, \ldots, d_s$: $\theta_1, \theta_2, \ldots, \theta_s$.

There are K linearly independent invariants of degree $n_1, n_2, \ldots, n_K$: $\varphi_1, \varphi_2, \ldots, \varphi_K$.

General polynomial invariant can be written as

$$P_0\left(\theta_1, \ldots, \theta_s\right) + \sum_{i=1}^{K} \varphi_i P_i\left(\theta_1, \ldots, \theta_s\right)$$

where $P_j(t_1, \ldots, t_s)$, $j = 0, 1, \ldots, K$ are arbitrary polynomials.

The structure of module of invariants $\mathcal{P}^G$ can be expressed as

$$\mathcal{P}^G = P[\theta_1, \theta_2, \ldots, \theta_s] \bullet (1, \varphi_1, \ldots, \varphi_K)$$

Alternative (Hilbert) interpretation of generating Molien function.

All generators of the ring of invariants are used as denominator invariants.

Numerator shows the existing relations between generators (syzygies of the first kind). relations between relations (syzygies of the second kind), ...

$$\frac{1 - \sum t^{f_i} + \sum t^{g_i} - \ldots \pm \sum t^{k_i}}{\prod (1 - t^{d_i})}$$

If Integrity Basis or system of generators and relations are known, the form of generating function follows.

The direct calculation of Molien function does not generally gives generating function in the form allowing symbolic interpretation.

Some useful properties of generating functions.

$$M^G(\Gamma_1 \oplus \Gamma_2 \leftarrow \Gamma_{\rm in}; t) = M^G(\Gamma_1 \leftarrow \Gamma_{\rm in}; t) + M^G(\Gamma_2 \leftarrow \Gamma_{\rm in}; t).$$

In particular (for regular representation)

$$\sum_j [\Gamma_j] M^G(\Gamma_j \leftarrow \Gamma_{\rm in}; t) = \frac{1}{(1-t)^{[\Gamma_{\rm in}]}}$$

$$M^G(\Gamma_{\rm fin} \leftarrow \Gamma_{\rm in1} \oplus \Gamma_{\rm in2}; t) =$$

$$\sum_{\Gamma_{f_1}, \Gamma_{f_2}} n^{\Gamma_{\rm fin}}_{\Gamma_{f_1}, \Gamma_{f_2}} M^G(\Gamma_{f_1} \leftarrow \Gamma_{\rm in}; t) M^G(\Gamma_{f_2} \leftarrow \Gamma_{\rm in}; t)$$

Representation of the orbit space in terms of invariant polynomials

Invariant polynomials for O and O_h action on $\{x, y, z\}$:

$$G_{O_h}(A_{1g} \leftarrow \{x, y, z\}; t) = \frac{1}{(1-t^2)(1-t^4)(1-t^6)}$$

$$G_O(A_1 \leftarrow \{x, y, z\}; t) = \frac{1+t^9}{(1-t^2)(1-t^4)(1-t^6)}$$

$$\theta_2 = x^2 + y^2 + z^2; \quad (1)$$

$$\theta_4 = x^4 + y^4 + z^4; \quad (2)$$

$$\theta_6 = x^2 y^2 z^2; \quad (3)$$

$$\varphi_9 = xyz(x^2 - y^2)(y^2 - z^2)(z^2 - x^2). \quad (4)$$

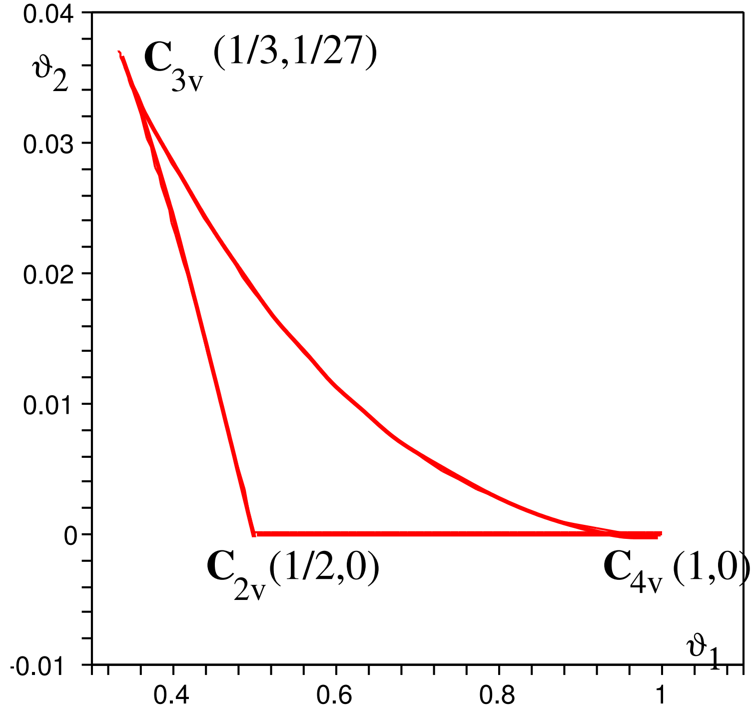
For group O the numerator invariant φ_9 is linearly independent but its square can be expressed through denominator invariants

$$(\varphi_9)^2 = \theta_6 \left(\frac{1}{2} (\theta_4)^3 - 27 (\theta_6)^2 - 9\theta_4\theta_6 - \frac{5}{4} (\theta_4)^2 + 5\theta_6 + \theta_4 - \frac{1}{4} \right)$$

This syzygy defines the boundary of the space of orbits in the invariant polynomial representation for the group O_h
(on the sphere $x^2 + y^2 + z^2 = 1$).

Orbits and strata for the action of O_h symmetry group on the classical rotational phase sphere.

Stabilizer	Number of points per orbit	Number of orbits per stratum	Comments
C_{4v}	6	1	Critical
C_{3v}	8	1	Critical
C_{2v}	12	1	Critical
C_s	24	∞	Open
C_s'	24	∞	Open
C_1	48	∞^2	Generic



Space of orbits of the O_h group action on the sphere. The boundary of the orbit space corresponds to a zero of $\varphi_9 = 0$ auxiliary invariant tensor for O group action, whose square is a polynomial of basic invariants.

