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Analysis of Rotation–Vibration Relative Equilibria on the Example of a Tetrahedral Four Atom Molecule

K. Efstathiou†, D. A. Sadovskii†, and B. I. Zhilinskii†

Abstract. We study relative equilibria (RE) of a nonrigid molecule, which vibrates about a well-defined equilibrium configuration and rotates as a whole. Our analysis unifies the theory of rotational and vibrational RE. We rely on the detailed study of the symmetry group action on the initial and reduced phase space of our system and consider the consequences of this action for the dynamics of the system. We develop our approach on the concrete example of a four-atomic molecule \( A_4 \) with tetrahedral equilibrium configuration, a dynamical system with six vibrational degrees of freedom. Further applications and illustrations of our results can be found in [van Hecke et al., Eur. Phys. J. D At. Mol. Opt. Phys., 17 (2001), pp. 13–35].

Key words. small vibrations, vibration-rotation of molecules, spherical top, relative equilibria, 1:1:1 resonant oscillator, normalization, reduction, bifurcations, orbit space, finite group action, reversing symmetry, Molien generating function, integrity basis

AMS subject classifications. 37J15, 37J35, 37J40, 81V55, 58D19

DOI. 10.1137/030600015

1. Introduction. This paper unifies modern methods of classical theory of symmetric Hamiltonian dynamical systems and quantum theory of molecules (and other isolated finite-particle systems). Considerable progress was achieved in both directions in the last decades and deep relations between these seemingly distant theories became evident. Significant effort by mathematicians and molecular physicists to converge the two fields resulted in the qualitative theory of highly excited quantum molecular systems based on recent mathematical developments. We join the two approaches and demonstrate what kind of concrete results can be immediately obtained in molecular systems [1, 2, 3, 4] by applying powerful methods of symmetric Hamiltonian systems [5, 6, 7, 8, 9, 10, 11]. We choose a concrete problem of rotation–vibration of a four-atomic molecule with tetrahedral equilibrium configuration [12, 13] in order to explain the details of our approach.

1.1. Vibrational relative equilibria or nonlinear normal modes. Montaldi, Roberts, and Stewart [14, 15, 16] gave a general description of periodic solutions near equilibria of symmetric Hamiltonian systems: the so-called nonlinear normal modes or relative equilibria (RE). They related the number of RE to the symmetry group of the system and showed, on several examples of bound systems of vibrating particles, that this number can be significantly larger than the number of vibrational degrees of freedom. This mathematical result was not fully

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appreciated by molecular physicists until it was reproduced by an alternate technique [17, 18, 19] based on the analysis of the reduced system in the so-called polyad approximation, a generalization of the approximation used for two-oscillator systems in [20, 21, 22, 23, 24, 25, 26, 27] and others. It was shown that fixed points of the symmetry group action on the reduced phase space correspond to vibrational RE. Later work [28, 29, 30]\(^1\) uncovered more fully the correspondence of both approaches and bridged the differences in their tools and terminology.

1.2. Rotational RE or stationary axes of rotation. Similar analysis of stationary points of the reduced rotational system [31, 32, 33, 34, 35, 36, 37, 38, 39, 40, 41, 42, 43] was initiated in molecular physics even before the analysis of vibrational RE. In terms of symmetric Hamiltonian systems [45, 46, 44], this analysis is equivalent to studying rotational RE [28, 29]. This was demonstrated in the recent study [12] of the rotational structure of the tetrahedral molecule \(P_4\) [47]\(^2\) where the energy of rotational RE is derived from the parameters of the internuclear potential. Our present analysis extends the method in [12] to rotation–vibration systems.

1.3. Applications in molecular physics and spectroscopy. Classical analysis of different kinds of RE is used for the description of molecular energy level spectra on the basis of the classical quantum correspondence principle, which links the topological description of the classical dynamical system to such qualitative aspects of quantum spectra as existence of bands, polyads, clusters, and their persistence under small modifications of parameters. Some of these qualitative characteristics are discussed in the present paper. Review articles [48, 49, 50, 51, 52, 53]\(^3\) give more examples of molecular applications and initiation to formal theory.

Much of the work in molecular spectroscopy is done using so-called effective model Hamiltonians \(H_{\text{eff}}\), which describe explicitly only a fraction of degrees of freedom of the system and treat other degrees effectively. In other words, \(H_{\text{eff}}\) describe reduced systems, where reduction is based on a model assumption of approximate separability and/or approximate dynamical symmetries. Equilibria (stationary points) of \(H_{\text{eff}}\) are RE of the initial system.

In practice, reduction often remains only an abstract theoretical possibility because parameters in the full initial molecular Hamiltonian are unknown. So, parameters of \(H_{\text{eff}}\) are simply fitted to experimental data. Classical analogues of such phenomenological model Hamiltonians can be constructed if excitation is sufficiently high to validate the classical limit. When, as it is often the case, only some degrees of freedom described by \(H_{\text{eff}}\) (e.g., rotation) can be meaningfully treated as classical, the rest (e.g., vibration) is kept quantum. The energies of such hybrid “semiquantum” systems are eigenvalues that depend on the dynamical variables of the classical subsystem. The most well-known example of semiquantum energy is the rotational energy surfaces of vibration-rotation systems [36, 35, 41].

\(^1\) The approach of Montaldi and Roberts is less oriented to the reduced problem and thus can be potentially extended to molecules in which separation of vibration and rotation and the introduction of the molecule-fixed frame is problematic. For the relatively rigid molecules, we consider their approach as being equivalent to ours.

\(^2\) Among the few different molecules of type \(A_4\), the phosphorus \(P_4\) is studied experimentally; see [47].

\(^3\) Our approach follows closely the ideas in [48, 49, 50], which review group actions and their applications in physics.
The semiquantum approach turned out to be very fruitful, and numerous vibration-rotation systems at low vibrational excitation were analyzed in great detail [37, 38, 18, 54, 55, 56, 42, 57, 43, 58]. In particular, typical (universal) modifications of the cluster structure of the energy level spectrum, or quantum bifurcations, were described in terms of modifications of the set of stationary points of the energy surfaces. Direct, explicit relation of these stationary points to classical RE was established recently in [58, 13]. Other important qualitative quantum phenomena include rearrangements (crossings) of energy level bands [59, 43, 60] and quantum monodromy [61, 62], which are interpreted as crossings of semiquantum energies and are also related to classical RE [60, 63, 64, 65].

1.4. Main idea. We combine recent theories of rotational RE and vibrational nonlinear normal modes in order to study the rotation–vibration problem. Using symmetry and topology, we find particular solutions (critical orbits) common to a whole class of model systems with given symmetry and with different potentials. Subsequently, we define a concrete potential, normalize the classical system, and construct explicitly the effective Hamiltonian $H_{\text{eff}}$. Using this Hamiltonian, we obtain quantitative predictions for concrete molecular models, which illustrate general qualitative results. We explain our approach in the example of rotation–vibration of the four-atomic homonuclear molecule $A_4$ with tetrahedral equilibrium configuration [47].

2. Basic aspects of the analysis. We review certain general definitions, which are used later in the paper, and give the plan of the analysis.

2.1. Symmetry group $T_d$ and its extensions. Along with translation and rotational symmetry, which are present for any isolated finite-particle system in the absence of external fields, each molecule possesses its own internal symmetry related to the existence of identical particles. The symmetry group of our system originates from the spatial symmetry group $T_d$ of the tetrahedral equilibrium configuration of $A_4$ and momentum reversal $T$, which in the original system sends $(q,p)$ to $(q,-p)$, and is discussed in more detail in section 3.1. Our initial Hamiltonian is invariant with respect to these symmetries. As an abstract group, $T_d$ is the permutation group of four identical objects. We use the Schönflies point group notation [67, 66], which is standard in molecular physics. Irreducible representations of $T_d$ are most frequently labeled in molecular physics as $A_1$, $A_2$ (one-dimensional), $E$ (two-dimensional), and $F_1$, $F_2$ (three-dimensional).

2.2. Vibrational degrees of freedom of an $A_4$ molecule. The $A_4$ molecule has six vibrational degrees of freedom, which constitute the nondegenerate “breathing” mode $A_1$, and the doubly and triply degenerate modes $E$ and $F_2$. The spectroscopic notation of these modes is $\nu_1^{A_1}$, $\nu_2^E$, $\nu_3^{F_2}$. We use a simplified notation for the coordinates and conjugate momenta of the modes given in Table 1 and we also use classical complex oscillator variables

$$z = q + ip, \quad \bar{z} = q - ip.$$  

The zero order vibrational Hamiltonian $H_0$ of $A_4$ represents a 1-oscillator, a 1:1 oscillator, and a 1:1:1 oscillator with frequencies $\omega_{A_1}$, $\omega_E$, and $\omega_{F_2}$, respectively.

2.3. Rotation–vibration Hamiltonian. Assuming that the static equilibrium configuration of $A_4$ about which the atoms are vibrating is well defined and the amplitudes of vibrations
Table 1
Notation for vibrational and rotational dynamical variables of the \( \text{A}_4 \) molecule. Expression of angular momenta \( j_\alpha \) in terms of dynamical variables of a two-dimensional oscillator (Schwinger representation) is used in this table and throughout the paper.

<table>
<thead>
<tr>
<th>Subsystem</th>
<th>Traditional notation</th>
<th>This paper</th>
</tr>
</thead>
<tbody>
<tr>
<td>F(_2) mode</td>
<td>( q_{F_2}^\alpha, p_{F_2}^\alpha, \alpha = x, y, z )</td>
<td>( q_i, p_i, i = 1, 2, 3 )</td>
</tr>
<tr>
<td>E mode</td>
<td>( q_{E_\alpha}^\alpha, p_{E_\alpha}^\alpha, \alpha = a, \text{or} 1, 2 )</td>
<td>( q_i, p_i, i = 4, 5 )</td>
</tr>
<tr>
<td>A(_1) mode</td>
<td>( q_{A_1}^\alpha, p_{A_1}^\alpha )</td>
<td>( q_\alpha, p_\alpha )</td>
</tr>
<tr>
<td>rotation momenta</td>
<td>( j_\alpha, \alpha = x, y, z )</td>
<td>( q_i, p_i, i = 6, 7 )</td>
</tr>
</tbody>
</table>

are small, we can separate molecular rotation and define the frame rotating with the molecule. The molecule is isolated, external fields are absent, and translation of the center of mass is therefore excluded.

To derive the rotation–vibration Hamiltonian \( H \), we can follow the procedure described in Chapter 11 of [1] and, more rigorously, in Chapter 7.10 of [68]. The molecule-fixed frame is related to the equilibrium configuration by the Eckart conditions. The kinetic energy \( T \) is a complicated function

\[
2T = \sum_i m_i \left[ \Omega \wedge (R_i^0 + r_i)^2 + \dot{r}_i^2 + 2\Omega (r_i \wedge \dot{r}_i) \right]
\]

of small vibrational displacement velocities and angular velocities defined with respect to this frame. The intramolecular potential \( U \) can be simply written in terms of vibrational coordinates. The Hamiltonian form requires rotational angular momenta \( j \), defined in the molecule-fixed frame, and vibrational coordinates \( q \) and momenta \( p \).

To put the initial Hamiltonian in the form suitable for normalization, we Taylor expand \( H = T(q, p, j) + U(q) \) in \( q \) and rescale \( (p, q) \) to bring the harmonic part to the standard form. We then express the components of \( j \) in terms of coordinates and momenta of the auxiliary two-dimensional harmonic oscillator in order to treat vibrational and rotational variables in the same way and use complex variables \( z \) in (2.1). The resulting formal power series expression

\[
H = \omega (H_0 + \epsilon H_1 + \epsilon^2 H_2 + \epsilon^3 H_3 + \cdots)
\]

is the starting point of the normal form transformation.

We use the concrete example of the phosphorus molecule \( \text{P}_4 \) with the tetrahedral equilibrium configuration and harmonic atom–atom bond potential [13] to illustrate our results. The only two molecular parameters in this example are the energy scale \( \omega \) and the dimensional smallness parameter \( \epsilon = (kmr)^{-1} \) in the series expansion. Here \( r \), \( m \), and \( k \) stand for the interatomic distance, the mass of the atoms, and the force constant of the potential, respectively. The values of \( \epsilon \) and \( \omega \) can be used as phenomenological parameters to reproduce experimental data qualitatively: \( \epsilon \approx 2 \times 10^{-2} \) and \( \omega \approx 329 \text{ cm}^{-1} \) for \( \text{P}_4 \) [13].

2.4. Reduced system. The approximate dynamical symmetry of the system with Hamiltonian (2.3) is defined by the zero order term \( H_0 \). We suppose that the frequencies \( \nu_{A_1}, \nu_E \), and \( \nu_{F_2} \) are incommensurate; i.e., we assume the absence of any resonances between different
vibrational modes. In such a case, we can introduce reduced phase spaces for each of the sub-systems simultaneously. The total reduced phase space is the product of these spaces. The normal form $H_{\text{eff}}$ is an effective rotation–vibration Hamiltonian describing polyads of nonresonant modes $A_1, E,$ and $F_2$. For simplicity, we neglect the $A_1$ mode (i.e., we set $q^{A_1} = p^{A_1} = 0$) and focus on modes $E$ and $F_2$.

2.4.1. Rotational subsystem; rotational space $S^2$. Conservation of the total angular momentum is the consequence of the isotropy of physical space (in the absence of external fields). The rotational dynamical variables $j_\alpha$ ($\alpha = 1, 2, 3$) are subjected to the constraint $j_1^2 + j_2^2 + j_3^2 = \text{const}$ and the rotational phase space is a two-dimensional sphere $S^2$, which can be constructed in the space $\mathbb{R}^3$ with coordinates $j_\alpha$. For the auxiliary two-dimensional oscillator, used to represent the momenta $v_j$ (Table 1), the restriction $j^2 = \text{const}$ is equivalent to fixing the sum of two actions.

2.4.2. $E$-mode subsystem, vibrational space $\mathbb{C}P^1 \sim S^2$. Exploiting the well-known equivalence of the two-dimensional 1:1 harmonic oscillator and an angular momentum system, we introduce vibrational angular momenta $v_1, v_2, v_3$ [69, 20, 21]. The internal structure of vibrational polyads formed by the doubly degenerate vibrational mode $E$ can be described in terms of these dynamical variables. The $E$-mode polyad sphere $S^2$ is defined by the equation

$$v_1^2 + v_2^2 + v_3^2 = n_e^2 = \text{const}$$

in the ambient space $\mathbb{R}^3$ with coordinates $(v_1, v_2, v_3)$. Any point on this sphere is uniquely represented by the values of $(v_1, v_2, v_3)$ if we keep in mind that $v_1^2 + v_2^2 + v_3^2$ is a constant. The diffeomorphic space $\mathbb{C}P^1$ can be defined in $C^2 = \{0\}$ using the equivalence class of points $z_4:z_5$. Two complex numbers $(z_4, z_5)$ can be used as coordinates on $\mathbb{C}P^1_{n_e}$ if their modules are restricted as

$$|z_4|^2 + |z_5|^2 = 2n_e$$

and all pairs $(z_4, z_5)$, which differ in a common phase factor $e^{i\phi}$, correspond to the same point of $\mathbb{C}P^1$. For example, coordinates $(v_1, v_2, v_3) = (0, 1, 0)$ and $(z_4, z_5) = (1, -i) = (e^{i\phi}, e^{i\phi - \pi/2})$ define the same point.

2.4.3. $F_2$-mode subsystem; vibrational space $\mathbb{C}P^2$. Generalization of the above construction for the $F_2$-mode 1:1:1 oscillator [17, 18, 70] leads to the reduced phase space $\mathbb{C}P^2_{nf}$. The approximate integral of motion equals

$$\frac{1}{2}(z_1 \bar{z}_1 + z_2 \bar{z}_2 + z_3 \bar{z}_3) = n_f \approx \text{const},$$

and $(z_1, z_2, z_3)$ can be used as coordinates on $\mathbb{C}P^2$. In fact, we can define a point on the $\mathbb{C}P^k$ space as an equivalence class of points on $C_{k+1}$ given by their homogeneous coordinates $z_1 : z_2 : \cdots : z_{k+1}$ or, equivalently, as a class of points on $(z_1, z_2, \ldots, z_{k+1}) \in C_{k+1}$ defined up to a common phase $(z_1, z_2, \ldots, z_{k+1}) \sim e^{i\phi}(z_1, z_2, \ldots, z_{k+1})$ and such that $|z_1|^2 + |z_2|^2 + \cdots + |z_{k+1}|^2$ is a constant.
2.4.4. Full reduced phase space \( \mathbb{C}P^2 \times \mathbb{C}P^1 \times S^2 \). Before reduction, our initial molecular system has five vibrational degrees of freedom (if the nondegenerate \( A_1 \) mode is neglected) and two auxiliary oscillatory degrees of freedom introduced to describe the rotational subsystem. Three independent reductions fix the strict integral of motion \( j \) (the amplitude of the total angular momentum) and polyad integrals \( n_e \) and \( n_f \) of the doubly degenerate mode \( E \) and the triply degenerate mode \( F_2 \). The reduced system is left with only four degrees of freedom. Reduction makes the topology of the reduced phase space more complicated. The total reduced space is a direct product of the rotational phase sphere, \( S^2_1 \), \( E \)-mode vibrational polyad sphere \( \mathbb{C}P^1_{n_e} \sim S^2 \), and \( F_2 \)-mode vibrational polyad phase space \( \mathbb{C}P^2_{nf} \). Omitting extra indexes and shortening the notation, we represent the topology of the reduced phase space simply as \( \mathbb{C}P^2 \times \mathbb{C}P^1 \times S^2 \), where \( S^2 \) and \( \mathbb{C}P^1 \) stand for the rotational and vibrational \( E \)-mode phase spaces, respectively.

2.4.5. Normal form. Once the Hamiltonian function \( H \) is in the oscillator form (2.3), we can normalize it using the standard Lie transform method [71, 72, 73, 74]. All odd orders [odd degrees in \( z, \bar{z} \)] vanish in the normal form

\[
\mathcal{H}_{\text{nf}} = \omega (H_0 + \epsilon^2 \mathcal{H}_2 + \epsilon^4 \mathcal{H}_4 + \epsilon^6 \mathcal{H}_6 + \cdots),
\]

which is a power series in \( \epsilon^2 \). To obtain the reduced Hamiltonian \( H_{\text{eff}} \), the terms \( \mathcal{H}_{2k} \) in (2.4) should be expressed as functions of basic invariant polynomials (of all generators of the algebra of invariant polynomials) on the reduced phase space \( \mathbb{C}P^2 \times \mathbb{C}P^1 \times S^2 \). Due to algebraic dependencies between generators (or “syzygies”) a special polynomial basis should be constructed. A general solution to this problem is provided by a Gröbner basis. Two more specialized polynomial bases—an integrity basis used in invariant theory, and a tensorial basis used by spectroscopists to represent effective Hamiltonians—can be used. We further discuss these bases in section 6.4.

2.5. Scheme of the analysis. Our analysis of a finite-particle quantum system includes several steps: (i) construction of the initial complete classical Hamiltonian \( H \) and of the corresponding quantum operator; (ii) reduction of \( H \), taking into account strict and approximate integrals of motion, i.e., the “model”; (iii) analysis of classical RE, relative periodic orbits, and invariant submanifolds;

(iv) interpretation in terms of quantum energy spectrum. Each step has a general part and a concrete part. Many important general results follow from the topology of the reduced phase space and the symmetry group action on it, i.e., from the model.

In the first half of the paper, which includes sections 4 and 5, we find as much information about our system as possible before any concrete interaction potential bounding the particles is introduced explicitly and even before any dynamics is studied. After establishing the topology of the reduced phase space \( \mathbb{C}P^2 \times \mathbb{C}P^1 \times S^2 \) and the invariance symmetry group \( T_d \times T \) of our system, we study the action of the group \( T_d \times T \) on \( \mathbb{C}P^2 \times \mathbb{C}P^1 \times S^2 \). To this end, we first consider the action on the individual factor spaces \( \mathbb{C}P^2 \), \( \mathbb{C}P^1 \), and \( S^2 \) and then extend it to the full reduced space. Time reversal \( T \) and other reversing symmetries, which include \( T \), are antisymplectic and should be treated differently from purely spatial symplectic symmetries.

We assume that the reduced Hamiltonian \( H_{\text{eff}} \) is a generic \( T_d \times T \) invariant Morse function on \( \mathbb{C}P^2 \times \mathbb{C}P^1 \times S^2 \). The RE of our system are stationary points of \( H_{\text{eff}} \), which exist anywhere...
case, RE are entirely defined by the finite symmetry $T$ suggest possible stabilities of RE. Considering Morse theory requirements, local symmetry, and local symplectic coordinates, we of the critical orbits of the factor spaces of (they are isolated fixed points of this action). The position of these orbits is independent of the interaction potential (and thus of the particular Hamiltonian). We combine information about critical orbits on each of the factor spaces of $C_2 \times \mathbb{C}P^1 \times S^2$ in order to find all critical orbits on the total space. Considering Morse theory requirements, local symmetry, and local symplectic coordinates, we suggest possible stabilities of RE.

Sections 6–9 focus on the dynamical analysis of the reduced system; concrete applications are presented in sections 10 and 11. As soon as the interaction potential and the Hamiltonian

---

Table 2

<table>
<thead>
<tr>
<th>Class$^4$</th>
<th>Structure$^5$</th>
<th>Description and comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>$C_1$</td>
<td>${1}$</td>
<td>Trivial subgroup.</td>
</tr>
<tr>
<td>$T$</td>
<td>${1, T}$</td>
<td>Momentum (or time) reversal, also denoted as $Z_2$.</td>
</tr>
<tr>
<td>$C_3$</td>
<td>${1, \sigma^0}$</td>
<td>Reflection in a plane, $T_d$ has six conjugated operations $\sigma^0$.</td>
</tr>
<tr>
<td>$T_d$</td>
<td>${1, T_d}$</td>
<td>Simultaneous reflection and time reversal, also denoted as $(\sigma T)$ or $(\sigma Z_2)$.</td>
</tr>
<tr>
<td>$C_2$</td>
<td>${1, C_2}$</td>
<td>Rotation by $\pi$ around one of axes $S^2_i$, $a = (x, y, z)$.</td>
</tr>
<tr>
<td>$T_2$</td>
<td>${1, T_2}$</td>
<td>Rotation by $\pi$ and time reversal, also denoted as $(C_2 T)$ or $(C_2 Z_2)$.</td>
</tr>
<tr>
<td>$C_3$</td>
<td>${1, C_3, C_3^2}$</td>
<td>Cyclic rotational subgroups corresponding to four different $C_3$ axes of the $T_d$ group.</td>
</tr>
<tr>
<td>$D_2$</td>
<td>${1, C_2^x, C_2^y, C_2^z}$</td>
<td>An invariant subgroup of the $T_d$ group.</td>
</tr>
<tr>
<td>$S_4$</td>
<td>${1, S_4, C_2, S_4^1}$</td>
<td>Cyclic groups generated by the $S_4$ operations $a = (x, y, z)$.</td>
</tr>
<tr>
<td>$T_4$</td>
<td>${1, T_{4+}, C_2, T_{4-}}$</td>
<td>Cyclic groups generated by the $S_4 \circ T = T_{4\pm}$ operations.$^9$</td>
</tr>
<tr>
<td>$C_2 \times T_2$</td>
<td>${1, C_2^x, T_2^a, T_2^b}$</td>
<td>(a, b, c) is one of the three cyclic permutations of $(x, y, z)$.$^6$</td>
</tr>
<tr>
<td>$C_3 \times T_2$</td>
<td>${1, \sigma^{x1}, T_2^a, T_2^{x2}}$</td>
<td>These correspond to six different choices of the $\sigma^{x1}$ symmetry plane.$^6,7,8$</td>
</tr>
<tr>
<td>$C_{2v}$</td>
<td>${1, C_2^x, \sigma^{x1}, \sigma^{x2}}$</td>
<td>Subgroup of $T_d$. Axis $a$ is one of $(x, y, z)$.$^7$</td>
</tr>
<tr>
<td>$C_2 \times T_3$</td>
<td>${1, C_2^x, T_3^{a1}, T_3^{a2}}$</td>
<td>Obtained from $C_{2v}$ by combining two reflections and time reversal.$^7,8$</td>
</tr>
<tr>
<td>$C_2 \times T$</td>
<td>${1, C_2, T, T_2}$</td>
<td>Direct product of $C_2^x$ and time reversal. Axis $a$ is one of $(x, y, z)$.$^6$</td>
</tr>
<tr>
<td>$C_3 \times T$</td>
<td>${1, \sigma, T, T_3}$</td>
<td>Corresponding to one of the six conjugated symmetry planes $\sigma$ of the $T_d$ group.$^9$</td>
</tr>
<tr>
<td>$C_3 \times T$</td>
<td>${1, C_3, C_3^2, T, C_3 T, C_3^{2T}}$</td>
<td>Direct product of $C_3$ and time reversal $T$ corresponding to four different axes $C_3$.</td>
</tr>
<tr>
<td>$C_3 \tau$</td>
<td>${1, 2C_3, 3\sigma}$</td>
<td>Conjugated subgroups of the spatial symmetry group $T_d$.</td>
</tr>
<tr>
<td>$C_3 \tau T_3$</td>
<td>${1, 2C_3, 3T_3}$</td>
<td>This group has $T_3$ instead of $\sigma_d$ in $C_{3\nu}$ and is isomorphic to $C_{3\nu}$ as an abstract group.$^8$</td>
</tr>
</tbody>
</table>

$^4$-$^8$See the footnotes to Table 3 on the following page.
Table 3
Classes of conjugated and invariant subgroups of the $T_d \times T$ group. Part II.

<table>
<thead>
<tr>
<th>Class</th>
<th>Structure</th>
<th>Description and comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>Subgroups of order 8</td>
<td></td>
<td></td>
</tr>
<tr>
<td>1</td>
<td>$D_2 \times T$</td>
<td>Direct product of the $D_2$ subgroup of $T_d$ and time reversal $T$.</td>
</tr>
<tr>
<td>2</td>
<td>$C_{3v} \times T$</td>
<td>Direct product of the $C_{3v}$ subgroup of $T_d$ and time reversal $a = (x, y, z)$.</td>
</tr>
<tr>
<td>3</td>
<td>$D_{2d}$</td>
<td>Conjugated subgroups of the spatial symmetry group $T_d$.</td>
</tr>
<tr>
<td>3</td>
<td>$D_{2d} \times T$</td>
<td>Isomorphic to $D_{2d}$ as an abstract group; two conjugated $C_2$ rotations and two conjugated $S_4$ operations of $D_{2d}$ are replaced for their products with $T$.</td>
</tr>
<tr>
<td>3</td>
<td>$S_4 \times T$</td>
<td>Direct product of the cyclic subgroup $S_4^a$ of $T_d$ and time reversal.</td>
</tr>
<tr>
<td>3</td>
<td>$S_4 \times T$</td>
<td>Isomorphic to $D_{2d}$ as an abstract group; has two conjugated $\sigma$ reflections and two conjugated $S_4$ operations of $D_{2d}$ replaced for their products with $T$.</td>
</tr>
<tr>
<td>Subgroups of order 12</td>
<td></td>
<td></td>
</tr>
<tr>
<td>1</td>
<td>$T$</td>
<td>Rotational subgroup of the $T_d$ group.</td>
</tr>
<tr>
<td>4</td>
<td>$C_{3v} \times T$</td>
<td>Direct product of a $C_{3v}$ subgroup of $T_d$ and time reversal.</td>
</tr>
<tr>
<td>Subgroups of order 16</td>
<td></td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>$D_{2d} \times T$</td>
<td>Direct product of one of the three $D_{2d}$ subgroups of $T_d$ and time reversal $T$.</td>
</tr>
<tr>
<td>Subgroups of index two (order 24)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>1</td>
<td>$T \times T$</td>
<td>Direct product of $T$ and time reversal, also denoted as $T \times Z_2$.</td>
</tr>
<tr>
<td>1</td>
<td>$T \times T$</td>
<td>Tetrahedral group, isomorphic to the permutation group $S_4$ as an abstract group.</td>
</tr>
<tr>
<td>1</td>
<td>$T \times T$</td>
<td>Another realization of $S_4$ obtained from $T_d$ by replacing all improper rotations, namely six $\sigma$ and six $S_4$ operations, for their products with time reversal $T$.</td>
</tr>
<tr>
<td>Complete group (order 48)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>1</td>
<td>$T_d \times T$</td>
<td>Direct product of $T_d$ and time reversal group $T$.</td>
</tr>
</tbody>
</table>

4The leftmost column gives the number of conjugated subgroups in the class.

5When all operations in the group correspond to the same rotation axis $a$, we do not specify the choice of the axis and omit index $a$.

6The operation $T_a = C_2 \circ T$ is rotation by $\pi$ around axes $a$ and time reversal; by convention $a = (x, y, z)$ is one of the axes $S_4$.

7In the $T_d$ group, reflection planes $\sigma^{a_1}$ and $\sigma^{a_2}$ intersect on axis $C_2^a$, where by convention $a$ is one of $(x, y, z)$; in the $O_h$ group these planes are called $\sigma_d$.

8The operation $T_a = \sigma \circ T$ is reflection in one of the six planes $\sigma_d$ and time reversal; in particular, $T_a^{a_1} = T \circ \sigma^{a_1}$. |

9The operations $T_a^a = T(S_a)^{-1} = T \circ (S_a)^{-1}$, where $a = (x, y, z)$, are operations $S_4$ or $S_4^{-1}$ combined with time reversal $T$. |
are introduced explicitly, the value of $H_{\text{eff}}$ at critical orbits is found. This gives analytic expressions for the energy of RE as a function of actions $N_e, N_f, J$. Using these energies, we characterize the multiplet of quantum states with quantum numbers $N_e, N_f, J$. We can also use the quantum analogue of $H_{\text{eff}}$ in order to compute energies of individual states. Using the concrete Hamiltonian, we can check the Morse indexes of all known RE and find, if necessary, additional RE which do not lie on critical orbits but are nevertheless required by Morse theory conditions.

3. Finite symmetry group of the system. We briefly review the structure of the tetrahedral group $T_d$ and its extension $T_d \times T$. This group and its subgroups can be considered as magnetic (or color) crystallographic symmetry groups; see Chapter 2 of [67]. Notation for such groups is not commonly established. Below we explain our conventions and describe the abstract group structure of $T_d \times T$ given by its subgroup lattice (see Tables 2 and 3). We distinguish only the nonconjugate subgroups of $T_d \times T$ and study certain sublattices corresponding to reduced or partial symmetry groups. This information is vital for understanding the stratification of different reduced phase spaces by the action of $T_d \times T$ and, in particular, for finding fixed points and invariant subspaces of this action.

3.1. Time reversal symmetry $T$. Momentum reversal symmetry $T$ is a nonsymplectic symmetry operation defined for the original physical 3-space coordinates and conjugate momenta as

$$(q, p) \rightarrow (q, -p).$$

We denote this operation as $T$, or simply as $Z_2$, and imply that its action in each particular context is either known or should be specified. We will distinguish the two types of behavior (two representations of $Z_2$) with regard to momentum reversal by “parity” indexes $g$ (gerade) and $u$ (ungerade), respectively.

The symmetry operation $T$ is also sometimes called time reversal. We like to make clear that our operation $T$ acts only on the phase space variables $(q, p)$ and does not involve time $t$. This implies that the action of $T$ on the extended phase space is

$$T : (q, p, t) \rightarrow (q, -p, t).$$

It can be seen that, even when the Hamiltonian of the system is invariant with regard to such operation $T$, the corresponding equations of motion are not. In fact, this is due to the fact that the action of $T$ on $(q, p)$ is antisymplectic. Operation $T$ is an example of reversing symmetries. Another commonly used definition of time reversal extends nontrivially our operation $T$ to time $t$:

$$T_t : (q, p, t) \rightarrow (q, -p, -t).$$

This operation preserves the flow of the system with $T$-invariant Hamiltonian function. In quantum mechanics, operation $T$ changes the signs of all commutator relations while $T_t$ preserves these signs.

Of course, one can use either $T$ or $T_t$ for the analysis, as long as one understands their action. For example, action of $T$ and $T_t$ on equilibria is the same, while their action on the
trajectories $\gamma : t \to (q,p)$ is different. Trajectories $T(\gamma)$ and $T_t(\gamma)$ coincide in the phase space but have different direction. Reversing direction is the result of $t \to -t$, which cannot be represented as a geometric transformation of the phase space. Since in most cases we do not work with extended phase spaces, we prefer to define $T$ as just another transformation of the phase space with coordinates $(q,p)$.

The action of $T \sim Z_2$ on vibrational normal mode coordinates and conjugate momenta is, of course, the same as on the 3-space $q$’s and $p$’s, and as we go to the complex variables

$$z = q - ip, \quad \bar{z} = q + ip,$$

this action becomes

$$(3.1a) \quad (z_1, z_2, z_3, z_4, z_5) \to (\bar{z}_1, \bar{z}_2, \bar{z}_3, \bar{z}_4, \bar{z}_5).$$

Note that this operation differs from plain “complex conjugation” as shown by

$$(3.1b) \quad z_1 + iz_2 \to \bar{z}_1 + i\bar{z}_2.$$  

Molecular angular momentum components $(j_1, j_2, j_3)$ are not invariant with respect to $Z_2$:

$$(3.1c) \quad (j_1, j_2, j_3) \to (-j_1, -j_2, -j_3).$$

This property of $(j_1, j_2, j_3)$ follows, of course, from the explicit Wilson–Howard definition of rotational angular momenta in terms of particle coordinates and momenta. At the same time, we can simply note that time reversal changes the direction of classical rotation and therefore changes signs of $(j_1, j_2, j_3)$.

### 3.2. Spatial finite symmetry $T_d$. The spatial symmetry group of the $A_4$ molecule is the point group of its tetrahedral equilibrium configuration $T_d$. This group, and cubic groups $O$ and $O_h$ (and to a lesser extent, $T$ and $T_h$) are well known to molecular physicists and crystallographers. It is generated by the three-fold rotation $C_3$ and the four-fold inversion rotation $S_4$. The latter can be realized as $C_4 \circ C_i$, a rotation $C_4$ by angle $\pi/2$ followed by a 3-space inversion $C_i$, or alternately as rotation by angle $-\pi/2$ followed by reflection in the plane orthogonal to the rotation axis. A particular realization of $T_d$ is given in Table 4 and is illustrated in Figure 1. We will use the three symmetry operations in Table 4 for explicit demonstrations later in the paper. Conventionally, axes $x$, $y$, and $z$ are chosen as $S_4^2$ axes. Three operations $S_4$ and three inverse operations $S_4^{-1}$ form a class of six conjugate elements. Three operations $C_2 = S_4^2$, which rotate by $\pi$ about the same axes, form a separate class. Operations $C_3$, which rotate by $\pm 2\pi/3$ about four diagonal axes, such as axis [1,1,1] in Table 4, form one class of eight elements. Finally, there is a class of six reflection planes denoted $\sigma$ or $C_s$; each element $C_s$ can be considered as a combination $C_2 \circ C_i$, where axis $C_2$ is orthogonal to the reflection plane.

### 3.3. Full finite symmetry group $T_d \times T$. The total symmetry group of our system is the tetrahedral group $T_d$ extended to include the time reversal operation $T$. We exploit the isomorphism $T_d \times T \sim O_h \sim O \times T$ to explain the notation for symmetry operations and different subgroups of $T_d \times T$. Table 5 summarizes correspondence of notation for the symmetry operations of the three groups.
The lattices of conjugate subgroups of the $O_h$ and $T_d \times T$ groups are shown in Figures 2 and 3, respectively, in order to compare the Schönflis notation for the classes of $O_h$ [67] to our notation of the $T_d \times T$ classes. The 33 classes of conjugate subgroups of $T_d \times T$ are arranged according to their order and are further described in Tables 2 and 3. Left superscripts in Figures 2 and 3 indicate, where necessary, the number of conjugate subgroups in the class. Invariant subgroups are unique in their class which needs, therefore, no such superscripts. Subgroups of $O_h$, which are distinguished by primes, $C_{2v}$, $C'_{2v}$, and $C''_{2v}$, $D_2$ and $D'_{2d}$, $D_2h$ and $D'_{2h}$, $D_2$ and $D'_{2h}$, $C_{2h}$ and $C'_{2h}$, $C_2$ and $C'_{2}$, $C_s$ and $C'_{s}$, are nonconjugate in $O_h$ but become conjugate in the larger group SO(3). Such notation is less informative in comparison with the $T_d \times T$ notation for the corresponding nonconjugate subgroups, which highlights the differences between the subgroups explicitly.

### 3.4. Sublattices corresponding to different images of $T_d \times T$ and broken symmetries.

The action of the symmetry group $T_d \times T$ on the vibrational $E$-mode polyad space $\mathbb{C}P^1$ is not effective; the invariant subgroup $D_2$ forms the kernel, and the image $(T_d \times T)/D_2$ is the group isomorphic (as an abstract group) to $C_{3v} \times T$ or $D_{3h}$, see Table 6. We compare the subgroup lattice of $(T_d \times T)/D_2$ in Figure 4, right, to the equivalent lattice of $D_{3h}$ (Figure 4, left) in order to better explain the action of $T_d \times T$ on $\mathbb{C}P^1$. When characterizing the subgroups of $(T_d \times T)/D_2$ we take into account their extension by the kernel $D_2$ in order to preserve the

---

**Table 4**

Matrix representations of basic operations of the $T_d$ group illustrated in Figure 1.

<table>
<thead>
<tr>
<th>Subgroup</th>
<th>A1</th>
<th>A2</th>
<th>F2</th>
<th>E</th>
<th>F1</th>
</tr>
</thead>
<tbody>
<tr>
<td>$C_{3[111]}$</td>
<td>1</td>
<td>1</td>
<td>$\begin{pmatrix} 0 &amp; 0 &amp; 0 \ 0 &amp; 1 &amp; 0 \ 1 &amp; 0 &amp; 0 \end{pmatrix}$</td>
<td>$\frac{1}{3} \begin{pmatrix} -1 &amp; -\sqrt{3} \ \sqrt{3} &amp; -1 \end{pmatrix}$</td>
<td>$\begin{pmatrix} 0 &amp; 0 &amp; 1 \ 0 &amp; 1 &amp; 0 \ 1 &amp; 0 &amp; 0 \end{pmatrix}$</td>
</tr>
<tr>
<td>$S_4^2$</td>
<td>1</td>
<td>-1</td>
<td>$\begin{pmatrix} 0 &amp; 1 &amp; 0 \ -1 &amp; 0 &amp; 0 \ 0 &amp; 0 &amp; -1 \end{pmatrix}$</td>
<td>$\begin{pmatrix} 1 , 0 &amp; \end{pmatrix}$</td>
<td>$\begin{pmatrix} 0 &amp; -1 , 0 \ 1 &amp; 0 , 0 \ 0 &amp; 0 , 1 \end{pmatrix}$</td>
</tr>
<tr>
<td>$C_{sxy}$</td>
<td>1</td>
<td>-1</td>
<td>$\begin{pmatrix} 0 &amp; 1 &amp; 0 \ 1 &amp; 0 &amp; 0 \ 0 &amp; 0 &amp; 1 \end{pmatrix}$</td>
<td>$\begin{pmatrix} 0 , 1 , 0 \ 1 , 0 , 0 \ 0 , 0 , 1 \end{pmatrix}$</td>
<td></td>
</tr>
</tbody>
</table>

---

**Figure 1.** Basic operations of the $T_d$ point group (left). The symmetry axis $C_2$ (dashed line) of the $O_h$ and $O$ groups is orthogonal to the $C_s$ reflection plane (shadowed) of $T_d$. This $C_2$ should not be confused with axis $C_2 = S_4^2$, which has the same orientation as axis $S_4$. Right: lattice of conjugate subgroups of the $T_d$ group. Left: superscripts give the number of conjugate subgroups in each class.

---

**Figure 2.** Figures 2 and 3, respectively, in order to compare the Schönflis notation for the classes of $O_h$ [67] to our notation of the $T_d \times T$ classes. The 33 classes of conjugate subgroups of $T_d \times T$ are arranged according to their order and are further described in Tables 2 and 3. Left superscripts in Figures 2 and 3 indicate, where necessary, the number of conjugate subgroups in the class. Invariant subgroups are unique in their class which needs, therefore, no such superscripts. Subgroups of $O_h$, which are distinguished by primes, $C_{2v}$, $C'_{2v}$, and $C''_{2v}$, $D_2$ and $D'_{2d}$, $D_2h$ and $D'_{2h}$, $D_2$ and $D'_{2h}$, $C_{2h}$ and $C'_{2h}$, $C_2$ and $C'_{2}$, $C_s$ and $C'_{s}$, are nonconjugate in $O_h$ but become conjugate in the larger group SO(3). Such notation is less informative in comparison with the $T_d \times T$ notation for the corresponding nonconjugate subgroups, which highlights the differences between the subgroups explicitly.

---

**Figure 3.** Figures 2 and 3, respectively, in order to compare the Schönflis notation for the classes of $O_h$ [67] to our notation of the $T_d \times T$ classes. The 33 classes of conjugate subgroups of $T_d \times T$ are arranged according to their order and are further described in Tables 2 and 3. Left superscripts in Figures 2 and 3 indicate, where necessary, the number of conjugate subgroups in the class. Invariant subgroups are unique in their class which needs, therefore, no such superscripts. Subgroups of $O_h$, which are distinguished by primes, $C_{2v}$, $C'_{2v}$, and $C''_{2v}$, $D_2$ and $D'_{2d}$, $D_2h$ and $D'_{2h}$, $D_2$ and $D'_{2h}$, $C_{2h}$ and $C'_{2h}$, $C_2$ and $C'_{2}$, $C_s$ and $C'_{s}$, are nonconjugate in $O_h$ but become conjugate in the larger group SO(3). Such notation is less informative in comparison with the $T_d \times T$ notation for the corresponding nonconjugate subgroups, which highlights the differences between the subgroups explicitly.

---

**Figure 4.** Basic operations of the $T_d$ point group (left). The symmetry axis $C_2$ (dashed line) of the $O_h$ and $O$ groups is orthogonal to the $C_s$ reflection plane (shadowed) of $T_d$. This $C_2$ should not be confused with axis $C_2 = S_4^2$, which has the same orientation as axis $S_4$. Right: lattice of conjugate subgroups of the $T_d$ group. Left: superscripts give the number of conjugate subgroups in each class.
In order to compare our present work to [70] we give in Figure 5 the correspondence of the higher symmetry group \( T_d \times T \) to the local symmetry group or stabilizer to the reduced polyad phase space \( \mathbb{C}P^2 \) of the doubly degenerate mode \( E \). Each element in \( D_{3h} \) is an image of four elements of \( T_d \times T \). In particular, the identity in \( D_{3h} \) is the image of the invariant subgroup \( D_3 \) of \( T_d \times T \).

Table 5

<table>
<thead>
<tr>
<th>( O_h )</th>
<th>( T_d \times T )</th>
<th>( O \times T )</th>
<th>( O_h )</th>
<th>( T_d \times T )</th>
<th>( O \times T )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1</td>
<td>1</td>
<td>( C_1 )</td>
<td>( T )</td>
<td>( T )</td>
</tr>
<tr>
<td>8C_4</td>
<td>8C_4</td>
<td>8C_3</td>
<td>8S_6</td>
<td>8(TC_4)</td>
<td>8(TC_3)</td>
</tr>
<tr>
<td>3C_2</td>
<td>3C_2</td>
<td>3C_2</td>
<td>3( \sigma_h )</td>
<td>3(TC_2)</td>
<td>3(TC_2)</td>
</tr>
<tr>
<td>6C_2</td>
<td>6( \sigma_d )</td>
<td>6C_2’</td>
<td>6( \sigma_d )</td>
<td>6(T( \sigma_d ))</td>
<td>6(TC_2)</td>
</tr>
<tr>
<td>6C_4</td>
<td>6S_4</td>
<td>6C_4</td>
<td>6S_4</td>
<td>6(TS_4)</td>
<td>6(TC_4)</td>
</tr>
</tbody>
</table>

Table 6

Homomorphism \( T_d \times T \to D_{3h} \), which defines the group of symmetry transformations of the vibrational reduced polyad phase space \( \mathbb{C}P^2 \) of the doubly degenerate mode \( E \). Each element in \( D_{3h} \) is an image of four elements of \( T_d \times T \). In particular, the identity in \( D_{3h} \) is the image of the invariant subgroup \( D_3 \) of \( T_d \times T \).

\[
\begin{align*}
\{ T_d \times T \} & \rightarrow D_{3h} \\
\{ 1, 3C_2 \} & \rightarrow 1 \\
\{ 8C_3 \} & \rightarrow 2C_3 \\
\{ 6S_4, 6\sigma_d \} & \rightarrow 3C_2 \\
\{ T, 3(TC_2) \} & \rightarrow \sigma_h \\
\{ 8(TC_3) \} & \rightarrow 2S_3 \\
\{ 6(TS_4), 6(T\sigma_d) \} & \rightarrow 3\sigma_v
\end{align*}
\]

4. Group action. When a group element acts on the point \( x \) on the space \( \mathcal{P} \), it can map \( x \) either to a different point \( x' \) on \( \mathcal{P} \) or to itself. In the latter case the group element belongs to the local symmetry group or stabilizer of \( x \). The set of points obtained from \( x \) by applying all group elements is called an orbit. Orbits of a finite group \( G \) are, obviously, finite sets, and the maximum number of points in an orbit of the \( G \) action equals the number of group elements or the order \( |G| \) of the group. If the stabilizer \( G_x \) of the point \( x \) is nontrivial, then the number of points in the orbit equals \( |G|/|G_x| \). In particular, if \( x \) is a fixed point of the group action, it forms a one-point orbit.

Out of all the orbits of the action of the group \( G \) on the space \( \mathcal{P} \), we distinguish critical orbits [75, 76]. The stabilizer of a point \( x \) on the critical orbit differs from that of any point in a sufficiently small open neighborhood of \( x \); i.e., points on critical orbits are isolated. As a consequence, these points must be stationary or critical points of any \( G \)-invariant function \( f(x) \) on \( \mathcal{P} \). When \( \mathcal{P} \) is a reduced phase space and \( f(x) \) is a reduced Hamiltonian \( H_{\text{red}} \), these points correspond to RE of the initial system. This makes finding critical orbits the primary purpose of our group action study [48, 49, 50]. In general, we also look for invariant subspaces...
Figure 2. Lattice of conjugate subgroups of the $O_h$ group. The order of all subgroups on the same row is indicated on the right of the graph.

Figure 3. Lattice of conjugate subgroups of the $T_d \times T$ group; cf. Figure 2. Shorthand notation $T_2$, $T_s$, and $T_4$ is used for stabilizers $TC_2$, $T \sigma_d$, and $T S_4$; the order of all subgroups on the same row is indicated on the right of the graph.

of the reduced phase space $\mathcal{P}$—and especially for the invariant subspaces whose stabilizer is a purely spatial symmetry subgroup of $G$.

The symmetry group $T_d$ was originally defined as a point group of transformations in the Euclidean 3-space $\mathbb{R}^3$ with coordinates $(x, y, z)$, which transform in the same way as components of the $F_2$ mode $(q_1, q_2, q_3)$. The action of $T_d$ is subsequently extended symplectically on $(p_1, p_2, p_3)$, which transform in the same way as $(q_1, q_2, q_3)$. This defines the action on $(z_1, z_2, z_3)$. At the same time, momentum reversal $T$ or $Z_2$ is introduced as an antisymplectic symmetry.

The $E$-mode variables and rotational variables $(j_1, j_2, j_3)$ transform according to the $E$ and $F_1$ irreducible representations of the $T_d$ group. The action of the symmetry group in these
representations is defined by the *image* of the initial symmetry group. To find the action of the symmetry group $T_d$ and its extension $T_d \times T$ on different components of the reduced phase space (the $F_2$-mode space $\mathbb{C}P^2$, the $E$-mode space $\mathbb{C}P^1$, and the rotational sphere $S^2$), we first need to know the image of our symmetry group in the corresponding representations. We find the image of the group in the particular representation $\Gamma$ by acting explicitly on the variables which realize $\Gamma$.

Group images and their actions can be very nontrivial even for finite symmetry groups and should be studied with care. Thus the action of spatial inversion on the reduced phase space of our system is equivalent to identity, and as a consequence, it suffices to consider pure rotations $C_4$ and $C_2$ of the $O$ group instead of operations $S_4$ and $C_4$ of the $T_d$ group. We will also see that the image of $T_d$ in the $E$ representation is a smaller group $C_{3v}$ and that its action on the $E$-mode reduced phase space $\mathbb{C}P^1$ is equivalent to that of a dihedral group $D_3$. We begin by explaining actions of $T_d \times T$ on the reduced phase spaces $\mathbb{C}P^2$, $\mathbb{C}P^1$, and $S^2$ and on the total reduced space $\mathbb{C}P^2 \times \mathbb{C}P^1 \times S^2$ with the action of the rotation group $SO(2)$ (or $C_{\infty}$) and its finite subgroups $C_k$, $k = 2, 3, 4, \ldots$, of which $C_2$ is a special case, and by explaining the action of time reversal $T$ (or $Z_2$). We use operations from Table 4 to illustrate group actions.

**4.1. Rotational subsystem: Action of $T_d \times T$ on $S^2$.** Unlike components of polar vectors $(x, y, z)$ and $(q_1, q_2, q_3)$, the angular momenta $(j_1, j_2, j_3)$ are invariant with regard to the 3-space inversion $C_i$ (i.e., they do not change sign). The image of $T_d$ in the $F_1$ representation realized by $(j_1, j_2, j_3)$ is an isomorphic group $O$ generated by pure rotations. (This group can...
As discussed in section 2.4.1, equation $j^2 = \text{const}$ defines the reduced rotational phase space $S^2$ as a sphere in the ambient space $\mathbb{R}^3$ with coordinates $(j_1, j_2, j_3)$. The action of $O \times T$ on this sphere is often represented in terms of the action of the $O_h$ group of transformations of the $\mathbb{R}^3$ space (see Figure 7). The $O_h$ notation, or even shorter $O$ group notation, is used in practically all applications [18, 39, 32, 33, 34] and remains preferred (at least for the study of a purely rotational system) because geometric transformations in $\mathbb{R}^3$ are very commonly known. On the other hand, the $T_d \times T$ notation properly reflects the actual symmetry of the system and is more adequate.

Any rotation $C_k$ acting on $S^2$ (as an element of the $O_h$ group of transformations of the ambient space $\mathbb{R}^3$) has two fixed points, which are the two diametrically opposite points of $S^2$ situated on the axis. The two points are mapped into each other by the $T$ operation (which acts as inversion in $\mathbb{R}^3$) and belong to one orbit. This orbit is critical. Reversing operations $C_k \circ T$ with $k > 2$ have no fixed points on $S^2$. The operation $T_2 = C_2 \circ T$ acts in $\mathbb{R}^3$ like a symmetry plane $\sigma$ orthogonal to the $C_2$ axis. The set of all points on $S^2$ invariant with regard to $T_2$ is a circle $S^1$, which is the intersection of $\sigma$ and $S^2$.

As a simple example, consider the action of the $C_2 \times T$ group on $S^2$ illustrated in Figure 6...
the orbit.

specific stabilizer in the class of conjugate stabilizers corresponds to two different points in

Table 7

Action of $T_d \times T$ on the rotational sphere $S^2$.

<table>
<thead>
<tr>
<th>$O_h$ stabilizer</th>
<th>$C_{4v}$</th>
<th>$C_{3v}$</th>
<th>$C_{2v}$</th>
<th>$C_s$</th>
<th>$C_s'$</th>
<th>$C_1$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$T_d \times T$ stabilizer</td>
<td>$S_d \wedge T_3$</td>
<td>$C_3 \wedge T_s$</td>
<td>$C_s \wedge T_2$</td>
<td>$T_2$</td>
<td>$T_s$</td>
<td>$C_1$</td>
</tr>
<tr>
<td>Points in orbit</td>
<td>6</td>
<td>8</td>
<td>12</td>
<td>24</td>
<td>24</td>
<td>48</td>
</tr>
<tr>
<td>Conjugate stabilizers</td>
<td>3</td>
<td>4</td>
<td>6</td>
<td>3</td>
<td>6</td>
<td>1</td>
</tr>
</tbody>
</table>

(with the $C_2$ axis along the $z$ axis). There are three types of orbits: a two-point orbit with stabilizer $C_2$, a one-dimensional stratum of two-point orbits with stabilizer $T_2$, and a two-
dimensional stratum with trivial stabilizer. The space of orbits is a punctured closed disc shown in Figure 6, right.

The action of $T_d \times T$ on $S^2$ is described in Table 7 and the space of orbits is shown in Figure 7. Out of 33 classes of the conjugate subgroups of this group, six appear as stabilizers (see Figure 8). There are 26 fixed points on $S^2$, which form three critical orbits with stabilizers $S_d \wedge T_3 \sim C_{4v}$, $C_3 \wedge T_s \sim C_{3v}$, $C_s \wedge T_2 \sim C_{2v}$. Note that, as in the case of any $C_k$ action, each specific stabilizer in the class of conjugate stabilizers corresponds to two different points in the orbit.

4.2. $E$-mode vibrational subsystem: Action of $T_d \times T$ on $\mathbb{C}P^1 \sim S^2$. We find the image of the spatial symmetry group $T_d$ in the $E$ representation by considering the action of

$T_d$ on the plane $\mathbb{R}^2$ with coordinates $(q_1, q_5)$ or on a complex plane with coordinates $(z_4, z_5)$. From Table 4 we can see that operation $C_2^z = (S_3^c)^2$ acts trivially on this plane, operation $C_3$ rotates by $2\pi/3$ about the origin, while operations $S_3^z$ and $C_s^{xy}$ have the same action on $\mathbb{R}^2$: they reflect with respect to the axis $\{q_5 = 0\}$ passing through the origin. It follows that the

image of $T_d$ is a group $D_3$ (or $C_{3v}$).

The action of the full symmetry group $T_d \times T$ on the reduced vibrational phase space $\mathbb{C}P^1$ is equivalent to that of $C_{3v} \times T$. The kernel of the homomorphism $T_d \times T \to C_{3v} \times T$
is $D_2$, i.e., the order four invariant subgroup of $T_d \times T$ described in Table 2. The action of $C_{3h}$ on the $E$-mode vibrational phase sphere $S^2 \sim \mathbb{C}P^1$ can be better visualized as the natural action of the point group $D_{3h}$ of transformations of the Euclidean 3-space $\mathbb{R}^3$ on a sphere embedded in this space. The correspondence between the $D_{3h}$ notation and symmetry operations of $T_d \times T$ is given in Figure 4 and Table 6.