Qualitative analysis of the invariant function depending on control parameters $H(a, b, ...; q_{\rm in})$.

a) To rewrite $H(a, b, ...; q_{\rm in})$ in terms of invariant polynomails

b) To check intersection of $H = const$ levels with the space of orbits and to find critical levels when the topology of intersection changes

c) To study the modification of the system of critical levels under variation of control parameters.

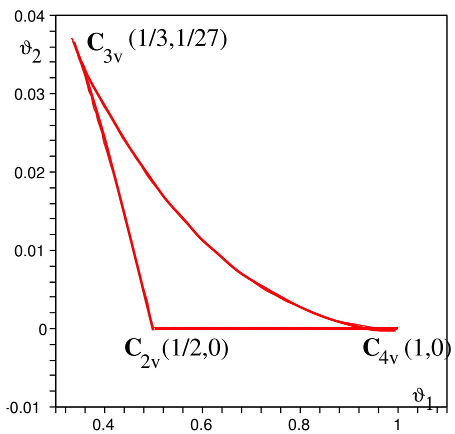
Example:

Phenomenological rotational Hamiltonian invariant under O_h written as an invariant polynomial of degree six has generically eigher

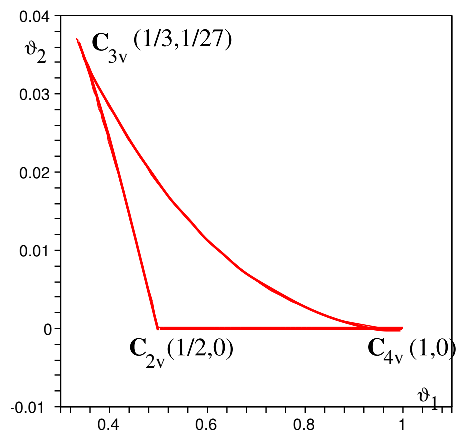
i) three orbits of stationary points: 6(8) minima, 8(6) maxima, 12 saddle points.

ii) four orbits of stationary points: 24 saddle points and three orbits (26 points) of stable stationary points.

To construct the space of orbits of O group one needs to use two charts (one for $\varphi_9 \geq 0$ and another for $\varphi_9 \leq 0$)



$\varphi_9 \leq 0$



$\varphi_9 \geq 0$

Space of orbits of the O group action on the sphere. The boundaries of two parts correspond to $\varphi_9 = 0$ and should be identified to get the whole orbit space (which is a topological sphere with three marked points).

Example: $\{x, y, z\}$ transform each under anti symmetric representation of Z_2 group.

Molien function for invariants depending on three auxiliary parameters (t_1, t_2, t_3) reads

$$\frac{1 + t_1 t_2 + t_2 t_3 + t_1 t_3}{(1 - t_1^2)(1 - t_2^2)(1 - t_3^2)}$$

It has the following meaning from the point of view of the “*Integrity basis*“ construction.

There are three quadratic algebraically independent (denominator) invariants,

$$\theta_1 = x^2, \quad \theta_2 = y^2, \quad \theta_3 = z^2,$$

and three quadratic linearly independent (numerator) invariants

$$\phi_1 = xy, \quad \phi_2 = xz, \quad \phi_3 = yz.$$

Using “denominator“ and “numerator“ invariants (forming so called integrity basis or homogeneous system of parameters) an arbitrary invariant can be written as

$$\mathcal{P}(\theta_1, \theta_2, \theta_3) + \sum_i \phi_i \mathcal{P}_i(\theta_1, \theta_2, \theta_3)$$

where $\mathcal{P}(p, q, r)$ is an arbitrary polynomial of its variables.

Numerator invariants enter only in linear fashion because their squares and products can be expressed in terms of denominator and numerator invariants. Such relations are named “syzygy“

$$(xy)^2 = x^2y^2 \Longleftrightarrow \phi_1^2 = \theta_1\theta_2$$

$$(xy)(xz) = x^2yz \Longleftrightarrow \phi_1\phi_2 = \theta_1\phi_3$$

Interpretation of Molien function in terms of generators and syzygies.

$$\frac{1+3t^2}{(1-t^2)^3} = \frac{1-6t^4+8t^6-3t^8}{(1-t^2)^6}$$

Generators: $g_1 = x^2, g_2 = y^2, g_3 = z^2, g_4 = xy, g_5 = xz, g_6 = yz$

There are

six syzygies of the first kind

$$s_a^1 = g_1g_2 - g_4^2, \quad s_b^1 = g_1g_3 - g_5^2, \quad s_c^1 = g_2g_3 - g_6^2$$

$$s_d^1 = g_4g_5 - g_1g_6, \quad s_e^1 = g_4g_6 - g_2g_5, \quad s_f^1 = g_5g_6 - g_3g_4$$

eight syzygies of the second kind

$$s_a^2 = g_5s_a^1 + g_6s_d^1 + g_1s_e^1; \quad \ldots$$

and three syzygies if the third kund

$$s_a^3 = g_6s_a^2 - g_5s_b^2 + g_2s_c^2 - g_1s_e^2 + g_4s_g^2 - g_4s_h^2, \quad \ldots$$

Explicit expressions for the coefficients of the Molien function expansion

$$g_{d_1:d_2:\dots:d_K}(t) = \frac{1}{(1-t^{d_1})(1-t^{d_2})\dots(1-t^{d_K})}. \tag{5}$$