All strata of the $T_d \times T$ action on the $E$-mode space $\mathbb{C}P^1 \sim S^2$ are described in Figure 9 and Table 8. The $D_{3h}$ analogy makes understanding this stratification straightforward. We can essentially use the approach in section 4.1 and, of course, earlier results for classical $C_{3v}$ symmetric rotational systems (see section 1), such as a triatomic molecule with equilateral equilibrium configuration. For example, any rotation in $D_{3h}$ has two fixed points on $S^2$; the particular $C_3$ rotation in Table 4 has fixed points with coordinates $v = (0, \pm 1, 0)$ or equally $(z_4, z_5) = (1, \mp i)$, which form one two-point critical orbit with stabilizer $T \wedge T_s$. The stabilizer of the two other critical orbits is $D_{2d} \times T$. Note that the points in the $T \wedge T_s$ orbit have exactly the same stabilizer (because $T \wedge T_s$ is an invariant subgroup), whereas the three points in each $D_{2d} \times T$ orbit have different conjugate stabilizers.

Dynamical variables of the reduced $E$-mode system and local canonical coordinates near points on critical orbits on $\mathbb{C}P^1$ can be classified using irreducible representations of both $T_d \times T$ and $D_{3h}$. Thus, vibrational angular momenta $\{v_1, v_2, v_3\}$ introduced in section 2.4.2 span the natural reducible representation $A_{2u} \oplus E_g$ of the $T_d \times T$ group (see section 7), which corresponds to $A''_2 \oplus E'$ of the $D_{3h}$ group. Table 9 gives the relation between the irreducible representations of the $T_d \times T$ group and its subgroup $(T_d \wedge T)/D_2$. This correspondence should be taken into account in order to study vibration-rotation dynamics on $\mathbb{C}P^1 \times S^2$, where the group $T_d \times T$ acts as $D_{3h}$ and $O_h$ on the vibrational subspace $\mathbb{C}P^1$ and rotational subspace $S^2$. We should warn the reader that $D_{3h}$ is not a subgroup of $O_h$. We simply use standard
The results of [17] for the symmetry groups $T$ and inversion is identity. It follows that the images of the correspondence is written initially for $O_h$ and its $D_{3d}$ subgroup and is further extended using the isomorphism $D_{3d} \leftrightarrow D_{3h}$.

Table 9

<table>
<thead>
<tr>
<th>$T_d \times T \rightarrow$</th>
<th>$(T_d \times T)/D_2 \sim O_h \rightarrow D_{3d} \sim D_{3h}$</th>
<th>$T_d \times T \rightarrow$</th>
<th>$(T_d \times T)/D_2 \sim O_h \rightarrow D_{3d} \sim D_{3h}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$A_{1g} \rightarrow A_{1g}$</td>
<td>$A'_1$</td>
<td>$A_{1u} \rightarrow A_{1u}$</td>
<td>$A''_1$</td>
</tr>
<tr>
<td>$A_{2g} \rightarrow A_{2g}$</td>
<td>$A'_2$</td>
<td>$A_{2u} \rightarrow A_{2u}$</td>
<td>$A''_2$</td>
</tr>
<tr>
<td>$E_g \rightarrow E_g$</td>
<td>$E'$</td>
<td>$E_u \rightarrow E_u$</td>
<td>$E''$</td>
</tr>
<tr>
<td>$F_{1g} \rightarrow A_{1g} \oplus E_g$</td>
<td>$A'_1 \oplus E'$</td>
<td>$F_{1u} \rightarrow A_{1u} \oplus E_u$</td>
<td>$A''_1 \oplus E''$</td>
</tr>
<tr>
<td>$F_{2g} \rightarrow A_{2g} \oplus E_g$</td>
<td>$A'_2 \oplus E'$</td>
<td>$F_{2u} \rightarrow A_{2u} \oplus E_u$</td>
<td>$A''_2 \oplus E''$</td>
</tr>
</tbody>
</table>

notation for irreducible representations of $O_h$ and $D_{3h}$.

4.3. $F_2$-mode vibrational subsystem: Action on $\mathbb{C}P^2$. Action of several different point symmetry groups on the $\mathbb{C}P^2$ space was studied by Zhilinskii [17]. An example of the extension to a larger group including the time reversal $T$ was given later in [70]. We summarize the results of [17] for the symmetry groups $O$ and $T_d$ and then take the $T$ element into account.

The action of $T_d$ on the 3-space with coordinates $(q_1, q_2, q_3)$, which span the irreducible representation $F_2$, is effective, and the image corresponds to the whole group. Of course, the same holds for $(p_1, p_2, p_3)$ and $(z_1, z_2, z_3)$. In order to verify that the action of $T_d \times T$ on the $\mathbb{C}P^2$ space is also effective [17], we can consider the representation realized by $(z_1, z_2, z_3, \bar{z}_1, \bar{z}_2, \bar{z}_3)$, act by operations in $T_d \times T$ (use (3.1a) and Table 4), and take the $\mathbb{C}P^2$ restrictions (section 2.4.3) into account. In particular, due to the common phase equivalence, points $(z_1, z_2, z_3)$ and $(\bar{z}_1, \bar{z}_2, \bar{z}_3)$, are the same on $\mathbb{C}P^2$; i.e., the image of the 3-space inversion is identity. It follows that the images of the $T_d$, $O$, and $O_h$ point symmetry groups are the same (up to an isomorphism between the stabilizers), and we can simply use the $O$ group whose elements are proper rotations.

For any rotation axis $C_k$, we should consider a point in $\mathbb{C}P^2$ lying on the axis and a subspace orthogonal to the axis. The former is obviously an isolated fixed point, while the latter is a $\mathbb{C}P^1 \sim S^2$ subspace of $\mathbb{C}P^2$, which contains other $C_k$ symmetric points. As an example, take rotation about axis $z_1$ that can be most easily understood in the coordinates $z_1, \zeta = \frac{1}{\sqrt{2}}(z_2 + iz_3), \zeta' = \frac{1}{\sqrt{2}}(z_2 - iz_3),$ subject to the same restriction

$$|z_1|^2 + |\zeta|^2 + |\zeta'|^2 = 1$$

and common phase identification

$$(z_1, \zeta, \zeta') \equiv (z_1 e^{i\phi}, \zeta e^{i\phi}, \zeta' e^{i\phi})$$

as the initial $(z_1, z_2, z_3)$ in section 2.4.3. When we rotate about $z_1$ by angle $\varphi \neq 0$ so that

$$(z_1, \zeta, \zeta') \rightarrow (z_1, \zeta e^{i\varphi}, \zeta' e^{-i\varphi}),$$
the fixed point coordinates should satisfy equations

\[(z_1, \zeta e^{i\phi}, \zeta' e^{-i\phi}) = (z_1 e^{i\phi}, \zeta e^{i\phi}, \zeta' e^{i\phi}).\]

For all \(\varphi \neq \pi\) (and in particular for all \(\varphi = 2\pi/k\) with \(k > 2\)) we have three isolated solutions

\[A : \zeta = \zeta' = 0, \quad B : z_1 = \zeta = 0, \quad \text{and} \quad C : z_1 = \zeta' = 0;\]

i.e., two of the three coordinates should vanish. When \(\varphi = \pi\) (rotation \(C_2\)) our equations become

\[(z_1, -\zeta, -\zeta') = (z_1 e^{i\phi}, \zeta e^{i\phi}, \zeta' e^{i\phi}).\]

We should take the point \((1, 0, 0)\) and the whole \(\mathbb{C}P^1\) subspace with \(z_1 = 0\). (Set \(\phi = \pi\) to show explicitly that \((0, z_2, z_3)\) and \((0, -z_2, -z_3)\) is the same point of this \(C_2\)-invariant subspace.)

The action of the entire symmetry group \(O\) on the reduced phase space \(\mathbb{C}P^2\) is obtained if we apply the above principle to every rotation in \(O\). The groups \(T_d\) and \(O\) have the same action on \(\mathbb{C}P^2\). The action of \(T_d \times T\) then can be found as an extension by adding the \(T\) element. Results are summarized in Figure 10 reproduced from [17] and in Tables 10–12. Action of \(O\) on \(\mathbb{C}P^2\) has five critical orbits (five zero-dimensional strata) characterized in Table 10. It is important to notice that each of the three points on the \(D_3\) orbit correspond to a different (but conjugate) stabilizer; the same is true for the four points on the \(D_4\) orbit. In

\begin{table}[h]
\centering
\begin{tabular}{|c|c|}
\hline
fixed point & stabilizer \tabularnewline
\hline
\hline
\(D_{2d} \times T\) & \(O\) & \(T_d \times T\) \tabularnewline
\hline
\(C_{3v} \times T\) & \(D_3 \times T\) \tabularnewline
\hline
\(S_4 \times T\) & \(C_3 \times T\) \tabularnewline
\hline
\(C_3 \times T\) & \(C_2 \times T\) \tabularnewline
\hline
\end{tabular}
\caption{Orbits of the \(O\) (and \(T_d \times T\)) group action on the complex projective space \(\mathbb{C}P^2\) according to Zhilinskii [17]. Colored areas represent nine \(C_2\)-invariant spheres, which belong to the classes of three and six spheres (according to their stabilizers).}
\end{table}
Table 10

Zero-dimensional strata of the CP² space under the action of the image of the \( T_d \times T \) (or \( O \times T \) or \( O_h \times T \)) group in the representation spanned by bilinear combinations of vibrational coordinates \( q \) and conjugate momenta \( p \), which transform according to the triply degenerate representation \( F_2 \) of point symmetry group \( T_d \), \( O \), or \( O_h \).

<table>
<thead>
<tr>
<th>Orbit stabilizer (^{10}) ( T_d ) or ( O_h )</th>
<th>Coordinates (^{11}) on CP²</th>
<th>Point stabilizer (^{10}) ( T_d ) or ( O_h )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( D_{2d} \times T ) ( D_4 \times T )</td>
<td>( (1,0,0) ) ( D_4^{(x)} \times T ) ( D_2^{(x)} \times T )</td>
<td>( (1,0,0) ) ( D_4^{(x)} \times T ) ( D_2^{(x)} \times T )</td>
</tr>
<tr>
<td>( (0,1,0) ) ( D_4^{(y)} \times T ) ( D_2^{(y)} \times T )</td>
<td>( (0,0,1) ) ( D_4^{(z)} \times T ) ( D_2^{(z)} \times T )</td>
<td></td>
</tr>
<tr>
<td>( C_{3v} \times T ) ( D_3 \times T )</td>
<td>( (1,1,1) ) ( D_3^{(c)} \times T ) ( C_3^{(c)} \times T )</td>
<td>( (1,1,1) ) ( D_3^{(c)} \times T ) ( C_3^{(c)} \times T )</td>
</tr>
<tr>
<td>( (1,1,1) ) ( D_3^{(d)} \times T ) ( C_3^{(d)} \times T )</td>
<td>( (1,-1,1) ) ( D_3^{(d)} \times T ) ( C_3^{(d)} \times T )</td>
<td></td>
</tr>
<tr>
<td>( (0,1,1) ) ( C_3 \times T ) ( D_3^{(d)} \times T ) ( C_3^{(d)} \times T )</td>
<td>( (0,1,1) ) ( C_3 \times T ) ( D_3^{(d)} \times T ) ( C_3^{(d)} \times T )</td>
<td></td>
</tr>
<tr>
<td>( C_3 \times T ) ( C_3 \times T ) ( C_3 \times T )</td>
<td>( (0,1,1) ) ( C_3 \times T ) ( D_3^{(d)} \times T ) ( C_3^{(d)} \times T )</td>
<td></td>
</tr>
<tr>
<td>( C_3 \times T ) ( S_\infty \times T )</td>
<td>( (0,1,1) ) ( S_\infty \times T ) ( S_\infty \times T )</td>
<td></td>
</tr>
</tbody>
</table>

The case of the \( C_4 \), \( C_3 \), and \( D_2 \) orbits, one stabilizer corresponds to two different orbit points. Zero-dimensional strata of the action of the symmetry group \( O \times T \) and \( T_d \times T \) (where \( T \) acts as in (3.1a)) remain the same, but their stabilizers become larger. The order of the symmetry group \( O \times T \) is twice that of \( O \) and the order of all stabilizers is doubled. The structure of critical orbits also remains exactly the same except for the stabilizers. Each zero-dimensional stratum again consists of one orbit.

At the same time, two-dimensional invariant topological spheres \( S^2 \) with stabilizers \( C_2^{(a)} \), \( a = \{x, y, z\} \), and \( C_3^{(a)} \), \( \alpha = 1, \ldots, 6 \), of the \( T_d \) action on CP² (see Figure 10) become further stratified due to the action of the \( T \)-extended group. Below we detail the action of \( O \times T \) (and \( T_d \times T \)) on these invariant manifolds.

Stratification of each of the three \( C_2 \)-invariant \( S^2 \) spheres is equivalent to the natural action of the \( D_{2h} \) point symmetry group (see Figure 11, left). The generic two-dimensional

\(^{10}\)We give notation for \( T_d \), and \( O \) or \( O_h \) groups.

\(^{11}\)Coordinates in terms of \((z_1, z_2, z_3), \eta = \exp(i\pi/3)\).
stratum has stabilizer $C_2$; three isolated (critical) two-point orbits with stabilizers $D_{2d} \wedge T$, $S_4 \wedge T$, and $C_{2v} \wedge T$ are described in Table 10; three one-dimensional strata with stabilizers $C_2 \wedge g$, where $g = T$, $T_2$, or $T_5$, are listed in Table 11. Together with isolated fixed points, these strata form $C_2 \wedge g$-invariant circles $S^1$.

Stratification of the six topological $S^2$ spheres with stabilizers $C_s^{(a)}$ deserves special comment. Each such sphere has one exceptional two-point critical orbit with stabilizer $C_3 v \wedge T$ (see Figure 12, left). This orbit cannot be found if we consider only those symmetry operations that act within the $C_s^{(a)}$-invariant sphere, its presence is due to the action of the symmetry group $T_d \times T$ on the entire $CP^2$ space. Disregarding the exceptional $C_3 v \wedge T$ orbit, we can identify the action of the symmetry group $T_d \times T$ within each $C_s^{(a)}$ sphere with the natural action of the $C_{2v}$ point group (on a sphere in a 3-space). This action has two critical one-point orbits with global stabilizers $D_{2d} \wedge T$ and $C_{2v} \wedge T$ (Table 10), which lie on the $C_2$ axis (horizontal axis of the leftmost sphere in Figure 12) and two different one-dimensional families of orbits with stabilizers $C_s \wedge g$, where $g = T$ or $T_2$ (Table 11). Except for the $C_{2v}$ and $D_{2d}$ points, all other points form two-point orbits of the spatial subgroup $C_2$. The $C_s \wedge g$ invariant circles combine respective one-dimensional strata and fixed points.

All two-dimensional invariant subspaces of the $T_d \times T$ group action on $CP^2$ are described in Table 12. In addition to the two types of invariant spheres $S^2$, this action has a number of other two-dimensional invariant subspaces whose stabilizers $T$, $T_2$, and $T_5$ include reversing symmetries. Generic stratum on the $T$, $T_2$, and $T_5$ invariant subspaces includes orbits with
Table 11
One-dimensional strata on the \( \mathbb{C}P^2 \) space under the same group action as in Table 10.

| Orbit stabilizer & Coordinates & Point stabilizer |
|------------------|-----------------|------------------|
| \( T_d \) & \( O \) or \( O_h \) & \( T_d \) |
| \( C_2 \wedge T \) & \( C_2 \wedge T \) & \( C_2^{(z)} \wedge T \) |
| \( C_2 \wedge T_2 \) & \( C_2 \wedge T_2 \) & \( C_2^{(z)} \wedge T_2 \) |
| \( C_2 \wedge T_s \) & \( C_2 \wedge T_2^{(d)} \) & \( C_2^{(z)} \wedge T_2^s \) |
| \( C_2 \wedge T \) & \( C_2^{(d)} \wedge T \) & \( C_2^{(z)} \wedge T_2 \) |
| \( C_2 \wedge T_2 \) & \( C_2 \wedge T_2^{(d)} \) & \( C_2^{(z)} \wedge T_2^s \) |

24, 8, and 4 points, respectively. The topology of all these subspaces is \( \mathbb{R}P^2 \).

4.4. Rotational structure of the \( E \) mode: Action on \( \mathbb{C}P^1 \times S^2 \sim S^2 \times S^2 \). The Hamiltonian that describes rotational structure of the \( E \)-mode polyads is defined on the four-dimensional reduced rotation–vibration phase space \( \mathbb{C}P^1 \times S^2 \), the direct product of the vibrational \( E \)-mode polyad space \( \mathbb{C}P^1 \) (polyad sphere) and rotational sphere \( S^2 \). We use

\[ \text{Here } a \neq 0, \pm 1, \infty, \text{ and } \eta = e^{i \varphi}, \text{ where } \varphi \neq k\pi/2. \]
information on the stratification of the individual factor spaces $\mathbb{C}P^1$ (section 4.2) and $\mathbb{S}^2$ (section 4.1) in order to find the stratification of $\mathbb{C}P^1 \times \mathbb{S}^2$.

Let $(v)$ and $(r)$ be points on $\mathbb{C}P^1$ and $\mathbb{S}^2$, respectively, and let $(v, r)$ denote points on the rovibrational (i.e., rotational-vibrational) space $\mathbb{C}P^1 \times \mathbb{S}^2$. The stabilizer $G_{v,r}$ of point $(v, r)$ is an intersection $G_v \cap G_r$ of stabilizers on $\mathbb{C}P^1$ and $\mathbb{S}^2$. In simple terms, the symmetry of $(v, r)$ can only be lower than that of its projections $(v)$ and $(r)$. The dimension of the stratum \{$(v, r)$\} on $\mathbb{C}P^1 \times \mathbb{S}^2$ is the sum of the dimensions of strata \{$(v)$\} and \{(r)\}. The stratum \{(v, r)\} on the product space is connected if both its projections \{$(v)$\} and \{(r)\} on the two factor subspaces are connected.

Most important and basic to our analysis are critical orbits $(v, r)$. Such orbits can either be nonconnected parts of a nonzero-dimensional stratum or belong to a stratum \{(v, r)\} of dimension zero. These latter strata occur when both strata \{(r)\} and \{(v)\} have dimension zero and there is no stratum of nonzero dimension with stabilizer $G_r \cap G_v$.

Using the lattice of conjugate subgroups of $\mathcal{T}_d \times \mathcal{T}$ in Figure 8, where we indicated all possible stabilizers $G_v$ and $G_r$, the reader can easily find the intersections $G_v \cap G_r$ and then look up the details of the structure of the particular subgroups in Table 2. Indeed, all subgroups of a given stabilizer $G$ are found by descending along the lattice paths which originated

\begin{table}[h]
\centering
\caption{Two-dimensional invariant subspaces of $\mathbb{C}P^2$ under the same group action as in Tables 10 and 11.}
\begin{tabular}{|c|c|c|c|c|}
\hline
Orbit stabilizer & Coordinates & Point stabilizer & Topology \\
\hline
$C_2$ & $C_2$ & \{(1, w, 0)\} & $S^2$ \\
& & \{(1, 0, w)\} & \\
& & \{(0, 1, w)\} & \\
$C_2$ & $C_2^{(d)}$ & \{(1, 1, w)\} & $S^2$ \\
& & \{(1, -1, w)\} & \\
& & \{(1, w, 1)\} & \\
& & \{(1, w, -1)\} & \\
& & \{(1, w, w)\} & \\
& & \{(1, w, -w)\} & \\
\hline
$T$ & $T$ & \{(1, a, b)\} & $\mathbb{R}P^2$ \\
& & \{(1, a, ib)\} & \\
& & \{(1, ia, b)\} & \\
& & \{(1, ia, ib)\} & \\
$T_2$ & $T_2$ & \{(1, w, w)\} & $\mathbb{R}P^2$ \\
& & \{(1, w, -w)\} & \\
& & \{(1, a\eta, \eta^2)\} & \\
& & \{(1, a\eta, -\eta^2)\} & \\
& & \{(1, \eta^2, a\eta)\} & \\
& & \{(1, -\eta^2, a\eta)\} & \\
& & \{(1, -\eta^2, a\eta)\} & \\
\hline
\end{tabular}
\end{table}

\footnote{We give notation for either the $T_d$, $O$, or $O_h$ group.}
\footnote{Here $a$, $b$ are real, $w$ is a complex number, and $\eta = e^{i\varphi}$.}
Intersection (correlation) of stabilizers of the $T_d \times T$ group action on the E-mode polyad phase space $\mathbb{C}P^1$ (left column) and on the rotational phase space $\mathbb{S}^2$ (top row). For information on the notation and structure of subgroups of $T_d \times T$ refer to Table 2. Critical orbits on $\mathbb{C}P^1 \times \mathbb{S}^2$ are underlined.

![Table 13](image)

4.4.1. Noncritical orbits. Generic points $(r)$ on $\mathbb{S}^2$ have stabilizer $G_r = C_1$ (rightmost column in Table 13). Obviously, these points lift to points $(v, r)$ with trivial symmetry $C_1$ regardless of the stabilizer $G_v$. The generic stratum \{v, r\} is of dimension four, has stabilizer $C_1$, and includes 48-point orbits.

Generic points $(v)$ on $\mathbb{C}P^1$ (bottom row in Table 13) have stabilizer $D_2$, which has three order-two subgroups $C_2$ with axes $\eta = \{x, y, z\}$. Intersection of $D_2$ with stabilizers $G_v$ equals $C_1$ in all cases except for the three conjugate subgroups $G^v_\eta = S_4^\eta \wedge T_3$. Intersection $G^v_\eta \cap D_2$ is the particular $C_2$ subgroup of $D_2$. The corresponding $C_2$ stratum on $\mathbb{C}P^1 \times \mathbb{S}^2$ includes 24-point orbits. Since $S_4^\eta \wedge T_3$ points on $\mathbb{S}^2$ are critical (fixed), this stratum has dimension two.

The stabilizer $G_v = D_3 \wedge T$ of the one-dimensional stratum on $\mathbb{C}P^1$ is an invariant subgroup of $T_d \times T$; its intersection with subgroups $G_r$ of the same class of conjugate subgroups of $T_d \times T$ results again in conjugate subgroups. For $G_r = S_3 \wedge T_3$ the intersection is $C_2 \times T_2$ and the stratum \{v, r\} has dimension one. If $G_r = T_2^b$, where $b = \{x, y, z\}$, we have a two-dimensional strata at $G$. The highest node, where the paths descending from $G_v$ and $G_r$ join, is the intersection $G_v \cap G_r$, i.e., the largest common subgroup of $G_v$ and $G_r$. All possible intersections are summarized in Table 13. We comment on them below starting with the low-symmetry strata.

For each space, strata of dimensions zero, one, and two are marked as 0D, 1D, and 2D; the number of different conjugate stabilizers in the same class of $T_d \times T$ is given in parentheses. Right superscripts define concrete conjugate stabilizers: $\eta$ and $\xi$ label axes $(x, y, z)$ for orbits on $\mathbb{C}P^1$ and $\mathbb{S}^2$, respectively; $(k)$ and $\beta$ distinguish stabilizers of orbits on $\mathbb{S}^2$ in the $C_3$ class and the $\sigma$ class; they can take four and six values, respectively.

17 $\eta = \xi$; axes $\eta$ and $\xi$ are the same.
18 $\eta \neq \xi$; axes $\eta$ and $\xi$ are different.
19 $\beta = \{\eta_1, \eta_2\}$; stabilizer of the orbits on $\mathbb{S}^2$ of index $(\beta)$ includes one of the two operations of index $\{\eta_1, \eta_2\}$; see text for examples.
20 $\beta \neq \{\eta_1, \eta_2\}$; stabilizer of the orbits on $\mathbb{S}^2$ of index $(\beta)$ does not include operations of index $\{\eta_1, \eta_2\}$.
family \{v, r\} of 24-point orbits with symmetry \(T_2^3\). If \(G_v = C_s \wedge T_2\), the intersection is again \(T_2\); i.e., isolated fixed points \(r\) on \(S^2\) with stabilizer \(C_s \wedge T_2\). Since the zero-dimensional stratum \(C_s \wedge T_2\) on \(S^2\) is the closure of the one-dimensional stratum \(T_2\) on \(S^2\), the entire \(T_2\) stratum \(\{v, r\}\) is connected. As a consequence, isolated points \((r)\) with stabilizer \(C_s \wedge T_2\) lift to noncritical points \((v, r)\) on the two-dimensional stratum on \(\mathbb{C}P^1 \times S^2\).

When both \(G_v\) and \(G_r\) are not invariant subgroups, the symmetry of the \(\{v, r\}\) stratum depends on the choice of the subgroup within the class of conjugate subgroups. In the case of \(G_v = D_2 \wedge T_s\) and \(G_r = T_s\) the intersection can be either \(T_s\) or \(C_1\). As shown in Table 2, the element \(C_{y}^3\), where \(a = \{x, y, z\}\), of \(D_2 \wedge T_s\) distinguishes a particular stabilizer in the class of three conjugate subgroups. This stabilizer has two \(T_s\) subgroups generated by \(T_s^{a_1}\) and \(T_s^{a_2}\). If, therefore, \(G_r\) is one of these two subgroups, then its intersection with \(G_v\) is nontrivial; otherwise \(G_v \cap G_r = C_1\). In the case of \(G_v = D_2 \wedge T_s\) and \(G_r = T_2\) the intersection is always trivial. On the other hand, intersection of \(G_v = D_2 \wedge T_s\) and \(C_3 \wedge T_s\) is always a nontrivial subgroup \(T_s\) because one of the two orthogonal symmetry planes \(T_s^{a_1, 2}\) in \(D_2 \wedge T_s\) always contains the particular axis \(C_3\) of \(C_3 \wedge T_s\). In other words, intersection of the set of two \(T_s\) elements in \(D_2 \wedge T_s\) and three \(T_s\) elements in \(C_3 \wedge T_s\) (which cross on the \(C_3\) axis) is never empty. Observe that the \(T_s\) stratum \(\{v, r\}\) has dimension two and is connected. All points in Table 13 that lift to this stratum become noncritical; the \(\{v, r\}\) parts of dimensions zero and one form the closure.

### 4.4.2. Critical orbits (strata of dimension zero)

Orbits that project on zero-dimensional strata of \(\mathbb{C}P^1\) and \(S^2\) and have unique stabilizers are critical. The six critical orbits on \(\mathbb{C}P^1 \times S^2\) are characterized below.

| Stabilizer on \(\mathbb{C}P^1\) | \(T \wedge T_s\) | \(D_{2d} \times T\) | \(D_{2d} \times T\) |
| Stabilizer \(\mathbb{C}P^1 \times S^2\) | \(C_3 \wedge T_s\) | \(S_4 \wedge T_s\) | \(C_2 \wedge T_2\) |
| Number of orbits | 2 | 2 | 2 |
| Number of points in orbit | 8 | 6 | 12 |

We explain how to find these orbits using Table 13.

Consider the stratum \(\{v\}\) with stabilizer \(G_v = T \wedge T_s\), which consists of one two-point orbit, and the stratum \(\{r\}\) with stabilizer \(G_r = C_3 \wedge T_s\), which consists of one eight-point orbit. Since each of the four conjugate subgroups \(G_r\) is a subgroup of \(G_v\), we have the zero-dimensional stratum \(\{v, r\}\) with stabilizer \(C_3 \wedge T_s\), which includes two eight-point orbits (all points on the orbit \(\{r\}\) lift to the same orbit \(\{v, r\}\)). If for the same \(\{v\}\) we consider \(\{r\}\) with stabilizer \(G_r = S_4 \wedge T_s\), the resulting 12-point orbit \(\{v, r\}\) has the stabilizer \(C_2 \times T_s\) and should, therefore, be part of a one-dimensional stratum. Indeed, as can be seen from Figure 8,

\[
T \wedge T_s \cap S_4 \wedge T_s = D_2 \wedge T_s \cap S_4 \wedge T_s = C_2 \times T_s.
\]

Consider now the stratum \(\{v\}\) with stabilizer \(G_v = D_{2d} \times T\), which again consists of one two-point orbit. The intersection of \(G_v\) with \(G_r = S_4 \wedge T_s\) can be the whole \(G_r\) (i.e., \(G_r\) can be the subgroup of \(G_v\) if both subgroups include the same element \(C_{y}^3\), where axis \(\eta\) can be \(x, y,\) or \(z\)). In this case we have a zero-dimensional stratum \(\{v, r\}\) with stabilizer \(S_4 \wedge T_s\), which includes two six-point orbits (all points on the six-point orbit \(\{r\}\) lift to the same orbit \(\{v, r\}\)). If for the same \(\{v\}\) we take \(\{r\}\) with stabilizer \(G_r = C_s \wedge T_2\), this latter stabilizer can
Intersection (correlation) of stabilizers of the $T_d$ group action on the $F_2$-mode vibrational phase space $\mathbb{C}P^2$ (left column), on the rotational phase space $S^2$ (top row, center), and on the $E$-mode vibrational phase space $\mathbb{C}P^1$ (top row, right). Critical orbits are underlined.

<table>
<thead>
<tr>
<th>Strata$^{21}$ on $\mathbb{C}P^2$</th>
<th>Strata$^{21}$ on $S^2$</th>
<th>Strata$^{21}$ on $\mathbb{C}P^1$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$0D; D_{2d}^{(\eta)}$ $\eta \leq 3$</td>
<td>$S_4^{(\eta')}$ $C_3^{(k')}$ $C_v^{(\beta')}$ $C_1$</td>
<td>$D_2$ $D_{2d}^{(\eta')}$ $D_2$</td>
</tr>
<tr>
<td>$0D; S_4^{(\eta)}$ $\eta \leq 3$</td>
<td>$S_4^{22}$ $C_1^{23}$</td>
<td>$C_2$ $S_4^{22}$ $C_2$</td>
</tr>
<tr>
<td>$0D; C_3^{(k)}$ $k \leq 4$</td>
<td>$C_1$ $C_3^{22}$ $C_1^{23}$ $C_1$</td>
<td>$C_3$ $C_s$ $C_1$</td>
</tr>
<tr>
<td>$0D; C_3^{(k)}$ $k \leq 4$</td>
<td>$C_1$ $C_3^{22}$ $C_1^{23}$ $C_1$</td>
<td>$C_3$ $C_1$ $C_1$</td>
</tr>
<tr>
<td>$0D; C_2^{(\eta)}$ $\eta \leq 3$</td>
<td>$C_2^{22}$ $C_1^{23}$</td>
<td>$C_2$ $C_2^{22}$ $C_2$</td>
</tr>
<tr>
<td>$2D; C_2^{(\eta)}$ $\eta \leq 3$</td>
<td>$C_2^{22}$ $C_1^{23}$</td>
<td>$C_2$ $C_2^{22}$ $C_2$</td>
</tr>
<tr>
<td>$2D; C_3^{(\beta)}$ $\beta \leq 6$</td>
<td>$C_1$ $C_1$ $C_3^{22}$ $C_1^{23}$</td>
<td>$C_1$ $C_3^{24}$ $C_1$</td>
</tr>
<tr>
<td>$4D; C_1$</td>
<td>$C_1$ $C_1$ $C_1$ $C_1$</td>
<td>$C_1$ $C_1$ $C_1$</td>
</tr>
</tbody>
</table>

again be a subgroup of $G_v$ if both share the same $C_s = \sigma$ element, which can be either $\sigma^{m}$ or $\sigma^{p2}$ (see Table 2). Since in this case $\{r\}$ consists of one 12-point orbit, the corresponding zero-dimensional $\{v, r\}$ stratum with stabilizer $C_s \times T_2$ contains two 12-point orbits.

4.5. Rotational structure of the $F_2$ mode: Action of $T_d$ and $T_d \times T$ on $\mathbb{C}P^2 \times S^2$. We now combine small-amplitude $F_2$-mode vibrations and rotation. The Hamiltonian of this system is a $(T_d \times T)$-invariant function on the six-dimensional reduced phase space $\mathbb{C}P^2 \times S^2$. The action of the full symmetry group $T_d \times T$ on $\mathbb{C}P^2 \times S^2$ can be found from that on the individual spaces $\mathbb{C}P^2$ and $S^2$ using the approach of the previous section; in particular, we

---

$^{21}$Strata of dimension $s$ are marked as $sD$, $s = 0, 1, 2, 4$. Classes of stabilizers of the strata are listed in $T_d$ notation. Indexes $\eta$, $k$, $\beta$ distinguish different stabilizers on $\mathbb{C}P^2$ within the same class; indexes $\eta'$, $k'$, $\beta'$ are used for $S^2$ or $\mathbb{C}P^1$. Refer to Table 2 for information on the notation and structure of subgroups of $T_d \times T$.

$^{22}$Identical subgroups of $T_d \times T$: axes $\eta$ and $\eta'$, $k$ and $k'$, or subgroups $\beta$ and $\beta'$ are the same, i.e., $\eta \equiv \eta'$, $k \equiv k'$, or $\beta \equiv \beta'$.

$^{23}$Different subgroups of $T_d \times T$ of the same class: axes $\eta$ and $\eta'$, $k$ and $k'$, or subgroups $\beta$ and $\beta'$ are different, i.e., $\eta \neq \eta'$, etc.

$^{24}$Subgroups $D_{2d}^{(\eta')}$, $C_{2v}^{(\eta')}$, $C_3^{(k')}$ include the symmetry plane $\beta'$.

$^{25}$$\beta'$ equals $\eta_1$ or $\eta_2$; the point projects on the disconnected zero-dimensional component of the $C_s^{(1)}$ or $C_s^{(2)}$ stratum on $\mathbb{C}P^2$; see section 4.5.1.
determine intersections of stabilizers from the subgroup lattice of $T_d \times T$.

Essential information can be obtained from the simpler study of the action of the spatial
symmetry group $T_d$ whose subgroup lattice is given in Figure 1. As shown in Table 14, the
action of $T_d$ on the rotation–vibration space $\mathbb{CP}^2 \times S^2$ creates strata of symmetry $S_4$, $C_2$, $C_3$, $C_s$, and $C_1$ (generic). Some strata, notably $C_s$, have disconnected components of different
dimension. By dimension of these strata, we mean the highest dimension of their components.
The $C_1$ stratum has dimension six, components of other strata can be of dimension zero
and two.

4.5.1. Strata and components of dimension zero (critical orbits). The $S_4$ stratum on
$\mathbb{CP}^2 \times S^2$ projects on the $S_4$ orbits on the rotational space $S^2$ and on the $D_{2d}$ or $S_4$ orbits
on the vibrational space $\mathbb{CP}^2$. Each $G_r = S_4^{(\eta)}$ stabilizer has two fixed points on $S^2$ (which
belong to the same orbit of the $T_d$ action). Each $G_v = D_{2d}^{(\eta)}$ stabilizer has one fixed point on
$\mathbb{CP}^2$ (see Table 10). Consequently, there are two points on $\mathbb{CP}^2 \times S^2$ with the same stabilizer

$$G_r \cap G_v = D_{2d}^{(\eta)} \cap S_4^{(\eta)} = S_4^{(\eta)}.$$  

The six points corresponding to three different conjugate stabilizers with $\eta = x, y, z$ form one
six-point orbit, which we label $A^{(4)}$. If for the same $G_r$ we take $G_v = S_4^{(0)}$, we combine two
points on $\mathbb{CP}^2$ (which are in the same orbit) with two points on $S^2$. It is important to observe
that the resulting four points on $\mathbb{CP}^2 \times S^2$ belong to two different orbits: one pair belongs to
orbit $B^{(4)}$ and another to orbit $C^{(4)}$. With three possible axes $\eta$ taken into account, orbits $B$
and $C$ contain six points each.

The above description of the $S_4$ orbits $B^{(4)}$ and $C^{(4)}$ can be easily verified on a concrete
example. Such examples are given in Table 15, where the $E$-mode coordinates $(z_4, z_5)$ should
at present be ignored. Consider a particular axis $\eta = z$ (axis 3). The two fixed points on the
$\mathbb{CP}^2$ space have coordinates (Table 10)

$$(4.1a) \quad (z_1, z_2, z_3) = (1, \pm i, 0),$$

and the coordinates of the two fixed points on the $S^2$ sphere are

$$ (4.1b) \quad (j_1, j_2, j_3) = (0, 0, \pm 1).$$

(For simplicity, here and in the rest of this section, we drop normalization factors, which
are not essential to our current discussion.) The group $T_d$ acts on $\mathbb{CP}^2$ and $S^2$ in such a way
that any operation in $T_d$ that interchanges the two points (4.1a) on $\mathbb{CP}^2$ interchanges the two
points (4.1b) on $S^2$. The $C_2$ rotation about axis $x$ (axis 1) is an example:

$$C_2^x : (z_1, z_2, z_3; j_1, j_2, j_3) \rightarrow (z_1, -z_2, -z_3; j_1, -j_2, -j_3).$$

As a result, no operation in $T_d$ maps points

$$B = (1, \pm i, 0; 0, 0, \pm 1) \quad \text{and} \quad C = (1, \pm i, 0; 0, 0, \mp 1)$$

of the $\mathbb{CP}^2 \times S^2$ space into each other; these points, therefore, belong to different orbits.
The three eight-point critical orbits of the $C_3$ stratum can be described analogously; cf. Table 15(b). Combination of the $C^{(k)}_{3v}$ point on $\mathbb{C}P^2$ and two $C^{(k)}_{3}$ points on $S^2$ gives two points on the $A^{(3)}$ orbit. With all four axes $C_3$ taken into account ($k = 1, \ldots, 4$), the orbit has eight points. The $B^{(3)}$- and $C^{(3)}$-type orbits of the $C_3$ action include points $(z, j)$ and $(z, -j)$, respectively, where $(z)$ and $(j)$ stand for the coordinates of the fixed point on $\mathbb{C}P^2$ and $S^2$.

The two critical fixed points of the $C^{(a)}_s$ action on $\mathbb{C}P^2 \times S^2$ are obtained when we combine the only isolated fixed point of the $C^{(a)}_s$ action on $\mathbb{C}P^2$ (see Table 10) with the two respective points on $S^2$ (recall that $C_s$ acts both on $\mathbb{C}P^2$ and on $S^2$ as operation $C_2$ of the $O$ group). In the particular case of $C^{(z)}_{2v}$ and its subgroup $C^{(xy)}_s$ (set $\eta = z$ and $\beta' = \eta_1 = xy$ in Table 14), we combine the $z = (1, -1, 0)$ fixed point of the $C^{(xy)}_s$ action on $\mathbb{C}P^2$ with two points $j = \pm(1, -1, 0)$ on $S^2$. For six conjugate elements $C_s$, we obtain a 12-point orbit, which is isolated from the rest of the $C_s$ stratum (because its projection on the $\mathbb{C}P^2$ space is isolated). This orbit is therefore critical.

### Table 15

Fixed points of the $T_3 \times T$ group action on the reduced phase space $\mathbb{C}P^2 \times \mathbb{C}P^1 \times S^2$.

| (a) Stabilizer $S^2_1$ (or $C_4$), $r_f = \sqrt{N_f}$, $r_c = \sqrt{2N_c}$, $r_j = J$. |
|---|---|---|---|---|---|---|---|---|
| Point | $z_1/r_f$ | $z_2/r_f$ | $z_3/r_f$ | $z_4/r_f$ | $z_5/r_c$ | $j_1/r_j$ | $j_2/r_j$ | $j_3/r_j$ |
| $A_1$ | 0 | 0 | $\sqrt{2}$ | 1 | 0 | 0 | 0 | 1 |
| $A_2$ | 0 | 0 | $\sqrt{2}$ | 1 | 0 | 0 | 0 | $-1$ |
| $A_4$ | 0 | 0 | $\sqrt{2}$ | 0 | 1 | 0 | 0 | 0 |
| $B_1$ | 1 | $i$ | 0 | 1 | 0 | 0 | 0 | 0 |
| $B_2$ | 1 | $-i$ | 0 | 1 | 0 | 0 | 0 | 0 |
| $B_4$ | 1 | $i$ | 0 | 0 | 1 | 0 | 0 | 0 |
| $C_1$ | 1 | $i$ | 0 | 1 | 0 | 0 | 0 | 0 |
| $C_4$ | 1 | $-i$ | 0 | 1 | 0 | 0 | 0 | 0 |
| $C_4$ | 1 | 0 | 0 | 1 | 0 | 0 | 0 | 0 |

| (b) Stabilizer $C_3 [111]$, $r_f = (\sqrt{2N_f})/\sqrt{3}$, $r_c = \sqrt{N_c}$, $r_j = \sqrt{3}J$, $\chi = \exp(2\pi i/3)$. |
|---|---|---|---|---|---|---|---|---|
| Point | $z_1/r_f$ | $z_2/r_f$ | $z_3/r_f$ | $z_4/r_f$ | $z_5/r_c$ | $j_1/r_j$ | $j_2/r_j$ | $j_3/r_j$ |
| $A_1$ | 1 | 1 | 1 | 1 | $i$ | 1 | 1 | 1 |
| $A_2$ | 1 | 1 | 1 | 1 | $i$ | $-1$ | $-1$ | $-1$ |
| $B_1$ | 1 | $\chi$ | $\bar{\chi}$ | 1 | $i$ | 1 | 1 | 1 |
| $B_2$ | 1 | $\chi$ | $\bar{\chi}$ | 1 | $i$ | $-1$ | $-1$ | $-1$ |
| $C_1$ | 1 | $\chi$ | $\bar{\chi}$ | 1 | $i$ | $-1$ | $-1$ | $-1$ |
| $C_2$ | 1 | $\chi$ | $\bar{\chi}$ | 1 | $i$ | 1 | 1 | 1 |

| (c) Stabilizer $C_{s}^{xy}$ (or $C_2$), $r_f = \sqrt{N_f}$, $r_c = \sqrt{2N_c}$, $r_j = J/\sqrt{2}$. |
|---|---|---|---|---|---|---|---|---|
| Point | $z_1/r_f$ | $z_2/r_f$ | $z_3/r_f$ | $z_4/r_f$ | $z_5/r_c$ | $j_1/r_j$ | $j_2/r_j$ | $j_3/r_j$ |
| $A_1$ | 1 | $-1$ | 0 | 1 | 0 | 1 | $-1$ | 0 |
| $A_2$ | 1 | $-1$ | 0 | 0 | 1 | $-1$ | 1 | 0 |
4.5.2. Strata of dimension two. Action of $T_4$ on $\mathbb{C}P^2 \times S^2$ creates two strata of dimension two, $C_2$ and $C_s$. The $C_s$ stratum has a disconnected component of dimension zero, described above. In both cases, we combine isolated fixed points on the rotational space $S^2$ and points on the invariant spheres $S^2 \subset \mathbb{C}P^2$. This is illustrated in Figure 11 and 12.

We describe first the $C_2$ stratum. Since $C_2 = S^2_4$, points with local symmetry $C_2$ and $S_4$ coincide on the rotational space $S^2_4$. In the particular example of $C^2_4 = (S^2_4)^2$ these points are given in (4.1b). We combine points on $S^2_4$ with points on the $C_2$-invariant sphere in $\mathbb{C}P^2$. In our $C^2_4$ example, these latter points are (see Table 12)

$$(z_1, z_2, z_3) = (1, w, 0), \quad \text{Re} \, w \neq 0.$$  

All points on $\mathbb{C}P^2 \times S^2$ with stabilizer $C^2_4$ are

$$(z_1, z_2, z_3; j_1, j_2, j_3) = (1, w, 0; 0, 0, \pm 1), \quad \text{Re} \, w \neq 0.$$  

Removing the above restriction on $w$ adds four critical points $(1, \pm i, 0; 0, 0, \pm 1)$ with stabilizer $S^2_4$ and produces two spheres shown in Figure 11, right. These are the only isolated critical points which remain on the $C_2$-invariant spheres when we add rotation; all other fixed points which lie on the $C_2$-invariant sphere of the purely vibrational system with phase space $\mathbb{C}P^2$ (i.e., when $j = 0$) disappear. For example, consider the two $D_{2d}$ points $z = (1, 0, 0)$ and $(0, 1, 0)$ with stabilizers $D^x_2$ and $D^y_2$, respectively (Table 10 and Figure 11, left). Their rotational coordinates should necessarily be $j = (1, 0, 0)$ and $(0, 1, 0)$, which project to points on $S^2$ with stabilizers $S^x_4$ and $S^y_4$, respectively.

A similar approach can be used to describe the $C_s$-invariant spheres (the two-dimensional component of the $C_s$ stratum) in the $\mathbb{C}P^2 \times S^2$ space shown in Figure 12, right. In this case, no critical points remain on the spheres when rotation is added and we lift from $\mathbb{C}P^2$ to $\mathbb{C}P^2 \times S^2$. As an example, consider the reflection plane $x = y$ whose action is given in Table 4. This operation has two fixed points on the rotational sphere $S^2_4$:  

$$(j_1, j_2, j_3) = (\pm 1, \mp 1, 0).$$  

(At these points, axial vector $j$ is orthogonal to the plane $x = y$.) Operation $C^{xy}_s$ is a combination of inversion and rotation by $\pi$ about axis $x = -y$, i.e., $(1, -1, 0)$. The points on the $\mathbb{C}P^1 \sim S^2$ subspace orthogonal to this axis have, therefore, coordinates (see Table 12)

$$(z_1, z_2, z_3) = (1, 1, w),$$  

and the points of the two $C_s$-invariant spheres $S^2$ in the six-dimensional space $\mathbb{C}P^2 \times S^2$ are

$$(z_1, z_2, z_3; j_1, j_2, j_3) = (1, 1, w; \pm 1, \mp 1, 0).$$  

Stabilizers of critical points, which are present on the $C_s$-invariant sphere when $j = 0$ (Figure 12, left), are such that these points become noncritical when rotation is added. Thus, the $C_{2v}$ point with $z = (1, 1, 0)$, which lies on the $C^{xy}_s$-invariant sphere of our example, has the stabilizer $C^s_2$ and must, therefore, combine with $j = (0, 0, 1)$ in order to have a higher stabilizer.
4.5.3. Extension by time reversal $T$. The action of the full group $T_d \times T$ on the $\mathbb{C}P^2 \times S^2$ space creates more strata. For our purposes, however, it is sufficient to observe that the system of critical orbits of $T_d \times T$ remains the same, as in the case of $T_d$, and to study the action of reversal operations on the invariant spheres with stabilizers $C_2$ and $C_s$.

Internal stratification of the $C_2$-invariant spheres in the $\mathbb{C}P^2 \times S^2$ space under the action of $T_d \times T$ is shown in Figure 11, right. It can be seen that the action of $T_d \times T$ on these spheres is equivalent to the natural action of the $C_{2v}$ group (whose axis $C_2$ is the vertical axis in Figure 11). In addition to the two isolated $S_4$ points, this action creates one-dimensional strata with stabilizers $C_2 \times T_2$ and $C_2 \times T_s$.

The $C_s$-invariant spheres also do not remain homogeneous when reversal operations are accounted for properly. The action of $T_d \times T$ on these spheres is equivalent to that of the group $C_h$ (whose reflection plane is the plane of Figure 12); it creates a $(C_s \land T_2)$-invariant circle on each $C_s$-invariant sphere in $\mathbb{C}P^2 \times S^2$.

4.6. Action on the vibrational subspace $\mathbb{C}P^2 \times \mathbb{C}P^1$. Description of combined small-amplitude $E$- and $F_2$-mode vibrations requires the six-dimensional reduced phase space $\mathbb{C}P^2 \times \mathbb{C}P^1$. The action of the $T_d \land T$ symmetry group on the $F_2$-mode subspace $\mathbb{C}P^2$ and on the whole of $\mathbb{C}P^2 \times \mathbb{C}P^1$ is effective. The action of $T_d \times T$ on the $E$-mode subspace is not effective; see Table 14: any point on this subspace is automatically $D_2$-invariant.

4.6.1. Critical orbits. All critical orbits on $\mathbb{C}P^2 \times \mathbb{C}P^1$ can be found and classified if we combine points from Tables 8 and 10 and determine the intersection of their stabilizers $G_f \cap G_e$ using the lattice from Figure 2, 3, or 8. To find whether the point (orbit) is critical, we consider the stratum with stabilizer $G_f \cap G_e$ and verify that we deal with an isolated point (orbit) using projections on the orbit spaces in Figures 9 and 10. As in the previous sections, we should combine points with identical stabilizers in order to determine the number of orbits and of points in the orbits. Concrete examples can be found in Table 15 if we ignore the rotational part (i.e., let $j = 0$). Results are summarized below.

Here the superscripts $^{(4)}$, $^{(3)}$, and $^{(2)}$ correspond to parts (a), (b), and (c) of Table 15; by $k+k$ we denote two $k$-point orbits.

4.6.2. Invariant subspaces of $\mathbb{C}P^2 \times \mathbb{C}P^1$. Three $D_{2d}$-invariant points on $\mathbb{C}P^2$ are the only points whose stabilizer includes $D_2$. Combining these points with the whole $E$-mode space $\mathbb{C}P^1 \sim S^2$ gives three $D_2$-invariant spheres $S^2$ in the six-dimensional space $\mathbb{C}P^2 \times S^2$. Six $C_s$-invariant spheres on $\mathbb{C}P^2$ combined with the $E$-space give 12 $C_s$-invariant spheres $S^2$ in $\mathbb{C}P^2 \times S^2$. The stabilizer $D_3$ of the $E$-mode space $\mathbb{C}P^1 \sim S^2$ has three conjugate $C_3^0$ subgroups with $a = \{x, y, z\}$. Consequently, there are three $C_2$-invariant subspaces $S^2_{(F)} \times S^2_{(E)}$. Points with higher symmetry lie on each of the above subspaces.
4.7. Action on the full reduced phase space \( \mathbb{C}P^2 \times \mathbb{C}P^1 \times S^2 \). In order to describe the simultaneous rotation and small amplitude \( E \)- and \( F_2 \)-mode vibrations of the \( A_4 \) molecule (rotational structure of all combination polyads \( nu_2 + mv_3 \)), we need the eight-dimensional total classical reduced phase space \( \mathbb{C}P^2 \times \mathbb{C}P^1 \times S^2 \). In this section, we find critical (fixed) points of the \( T_d \times T \) action on \( \mathbb{C}P^2 \times \mathbb{C}P^1 \times S^2 \) by combining points on the three factor spaces. Fortunately, most of the work has already been done in the previous sections. We can take critical orbits \( A, B, \) and \( C \) on \( \mathbb{C}P^2 \times S^2 \) found in section 4.5 and combine them with critical orbits of the \( T_d \times T \) action on the \( E \)-mode space \( \mathbb{C}P^1 \) while matching the stabilizers carefully. It can be seen in the examples of Table 15 that orbits \( A, B, \) and \( C \) are duplicated in the presence of \( E \)-mode vibrations. Indexes 1 and 2 distinguish two different possible projections \((z_5, z_6)\) on the \( E \)-mode space \( \mathbb{C}P^1 \). We use shorter \( T_d \) notation for stabilizers in Table 15.

Extending the symmetry group \( T_d \) by the time reversal \( T \) does not modify the critical orbits; it merely doubles the order of stabilizers, which become \( S_4 \wedge T_s, C_3 \wedge T_s, \) and \( C_s \times T_2 \). We comment briefly on these orbits.

The orbit stabilizer is defined as a class of conjugate subgroups; the point stabilizer is an individual subgroup in that class. As before, we match concrete point stabilizers. The \( S_4 \) operation has \((1 + 2), 2, \) and \( 2 \) fixed points on the \( F_2 \)-mode space \( \mathbb{C}P^2 \), \( E \)-mode space \( \mathbb{C}P^1 \), and rotational sphere \( S^2 \), respectively. The \( 3 \times 2 \times 2 = 12 \) points on \( \mathbb{C}P^2 \times \mathbb{C}P^1 \times S^2 \) with the stabilizer \( S_4 \) are listed in Table 15. To complete orbits of the \( T_d \) group action we should add points with stabilizers \( S_4^4 \) and \( S_4^2 \) (which are obtained from the given points using symmetry operations \( R \) such that \( S_4^4 = R \circ S_4^4 \circ R^{-1} \)). The total of 36 points can split into six orbits with stabilizer \( S_4 \). In particular, points \( A_1 \) and \( A'_1 \) in Table 15 belong to the same six-point orbit (which also includes two points with stabilizer \( S_4^4 \) and two points with stabilizer \( S_4^2 \)).

A similar argument shows that there are 12 points on \( \mathbb{C}P^2 \times \mathbb{C}P^1 \times S^2 \) for each of the four conjugate stabilizers \( C_4^{(k)} \) (Table 15(b), where points \( A', B', \) and \( C' \) are omitted for brevity). The total of \((3 \times 2 \times 2) \times 4 = 48 \) points on \( \mathbb{C}P^2 \times \mathbb{C}P^1 \times S^2 \) is made up of six eight-point orbits with stabilizer \( C_4 \).

The remaining two critical orbits on \( \mathbb{C}P^2 \times \mathbb{C}P^1 \times S^2 \) have stabilizer \( C_s \). We construct these orbits by taking points with stabilizer \( C_s^4 \) on the \( \mathbb{C}P^2 \times S^2 \) subspace (section 4.5) and combining them with the appropriate two \( D_{2d} \) points on the \( E \)-mode space \( \mathbb{C}P^1 \) (see Table 15(c)), as in the case of the stabilizer \( S_4 \). For six conjugate subgroups \( C_s \) we have 24 critical points on (the zero-dimensional component of) the \( C_s \) stratum of \( \mathbb{C}P^2 \times \mathbb{C}P^1 \times S^2 \), which separate into two 12-point orbits.

5. Prediction of RE. This section is a reward for our painstaking study of the \( T_d \times T \) group action on \( \mathbb{C}P^2 \times \mathbb{C}P^1 \times S^2 \). The reduced Hamiltonian \( H_{\text{eff}} \) is a \((T_d \times T)\)-invariant function on \( \mathbb{C}P^2 \times \mathbb{C}P^1 \times S^2 \) and it must have stationary points at all critical orbits of the \( T_d \times T \) action, which we found in the previous section (Table 15). Stationary points of \( H_{\text{eff}} \) are equilibria of the reduced system and are RE of the initial system with six vibrational degrees of freedom.\(^{26}\)

\(^{26}\)In order to simplify the analysis of the reduced system for \( P_4 \), the \( A_1 \)-mode subsystem is excluded in [13] by setting \( q^{A_1} = p^{A_1} = 0 \) and \( n_0 = 0 \); the model potential function was developed to cubic terms only. The number of degrees of freedom can be counted in several ways. Translational degrees of freedom can be trivially separated. Out of three rotational degrees of freedom, two can be reduced to account for the preservation of
RE correspond to families of special 3-tori in the initial phase space (see footnote 26) and are characterized entirely by symmetry and the values of the three integrals \(n_f, n_e,\) and \(j\). The value of \(H_{\text{eff}}\) (energy) at RE and stability of RE are the primary characteristics of our system. Table 15 becomes, therefore, our most important result in view of practical applications. (Note that RE forming one symmetry group orbit are equivalent and it suffices to analyze stability and energy for one RE in the orbit.)