The coefficient C_N in the formal series

$$g_{d_1:d_2:\dots:d_K}(t) = \sum_N C_N t^N, \tag{6}$$

can in its turn be represented in the form

$$C_N = a_{K-1}N^{K-1} + a_{K-1}N^{K-1} + \dots + a_0 + \text{oscillatory part}, \tag{7}$$

with a_j being the polynomials of d_i exposants

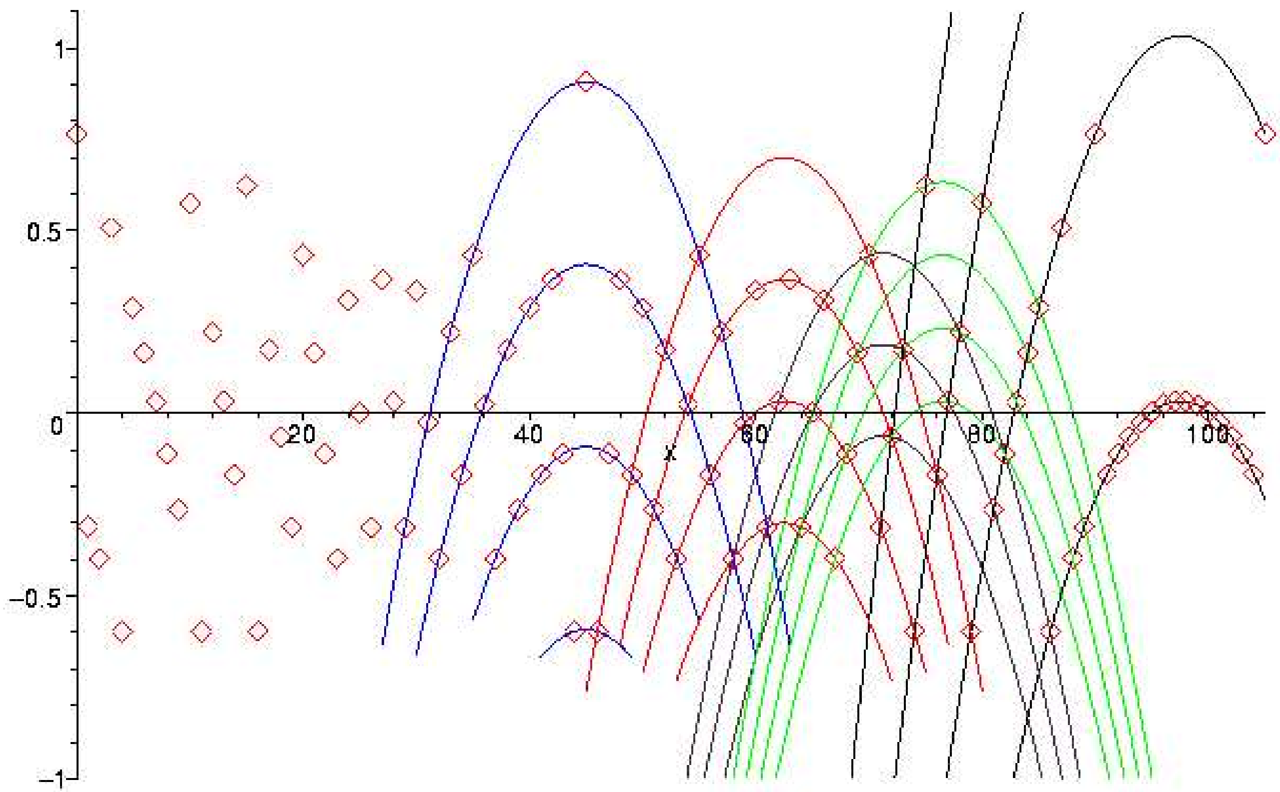
$$a_{K-1-i}(d_1, d_2, \ldots, d_K) \sim \frac{1}{(K-1-i)!} Todd_i([d_1, d_2, \ldots, d_K]). \quad (8)$$

$$a_{K-1} = \frac{1}{(K-1)! \prod d_i}; \quad a_{K-2} = \frac{\sum d_i}{2(K-2)! \prod d_i};$$

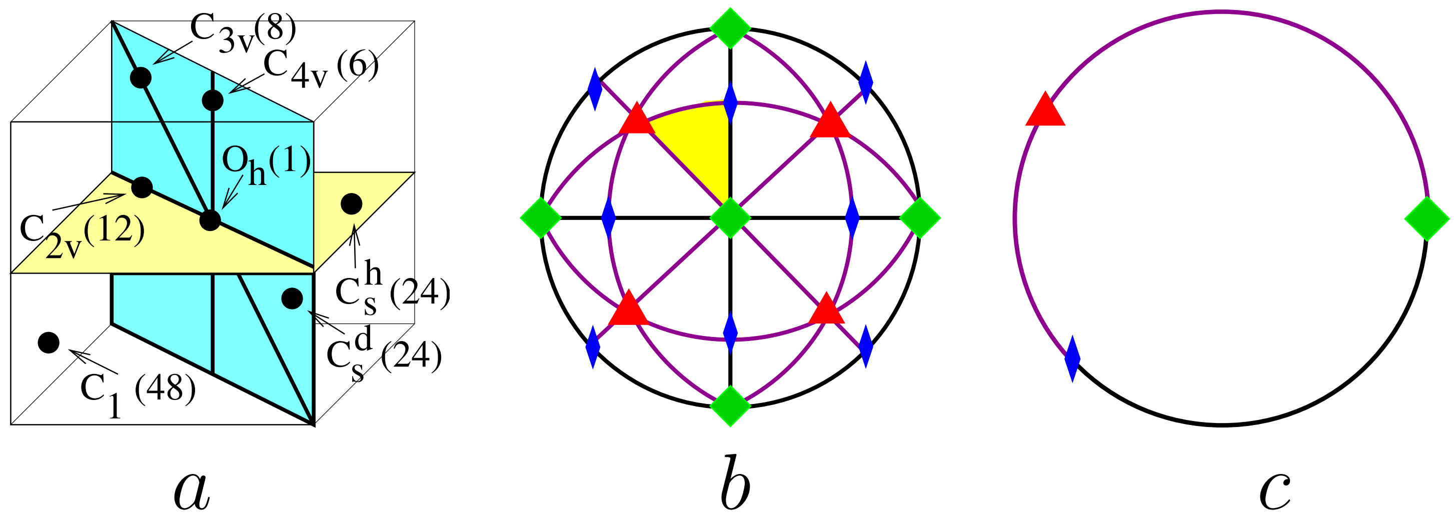
$$a_{K-3} = \frac{3\left(\sum d_i\right)^3 - \sum d_i \sum d_i^2}{48(K-4)! \prod d_i}; \qquad a_{K-4} = \frac{3\left(\sum d_i\right)^2 - \sum d_i^2}{24(K-3)! \prod d_i};$$

$$\ldots$$

The oscillatory part of the number of state function has complicated form related to the problem of counting the lattice points of rational polyhedra 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.



Oscillatory part of the $C(N)$ for $d_1 = 3, d_2 = 5, d_3 = 7$ generating function.

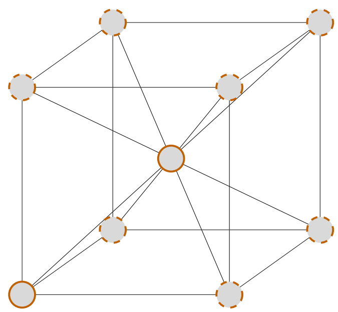


Construction of the orbifold for the 3D-point group O_h acting on two dimensional sphere.

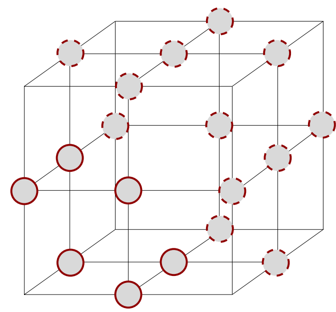
(a) - Action of the group O_h on the 3D-space.

(b) - Schematic view of the action of O_h group on two-dimensional sphere.

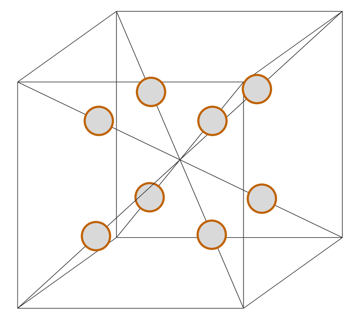
(c) - Representation of the orbifold $*432$ as a disk with three special points on its boundary.



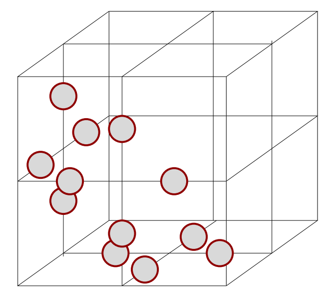
$O_h = m\bar{3}m$; a



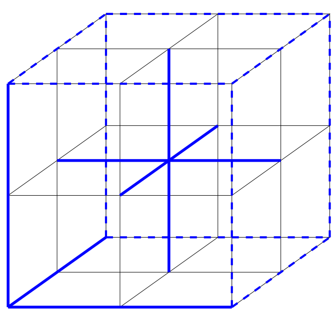
$D_{4h} = 4/mmm$; b



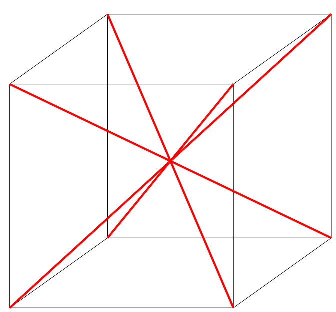
$D_{3d} = \bar{3}m$; c



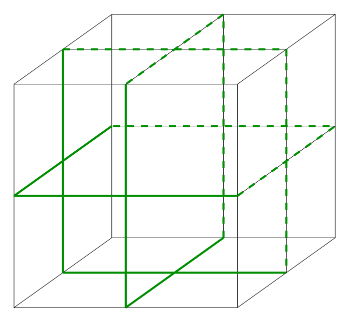
$D_{2d} = \bar{4}m2$; d



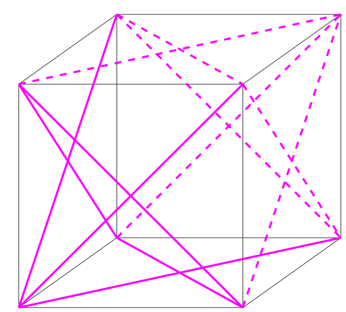
$C_{4v} = 4mm$; e



$C_{3v} = 3m$; f

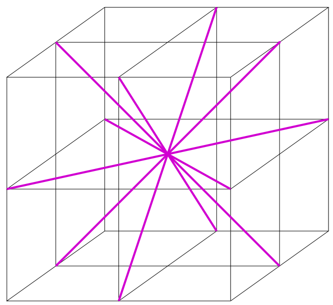


$C_{2v} = mm2$; g

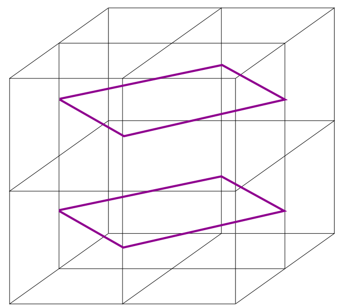


$C_{2v} = mm2$; h

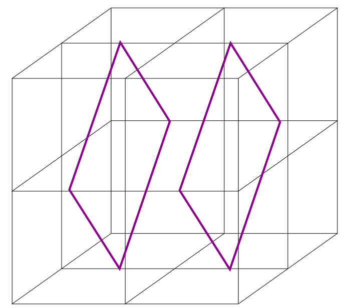
Different strata for $Im\bar{3}m$ Bravais group.