In this section, we are preoccupied with general understanding and description of possible functions \(H_{\text{eff}}\). In particular, we want to know if such functions can have stationary points only on critical orbits, i.e., have the minimum number of stationary points. We place RE on critical group orbits and suggest possible stability. Assuming that \(H_{\text{eff}}\) is a Morse function on the space \(\mathbb{CP}^2 \times \mathbb{CP}^1 \times S^2\), we make sure that possible sets of stationary points satisfy Morse inequalities for this space and its invariant subspaces. We then find the simplest possible set (or sets) of RE, which correspond to the simplest Morse Hamiltonian(s) on \(\mathbb{CP}^2 \times \mathbb{CP}^1 \times S^2\) invariant with respect to the symmetry group of the system \(T_d \times T\). We can expect that at low perturbation (or excitation) our \(H_{\text{eff}}\) is such a simplest function.

The main purpose of this paper is the analysis of the complexity of the set of RE of systems combined of different subsystems. Our first observation in this context follows directly from the group action study in section 4. The RE set of the entire system is far from being a simple combination of the RE of the subsystems. As an example, take the \(F_2\)- and \(E\)-mode subsystems, which have 9 and 27 RE, respectively. These RE are also known as “nonlinear normal modes” [14, 15, 16]. They combine nonlinearly; there are 48 RE of the combined \(E-F_2\) system corresponding to critical orbits on the \(\mathbb{CP}^2 \times \mathbb{CP}^1\) phase space (see section 4.6).

Finding critical orbits on high-dimensional spaces constructed as a direct product of simpler spaces is greatly facilitated by tracing the correlation between critical orbits on subspaces and those on the complete space (for example, see section 4.5, Figures 11 and 12). Our second main observation is that the simplest \((T_d \times T)\)-invariant Morse-type function \(H_{\text{eff}}\) with stationary points placed exclusively on critical orbits can be defined on individual subspaces \(S^2, \mathbb{CP}^1,\) and \(\mathbb{CP}^2\). However, when we go to a product space, such as \(\mathbb{CP}^2 \times S^2\), the situation becomes more complicated and there must be RE (stationary points of \(H_{\text{eff}}\)) lying on noncritical group orbits.

### 5.1. Consequences of local symmetry for linear stability.

We can use our results on the critical orbits of the \(T_d \times T\) group action on \(\mathbb{CP}^2 \times \mathbb{CP}^1 \times S^2\) to find the position of corresponding RE and compute their energy for any given Hamiltonian \(H_{\text{eff}}\). To find more about these RE without using any concrete \(H_{\text{eff}}\), we should classify small phase space displacements \(x\) from them (coordinates on the tangent plane) according to the irreducible representations of their stabilizers. In this work, we are interested in one particular kind of group action, which

the length of the angular momentum vector and its projection on a laboratory fixed frame. This leaves six vibrational degrees of freedom and one rotational degrees of freedom, sometimes called “internal” degrees of freedom. However, we replace internal rotational degrees of freedom with two constrained oscillatory degrees of freedom, so there is a total of eight initial degrees of freedom (and a phase space of dimension 16), of which two represent one physical rotational degrees of freedom, and one representing the \(A_1\) mode is ignored. Reduction with respect to all integrals \(n_a, n_f, n_e,\) and \(j\) leads to the reduced system on the space \(\mathbb{CP}^2 \times \mathbb{CP}^1 \times S^2\) with four degrees of freedom. The corresponding dynamical symmetry is \(T^3\). If we neglect \(n_a\) by setting \(q^{A_1} = p^{A_1} = 0\) before reduction, we restrict the initial system to seven degrees of freedom, and the dynamical symmetry is \(T^3\).
is induced on $\mathbb{C}P^2 \times \mathbb{C}P^1 \times S^2$ by spatial and reversal symmetries of the initial molecular rotation–vibration system. This action can be studied in the example of the $SO(2)$ group (axial symmetry) and its discrete cyclic subgroups $C_k$ (rotation by $2\pi/k$ with $k = 2, 3, 4, \ldots$) acting on the initial coordinates of our system as groups of transformations.

We begin by describing a number of nondegenerate equilibria $e$ with nontrivial stabilizers $G_e = C_k$ and corresponding $G_e$-invariant local quadratic Hamiltonians $H_0$ such that $H_0(e) = 0$. The local symmetry of $e$ results in certain restrictions on $H_0$ and on the stability. We compute the Hessian matrix $\partial^2 H_0 / \partial x^2$. Displacements that transform according to different rows of the same irreducible representation $\Gamma_e$ form a degenerate eigenvalue block of $\partial^2 H_0 / \partial x^2$. The number of negative eigenvalues of this matrix, or the Morse index, enters in Morse inequalities in section 5.2; the Poincaré index gives the sign of $\det(\partial^2 H_0 / \partial x^2)$. In order to determine the stability of $e$, we consider $H_0$ as a Hamiltonian, establish local symplectic structure $J$, and compute the eigenvalues of the corresponding Hamiltonian matrix $J \partial^2 H_0 / \partial x^2$. Hamiltonian stability and the Morse index are related unambiguously only in the case of dimension two (reduced system with one degree of freedom). The Poincaré index, which can be computed from the Morse index, gives some characteristics of linear Hamiltonian stability in systems with any degrees of freedom. Subsequently, we use our results to study the RE of our system.

5.1.1. $C_k$-invariant quadratic Hamiltonians on $\mathbb{R}^2$. We define the action of the rotation group $SO(2)$ on the real variables $(x_1, x_2)$ using the $2 \times 2$ orthogonal matrix

$$M_m(\varphi) = \begin{pmatrix} \cos m\varphi & \sin m\varphi \\ -\sin m\varphi & \cos m\varphi \end{pmatrix}, \quad m = 0, 1, 2, \ldots,$$

and consider quadratic functions $H_0(x_1, x_2)$, which are invariant with respect to $SO(2)$ or its discrete subgroups $C_k$ (rotation by $\varphi = 2\pi/k$). For each given $m$ we take $k > m$. Furthermore, it suffices to consider $k \leq 2m$. The point $e = (x_1, x_2) = 0$ is a critical orbit and, therefore, an equilibrium of $H_0$. If the two displacements $(x_1, x_2)$ about $e$ transform as components of a two-dimensional real irreducible representation, then $e$ can only be a minimum or a maximum of $H_0$ with signature $(++)$ or $(--)$ (Morse index 0 or 2), respectively, but not a saddle $(-+)$ with index 1.

Invariants of our $SO(2)$ action are constructed using combinations

$$\xi = x_1 + ix_2 \quad \text{and} \quad \bar{\xi} = x_1 - ix_2,$$

which transform as conjugate irreducible one-dimensional complex representations $\pm m$ of $SO(2)$. The pair $(x_1, x_2)$ realizes a two-dimensional representation of $SO(2)$, which is irreducible over reals. Descending to $C_k$, we should check whether this representation remains irreducible (over reals). For $m = 1$ and $m = 2$ this is the case for all $k \neq 2$ and $k \neq 4$, respectively. When $m = 2$ and $k = 4$, the image of $C_4$ becomes $C_2$. The corresponding quadratic forms are given in Table 16. We can see that the case $k = 2m$ is stable (elliptic) when $c^2 - ab < 0$ or unstable (hyperbolic) otherwise, while the $k \neq 2m$ equilibrium is always stable.
Invariant local quadratic Hamiltonians with one and two degrees of freedom encountered in our study. The action of $C_k$ on the phase plane $\mathbb{R}^2$ with coordinates $(x_1, x_2)$ is given by the $2 \times 2$ orthogonal matrix $M_m(\varphi)$ with $\varphi = 2\pi/k$; the action of $C_k$ on the phase space $\mathbb{R}^4$ with coordinates $(x_1, x_2, x_3, x_4)$ is defined by $\text{diag}(M_{m'}, M_{m''})(\varphi)$. The action of the subgroups of $T_d \times T$ on the local coordinates $(x_1, x_2, y_1, y_2)$ is given in Table 18.

<table>
<thead>
<tr>
<th>Stabilizer</th>
<th>$C_k$-invariant quadratic form</th>
<th>Eigenvalues$^{27,28}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$C_{2m}$</td>
<td>$\frac{1}{2}ax^2 + \frac{1}{2}by^2 + cxy$</td>
<td>$[\pm \sqrt{a^2 - ab}], \frac{1}{2}(a + b \pm D_{abc})$</td>
</tr>
<tr>
<td>$C_{2m+1}$</td>
<td>$\frac{1}{2}a(x^2 + y^2)$</td>
<td>$[\pm ia], {a, a}$</td>
</tr>
</tbody>
</table>

Case A: $m' = 1$, $m'' = 1$, and $\omega = dx_1 \wedge dy_1 + dx_2 \wedge dy_2$

<table>
<thead>
<tr>
<th>$C_k$</th>
<th>$C_k$-invariant quadratic form</th>
<th>Eigenvalues$^{27,28}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$C_k(k &gt; 2)$</td>
<td>$\frac{1}{2}a'x_1^2 + \frac{1}{2}a''x_2^2 + \frac{1}{2}b'y_1^2 + \frac{1}{2}b''y_2^2$</td>
<td>$[\pm \sqrt{a^2 - ab} \pm id, \pm \sqrt{a^2 - ab} \pm id]$</td>
</tr>
<tr>
<td></td>
<td>+ $c(x_1y_1 + x_2y_2) + d(x_1x_2 - x_2y_1)$</td>
<td>$\frac{1}{2}{a + b \pm D_{abcd}} \times 2$</td>
</tr>
</tbody>
</table>

Case A with extended symmetry $T_6 = C_6 \times T$, where $T : (x_1, x_2, y_1, y_2) \to (x_1, x_2, -y_1, -y_2)$

| $T_2$            | $\frac{1}{2}a'(x_1^2 + x_2^2) + \frac{1}{2}b'(y_1^2 + y_2^2)$ | No simple restrictions |
|                  | + $(x_1y_1 + x_2y_2) + (x_1x_2 - y_1y_2)$ | $\frac{1}{2}\{b' + b'' \pm D_{uv'}d', a' + a'' \pm D_{u'a'c}\}$ |

Case B with full symmetry and $\omega = dx_1 \wedge dy_1 + dx_2 \wedge dy_2$

| $C_3, C_4$       | $\frac{1}{2}a'(x_1^2 + y_1^2) + \frac{1}{2}a''(x_2^2 + y_2^2)$ | $[\pm i\sqrt{a' - a''}, \pm i\sqrt{a'' - a'}], \{a', b', a'', b''\}$ |
|                  | + $c(x_1x_2 - y_1y_2) + d(x_1x_2 + y_1y_2)$ | $\frac{1}{2}\{a' + a'' \pm D_{a'a'c}\} \times 2$ |

$5.1.2. \textbf{C}_k$-invariant quadratic Hamiltonians on $\mathbb{R}^4$. We define the action of the $SO(2)$ group on the four-plane $\mathbb{R}^4$ with coordinates $(x_1, x_2, x_3, x_4)$ using the matrix $(M_{m'}^0, M_{m''}^0)$, where the submatrices $M_{m'}$ and $M_{m''}$ act on the $(x_1, x_2)$-subspace and the $(x_3, x_4)$-subspace,

$^{27}$Eigenvalues of the Hamiltonian and Hessian matrices are given in square $[ ]$ and curly $\{}$ brackets, respectively; $\times 2$ indicates multiplicity.

$^{28}\Delta = \sqrt{4(c^2 + d^2) - (a' + a'')^2}$, $D_{abcd} = \sqrt{(a - b)^2 + 4(c^2 + d^2)}$, $D_{abc} = D_{a'bc}$. 


representations of $SO(2)$ is lowered to $C$ together with their conjugates $\bar{\xi}$ and $\bar{\eta}$. The four variables $\xi, \eta, \bar{\xi}, \bar{\eta}$ realize irreducible representations $m', m'', -m', -m''$, respectively. We consider several situations of interest to our later study.

In the case of $m' = 1$ and $m'' = 2$, we have two quadratic $SO(2)$ invariants $\frac{1}{2}\xi\bar{\xi}$ and $\frac{1}{2}\eta\bar{\eta}$. When $SO(2)$ is lowered to $C_3$, we also have $\xi\eta$ and $\bar{\xi}\bar{\eta}$, which transform like $\exp(\pm 3i\varphi)$. Similarly, $\eta^2$ and $\bar{\eta}^2$ transform like $\exp(\pm 4i\varphi)$ and are the two extra invariants in the case of $C_4$.

In the case of $m' = m'' = 1$ (and generally for $m' = m''$), our $SO(2)$ action has four quadratic invariants: the familiar $\frac{1}{2}\xi\xi, \frac{1}{2}\eta\eta$, and the cross terms $\xi\bar{\eta}, \eta\bar{\xi}$. The same four remain if $SO(2)$ is lowered to $C_k$ and $k > 2$. When $k = 2$, each coordinate $x_i$ realizes real one-dimensional irreducible antisymmetric representation. All 10 quadratic monomials $x_jx_k$ are, therefore, $C_2$-invariant.

Generic $C_k$-invariant real quadratic forms in $(x_1, x_2, x_3, x_4)$ constructed using the above invariants are presented in Table 16. As can be seen from this table, Hamiltonian stability of $e = (0, 0, 0, 0)$ depends on $m', m'', k$, and the symplectic form $\omega$. The eigenvalues of the Hessian at $(0, 0, 0, 0)$, which are also given in Table 16, are used in the Morse theory analysis. Furthermore, we can see that additional symmetry, such as the time reversal extension for case $A$ critical orbits (see sections 4.3, 4.5.3 and Table 15), can simplify the situation quite radically.

5.1.3. Points on $S^2$ and $CP^1$. Consider a nondegenerate critical point $e$ with stabilizer $G_e$ on the 2-sphere $S^2$ or on the diffeomorphic space $CP^1$. The group $G_e$ is defined as a group of transformations of the ambient Euclidean space $\mathbb{R}^3$, which embeds $S^2$ (see section 4). We want to know how $G_e$ acts on the 2-plane $\mathbb{R}^2(e)$ tangent to $S^2$ or $CP^1$ at $e$. It suffices to consider the circle group $G_e = SO(2)$ and its subgroups $C_k$. A straightforward computation shows that the image of $SO(2)$ and $C_k$ in the representation spanned by the Euclidean coordinates $(x, y)$ on $\mathbb{R}^2(e)$ is again $SO(2)$ and $C_k$ and that $x \pm iy$ span representations $\pm 1$. Then, following section 5.1.1, the point $e$ on $S^2$ and $CP^1$ with stabilizer $C_k$, $k > 2$, is always stable; points with stabilizer $C_2$ can also be unstable.

5.1.4. Points on $CP^2$. As before, we study a special case of the group action on the $CP^2$ space induced by the natural action (vector representation) of the group $SO(2)$ and its subgroups $C_k$ on the complex 3-space with coordinates $(z_1, z_2, z_3)$. This action is defined by a $3 \times 3$ orthogonal matrix $M$. The action on the corresponding real 6-space with coordinates $(q_1, q_2, q_3, p_1, p_2, p_3)$ is given by the matrix $\begin{pmatrix} M & 0 \\ 0 & \frac{1}{M} \end{pmatrix}$ with one copy of $M$ acting on the $q$ space and the other on the $p$ space. The above action of $SO(2)$ with the symmetry axis $z_3$, and of the corresponding discrete subgroups $C_k$ with $k > 2$, on $CP^2$ has three isolated fixed points (see section 4.3 and [17]):

$$A = (0, 0, 1), \quad B = (1, \pm i, 0).$$
the point is isolated. It is also useful to recall that the stabilizer of the pair, respectively; 1:1 indicates resonance, c

displacement from point of the T

We can see right away that four small real quantities (in Table 15 we use notation B, C for points of type B.) In the C_2 case, only the A-type fixed point is isolated. It is also useful to recall that the stabilizer of the A points in the case of the T_d × T action on CP^2 includes T (see Table 10) and that C_k can be extended easily to T_k = C_k × T.

Any C_k-invariant Morse Hamiltonian H on CP^2 has nondegenerate stationary points of types A and B. Let z be one of these points and let CP^2 \sim \mathbb{R}^4_{(z)} be the plane tangent to CP^2 at z. This plane is a chart of CP^2 with four real displacement coordinates (q', p', q'', p''). The zero order H_0(q', p', q'', p'') of the Taylor expansion of H near z is a nondegenerate quadratic form. We study the action of C_k on (q', p', q'', p'') and find which generic forms in Table 16 correspond to H_0. Table 17 gives the summary of the results.

The action of C_k on \mathbb{R}^4_{(z)} can be found by direct computation; see also section 10. The matrix of the rotation about axis z_3 by an arbitrary angle \varphi is

$$M(\varphi) = \begin{pmatrix} \cos \varphi & \sin \varphi & 0 \\ -\sin \varphi & \cos \varphi & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$  

We can see right away that four small real quantities (q_1, q_2), and (p_1, p_2), which define a displacement from point A (in the appropriate chart of CP^2),

d_A = (q_1 + ip_1, q_2 + ip_2, 1)

transform like two copies of the real two-dimensional representation ±1 of the group SO(2). Consequently, the forms of case A in Table 16 with (x_1, x_2, y_1, y_2) corresponding to (q_1, q_2, p_1, p_2) represent generic C_k and (C_k × T)-invariant Morse functions locally at point A. The C_2 × T form can be further simplified if we consider the full C_2 × T stabilizer of the actual fixed point of the T_d × T action. In that case H_0 has only four terms q_1^2, q_2^2, p_1^2, and p_2^2. Hamiltonian (linear) stability analysis of the A-type equilibria in the case of the full T_d × T action is straightforward (see Table 17) because the linearized system separates in initial phase space coordinates and the analysis reduces to combining two systems with one degree of freedom.

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Table 17

<table>
<thead>
<tr>
<th>Equilibrium^{29}</th>
<th>( \partial^2 H_0 )</th>
<th>( \mathcal{J} \partial^2 H_0 )</th>
<th>Equilibrium^{29}</th>
<th>( \partial^2 H_0 )</th>
<th>( \mathcal{J} \partial^2 H_0 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>A ( C_2 \times T )</td>
<td>No simple restrictions</td>
<td></td>
<td>B ( C_3 )</td>
<td>4, 2, 0</td>
<td>ii</td>
</tr>
<tr>
<td>( C_2 \times T )</td>
<td>4, 2, 0</td>
<td>ii</td>
<td></td>
<td>2</td>
<td>c</td>
</tr>
<tr>
<td></td>
<td>3, 1</td>
<td>ir</td>
<td></td>
<td>( C_4 )</td>
<td>4, 2, 0</td>
</tr>
<tr>
<td></td>
<td>2</td>
<td>rr</td>
<td></td>
<td>3, 1</td>
<td>ir</td>
</tr>
<tr>
<td>A ( C_k \times T ), ( k &gt; 2 )</td>
<td>4, 0</td>
<td>ii</td>
<td>( 1:1 )</td>
<td></td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>rr</td>
<td>( 1:1 )</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Any C_k-invariant Morse Hamiltonian H on CP^2 has nondegenerate stationary points of types A and B. Let z be one of these points and let CP^2 \sim \mathbb{R}^4_{(z)} be the plane tangent to CP^2 at z. This plane is a chart of CP^2 with four real displacement coordinates (q', p', q'', p''). The zero order H_0(q', p', q'', p'') of the Taylor expansion of H near z is a nondegenerate quadratic form. We study the action of C_k on (q', p', q'', p'') and find which generic forms in Table 16 correspond to H_0. Table 17 gives the summary of the results.

The action of C_k on \mathbb{R}^4_{(z)} can be found by direct computation; see also section 10. The matrix of the rotation about axis z_3 by an arbitrary angle \varphi is

$$M(\varphi) = \begin{pmatrix} \cos \varphi & \sin \varphi & 0 \\ -\sin \varphi & \cos \varphi & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$  

We can see right away that four small real quantities (q_1, q_2), and (p_1, p_2), which define a displacement from point A (in the appropriate chart of CP^2),

d_A = (q_1 + ip_1, q_2 + ip_2, 1)

transform like two copies of the real two-dimensional representation ±1 of the group SO(2). Consequently, the forms of case A in Table 16 with (x_1, x_2, y_1, y_2) corresponding to (q_1, q_2, p_1, p_2) represent generic C_k and (C_k × T)-invariant Morse functions locally at point A. The C_2 × T form can be further simplified if we consider the full C_2 × T stabilizer of the actual fixed point of the T_d × T action. In that case H_0 has only four terms q_1^2, q_2^2, p_1^2, and p_2^2. Hamiltonian (linear) stability analysis of the A-type equilibria in the case of the full T_d × T action is straightforward (see Table 17) because the linearized system separates in initial phase space coordinates and the analysis reduces to combining two systems with one degree of freedom.

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\(^{29}\)Type and local symmetry (stabilizer) of equilibria on CP^2; see section 5.1.4 and Table 15 and compare to Table 16.

\(^{30}\)Possible Morse index derived from the corresponding Hessian eigenvalues in Table 16.

\(^{31}\)Possible eigenvalues of the Hamiltonian matrix: \( i \) and \( r \) stand for the imaginary and the real eigenvalue pair, respectively; \( 1:1 \) indicates resonance, \( c \) denotes four complex eigenvalues.
When we use the same approach for
\[ d_B = (1, i + q_2 + ip_2, q_3 + ip_3) = (1, i + z_2, z_3), \]
we should project the transformed vector
\[ M(\varphi)d_B = (e^{i\varphi} + z_2 \sin \varphi, ie^{i\varphi} + z_2 \cos \varphi, z_3) \]
back to the initial chart of \( \mathbb{CP}^2 \) and Taylor expand to the first order in \((q_2, p_2, q_3, p_3)\),
\[ M(\varphi)d_B \big|_{\text{chart}} = \left[e^{i\varphi} + z_2 \sin \varphi\right]^{-1} M(\varphi)d_B \]
\[ \approx (1, i + e^{-2i\varphi}z_2, e^{-i\varphi}z_3). \]

We can now see that \((q_3, p_3)\) and \((q_2, p_2)\) realize representations \(\pm 1\) and \(\pm 2\) of \(\text{SO}(2)\), respectively. Therefore, quadratic forms of case \(B\) in Table 16 with \((x_1, y_1, x_2, y_2)\) corresponding to \((q_2, p_2, q_3, p_3)\) represent generic \(C_k\)-invariant Morse functions locally at point \(B\). For all points \(B^{(k)}\) with \(k > 3\), linearization separates in the initial coordinates \((q_2, p_2)\) and \((q_3, p_3)\). As in case \(A\), stability analysis of these equilibria is simple. Point \(B^{(3)}\) turns out to be the only interesting case, where the localized system is intrinsically four-dimensional; cf. [97].

5.1.5. Stability analysis of stationary points on \( \mathbb{CP}^2 \) in the presence of \( T_d \times T \). In the previous section, we showed that linear stability of stationary points on \( \mathbb{CP}^2 \) (vibrational RE) can be predicted by analyzing possible local Hamiltonians for RE whose stabilizer is an \(\text{SO}(2)\) group or a discrete cyclic subgroup \(C_k\) of this group. For the five types of vibrational RE labeled \(A^{(2)}, A^{(3)}, B^{(3)}, A^{(4)},\) and \(B^{(4)}\) (see Table 15) we take subgroups \(C_2, C_3,\) and \(C_4\), respectively. The latter can be regarded as the principal symmetry operations of the respective stabilizers \(C_{2v} \times T, C_{3v} \times T, C_5 \wedge T, D_{2d} \times T,\) and \(S_4 \wedge T\). At the same time, prediction of stability of these RE can be further improved if we account for the full stabilizers.

To this end we proceed as before in section 5.1.4. We define local displacement coordinates \((x_1, y_1, x_2, y_2)\) near the stationary point on \( \mathbb{CP}^2 \) and determine the action of the full stabilizer \(G\) on these coordinates. Knowing the action, we find the representation of \(G\) realized by \((x_1, y_1, x_2, y_2)\) and construct the typical \(G\)-invariant quadratic form \(H(x_1, y_1, x_2, y_2)\). We choose \((x_1, y_1, x_2, y_2)\) so that the local 2-form is \(dx_1 \wedge dy_1 + dx_2 \wedge dy_2\) and consider \(H(x_1, y_1, x_2, y_2)\) as a Hamiltonian function of local linearization near the RE.

In order to define \((x_1, y_1, x_2, y_2)\) we rotate the initial coordinates \((z_1, z_2, z_3)\) so that in the new coordinates \((z'_1, z'_2, z'_3)\) the principal symmetry axis of the stabilizer becomes axis \(z'_1\). The direction of the two other axes can be chosen as shown below:

<table>
<thead>
<tr>
<th>Stabilizer</th>
<th>((z_1, z_2, z_3))</th>
<th>Map</th>
<th>((z'_1, z'_2, z'_3))</th>
</tr>
</thead>
<tbody>
<tr>
<td>(D^{(3)}_{2d} \times T)</td>
<td>(\sqrt{2}m(1, 0, 0))</td>
<td>(E)</td>
<td>(\sqrt{2}m(1, 0, 0))</td>
</tr>
<tr>
<td>(S^{(2)}_1 \wedge T^{(9)})</td>
<td>(\sqrt{2}m(1, 0, i))</td>
<td>(E)</td>
<td>(\sqrt{2}m(1, 0, i))</td>
</tr>
<tr>
<td>(C^{(2)}_{3v} \times T)</td>
<td>(\sqrt{2}m(1, 1, 0))</td>
<td>(M_2)</td>
<td>(\sqrt{2}m(1, 0, 0))</td>
</tr>
<tr>
<td>(C^{(11)}_{3v} \times T)</td>
<td>(\sqrt{2}m(1, 1, 1))</td>
<td>(M_2)</td>
<td>(\sqrt{2}m(1, 0, 0))</td>
</tr>
<tr>
<td>(C^{(11)}_{3v} \wedge T)</td>
<td>(\sqrt{4}m(1, 0, 0))</td>
<td>(\sqrt{4}m(1, 0, 0))</td>
<td>(\sqrt{4}m(0, 1, i))</td>
</tr>
</tbody>
</table>

where \(z' = Mz\), \(E = \text{diag}(1, 1, 1)\),
\[
M_1 = \begin{pmatrix}
\frac{\sqrt{2}}{2} & \frac{\sqrt{2}}{2} & 0 \\
\frac{\sqrt{2}}{2} & \frac{\sqrt{2}}{2} & 0 \\
0 & 0 & 1 \\
\end{pmatrix}, \quad \text{and} \quad M_2 = \begin{pmatrix}
\frac{1}{2} & \frac{1}{\sqrt{6}} & \frac{1}{\sqrt{3}} \\
\frac{1}{\sqrt{6}} & \frac{1}{2} & \frac{1}{\sqrt{3}} \\
\frac{1}{\sqrt{3}} & \frac{1}{\sqrt{6}} & \frac{1}{2} \\
\end{pmatrix}.
\]
Using the approach in section 5.1.4, we can show that the position of the RE in the new coordinates \((z_1', z_2', z_3')\) is \((1, 0, 0)\) for type \(A\) and \((0, 1, \pm i)\) for type \(B\). We define displacement vectors

\[
d_A = (z_1, x_1 + iy_1, x_2 + iy_2),
\]

with \(z_1 = \sqrt{2n - |z_2|^2 - |z_3|^2}\), and

\[
d_B = (x_1 + iy_1, z_2, i\sqrt{n} + \sqrt{2}x_2 + iy_2/\sqrt{2}),
\]

with \(z_2' = \sqrt{n - |z_1'|^2 - |z_3'|^2}\). Note that, instead of projecting on an \(\mathbb{R}^4_{(x, y)}\) chart of \(\mathbb{C}P^2\) as we do in section 5.1.4, we represent the points of \(\mathbb{C}P^2\) by fixing the total phase of \((z_1', z_2', z_3')\) so that \(\text{Im}(z_1') = 0\) in the case of \(d_A\) and \(\text{Im}(z_2') = 0\) in the case of \(d_B\) (cf. section 2.4.3).