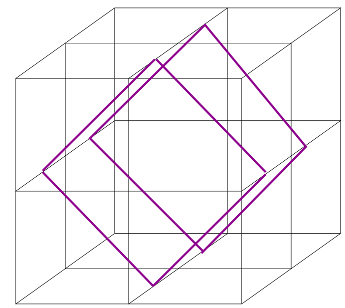
$C_{2v} = mm2; h$



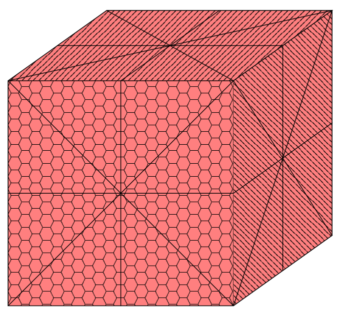
$C_2 = 2; i$



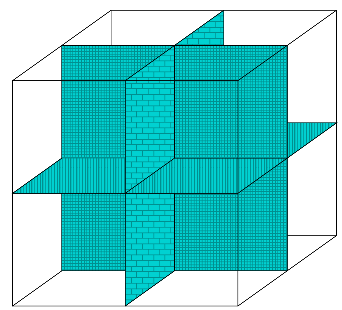
$C_2 = 2; i$



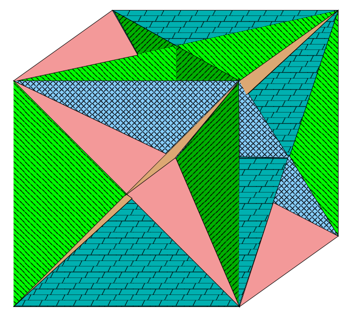
$C_2 = 2; i$



$C_s = m; j$

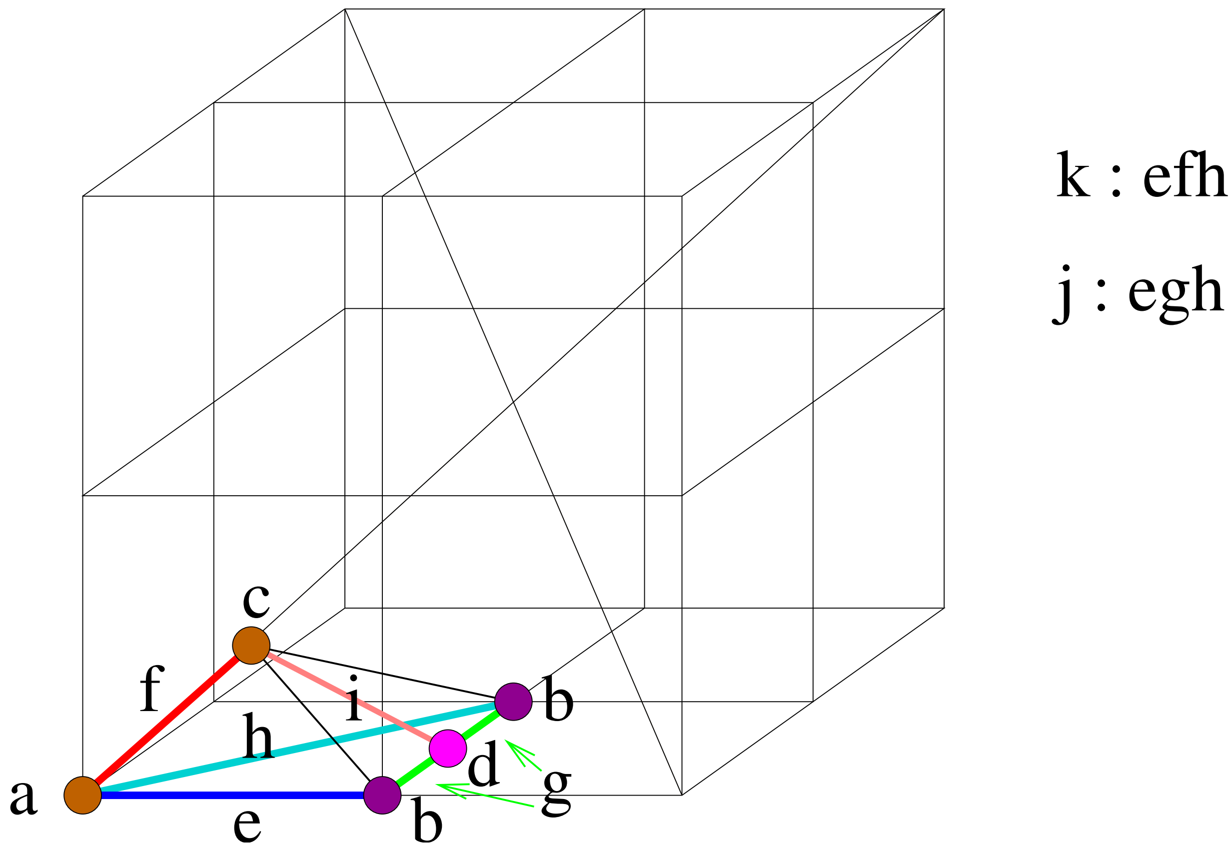


$C_s = m; j$

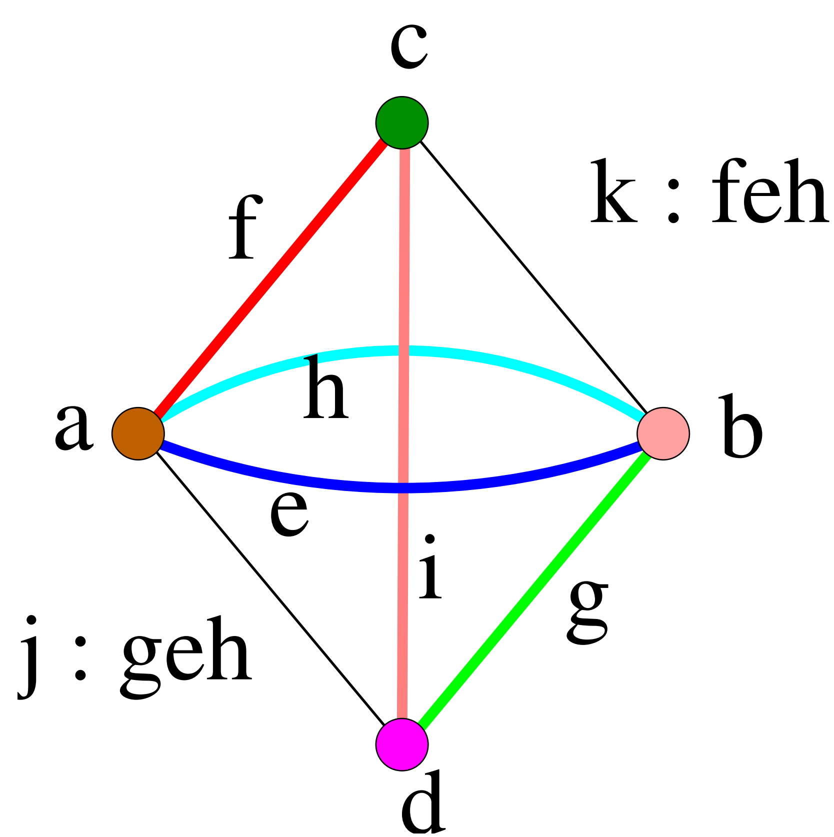


$C_s = m; k$

Different strata for $Im\bar{3}m$ Bravais group.



Double cell and orbifold for $Im\bar{3}m$ three-dimensional Bravais group.



Schematic representation of orbifold for $Im\bar{3}m$ three-dimensional Bravais group.

Extension to “band structures“.

Two types of variables “slow“ q^{Γ_s} and “fast“ Q^{Γ_f}.

Fast - discrete, quantum

Slow - continuous, classic.

Fibre bundle description. Matrix symbol over base space of classical variables.

Low coupling - isolated bands - eigenline bundles of the matrix symbol.

Each line bundle is characterized by the topological invariant - Chern number.

Symmetry of the problem imposes restrictions on the possible values of Chern numbers and on their possible modifications.

Example

Two bands of E type in the presence of O symmetry group form vector bundle of rank 2 with $c_a + c_b = 0$.

They can decompose into two eigenline bundles with

$$c_i = \pm 4 \bmod 12$$

For two A_1 bands :

$$c_i = \pm 24k,$$

for A_1 and A_2 bands :

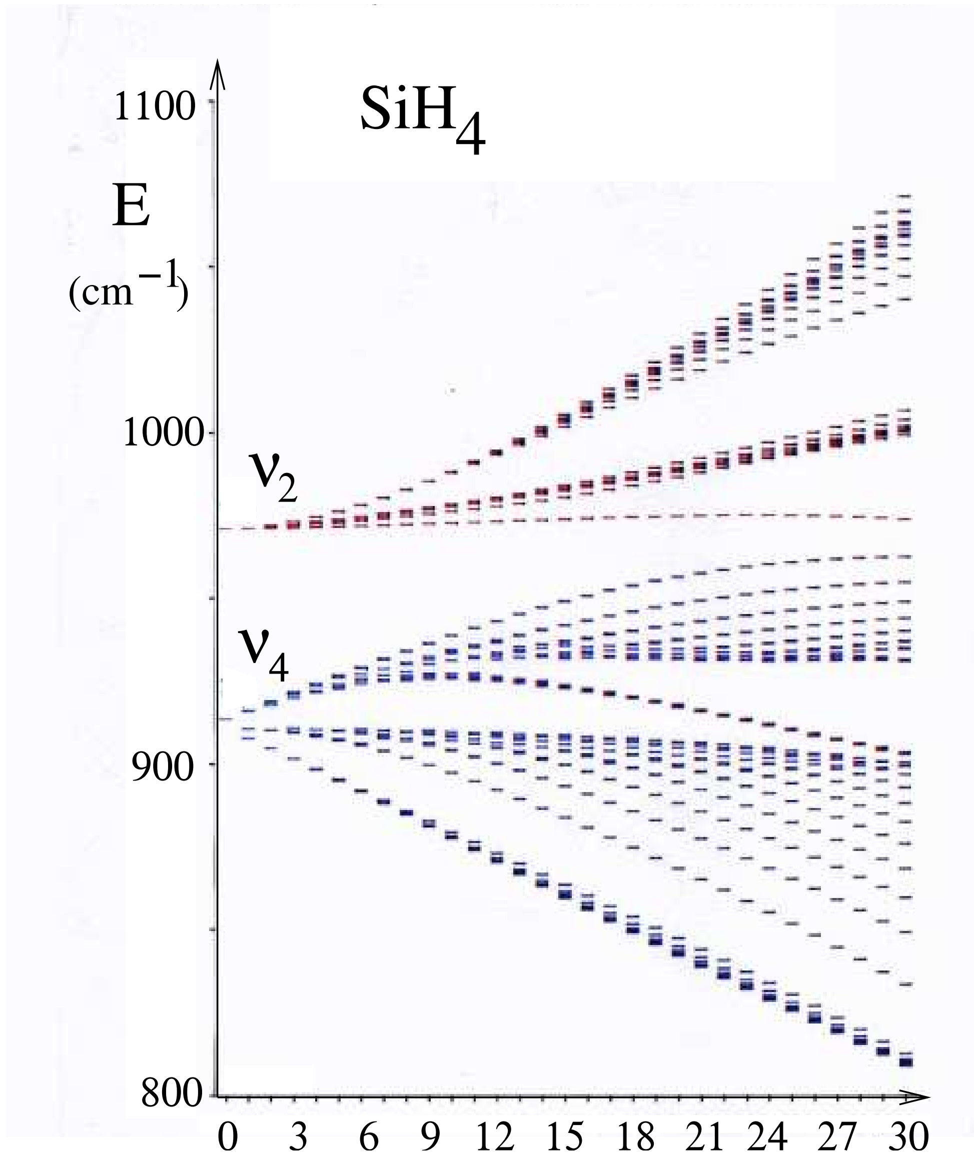
$$c_i = \pm 12k.$$

Qualitative description.