Each symmetry operation \(R\) in the stabilizer \(G\) is realized initially as a linear transformation of the space \(\mathbb{R}^3\) defined by a real matrix \(M_R\). The same transformation applies to \(\mathbb{C}^3\) with coordinates \((z_1', z_2', z_3')\). To realize this transformation on \(\mathbb{C}P^2\), we should correct or restore the phase of \(M_R z'\) in order to obey our phase condition. Therefore we define

\[
Rd_A = \frac{[M_R z_1']}{|[M_R z_1']|} M_R d_A \quad \text{and} \quad Rd_B = \frac{[M_R z_2']}{|[M_R z_2']|} M_R d_B.
\]

To find the action on \((x, y)\) we Taylor expand \(Rd_A\) and \(Rd_B\) at \((x, y) = 0\) and compare them to the initial vectors \(d_A\) and \(d_B\). Results are summarized in Table 18. As can be concluded from this table, displacements \((x, y)\) realize the following representations of the respective stabilizers:

<table>
<thead>
<tr>
<th>Point</th>
<th>Stabilizer</th>
<th>Representation spanned by ((x, y))</th>
</tr>
</thead>
<tbody>
<tr>
<td>(A^{(2)})</td>
<td>(C_{2v} \times T)</td>
<td>(A_{2g}(x_1) \oplus A_{2u}(y_1) \oplus B_{1g}(x_2) \oplus B_{1u}(y_2))</td>
</tr>
<tr>
<td>(A^{(3)})</td>
<td>(C_{3v} \times T)</td>
<td>(E_g(x_1, x_2) \oplus E_u(y_1, y_2))</td>
</tr>
<tr>
<td>(B^{(3)})</td>
<td>(C_3 \wedge T)</td>
<td>(E(x_1, y_1) \oplus E(x_2, -y_2))</td>
</tr>
<tr>
<td>(A^{(4)})</td>
<td>(D_{2d} \times T)</td>
<td>(E_g(x_1, x_2) \oplus E_u(y_1, y_2))</td>
</tr>
<tr>
<td>(B^{(4)})</td>
<td>(S_4 \wedge T_2)</td>
<td>(B_1(y_2) \oplus B_2(x_2) \oplus E(x_1, y_1))</td>
</tr>
</tbody>
</table>

Here we denote irreducible representations of \(T\)-extended groups using notation of corresponding point groups [66].

The above decomposition of representations realized by local displacements into irreducible representations makes construction of local quadratic Hamiltonians straightforward. In the case of \(A^{(4)}\) and \(B^{(4)}\) RE, all quadratic invariants are just linear combinations of scalar squares of displacements transforming according to different irreducible representations, such as \([E_g(x_1, x_2)]^2 = x_1^2 + x_2^2\), etc. The case of \(B^{(3)}\) is the only case where a scalar product of two different displacements transforming according to the same irreducible representation \(E\) occurs. Generic local quadratic Hamiltonians for each RE are listed in Table 16. The brute-force way to find these Hamiltonians is by projecting the most general homogeneous second degree polynomial in \((x_1, x_2, y_1, y_2)\) using the operator \(|G|^{-1} \sum_{R \in G} R\), where \(G\) is the stabilizer of the RE in question.
Table 18
Action of stabilizers on local displacements from the stationary points on \( \mathbb{C}P^2 \).

### Action of \( D_{2d}^{(x)} \times T \) on \( E_y \oplus E_u \)

<table>
<thead>
<tr>
<th>( R )</th>
<th>( Rx_1 )</th>
<th>( Rx_2 )</th>
<th>( Ry_1 )</th>
<th>( Ry_2 )</th>
<th>( \mathcal{T} )</th>
<th>( Rx_1 )</th>
<th>( Rx_2 )</th>
<th>( Ry_1 )</th>
<th>( Ry_2 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( E )</td>
<td>( x_1 )</td>
<td>( x_2 )</td>
<td>( y_1 )</td>
<td>( y_2 )</td>
<td>( x_1 )</td>
<td>( x_2 )</td>
<td>( -y_1 )</td>
<td>( -y_2 )</td>
<td></td>
</tr>
<tr>
<td>( C_{x}^{2} )</td>
<td>( -x_1 )</td>
<td>( -x_2 )</td>
<td>( -y_1 )</td>
<td>( -y_2 )</td>
<td>( T_{x}^{y} )</td>
<td>( -x_1 )</td>
<td>( -x_2 )</td>
<td>( y_1 )</td>
<td>( y_2 )</td>
</tr>
<tr>
<td>( C_{y}^{2} )</td>
<td>( -x_1 )</td>
<td>( -x_2 )</td>
<td>( -y_1 )</td>
<td>( -y_2 )</td>
<td>( T_{y}^{x} )</td>
<td>( -x_1 )</td>
<td>( -x_2 )</td>
<td>( y_1 )</td>
<td>( y_2 )</td>
</tr>
<tr>
<td>( \sigma^x )</td>
<td>( x_2 )</td>
<td>( x_1 )</td>
<td>( y_2 )</td>
<td>( y_1 )</td>
<td>( T_{y}^{y} )</td>
<td>( x_2 )</td>
<td>( x_1 )</td>
<td>(-y_2 )</td>
<td>(-y_1 )</td>
</tr>
<tr>
<td>( \sigma_y )</td>
<td>( -x_2 )</td>
<td>(-x_1 )</td>
<td>(-y_2 )</td>
<td>(-y_1 )</td>
<td>( T_{y}^{y} )</td>
<td>(-x_2 )</td>
<td>(-x_1 )</td>
<td>( y_1 )</td>
<td>( y_2 )</td>
</tr>
<tr>
<td>( S_1 )</td>
<td>( x_2 )</td>
<td>(-x_1 )</td>
<td>(-y_2 )</td>
<td>(-y_1 )</td>
<td>( S_1 ) ( \mathcal{T} )</td>
<td>( x_2 )</td>
<td>(-x_1 )</td>
<td>(-y_2 )</td>
<td>(-y_1 )</td>
</tr>
<tr>
<td>( S_1^{-1} )</td>
<td>( -x_2 )</td>
<td>(-x_1 )</td>
<td>(-y_2 )</td>
<td>(-y_1 )</td>
<td>( S_1^{-1} ) ( \mathcal{T} )</td>
<td>( -x_2 )</td>
<td>(-x_1 )</td>
<td>( y_1 )</td>
<td>( y_2 )</td>
</tr>
</tbody>
</table>

### Action of \( C_{2z}^{(x)} \times T \) on \( A_{2y} \oplus A_{2a} \oplus B_{1y} \oplus B_{1u} \)

### Action\(^{32}\) of \( C_{3z}^{(111)} \times T \) on \( E_y \oplus E_u \)

### Action\(^{32}\) of \( C_{3z}^{(111)} \) \( \times T \) on \( E \oplus E \)

### Action\(^{32}\) of \( C_{3z}^{(111)} \) \( \times T \) on \( E \oplus E \)

---

\(^{32}\) Notation \( a = 1/2, b = \sqrt{3}/2.\)
5.2. Application of Morse theory. Simplest Morse Hamiltonians. Consider a manifold $P$ whose topology is described by $\dim P + 1$ Betti numbers $b_k$. Particularly useful is the combination of these numbers, called the Euler characteristics $\Sigma$. A Morse function $f$ on $P$ is smooth and has only nondegenerate stationary points. Let $c_k$ be the number of stationary points of $f$ of Morse index $k$. The set of $\dim P$ Morse inequalities

$$\sum_{k=0}^{s} (-1)^{s-k} c_k \geq \sum_{k=0}^{s} (-1)^{s-k} b_k, \quad 0 \leq s < \dim P,$$

and the Euler–Poincaré equation

$$\sum_{k=0}^{\dim P} (-1)^k c_k = \sum_{k=0}^{\dim P} (-1)^k b_k = \Sigma,$$

express the relation between $c_k$ and topological invariants $b_k$ and $\Sigma$.

In the presence of a nonfree action of group $G$ on $P$, all isolated points on the critical orbits of this action must be stationary points of $f$. The Morse function $f$ with a minimal possible number of stationary points on $P$ (in the presence of the specific group action) represents a class of simplest Morse functions. In the most trivial situations, such functions would have stationary points only on the isolated critical points. We should, therefore, check whether (and how) placing stationary points exclusively on the isolated points of critical orbits can satisfy the above Morse theory requirements. Table 19 gives Betti numbers for $S^2$ and $CP^2$ and suggests systems of stationary points on the vibrational spaces $CP^2$ and $CP^1$ and the rotational space $S^2$ satisfying Morse theory in the presence of the $T_d \times T$ group action. We begin with the simplest Morse Hamiltonians on each factor space of the total reduced phase space $CP^2 \times CP^1 \times S^2$. Such Hamiltonians describe isolated $F_2$-mode or $E$-mode vibrational systems (polyads) or pure rotation.

5.2.1. Morse functions on the rotational space $S^2$. Among the 26 fixed points of the $T_d \times T$ action on $S^2$ (Table 7), six points with stabilizer $S_4 \wedge T$ and eight points with stabilizer $C_3 \wedge T$ should be elliptic. The Morse conditions are satisfied if the 12 points with stabilizer $C_3 \times T_2$ are hyperbolic (unstable): $6 - 12 + 8 = 2$. The two simplest Morse Hamiltonians differ in sign: one has six maxima and eight minima while the other has this structure turned upside-down. If the internuclear adiabatic potential of the $A_4$ molecule can be well approximated as a sum of six pairwise interaction terms and all vibrations are frozen, then the minima are located at the six $S_4$ points [12] as shown in Figure 13, left.

We like to note that stationary points of simplest Morse functions of purely rotational systems (rotational RE of nonrigid bodies) should not necessarily be fixed points on $S^2$. Thus in the case of the lowest possible symmetry of such systems $T$ (no spatial symmetry), neither of the three pairs of equivalent RE has a fixed position on $S^2$. Another example is the $C_2 \times T$ system in Figure 6: four (two pairs) of its six RE can lie anywhere on the invariant circle.

5.2.2. Morse functions on the $E$-mode phase space $CP^1$. Critical orbits of the $T_d \times T$ action on $CP^1$ are presented in Figure 9 and Table 8. The two equivalent $T \wedge T_s (C_{3v})$ points should be elliptic. The Morse conditions are satisfied if, out of the two three-point orbits with stabilizer $D_{2d} \times T$, one contains elliptic points and the other hyperbolic points. The freedom
Table 19

Betti numbers $b_k$ and Euler–Poincaré characteristics $\Sigma$ for the spaces $\mathbb{C}P^2$ and $\mathbb{C}P^1 \sim S^2$ (top). Number and type of stationary points of the simplest Morse function on the $F_2$-mode space $\mathbb{C}P^2$, $E$-mode space $\mathbb{C}P^1$, and rotational sphere $S^2$ in the presence of the symmetry group $T_d \times T$. The frame indicates additional stationary points of the possible nonsimplest Morse function on $\mathbb{C}P^2$.

<table>
<thead>
<tr>
<th>Space</th>
<th>$b_0$</th>
<th>$b_1$</th>
<th>$b_2$</th>
<th>$b_3$</th>
<th>$b_4$</th>
<th>$b_5$</th>
<th>$b_6$</th>
<th>$\Sigma$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\mathbb{C}P^1 \sim S^2$</td>
<td>1</td>
<td>0</td>
<td>1</td>
<td></td>
<td>0</td>
<td>1</td>
<td></td>
<td>2</td>
</tr>
<tr>
<td>$\mathbb{C}P^2$</td>
<td>1</td>
<td>0</td>
<td>1</td>
<td>0</td>
<td>0</td>
<td>1</td>
<td></td>
<td>3</td>
</tr>
<tr>
<td>$\mathbb{C}P^1 \times S^2$</td>
<td>1</td>
<td>0</td>
<td>2</td>
<td>0</td>
<td>0</td>
<td>1</td>
<td>4</td>
<td></td>
</tr>
<tr>
<td>$\mathbb{C}P^2 \times S^2$</td>
<td>1</td>
<td>0</td>
<td>2</td>
<td>0</td>
<td>0</td>
<td>1</td>
<td>4</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Space</th>
<th>$c_0$</th>
<th>$c_1$</th>
<th>$c_2$</th>
<th>$c_3$</th>
<th>$c_4$</th>
<th>$c_5$</th>
<th>$c_6$</th>
<th>$\Sigma$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\mathbb{C}P^1$</td>
<td>$3D_{2d} \times T$</td>
<td>$3D_{2d} \times T$</td>
<td>$2T \wedge T_s$</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>2</td>
</tr>
<tr>
<td>$S^2$</td>
<td>$6S_4 \wedge T_s$</td>
<td>$12C_3 \wedge T_s$</td>
<td>$8C_3 \wedge T_s$</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>2</td>
</tr>
<tr>
<td>$\mathbb{C}P^2$</td>
<td>$4C_{3v} \times T$</td>
<td>$6C_{2v} \times T$</td>
<td>$8C_3 \wedge T_s$</td>
<td>$6S_4 \wedge T_s$</td>
<td>$3D_{2d} \times T$</td>
<td></td>
<td></td>
<td>3</td>
</tr>
<tr>
<td>$\mathbb{C}P^2$</td>
<td>$4C_{3v} \times T$</td>
<td>$6C_{2v} \times T$</td>
<td>$3D_{2d} \times T$</td>
<td>$6C_3 \wedge T_s$</td>
<td>$6C_4 \wedge T_s$</td>
<td>$6S_4 \wedge T_s$</td>
<td></td>
<td>3</td>
</tr>
<tr>
<td>$\mathbb{C}P^2 \times S^2$</td>
<td>$8C(3)$</td>
<td>$12C_4$</td>
<td>$6C(4)</td>
<td>6A(4)$</td>
<td>$12A(2)$</td>
<td>$8A(3)$</td>
<td>$8B(3)$</td>
<td>$12C_4$</td>
</tr>
</tbody>
</table>

Figure 13. Simplest purely rotational (left) and $E$-mode vibrational (right) Morse Hamiltonians (often called energy surfaces) of the $A_4$ molecule as functions on the phase spaces $S^2$ and $S^2 \sim \mathbb{C}P^1$. The bounding potential of the $A_4$ molecule is approximated as a sum of pairwise harmonic atom–atom interaction terms; see [12].

of choice is limited to having two maxima and three minima or vice versa. As before, we can predict which of the two possibilities is realized in $A_4$ using the simple atom–atom vibrational potential of [12, 13]. It turns out that at fixed action $n_e$ the two $C_{3v}$-symmetric $\text{RE}$ have maximum energy; see Figure 13. Note that the same happens in the case of the $E$ mode of the $A_3$ molecule, such as $\text{H}_3^+$ [19], whose equilibrium configuration is an isosceles triangle.

5.2.3. Morse functions on the $F_2$-mode phase space $\mathbb{C}P^2$. Among the fixed points of the $T_d \times T$ action on $\mathbb{C}P^2$ (see Tables 10 and 17) only points with stabilizers $C_{2v} \wedge T$ and $S_4 \wedge T_2$ ($D_2$ and $C_1$ in the short notation) can have odd Morse indexes. Table 19 demonstrates how Morse inequalities for $\mathbb{C}P^2$ are satisfied if stationary points lie only on the critical orbits. We can interchange points of indexes $1 \leftrightarrow 3$ or/and $0 \leftrightarrow 4$ to obtain other possible simplest Morse functions. Table 20 shows how this simplest set of stationary points respects Morse
Table 20
Stationary points of the \((T_d \times \mathcal{T})\)-invariant Morse Hamiltonians on \(\mathbb{C}P^2\) (see Table 19) projected on the \(C_2\)- and \(C_s\)-invariant spheres.

<table>
<thead>
<tr>
<th>Stabilizer of orbit</th>
<th>Signature (index) on (\mathbb{C}P^2)</th>
<th>Number of points on (S^2)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Simplest Morse Hamiltonian:</td>
<td></td>
<td></td>
</tr>
<tr>
<td>(C_2) (D_{2d} \times \mathcal{T})</td>
<td>([++++]) (0) ([++]) (0)</td>
<td>2</td>
</tr>
<tr>
<td>(S_4 \land \mathcal{T})</td>
<td>([++++]) (1) ([+-]) (1)</td>
<td>2</td>
</tr>
<tr>
<td>(C_{2v} \land \mathcal{T})</td>
<td>([+-+] (3) ([-] (2)</td>
<td>2</td>
</tr>
<tr>
<td>(C_s) (D_{2d} \times \mathcal{T})</td>
<td>([+++] (0) ([++]) (0)</td>
<td>1</td>
</tr>
<tr>
<td>(C_{2v} \land \mathcal{T})</td>
<td>([++++]) (3) ([+-]) (1)</td>
<td>1</td>
</tr>
<tr>
<td>(C_{3v} \times \mathcal{T})</td>
<td>([-++] (2) ([-] (2)</td>
<td>2</td>
</tr>
</tbody>
</table>

| Nonsimplest Morse Hamiltonian: |
| \(C_2\) \(D_{2d} \times \mathcal{T}\) | \([++-\] (2) \([-+\] (1) | 2 |
| \(S_4 \land \mathcal{T}\) | \([+++\] (0) \([++]\) (0) | 2 |
| \(C_{2v} \land \mathcal{T}\) | \([+-+\] (3) \([-\] (2) | 2 |
| \(C_s\) \(D_{2d} \times \mathcal{T}\) | \([++-\] (2) \([-+\] (1) | 1 |
| \(C_{2v} \land \mathcal{T}\) | \([++++]\) (3) \([+-]\) (1) | 1 |
| \(C_s \land \mathcal{T}_2\) | \([++++]\) (1) \([++\] (0) | 2 |
| \(C_{3v} \times \mathcal{T}\) | \([-++\] (2) \([-\] (2) | 2 |

Figure 14. Position of RE (left) and vibrational \(F_2\)-mode Hamiltonian (right) of the \(A_4\) molecule restricted to the \(C_s\)-invariant sphere in the phase space \(\mathbb{C}P^2\). White circles denote extra (nonfixed) RE; other markers correspond to fixed points in Figure 12 (left). The bounding potential of \(A_4\) is approximated as a sum of pairwise atom–atom harmonic interaction terms [13].

5.2.4. Morse functions on combined spaces. The Betti numbers \(b_k\) and Euler characteristics \(\Sigma\) for the smooth manifold \(P\), which is a product \(P' \times P''\), follow from those for factor
spaces $P'$ and $P''$, 

$$b_k = \sum_{i+j=k} b'_i b''_j, \quad \Sigma = \sum_{k=0}^{\dim P} (-1)^k b_k,$$

where indexes $i$, $j$, and $k$ go from 0 to $\dim P'$, $\dim P''$, and $\dim P = \dim P' + \dim P''$, respectively. In many cases we can analyze RE on $P$ by combining the rules for $P'$ and $P''$; the most interesting case turns out to be that of $\mathbb{C}P^2 \times S^2$ ($F_2$-mode vibration and rotation).

Satisfying Morse conditions on invariant subspaces becomes increasingly important in high dimensions. Thus, even before attempting to consider whether the “minimum” set of the 12 $A_4^{C_2}$, six $(A, B, C)^{C_4}$, and eight $(A, B, C)^{C_3}$ stationary points (see Table 15—ignore indexes $1, 2$) satisfies all conditions for $\mathbb{C}P^2 \times S^2$, we can check if this set works for the subspaces of $\mathbb{C}P^2 \times S^2$. Going back to section 4.5 and Figure 12, we conclude immediately that our set is incomplete. Indeed, we should expect at least two stationary points (a maximum and a minimum) on each of the twelve $C$-invariant spheres in $\mathbb{C}P^2 \times S^2$—yet none of the fixed points of the $T_d \times T$ action lies on these spheres. Therefore, the set of stationary points on the $\mathbb{C}P^2 \times S^2$ space (rotation–vibration RE) includes necessarily at least two 12-point noncritical $C$-orbits. Adding these 24 points, the simplest Morse function on $\mathbb{C}P^2 \times S^2$ can be constructed; one possibility is presented in the last row of Table 19. This function corresponds to the Coriolis-dominated structure, which we will discuss on the example in section 11.

5.3. RE in the initial phase space. RE of the $A_4$ molecule in the initial phase space can be largely, and in some cases entirely, reconstructed using the qualitative information on the symmetry group action on the reduced phase space $\mathbb{C}P^2 \times \mathbb{C}P^1 \times S^2$ and stationary points of the reduced Hamiltonian. Thus all purely rotational RE of a tetrahedral molecule correspond to the stationary rotation around the symmetry axis of their stabilizers. For the $S_4 \times T$ stabilizer we take axis $C_1$, and for $C_n \times T_2$ we take the $C_2$ axis orthogonal to the symmetry plane. Vibrational RE of the $E$- and $F_2$-mode systems form families of basic periodic orbits in the initial phase space parameterized by the values of integrals $n_e$ and $n_f$. Rotation–vibration RE of our system are labeled by the values of integrals $j$, $n_e$, and $n_f$ and can be reconstructed as appropriate combinations of the periodic motions of the subsystems, which correspond to the combined stationary points on the reduced phase space $\mathbb{C}P^2 \times \mathbb{C}P^1 \times S^2$ (see Table 15) and which become 3-tori (see footnote 26) in the original phase space of the system. We will characterize these RE in more detail and illustrate the results on the concrete example of the $A_4$ molecule introduced in section 2.3 and [13].

5.3.1. RE of the $E$-mode system. Neglecting rotation and interaction with other vibrational modes, the $E$-mode system can be described by the Hamiltonian

$$(5.1a) \quad H = \omega_e [H_0 + V(q)],$$

where

$$(5.1b) \quad H_0 = \frac{1}{2} \sum_{i=1}^{2} (q_{E_i}^2 + p_{E_i}^2) = \frac{1}{2} (p_{E_1}^2 + p_{E_2}^2) + V_0$$
is the Hamiltonian of the 1:1 harmonic oscillator, and the anharmonic part of the $D_3$ symmetric potential equals

$$V(q) = \varepsilon \left( \frac{1}{3} q_{E_1}^2 - q_{E_2}^2 \right) q_{E_1} + \cdots.$$  

(5.1c)

The potential $V_0 + V$ is shown in Figure 15. We can see that to the lowest order in $\varepsilon$ our $E$-mode system is equivalent to the Hénon–Heiles oscillator, which has the same symmetry $D_3 \times T \sim D_{3h}$. (Note that the $E$-mode system of triatomic molecules with the equilateral triangle equilibrium, e.g., $H_3^+$ [19], also has the same symmetry and the same lowest order Hamiltonian.) In our $A_4$ example [13], $\varepsilon = -\frac{3\sqrt{3}}{4} \epsilon$ and $\omega_e = \omega$.

The RE of the $E$-mode system are, of course, reconstructed in the same way as the RE of the Hénon–Heiles oscillator [77, 14, 15, 16, 18, 19, 78]. We represent trajectories of this system at a given fixed energy $h$ using their projection in the configuration space, a plane $\mathbb{R}^2_q$ with coordinates $(q_{E_1}, q_{E_2})$. To distinguish between trajectories with the same coordinate...
image, we specify their direction. The boundary of the classical motion is the $h$-level set of $V_0(q) + V(q)$. (We consider small amplitudes and are not interested in the unbounded motion of the Hénon–Heiles system at large energies.)

The symmetry group $T_d \times T$ acts on $\mathbb{R}^2_q$ (see section 4.2) like the planar point group $D_3$. Operations in this group $\{1, 2C_3, 3C_2\}$ act naturally on the RE projections in the $\mathbb{R}^2_q$ space. The time reversal $T$ acts trivially on the coordinate space $\mathbb{R}^2_q$ while changing signs of the momenta $p$ and thus reversing the flow of the dynamical system. It follows that $T$ changes the direction of the periodic trajectories and of their image in $\mathbb{R}^2_q$. All we should do in order to reconstruct qualitatively the projection of the RE in $\mathbb{R}^2_q$ is to suggest two curves with stabilizer $T \wedge T_s$ and two groups of three curves with stabilizer $D_{2d} \times T$ (see critical orbits in Table 8).

In [77, 14, 15, 16] these RE are called $\Pi_7, \Pi_8$, $\Pi_{3,4,5}$, and $\Pi_{6,7,8}$, respectively.

Since the group $(T \wedge T_s)/D_2 = \{1, 2C_3, 2(C_2T)\}$ does not include the time reversal $T$ itself, the two periodic trajectories $\Pi_{7,8}$ are mapped into each other by $T$ and share the same image in $\mathbb{R}^2_q$. The image is a closed $C_3$-invariant loop shaped as a smoothed equilateral triangle (Figure 15, right). It is easy to check that any of the three reflections $C_2$ also map $\Pi_7 \leftrightarrow \Pi_8$, while the operations $C_2T$ leave them invariant. The trajectories $\Pi_{3,4,5}$ and $\Pi_{6,7,8}$ project on lines (degenerate loops) in $\mathbb{R}^2_q$ because their stabilizer $(D_{2d} \times T)/D_2 = C_2 \times T$ includes time reversal $T$. Such lines should necessarily begin and end on the boundary of the motion, where the trajectory has a turning point and approaches the boundary at a right angle. This leaves two possibilities (Figure 15, right): three straight lines on the three $C_2$ axes and three curved lines, each intersecting one of the $C_2$ axes at a right angle.

5.3.2. RE of the $F_2$-mode system. Neglecting rotation and interaction with other vibrational modes, the $F_2$-mode system can be described by the Hamiltonian

$$H = \omega_f[H_0 + \epsilon V_1(q) + \epsilon^2 V_2(q, p) + \cdots]$$

where

$$H_0 = \frac{1}{2} \sum_{i=1}^{3} (q_i^2 + p_i^2) = \frac{1}{2} (p_1^2 + p_2^2 + p_3^2) + V_0$$

is the Hamiltonian of the 1:1:1 harmonic oscillator and

$$V_1(q) = q_1 q_2 q_3$$

is the lowest order anharmonic part of the $T_d$ symmetric potential. The potential $V_0 + \epsilon V_1$ illustrated in Figure 16 appears as a direct three-dimensional analogue of the two-dimensional Hénon–Heiles potential in (5.1c). However, the (small) fourth degree term

$$V_2(q) = q_1^4 + q_2^4 + q_3^4$$

should also be included for the more general description of the reduced system [98]. (Note that any $T_d$ symmetric potential can be written as a polynomial in $V_0$, $V_1$, and $V_2$.) In the concrete potential of the $A_4$ molecule [13], we have

$$V(q) = V_0 + \epsilon \frac{3}{2 (2)!^4} V_1 + \epsilon^2 \left( \frac{7 \sqrt{2}}{64} V_2 - \frac{5 \sqrt{2}}{16} V_0^2 \right).$$
Figure 16. Qualitative representation of the equipotential surface of the $F_2$-mode system (top left). Non-linear normal modes (RE) of the three-dimensional analogue of the Hénon-Heiles oscillator ($F_2$-mode system) reconstructed for $\epsilon = 1$ and energy $H_0 = 0.118$. 

$V(q)$ 

$D_{2d} \times T$ 

$C_{3v} \times T$ 

$C_{2v} \times T$ 

$C_3 \times T_s$ 

$S_4 \times T_2$ 

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while $\omega_f = \sqrt{2}\omega_c$. The molecular $F_2$-mode Hamiltonian $H_2$ also contains the kinematic term $\epsilon^2 \frac{1}{8} [\mathbf{p} \times \mathbf{q}]^2$ related to the angular momentum induced by the $F_2$-mode vibrations.

The RE of the $F_2$-mode system in Figure 16 (cf. Figure 8 in [18] and [98]) can be reconstructed qualitatively using the method in the previous section. We project trajectories of this system in the configuration space $\mathbb{R}^3_q$, where they stay inside a tetrahedral cavity bounded by the $h$-level of $V(q)$; see Figure 16, top left. We classify curves in this cavity by their stabilizers. RE with stabilizers $D_{2d} \times T$, $C_{3v} \times T$, and $C_{2v} \times T$ ($D_4$, $D_3$, and $D_2$ in the shorthand notation of section 4.3) are $T$-invariant. They project to lines in $\mathbb{R}^3_q$, which are passed in both directions. Like $\Pi_7$ (see Figure 16), which brings the circular symmetry down precisely to $\epsilon p q$, while $\omega$ also contains the kinematic term $\epsilon^2 \frac{1}{8} [\mathbf{p} \times \mathbf{q}]^2$ related to the angular momentum induced by the $F_2$-mode vibrations.

The RE of the Hénon–Heiles system, the $D_{2d} \times T$ and $C_{3v} \times T$ RE lie on the corresponding symmetry axes $C_4$ and $C_3$. The $C_{2v} \times T$ RE lie in the symmetry planes $C_s$ and are slightly curved; they resemble, therefore, $\Pi_{4,5,6}$. RE with stabilizers $S_4 \times T_5$ and $C_3 \times T_5$ are similar to the “circular” RE $\Pi_{7,8}$. They project on closed directed curves in $\mathbb{R}^3_q$. In the crudest approximation, these RE can be represented as circles lying in the plane orthogonal to the respective axes $C_4$ and $C_3$. The $S_4 \times T_5$ RE develops a characteristic “bow tie” twist (see Figure 16), which brings the circular symmetry down precisely to $S_4 \times T_5$. The $C_3 \times T_5$ RE has a triangular shape similar to that of $\Pi_{7,8}$ and bends slightly out of plane like the trim on a skullcap. We can further observe that the energy–action characteristics of the $F_2$-mode RE (see Table 19 and sections 5.1.4 and 5.2.3) also shows a certain similarity to the $E$-mode system: At given fixed action $n_f$, the energy of “circular” RE tends to be higher than that of “linear” RE.

5.4. Quantum predictions. Quantum manifestations of RE are very familiar to physicists working on highly excited rotating molecules [31, 32, 33, 34, 18]. Within our more general context we should consider these manifestations for reduced phase spaces of dimension greater than two and products of two (or more) reduced phase spaces with two (or more) dynamical integrals of motion. The latter are quantized, and the corresponding quantum numbers label polyads or multiplets of quantum levels whose internal structure (at given fixed values of integrals) is analyzed using RE. In our system we have three dynamical integrals $J$, $n_q$, and $n_f$, and three corresponding quantum numbers $J$, $N_q$, and $N_f$, which all take integer values.

5.4.1. Systems with one dynamical integral. The most well-known quantum “signature” of classical RE is the presence of quantum states localized predominantly near one particular stable RE (a basic stable periodic orbit). In the simplest situation, all nodes of the quantum wavefunction lie along the periodic orbit, and the number of nodes $N$ (up to Maslov’s correction $\mu$ negligible in the classical limit of large $N$) equals $(2\pi)^{-1}$ times the action integral taken along the orbit that in turn equals the value of the dynamical integral $n$ for the particular RE and energy $h$,

$$N + \mu = n(h) = \frac{1}{2\pi} \oint_{H(p,q)=h} p dq,$$

where $\mu = K/2$ for a $K$-dimensional harmonic oscillator. The energy of such a state is as close to $h$, i.e., to the classical maximum or minimum energy, as possible. With excitation of oscillations about the RE growing, the nodal pattern becomes less trivial and localization disappears eventually.
Stable RE manifest themselves clearly in the structure of the energy levels. The energy level structure largely depends on the dimension of the reduced phase space $P$ and the symmetry present. The reduced system near a stable RE on $P$ can be represented as a nonlinear oscillator of dimension $\frac{1}{2} \dim P$. If the area of classical stability in the phase space is sufficiently large (compared to $\hbar$) we can even observe a “family” of states. If $\frac{1}{2} \dim P > 1$, the harmonic oscillator frequencies can be (partially) degenerate due to the local symmetry of the RE. In the case of $k$ equivalent RE, our reduced system is represented locally as a $k$-well oscillator. The depth of the wells (or the height of the barrier) is determined by the stability of the RE. We observe $k$-level quasi-degenerate quantum states or clusters. The cluster, which is closest in energy to the classical RE limit, has the smallest splitting.

We should well distinguish the quasi-degeneracy of quantum states caused by the degeneracy of the local oscillator system and by the presence of several equivalent (by symmetry) stable RE, respectively. We also recall that the presence of the symmetry group with multi-dimensional (degenerate) irreducible representations can further complicate the analysis of the energy level patterns because quantum states with wavefunctions transforming according to rows of the same irreducible representation are strictly degenerate.

### 5.4.2. Examples of simple cluster structures

The most well-known molecular example of the correspondence between quantum energy levels and classical RE is the structure of individual (isolated) rotational multiplets (section 1.2). In this case $P \sim S^2$, $\frac{1}{2} \dim P = 1$. We observe simple regular sequences of rotational clusters. Near the limiting RE energy, the system of almost equidistant sequences resembles a $k$-well one-dimensional harmonic oscillator; the energy separation between the RE and the closest (first) cluster is approximately half the distance between the clusters, i.e., half-quantum.

The $2J + 1$ multiplet of the ground vibrational state of a spherical top molecule [31, 32, 33, 34, 79] has six-fold and eight-fold clusters corresponding to stable RE (stable stationary axes of rotation) with stabilizers $C_4$ and $C_3$, respectively. The energy region near the unstable RE with stabilizer $C_s$ separates the two cluster systems. In the case of $A_4$ (section 5.2) the six-fold clusters lie at the bottom energies.

Asymmetric top molecules, such as H$_2$O, have three paired RE. The RE in each pair correspond to classical rotation about one of the principal inertia axes in two different directions and are related by time reversal. Four RE (in two pairs) are stable and rotational levels form respective two-fold clusters (doublets).

A similar cluster structure is known for vibrational systems with $P \sim S^2$, such as the $E$-mode system in H$_3^+$ [19], and in $A_4$ (section 5.2 and 5.3.1). Vibrational polyads of these systems are labeled by quantum number $N_e = 0, 1, \ldots$ and contain $N_e + 1$ levels (to complete the rotational analogy use $J_e = \frac{1}{2} N_e$); two-fold and three-fold clusters lie near the top and bottom polyad energies, respectively. These $E$-mode clusters are formed when vibrational excitation is high enough to have at least five quantum states in the polyad ($N_e > 4$). Other vibrational systems with reduced phase space $S^2$ include a number of triatomic molecules with nearly 1:1 resonant stretching vibrations, notably H$_2$O and O$_3$ [22, 23, 24, 25, 26, 27]. The so-called local modes of these molecules are nothing else but a pair of stable equivalent RE, which bifurcates (very early) from the initial “normal mode” RE as the polyad quantum number $n$ rises. The corresponding “local mode states” form doublets; they are commonly
associated with vibrations localized on the particular atom–atom bond.

5.4.3. Quantum $F_2$-mode system. So far in this section, we have summarized the fundamentals of quantum interpretation of RE that are largely known. New aspects begin here. The reduced phase space $P \sim CP^2$ of the $F_2$-mode system is a compact space of real dimension four, and $\frac{1}{2} \dim P = 2$. This means that we have a finite number of quantum states in each polyad with quantum number $N_f = 0, 1, \ldots$ and that the number of states is given by a polynomial in $N_f$ of degree 2. More precisely, the polyads of the 1:1:1 oscillator have $\frac{1}{2}(N_f + 1)(N_f + 2)$ states.

Predicting and understanding the internal structure of the $F_2$-mode polyads begins with the RE analysis. Taking into account Morse theory requirements for $CP^2$ (see section 5.1.4 and Table 17) and its $C_s$- and $C_2$-invariant symplectic subspaces $S^2$ (section 5.2.3) we can suggest stability of the set of RE in the second to last row of Table 19. One possibility is given below.

<table>
<thead>
<tr>
<th>RE</th>
<th>Stabilizer</th>
<th>Signature</th>
<th>Stability</th>
<th>Type</th>
</tr>
</thead>
<tbody>
<tr>
<td>6C_p</td>
<td>$S_4 \wedge T_2$</td>
<td>[----]</td>
<td>ii</td>
<td>B, $C^{(4)}$</td>
</tr>
<tr>
<td>12C_s</td>
<td>$C_3 \wedge T_2$</td>
<td>[-----]</td>
<td>ir</td>
<td>Not fixed</td>
</tr>
<tr>
<td>8C_3</td>
<td>$C_3 \wedge T_3$</td>
<td>[+++]</td>
<td>c</td>
<td>B, $C^{(3)}$</td>
</tr>
<tr>
<td>3D_4</td>
<td>$D_{3d} \wedge T$</td>
<td>[+-+]</td>
<td>rr 1:1</td>
<td>$A^{(4)}$</td>
</tr>
<tr>
<td>6D_2</td>
<td>$C_{2v} \wedge T$</td>
<td>[+++]</td>
<td>ir</td>
<td>$A^{(2)}$</td>
</tr>
<tr>
<td>4D_3</td>
<td>$C_{3v} \wedge T$</td>
<td>[+++]</td>
<td>ii 1:1</td>
<td>$A^{(3)}$</td>
</tr>
</tbody>
</table>

Here, as in Table 17, we use $i$ and $r$ to mark imaginary and real eigenvalue pairs of the local linearized Hamiltonian; $c$ stands for four complex eigenvalues.

Using only $N_f$ and energy $H$ is insufficient to untangle the rich energy level spectrum of the polyad. Since the system is not integrable (there is no third global integral), all we can do is label localized states of different kinds with different sets of additional “good” quantum numbers. When the local approximation separates into the $i$ and/or $r$ subsystems, quantum analysis becomes straightforward. Thus, near the two stable (elliptic) RE, which are denoted $ii$, our system can be represented as a two-dimensional oscillator.

At the minimum polyad energy $H(A^{(3)})$ we have an oscillator with four equivalent equilibria or “wells.” Near each equilibrium it is described as a two-dimensional $D_3$ symmetric oscillator with 1:1 resonant harmonic frequencies. In other words, we encounter a four-fold analogue of the Hénon–Heiles system. Provided that the $A^{(3)}$ RE is sufficiently stable (the wells are deep) we may expect to find a series of “small polyads” labeled by an additional “good” quantum number $\tilde{N} = 0, 1, \ldots \ll N_f$. The structure is similar to that already discussed for the $E$-mode system, albeit the number of levels is quadrupled. In particular, the first level with $\tilde{N} = 0$ (the lowest level in the polyad) is a four-fold cluster. At the maximum polyad energy $H(B^{(4)})$ we find a six-well two-dimensional oscillator. The wells are $C_4$ symmetric and have two frequencies which are, in general, incommensurate. The level system associated with the $B^{(4)}$ RE can be described using two additional local quantum numbers $\tilde{N}'$ and $\tilde{N}''$; the first level (the highest level in the polyad) is a six-fold cluster.

5.4.4. Combined systems with several dynamical integrals. Multiplets of combined systems are labeled with several quantum numbers. For example, rotation–vibration multiplets of the $F_2$-mode system are labeled with a pair of numbers $(J, N_f)$ and contain $\frac{1}{2}(N_f + 1)(N_f + 2)(2J + 1)$ states. The structure of such multiplets can be analyzed using our results for
the individual subsystems, the principles of combining rotational and vibrational RE, and, of course, the set of critical orbits of the $T_d \times T$ action given in Table 15. The new idea here is that we can continue to distinguish between the two kinds of motion, rotation and vibration, while both of them are treated classically.

In typical molecules, vibrational and rotational quanta differ by a magnitude, and the common experimental situation is that $J \gg N_f$. In this limit, it is often possible to separate the whole rotational–vibrational polyad into bands, branches, or, in the terminology of [80],33 vibrational components and consider the latter for different $J$ at fixed $N_f$ (or/and $N_e$). How do RE reflect this band structure? The answer is simple: points in Table 15 with the same rotational coordinates $(j_1, j_2, j_3)$ give different classical limits within the same component. Thus the $F_2$-mode system has three kinds of bands $A$, $B$, and $C$.

We recall that $F_2$-mode vibrations induce angular momentum $\pi$. Rotational multiplets of the $F_2$-mode polyads are split into branches due to the Coriolis coupling of $J$ and $\pi$ and are labeled with the additional “good” quantum number $R$ of the angular momentum $J + \pi$ [81]. The $N_f = 1$ fundamental state has $\pi = 1$. This state splits into three branches with $R = J - 1$, $J$, and $J + 1$, which diverge linearly as $J$ increases. The “circular” RE of type $B, C$ (see section 5.3.2) have maximal angular momentum $\pi$ and are the classical limit for the $R = J \pm 1$ branches; the $A$-type RE have zero momentum and give the limit of the $R = 0$ branch. Provided that we add the two extra nonfixed RE of symmetry $C_s \wedge T_2$ (see section 5.2.4), each classical limit branch has three types of RE with shorthand labels $C_1$, $C_2$, and $C_3$; the internal structure of branches can be analyzed like that of an isolated rotational state in section 5.2.1.

Similar analysis for the $E$-mode system shows that it has two types of branches $A_1$ and $A_2$ (see Table 15—ignore the $F_2$ part $(z_1, z_2, z_3)$ and use time reversal where necessary). In particular, the $N_e = 1$ state has two branches. The splitting between them is determined by higher order rotation–vibration interactions.

The number of vibrational states and, correspondingly, the number of quantum branches, increases with vibrational excitation. The number of critical orbits and of corresponding rotational–vibrational RE remains the same. Quantum branches that lie at “intermediate energies” far from the limit given by the RE can be considered in the same way as quantum states at intermediate energies of purely vibrational polyads (sections 5.4.2 and 5.4.3), i.e., as states with more complex vibrational localization. The RE analysis of the rovibrational structure is simpler for low vibrational polyads.

The number of quantum states in each band and possible intersections of bands (vibrational components) which can change this number is the subject of further qualitative study of bands. This study is beyond the scope of the present basic RE analysis. We mention only that each band can be assigned a topological index (Chern index) [82], which gives the difference between the number of states $2J + 1$ of an isolated rotational multiplet and the number of states in the band. The sum of these indexes over all components of the polyad equals zero. Thus the number of states in the Coriolis branches of the $F_2$-mode fundamental state equals $2R + 1$ and the indexes are $\pm 2$ and $0$. In the $E$-mode polyads the indexes can equal only 2 or 4 modulo 6 [80].

33Note that the index introduced in this work equals one-half of the Chern index introduced in [82].
6. Dynamical invariants of the reduced system. In the previous sections we analyzed the action of the symmetry group on the reduced phase space of our system and predicted its RE entirely on the basis of this analysis. We defined RE explicitly (Table 15) in terms of coordinates \( (z, \bar{z}) \) of the initial system (2.1). Any given reduced Hamiltonian \( H_{\text{eff}} \) can be expressed in terms of \( (z, \bar{z}) \) and the energy–action characteristics of fixed RE can be computed. Stability of RE can be determined using local expansions of \( H_{\text{eff}} \). Those RE whose position on the reduced phase space changes (as a function of energy or parameters) are found as conditional extrema of \( H_{\text{eff}}(z, \bar{z}) \) on the reduced phase space.

The use of initial coordinates \( (z, \bar{z}) \) has, however, obvious limitations. These coordinates are not well suited to studying dynamics on the reduced phase space \( \mathbb{C}P^2 \times \mathbb{C}P^1 \times S^2 \). The more appropriate way to analyze the reduced system is in terms of dynamically invariant functions, which can be constructed of \( (z, \bar{z}) \) [44]. In the following sections we show how invariant polynomials in \( (z, \bar{z}) \) can be used to describe the reduced system. We will use invariants to (i) express the reduced Hamiltonian \( H_{\text{eff}} \) most compactly and unambiguously, (ii) define nonlinear coordinates on the reduced phase space \( \mathbb{C}P^2 \times \mathbb{C}P^1 \times S^2 \), (iii) describe the action of the symmetry group \( T_d \times T \) on this space, (iv) describe the dynamics of the reduced system, and (v) characterize RE in terms of both their position on \( \mathbb{C}P^2 \times \mathbb{C}P^1 \times S^2 \) and stability.

We consider appropriate dynamical symmetry and its reduction in order to introduce dynamical invariants of degree 2 in \( (z, \bar{z}) \) (section 6.2 and Table 21), which generate the ring of all invariant polynomials. All terms in \( H_{\text{eff}} \) can be expressed as various powers of these generators. In section 6.3 we describe the structure of the ring of invariant polynomials using the Molien generating function, and later in section 6.4 we define an integrity basis in order to represent uniquely each invariant polynomial in this ring. In particular, all remaining dependence on the \( A_1 \) variables is expressed as a power series in the 1-oscillator action \( n_a \).

This happens because the \( A_1 \) vibration does not change the geometry of the molecule.

6.1. Reduction of the initial rovibrational system and normal form \( H_{\text{eff}} \). The zero order Hamiltonian of our system is a sum of three harmonic oscillators,

\[
H_0 = \omega_{A_1} n_a + \omega_E n_e + \omega_{F_2} n_f + 0 j,
\]

(6.1a)

where \( n_a, n_e, n_f, \) and \( j \) represent oscillators with degeneracy 1, 2, 3, and 2, respectively. Explicit definition in terms of initial symplectic variables \( (z, \bar{z}) \) is given in Table 21. The first three oscillators describe the \( A_1, E, \) and \( F_2 \) vibrational modes, respectively. The reduced rotational subsystem is lifted to an auxiliary degenerate two-oscillator system with dynamical variables \( (z_6, z_7, \bar{z}_6, \bar{z}_7) \), which is more convenient in computations.

The complete initial rotation–vibration Hamiltonian \( H \) is a power series in dynamical variables \( (z, \bar{z}) \),

\[
H = H_0 + \epsilon H_1 + \epsilon^2 H_2 + \cdots,
\]

(6.1b)

where \( \epsilon \) is a smallness parameter, and different perturbation terms are characterized below.
It follows that all monomials in \((z, \bar{z})\) that are invariant with respect to \(\varphi\) are of even total degree and have the same degree in \(z\) and \(\bar{z}\), e.g., \(z_1 \bar{z}_j, z_1z_j \bar{z}_m \bar{z}_i\), etc. Furthermore, all invariant polynomials can be expressed using quadratic monomials of the form \(z \bar{z}\) (or similar homogeneous polynomials of degree 2), which generate the multiplicative ring \(\mathcal{R}\) of all polynomials.

### Table 21

<table>
<thead>
<tr>
<th>Definition (n_a)</th>
<th>Definition (n_f)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(\frac{1}{2}(z_a \bar{z}_a))</td>
<td>(\frac{1}{2}(z_1 \bar{z}_1 + z_2 \bar{z}_2 + z_3 \bar{z}_3))</td>
</tr>
<tr>
<td>(j) (\frac{1}{2}(z_6 \bar{z}_6 + z_7 \bar{z}_7))</td>
<td>(x_3) (\frac{1}{2}(z_1 \bar{z}_1 - z_2 \bar{z}_2))</td>
</tr>
<tr>
<td>(j_2) (\frac{1}{2}(z_6 \bar{z}_7 + z_7 \bar{z}_6))</td>
<td>(n_3) (\frac{1}{2}(z_3 \bar{z}_3))</td>
</tr>
<tr>
<td>(j_3) (\frac{1}{2}(z_6 \bar{z}_7 - z_7 \bar{z}_6))</td>
<td>(s_1) (\frac{1}{2}(z_2 \bar{z}_4 + z_3 \bar{z}_2))</td>
</tr>
<tr>
<td>(j_4) (\frac{1}{2}(z_6 \bar{z}_6 - z_7 \bar{z}_7))</td>
<td>(t_1) (\frac{1}{2}(z_2 \bar{z}_3 - z_3 \bar{z}_2))</td>
</tr>
<tr>
<td>(n_c) (\frac{1}{2}(z_4 \bar{z}_4 + z_5 \bar{z}_5))</td>
<td>(s_2) (\frac{1}{2}(z_1 \bar{z}_3 + z_3 \bar{z}_1))</td>
</tr>
<tr>
<td>(v_1) (-\frac{1}{2}(z_4 \bar{z}_5 - z_5 \bar{z}_4))</td>
<td>(t_2) (\frac{1}{2}(z_3 \bar{z}_1 - z_1 \bar{z}_3))</td>
</tr>
<tr>
<td>(v_2) (\frac{1}{2}(z_5 \bar{z}_5 - z_4 \bar{z}_4))</td>
<td>(s_3) (\frac{1}{2}(z_1 \bar{z}_2 + z_2 \bar{z}_1))</td>
</tr>
<tr>
<td>(v_3) (\frac{1}{2}(z_4 \bar{z}_5 + z_5 \bar{z}_4))</td>
<td>(t_3) (\frac{1}{2}(z_1 \bar{z}_2 - z_2 \bar{z}_1))</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Order</th>
<th>Degree</th>
<th>Type of the term</th>
</tr>
</thead>
<tbody>
<tr>
<td>(\epsilon)</td>
<td>(z^3)</td>
<td>Cubic anharmonic terms</td>
</tr>
<tr>
<td>(\epsilon^2)</td>
<td>(z^4)</td>
<td>Quartic anharmonic terms</td>
</tr>
<tr>
<td></td>
<td>(z^2 j)</td>
<td>Coriolis interaction</td>
</tr>
<tr>
<td></td>
<td>(j^2)</td>
<td>“Rigid rotor” rotation</td>
</tr>
</tbody>
</table>

When the frequencies \(\omega_{A_1}, \omega_E, \) and \(\omega_{E_1}\) are incommensurate, \(n_a, n_c,\) and \(n_f\) can be regarded as three approximate integrals of motion with values \(N_a\) (see footnote 26), \(N_c,\) and \(N_f,\) respectively. The fourth integral \(j\) with the value \(J\) is the amplitude of the total angular momentum, which is strictly conserved.

We can now reduce (normalize) perturbations \(H_1, H_2,\) etc. in (6.1b) by removing all terms which do not Poisson commute with integrals \(n_f, n_c,\) and \(j.\) (Note that a priori \(\{H, j\} = 0\) since \(j\) is a strict integral.) In other words, we reduce the action of the dynamical 4-torus symmetry group \(T^4\) (see footnote 26) on the initial 16-dimensional phase space with coordinates \((z, \bar{z})\). This group is defined by the flow of four Hamiltonian vector fields \(X_{n_f}, X_{n_c}, X_{n_a},\) and \(X_j.\) The normalized Hamiltonian \(H_{\text{eff}},\) also called the reduced and/or effective Hamiltonian, or simply the normal form, is invariant with regard to this flow.

### 6.2. Invariant polynomials of the oscillator symmetry.

The dynamical symmetry of each oscillator subsystem has the form

\[
\varphi : \mathbb{R}^1 \times C_k \rightarrow C_k : (t, z) \rightarrow \exp(it) z, \tag{6.2a}
\]

where dimension \(k\) can be 3 (\(F_2\) mode), 2 (\(E\) mode and rotation), or 1 (\(A_1\) mode). The conjugate vector \(\bar{z}\) transforms, of course, as follows:

\[
(t, \bar{z}) \rightarrow \exp(-it) \bar{z}. \tag{6.2b}
\]

It follows that all monomials in \((z, \bar{z})\) that are invariant with respect to \(\varphi\) are of even total degree and have the same degree in \(z\) and \(\bar{z}\), e.g., \(z_1 \bar{z}_j, z_1z_j \bar{z}_m \bar{z}_i\), etc. Furthermore, all invariant polynomials can be expressed using quadratic monomials of the form \(z \bar{z}\) (or similar homogeneous polynomials of degree 2), which generate the multiplicative ring \(\mathcal{R}\) of all polynomials.
invariant with respect to $\varphi$. Since $\varphi$ is a flow of the vector field of the linearized system with Hamiltonian
\[
H_0 = \frac{1}{2} \bar{z} \dot{z} = \frac{1}{2} (z_1 \bar{z}_1 + z_2 \bar{z}_2 + \cdots + z_k \bar{z}_k),
\]
all polynomials in this ring Poisson commute with $H_0$, which is an integral of motion for the reduced system.

Generators are defined explicitly in Table 21. In the case of the rotational subsystem, the generators are the familiar components $j_1, j_2, j_3$ of the angular momentum whose amplitude $j$ is a constant. Since the reduced phase space of the 1:1 oscillator and that of the rotator are diffeomorphic, $CP^1 \sim S^2$, the generators $v_1, v_2, v_3$ for the $E$-mode polyads can also be considered as components of an angular momentum with fixed amplitude $\frac{1}{2} n_e$ [69]. The reduced $F_2$-mode oscillator system is described by nine linearly independent generators. The integral of motion $n_f$, and polynomials $x_3$ and $n_3$, are combinations of the actions of the individual oscillators,
\[
n_k = \frac{1}{2} z_k \bar{z}_k, \quad k = 1, 2, 3.
\]

Invariants $s$ and $t$ can be considered as inner and exterior products of 2-vectors,
\[
s_\alpha = \frac{1}{2} (z_\beta, \bar{z}_\beta) \cdot (z_\gamma, \bar{z}_\gamma), \quad t_\alpha = \frac{i}{2} (z_\beta, \bar{z}_\beta) \wedge (z_\gamma, \bar{z}_\gamma).
\]

This construction of invariants goes back to Weyl [83].