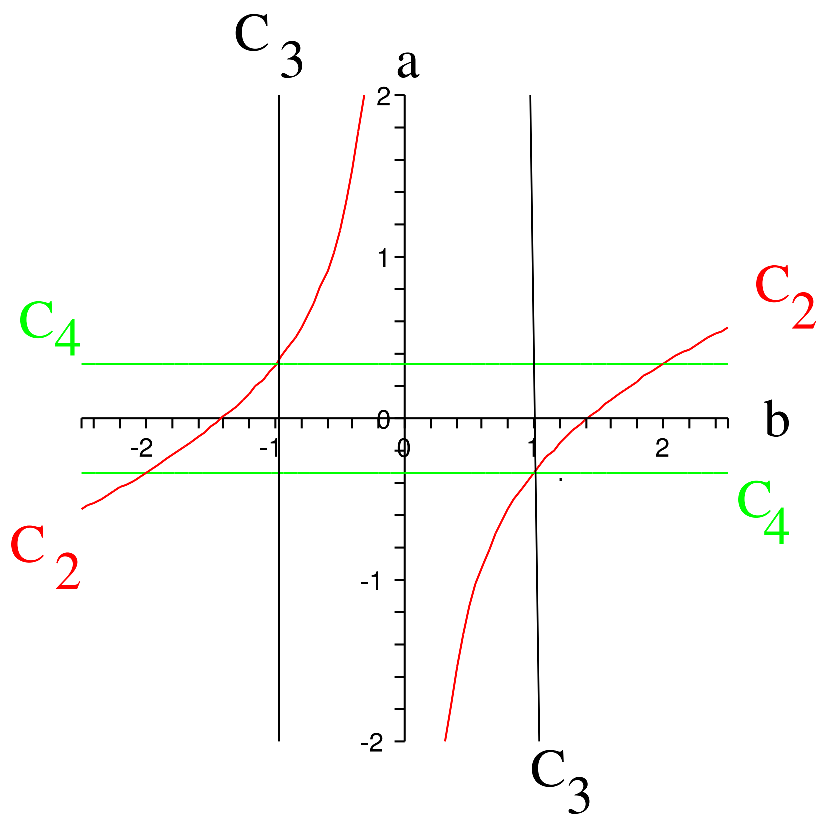
To study family of objects (or models) depending on a number of control parameters.

To find characteristics which are defined almost everywhere (i.e. for almost all values of control parameters) and are piece-wise constant on the space of control parameters.

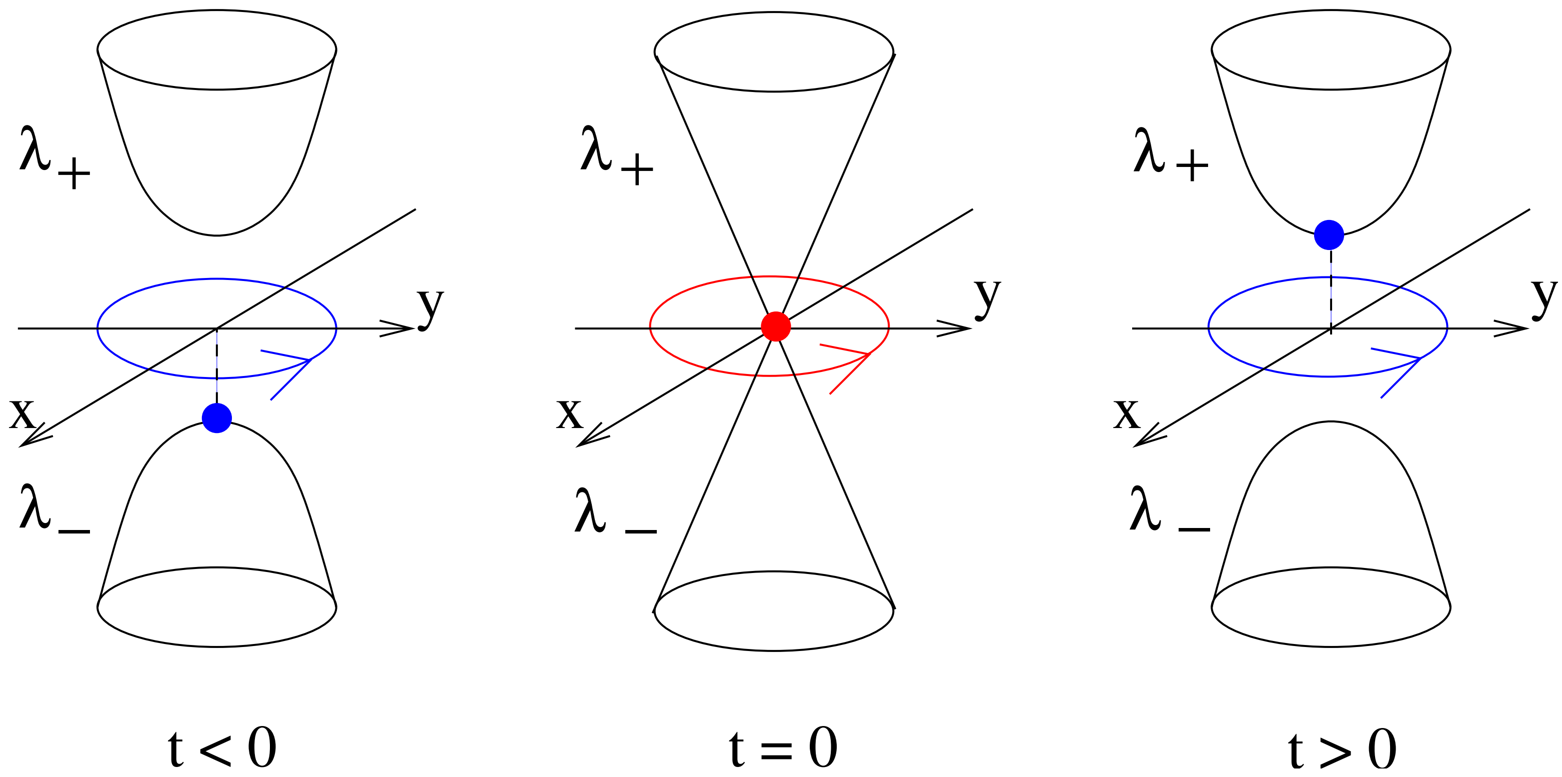
$\Rightarrow$ The qualitative description assumes the splitting of the space of control parameters into disconnected regions by a codimension one boundary and assumes equally the existence of internal boundaries of higher codimension.


SiH$_4$
E
(cm^{-1})
1100
1000
900
800
ν_2
ν_4
0 3 6 9 12 15 18 21 24 27 30

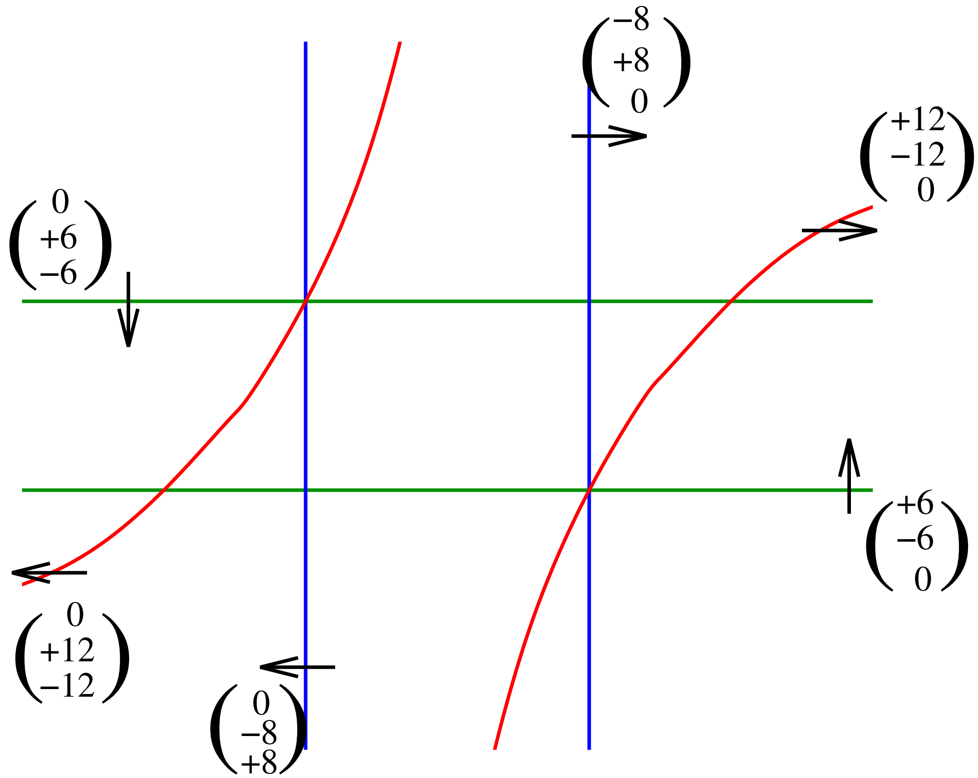
Reduced rovibrational energy for lowest vibrational bands ν_4 (F_2 symmetry type) and ν_2 (E symmetry type) of SiH_4 tetrahedral molecule (T_d point symmetry group). Two rearrangements of energy level between bands are seen on this diagram reconstructed from experimental data. Under J increase one group of energy levels goes from upper branch of ν_4 mode to the middle branch, and at approximately the same J values another group of energy levels passes from the lower branch of ν_2 mode to the upper branch of ν_4 mode.



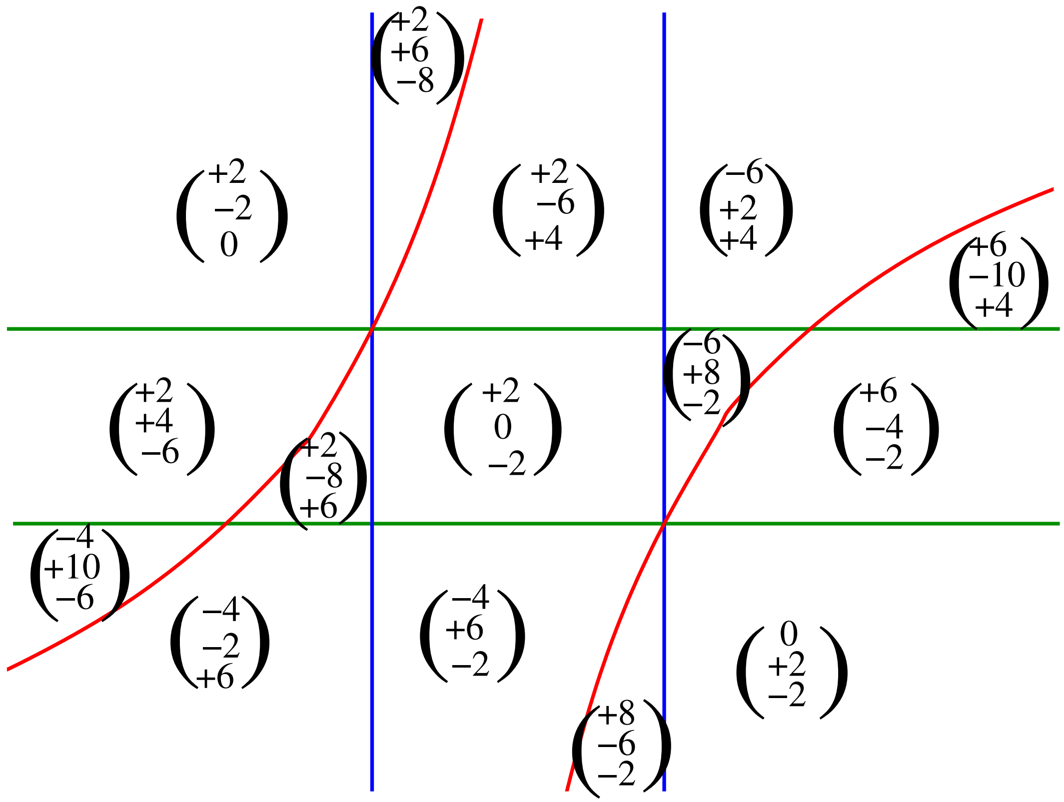
Degeneracy points (on C_2, C_3, C_4 orbits) in the space of control parameters (a, b) for the Hamiltonian for two bands forming E representation of O group.



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



Chern diagram for three state model. Each degeneracy line (the boundary of the iso-Chern domain) is associated with a three component column giving Delta Chern for each of three bands and with an arrow indicating the direction of the path in the control parameter space associated with the indicated modification of Chern numbers.



Iso-Chern diagram for three state model. Blue lines - boundaries with degeneracy points at C_4 positions. Green lines - boundaries with degeneracy points at C_3 positions. Red lines - boundaries with degeneracy points at C_2 positions. Each open iso-Chern domain is characterized by three Chern numbers associated with three bands arranged according to their energy. Upper, middle and lower numbers in each symbol give respectively Chern numbers for the band with higher, middle and lower energy.