6.3. Generating function for oscillator symmetry. Once the action of the dynamical symmetry on the initial phase space $C_k$ of the $k$-oscillator is defined explicitly in (6.2) we can compute the Molien generating function $g(\lambda)$, a heuristic tool [48, 49, 50, 84] suggesting certain structural characteristics of the ring of invariant polynomials in $(z, \bar{z})$. The function $g(\lambda)$ can be obtained directly from the Molien theorem [83]
\[
g(\lambda) = \frac{1}{2\pi} \int_0^{2\pi} \frac{dt}{\det(1 - \lambda U_t)},
\]
where the $2k \times 2k$ matrix $U_t$ represents the action of the dynamical symmetry in (6.2) on both $z_1, \ldots, z_k$ and $\bar{z}_1, \ldots, \bar{z}_N$, i.e., on all phase space variables used to construct invariants. We can see from (6.2) that $U_t$ is a diagonal matrix
\[
U_t = \text{diag}(e^{it}, \ldots, e^{it}, e^{-it}, \ldots, e^{-it}),
\]
and that
\[
g(\lambda) = \frac{1}{2\pi} \int_0^{2\pi} \frac{dt}{(1 - \lambda e^{it})^k(1 - \lambda e^{-it})^k}.
\]

After changing to the complex unimodular variable
\[
\theta = \exp(it), \quad dt = \frac{d\theta}{i\theta},
\]
the integral (6.5) becomes a Cauchy integral

\[ g(\lambda) = \frac{1}{2\pi i} \oint_{|\theta|=1} \frac{\theta^{k-1} d\theta}{(1 - \lambda \theta)^k (\theta - \lambda)^k}. \]  

Here we note that the formal real variable \( \lambda \) is used in Taylor series expansions of \( g(\lambda) \) and the value of \( \lambda \) can be assumed arbitrarily small. In particular, we can have \( |\lambda^{-1}| > 1 \). Since our integral has a single pole \( \theta = \lambda \) of order \( k \geq 1 \) within the unit circle \( |\theta| = 1 \), the Cauchy integral formula yields

\[ g(\lambda) = \frac{1}{(k-1)!} \left. \frac{\partial^{k-1}}{\partial \theta^{k-1}} (1 - \lambda \theta)^k \right|_{\theta=\lambda}, \]  

and in particular,\(^{34}\)

\[
\begin{align*}
(6.9a) \quad g_{C_1}/S_1(\lambda) &= 1/(1 - \lambda^2), \\
(6.9b) \quad g_{C_2}/S_1(\lambda) &= (1 + \lambda^2)/(1 - \lambda^2)^3, \\
(6.9c) \quad g_{C_3}/S_1(\lambda) &= (1 + 4\lambda^2 + \lambda^4)/(1 - \lambda^2)^5, \\
(6.9d) \quad g_{C_k}/S_1(\lambda) &= \sum_{s=0}^{k-1} \binom{k-1}{s} \lambda^{2s} / (1 - \lambda^2)^{2k-1}.
\end{align*}
\]

Here the formal variable \( \lambda \) represents any of the variables \( z \) and \( \bar{z} \). Since all invariants are of even degree in \( z \) and \( \bar{z} \), the degree in \( \lambda \) is also even. We can, therefore, change to variable

\[ \mu = \lambda^2, \]

which represents generators in Table 21. We can also omit one factor \( (1 - \lambda^2) \) in the denominator of (6.9) that represents the principal oscillator invariant. Then

\[
\begin{align*}
(6.10a) \quad g_{C_1}(\mu) &= (1 + \mu)/(1 - \mu)^2, \\
(6.10b) \quad g_{C_2}(\mu) &= (1 + 4\mu + \mu^2)/(1 - \mu)^4.
\end{align*}
\]

### 6.4. Integrity basis.

All functions invariant with respect to the dynamical symmetry (6.2a), and in particular the reduced Hamiltonian (the normal form) \( H_{\text{eff}} \) in (2.4), can be expressed in terms of generator invariants in Table 21. Coefficients \( c_k \) in the Taylor series for the corresponding Molien function \( g(\lambda) \) at \( \lambda = 0 \) give the total number of linearly independent invariant polynomials of degree \( k \). Even though the generators themselves are linearly independent, there are algebraic relations between them and the representation of \( c_k \) invariants of degree \( k \) in terms of such generators is not unique.

For example, the components of the angular momentum obey the relation

\[ j_1^2 + j_2^2 + j_3^2 = j^2 = \text{const}. \]

---

\(^{34}\)Alternative derivation of generating functions (6.9) was given in [84].
Due to this relation, the ring of all invariant polynomials generated multiplicatively by \((j_1, j_2, j_3)\) is not free. To express any member of this ring unambiguously we can use monomials of the type \(j_1^a j_2^b j_3^c\), where \(a\) and \(b\) are arbitrary nonnegative integers and \(c\) equals 0 or 1. In other words, the ring generated by \((j_1, j_2, j_3)\) has the structure \([48, 49, 50]\)

\[
\mathcal{R}(j_1, j_2) \cdot \{1, j_3\},
\]

where \(\mathcal{R}\) is a polynomial ring generated freely by \(j_1\) and \(j_2\). This structure is described by the Molien generating function

\[
g_j = (1 + \mu_j)/(1 - \mu_j)^2,
\]

where the formal variable \(\mu_j\) represents any of \((j_1, j_2, j_3)\), the two denominator factors \((1 - \mu_j)\) suggest two main (or principal) invariants of degree 1 in \((j_1, j_2, j_3)\), while numerator terms 1 and \(\mu_j\) suggest auxiliary invariants of degrees 0 and 1. Such decomposition of generators into principal and auxiliary is called integrity basis.\(^{35}\) Our example shows that the choice of such basis is not unique. Thus we can equally use \((j_2, j_3)\) and \(j_1\). Similarly, all \(E\)-mode invariant polynomials constitute the ring

\[
\mathcal{R}(v_2, v_3) \cdot \{1, v_1\}
\]

described by the generating function

\[
g_e = (1 + \mu_e)/(1 - \mu_e)^2.
\]

Note that \(v_1\) changes sign under time reversal \(T\), while \(v_2\) and \(v_3\) are \(T\)-invariant. Choosing \(v_1\) as an auxiliary (numerator) invariant is convenient for further symmetrization with respect to \(T\).

The choice of the integrity basis is more difficult in the case of the 1:1:1 oscillator system (\(F_2\) mode) with the reduced space \(\mathbb{CP}^2\).\(^{36}\) There are nine quadratic relations ("syzygies" of the first order) among the generators,

\[
\begin{align*}
(6.13a) \quad & t_1^2 + s_1^2 - 4n_3n_2 = 0, \quad t_1t_2 - s_1s_2 + 2s_3n_3 = 0, \quad s_2t_3 + s_3t_2 + 2n_1t_1 = 0, \\
(6.13b) \quad & t_2^2 + s_2^2 - 4n_3n_1 = 0, \quad t_1t_3 - s_1s_3 + 2s_2n_2 = 0, \quad s_1t_3 + s_3t_1 + 2n_2t_2 = 0, \\
(6.13c) \quad & t_3^2 + s_3^2 - 4n_1n_2 = 0, \quad t_2t_3 - s_2s_3 + 2s_1n_1 = 0, \quad s_1t_2 + s_2t_1 + 2n_3t_3 = 0,
\end{align*}
\]

as well as other relations of higher degree. The Molien generating function

\[
g_f = (1 + 4\mu_f + \mu_f^2)/(1 - \mu_f)^4,
\]

with \(\mu_f\) representing any of the generators \(\{x_3, n_3, s, t\}\), suggests that all four principal invariants can be chosen from \(\{x_3, n_3, s, t\}\) and that there should be four auxiliary invariants of

\(^{35}\)Such decomposition is known as integrity basis [83], homogeneous system of parameters [110], or Hironaka decomposition [111].

\(^{36}\)The number of principal and auxiliary invariants and their degrees in \((x, z)\) can be deduced from the Molien generating function. This function, however, does not suggest the explicit construction of the generators, which may not be unique or may not be possible at all.
The choice of four main invariants is far from arbitrary. One possible representation of the structure of this ring is

$$R(x_3, s_1, s_2, s_3) \cdot \{1, n_3, n_3^2, t_1, t_2, t_3\}.$$ 

If we use this integrity basis, relations (6.13) should, of course, be rewritten in order to replace $n_1$ and $n_2$ as

$$n_1 = \frac{1}{2}(n_f - n_3 + x_3), \quad n_2 = \frac{1}{2}(n_f - n_3 - x_3).$$

To obtain an unambiguous expression of the reduced rotation–vibration Hamiltonian $H_{\text{eff}}$ defined on $\mathbb{C}P^2 \times \mathbb{C}P^1 \times S^2$, we should combine the three integrity bases introduced above. The direct multiplication of the three rings is described by the generating function

$$g = gfg_3g_j = \frac{1}{2}(n_f - n_3 + x_3), \quad n_2 = \frac{1}{2}(n_f - n_3 - x_3).$$

where $\mu$ and $\bar{\mu}$ stand for $T$-invariants and $T$-covariants. We can use main invariants

$$R(x_3, s_1, s_2, s_3, v_2, v_3, j_1, j_2)$$

and auxiliary invariants

$$\{1, v_1, j_3, n_3, n_3^2, t_1, t_2, t_3, v_1 j_3, n_3 v_1, n_3^2 v_1, t_1 v_1, t_2 v_1, t_3 v_1, n_3 j_3, n_3^2 j_3, t_1 j_3, t_2 j_3, t_3 j_3, n_3 v_1 j_3, n_3^2 v_1 j_3, t_1 v_1 j_3, t_2 v_1 j_3, t_3 v_1 j_3\}.$$

All polynomials in the above integrity basis are chosen to be either invariant or pseudoinvariant (change sign) with respect to the time reversal $T$; the pseudoinvariants are underlined. This helps further symmetrization in section 7. Of course, we should multiply our ring by all integrals $R(n_f, n_e, j)$. More rigorously, we should first express the normalized Hamiltonian $H_{\text{nr}}$ in terms of the above integrity basis and $R(n_f, n_e, j)$, and only then we replace $n_f$, $n_e$, $j$ with their constant values $N_f$, $N_e$, and $J$, and thus obtain the reduced Hamiltonian $H_{\text{eff}}$.

7. Dynamical invariants symmetrized with respect to finite symmetries. While the integrity basis introduced above in section 6.4 serves the purpose of dynamical (oscillator) symmetry reduction, further modifications should, in principle, follow in order to take the finite symmetry of our system into account. In particular, a symmetrized basis allows us to express (2.4) using the minimum number of (linearly independent) terms whose coefficients can be treated by spectroscopists as free phenomenological (or “adjustable”) parameters.

7.1. Symmetry properties of dynamical invariants. We first find the action of the symmetry group $T_d \times T$ on the generators in Table 21. Before considering $T_d \times T$, we explain the action of two basic symmetry elements, the rotation $C_k$ and the time reversal $T$. 
7.1.1. Spatial axial symmetry. Consider a rotation \( C_\varphi \) of the Euclidean 3-space about axis 1 by angle \( \varphi \), which equals \( 2\pi/k \) in the case of the discrete operation \( C_k \) with \( k = 2, 3, \ldots \). The action of \( C_\varphi \) on the coordinates \((q_1,q_2,q_3)\) is defined by the familiar \( 3 \times 3 \) orthogonal matrix

\[
(7.1) \quad \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos \varphi & \sin \varphi \\ 0 & -\sin \varphi & \cos \varphi \end{pmatrix}, \quad \begin{pmatrix} M(\varphi) = \end{pmatrix}.
\]

Components of the angular momentum \((j_1,j_2,j_3)\) also transform according to this matrix.

To understand the action of \( C_\varphi \) on the \( \mathbb{C}P^1 \)-mode reduced space \( \mathbb{C}P^1 \), consider the rotation of the complex plane with coordinates \((z_1,z_2)\) defined by matrix \( M(\varphi) \) in (7.1) (recall that we rotate the \((q_1,q_2)\) and \((p_1,p_2)\) planes simultaneously) and show that the corresponding rotation of the 3-space with coordinates \((v_1,v_2,v_3)\) defined in Table 21 is given by the \( 3 \times 3 \) matrix in (7.1). It follows that for the 2-sphere \( \mathbb{S}^2 \), which is defined as \( v_1^2 + v_2^2 + v_3^2 = \frac{1}{2}N^2 \) and is isomorphic to \( \mathbb{C}P^1 \), axis \( v_1 \) is the corresponding symmetry axis of rotation. It can be equally verified that (due to the particular choice of variables \((j_1,j_2,j_3)\) in Table 21) similar rotation of the \((z_0,z_7)\) plane corresponds to the symmetry axis \( j_3 \).

To find how \( C_\varphi \) acts on the \( \mathbb{C}P^2 \) space, we can rotate the complex space \( C_3 \) with coordinates \((z_1,z_2,z_3)\) using the matrix

\[
\begin{pmatrix} M(\varphi) \cos \varphi & \sin \varphi \\ 0 & 1 \end{pmatrix},
\]

where \( M(\varphi) \) is the \( 2 \times 2 \) matrix in (7.1), and show by a direct calculation that the action of this operation on the invariants

\[
\begin{pmatrix} x_3 \\ s_3 \end{pmatrix}, \quad \begin{pmatrix} s_2 \\ s_1 \end{pmatrix}, \quad \begin{pmatrix} t_1 \\ t_2 \end{pmatrix}, \quad n_3, \quad t_3,
\]

is given by the matrix \( \text{diag}(M(2\varphi),M(\varphi),M(\varphi),1,1) \), i.e., that these invariants realize representations of the \( \text{SO}(2) \) group of indexes \( \pm 2, \pm 1, \pm 1, 0, \) and \( 0, \) respectively.

7.1.2. Time reversal symmetry \( T \) (or \( Z_2 \)). Recalling the action of \( T \) on the initial vibrational variables \((z,\bar{z})\), we can see that vibrational generators \( v_2, v_3, s_1, s_2, s_3, x_3, \) and \( n_3 \) defined in Table 21 are invariants of the \( Z_2 \) action, while \( v_1, t_1, t_2, \) and \( t_3 \) are covariants,

\[
\begin{align*}
(7.2a) & \quad (s_1, s_2, s_3) &\rightarrow& \quad (s_1, s_2, s_3), \\
(7.2b) & \quad (x_3, n_3, v_2, v_3) &\rightarrow& \quad (x_3, n_3, v_2, v_3), \\
(7.2c) & \quad (t_1, t_2, t_3, v_1) &\rightarrow& \quad (-t_1, -t_2, -t_3, -v_1).
\end{align*}
\]

Integrity basis polynomials in section 6.4 are chosen as either \( T \)-invariant or \( T \)-covariant (antisymmetric or antisymmetric with respect to \( T \)). We can easily symmetrize this basis with respect to \( T \) by taking squares of the principal \( T \)-covariants \( j_1 \) and \( j_2 \) and excluding all auxiliary covariants. The corresponding transformation of the generating function \( g_{fg_e g_j} \) \cite{48, 49, 50} begins with multiplying by

\[
(1 + \lambda)^2/(1 + \lambda)^2 = (1 + \bar{\mu}_j)^2/(1 + \bar{\mu}_j)^2
\]
(to transform the denominator) followed by expanding the numerator and sorting out all numerator terms which represent \( T \)-invariants. The resulting generating function

\[
(7.3) \quad \frac{1 + \mu + 19\mu^2 + 6\mu^3 + 19\mu^4 + \mu^5 + \mu^6}{(1 - \mu)^6(1 - \mu^2)^2},
\]

where \( \mu \) replaces any of formal variables \( \{ \mu_f, \mu_e, \mu_j \} \) and \( \{ \bar{\mu}_f, \bar{\mu}_e, \bar{\mu}_j \} \) for \( T \)-invariants and \( T \)-covariants, respectively, describes polynomials on the phase space \( \mathbb{C}P^2 \times \mathbb{C}P^1 \times S^2 \), which are invariant with regard to both dynamical and time reversal symmetry. The detailed expression for the numerator of (7.3) shows the origin of the auxiliary integrity basis invariants:

\[
1 + \mu_f + \mu_f^2 + 3\mu_f\bar{\mu}_e + 3\bar{\mu}_e\mu_j + 9\mu_f\bar{\mu}_j + 3\bar{\mu}_j^2 \\
+ 3\mu_f\bar{\mu}_j^2 + 3\mu_f\bar{\mu}_e\bar{\mu}_j + 3\bar{\mu}_j^2\mu_e + 3\mu_f^2\mu_j + 3\mu_f^2\bar{\mu}_j^2 \\
+ 9\mu_f\bar{\mu}_e\bar{\mu}_j^2 + 3\mu_f\bar{\mu}_j^3 + \mu_f\mu_j^3 + \mu_f\bar{\mu}_e\mu_j^3 + \mu_f^2\mu_e\bar{\mu}_j^3.
\]

### 7.1.3. Finite symmetry \( T_d \times T \).

The action of \( T_d \times T \) on the dynamical variables in Table 21 can, in principle, be found on the basis of sections 7.1.1 and 7.1.2 if we introduce an appropriately rotated coordinate frame to study each particular axial symmetry element of the \( T_d \) group. Otherwise we can consider tensor products

\[
[z^E \times \bar{z}^E]^\Gamma \quad \text{and} \quad [z^{F_2} \times \bar{z}^{F_2}]^{\Gamma'}
\]

of vectors \( z^{F_2} = (z_1, z_2, z_3) \) and \( z^E = (z_4, z_5) \) that transform according to irreducible representations \( \Gamma \) or \( \Gamma' \) of \( T_d \) (and \( T_d \times T \)) and express these products in terms of invariants in Table 21. A straightforward calculation using Clebsch–Gordan coefficients for cubic groups \([85, 86, 87, 88, 89, 90, 91, 92, 93]^{37}\) gives

\[
n_e = \frac{\sqrt{2}}{2} [z^E \times \bar{z}^E]^A_1, \\
v_1 = -i\frac{\sqrt{2}}{4} [z^E \times \bar{z}^E]^A_2, \\
(v_2, v_3) = \frac{\sqrt{2}}{4} [z^E \times \bar{z}^E]^E, \\
n_f = \frac{\sqrt{3}}{2} [z^{F_2} \times \bar{z}^{F_2}]^A_1, \\
\left(\frac{3n_3 - n_f}{\sqrt{3}}, x_3\right) = -\frac{1}{\sqrt{2}} [z^{F_2} \times \bar{z}^{F_2}]^E, \\
(t_1, t_2, t_3) = -\frac{i}{\sqrt{2}} [z^{F_2} \times \bar{z}^{F_2}]^{F_1}, \\
(s_1, s_2, s_3) = -\frac{1}{\sqrt{2}} [z^{F_2} \times \bar{z}^{F_2}]^{F_2}.
\]

\[^{37}\text{Our parameters } h_{ff}^{\Omega(K, \Gamma)} \text{ correspond to } t_{ff}^{\Omega(K, \Gamma)} \text{ in [92] times a constant (see [13]). The values of parameters are in spectroscopic units of energy, } \text{cm}^{-1}.\]
The transformation properties of the generators now can be obtained explicitly from the matrices in Table 4 and equations in section 7.1.2. In particular, \((t_1, t_2, t_3)\) and \((s_1, s_2, s_3)\) realize irreducible representations \(F_{1u}\) and \(F_{2g}\) of \(T_d \times T\). We can further note that the components of the 3-vectors \(q^2\), \(p^2\), and \(z^2 = q^2 - ip^2\) transform according to the irreducible representation of index 1 of the 3-space rotation group \(SO(3)\). We can also show that

\[ n_f, \quad (t_1, t_2, t_3), \quad \text{and} \quad \left( s_1, s_2, s_3, \frac{3n_3 - n_f}{\sqrt{3}}, x_3 \right) \]

transform according to the irreducible representations of \(SO(3)\) of indexes 0, 1, and 2, respectively.

Variables \((j_1, j_2, j_3)\) are components of the total angular momentum, which is an axial vector transforming according to the irreducible representation 1 of the \(SO(3)\) group and \(F_1\) of the \(O\) group. We can see from (3.1c) that \((j_1, j_2, j_3)\) realize an irreducible representation \(F_{1u}\) of \(T_d \times T\). (This \(O_h\)-like notation should not be confused with \(F_{1g}\), which is the representation of the spatial group \(O_h \subset O(3)\) realized by \((j_1, j_2, j_3)\).)

7.2. Symmetrized integrity basis. Once the symmetry properties of the dynamical variables are established, the integrity basis in sections 6 and 7.1.2 can be symmetrized with regard to the finite group \(T_d \times T\) and can be used to describe the ring of all polynomials invariant with regard to \(T_d \times T\).

7.2.1. Symmetrized basis for the rotational subsystem. The ring \(R\) of polynomials in \(\{j_1, j_2, j_3\}\) invariant with respect to the action of \(T_d \times T\) has the same structure as the ring of polynomials in \(\{x, y, z\}\) invariant with respect to the action of the \(O_h\) group of transformations of \(\mathbb{R}^3\). In both cases we construct an integrity basis using the components of the triply degenerate irreducible representation \(F_{1u}\) realized by \(\{j_1, j_2, j_3\}\). The Molien generating function \(g(A_{1g}, F_{1u}; \lambda)\) in Table 22 indicates that the ring \(R\) is freely generated by three invariants \(j^2\), \(r_4\), and \(r_6\) of degree 2, 4, and 6, respectively. (In molecular literature these invariants have several definitions, such as \(\Omega_4\) and \(\Omega_6\) in [31, 79] and \(R^{3(4, A_1)}\) and \(R^{6(6, A_1)}\) in [85, 86, 87, 88, 89].) Thus, up to degree 6 in \(j\), a purely rotational effective Hamiltonian of a tetrahedral (or octahedral) molecule has only six parameters corresponding to terms \(j^2\), \(j^4\), \(r_4\), \(j^6\), \(j^2r_4\), and \(r_6\).

To express terms in the reduced rotation–vibration Hamiltonian we also need to construct \(\Gamma\)-covariants (i.e., polynomials that transform according to representation \(\Gamma\)) for all irreducible representations \(\Gamma\) of \(T_d \times T\). Corresponding Molien generating functions \(g(\Gamma, F_{1u}; \lambda)\) have, of course, the same denominator as \(g(A_{1g}, F_{1u}; \lambda)\) but also have a numerator \(\text{num}(\Gamma)\) which describes auxiliary \(\Gamma\)-covariants. The ring of \(\Gamma\)-covariants is a product of freely generated \(R(j^2, j^4, r_4, r_6)\) and a finite set of numerator \(\Gamma\)-covariants. One possible explicit choice of these covariants is suggested in Table 22. (See [94] for the discussion of integrity bases for point groups.)
Table 22

Molien functions and possible explicit definition for invariants \((\Gamma = A_{1u})\) and \(\Gamma\)-covariants of the action of the \(O_h\) group (and of the isomorphic group \(T_d \times T\)) constructed from the components \(\{x, y, z\}\) of the triply degenerate irreducible representation \(F_{1u}\).

<table>
<thead>
<tr>
<th>(K)</th>
<th>(\Gamma)</th>
<th>(num(\Gamma))</th>
<th>Invariants and (\Gamma)-covariants</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>(A_{1g})</td>
<td>1</td>
<td>(x^2 + y^2 + z^2)</td>
</tr>
<tr>
<td>4</td>
<td>(A_{1u})</td>
<td>(\lambda^0)</td>
<td>(x^2 + y^2 + z^2)</td>
</tr>
<tr>
<td>6</td>
<td>(A_{2u})</td>
<td>(\lambda^3)</td>
<td>(x^2 y^2 z^2)</td>
</tr>
<tr>
<td>9</td>
<td>(A_{2g})</td>
<td>(\lambda^6)</td>
<td>(xyz(x^2 - y^2)(y^2 - z^2)(z^2 - x^2))</td>
</tr>
<tr>
<td>3</td>
<td>(E_g)</td>
<td>(\lambda^2 + \lambda^4)</td>
<td>({\sqrt{3}(y^2 - z^2), y^2 + z^2 - 2x^2})</td>
</tr>
<tr>
<td>4</td>
<td>(\lambda^6 + \lambda^7)</td>
<td>(xy z{\sqrt{3}(y^2 - z^2), y^2 + z^2 - 2x^2, \sqrt{3}(z^2 - y^2)})</td>
<td></td>
</tr>
<tr>
<td>6</td>
<td>(F_{1g})</td>
<td>(\lambda^4 + \lambda^6 + \lambda^8)</td>
<td>({(y^2 - z^2)y z, (z^2 - x^2)z x, (x^2 - y^2)y x})</td>
</tr>
<tr>
<td>3</td>
<td>(F_{2u})</td>
<td>(\lambda^3 + \lambda^5)</td>
<td>({x, y, z})</td>
</tr>
<tr>
<td>4</td>
<td>(F_{2g})</td>
<td>(\lambda^2 + \lambda^4 + \lambda^6)</td>
<td>({y z, x z, x y})</td>
</tr>
<tr>
<td>5</td>
<td>(\lambda^3 + \lambda^5 + \lambda^7)</td>
<td>({x y z, y^2 z x, z^2 x y})</td>
<td></td>
</tr>
<tr>
<td>6</td>
<td>(\lambda^3 + \lambda^5 + \lambda^7)</td>
<td>({x y z, y^2 z x, z^2 x y})</td>
<td></td>
</tr>
</tbody>
</table>

7.2.2. Symmetrized basis for the \(E\)-mode subsystem. The three components \(\{v_1, v_2, v_3\}\) of the induced vibrational angular momentum of the \(E\)-mode transform according to the reducible representation \(A''_1 \oplus E'\) of \(D_{3h}\) (\(v_1\) transforms according to \(A''_1\) and \(v_2, v_3\) span the doubly degenerate irreducible representation \(E'\)). The structure of the integrity basis for the invariant and \(\Gamma\)-covariant polynomials in \(\{v_1, v_2, v_3\}\), i.e., for the functions on the vibrational \(E\)-mode phase space \(\mathbb{C}P^1 \sim S^2\), is described by the Molien functions \(g(A''_1, A''_1 \oplus E'; \mu, \lambda)\) and \(g(\Gamma, A''_1 \oplus E'; \mu, \lambda)\) in Table 23.

Table 23 also suggests the explicit form of the integrity basis polynomials. One of the principal second degree invariants is, of course, the oscillator integral \(\frac{1}{2} n_\ell = v_1^2 + v_2^2 + v_3^2\). We also note that the cubic invariant \(v_3^2 - 3v_2 v_1^2\) represents the three-fold symmetry and that the reduced vibrational \(E\)-mode Hamiltonian should go up to degree 6 in the initial variables.

---

38 Maximum index of the irreducible representation of \(SO(3)\).
39 Molien function for \(\Gamma\)-covariants \(g(\Gamma, F_{1u}; \lambda)\) equals
\[
\frac{num(\Gamma)}{(1 - \lambda^2)(1 - \lambda^4)(1 - \lambda^6)} = num(\Gamma) g(A_{1g}, F_{1u}; \lambda).
\]
40 Axes \(\{x, y, z\}\) correspond to symmetry axes \(C_4\).
Molien functions and possible explicit definition for invariants and $\Gamma$-covariants of the action of the $D_{3h}$ group (and of the isomorphic group $(T_d \times T)/D_2$) constructed from the components $z \oplus \{x, y\}$ of the representation $A_1' \oplus E'$. 

<table>
<thead>
<tr>
<th>$\Gamma$</th>
<th>num($\Gamma$) $^{41, 42}$</th>
<th>Invariants and $\Gamma$-covariants $^{43, 44}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$A_1'$</td>
<td>1</td>
<td>$x^2 + y^2 + z^2$, $z^3$, $x^3 - 3xy^2$</td>
</tr>
<tr>
<td>$A_2''$</td>
<td>$\mu$</td>
<td>$z$</td>
</tr>
<tr>
<td>$A_2'$</td>
<td>$\lambda^3$</td>
<td>$3g x^2 - y^3$</td>
</tr>
<tr>
<td>$E'$</td>
<td>$\lambda + \lambda^2$</td>
<td>${x, y}, {y^2 - x^2, 2xy}$</td>
</tr>
<tr>
<td>$E''$</td>
<td>$\mu(\lambda + \lambda^2)$</td>
<td>${zy, -xz}, {2xyz, z(x^2 - y^2)}$</td>
</tr>
</tbody>
</table>

Molien generating functions for invariants $(\Gamma = A_{1q})$ and $\Gamma$-covariants of the action of the $O_h$ group (and of the isomorphic group $T_d \times T$) constructed from the components $\{x, y, z\}$ of the triply degenerate irreducible representation $F_{2g}$. 

<table>
<thead>
<tr>
<th>$\Gamma$ $^{45}$</th>
<th>num($\Gamma$) $^{46, 47}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$A_{1q}$</td>
<td>$1 + \lambda^3 + \lambda^4 + \lambda^5 + \lambda^6 + \lambda^9$</td>
</tr>
<tr>
<td>$A_{2g}$</td>
<td>$2\lambda^3 + \lambda^4 + \lambda^5 + 2\lambda^6$</td>
</tr>
<tr>
<td>$E_{1q}$</td>
<td>$\lambda + 2\lambda^2 + \lambda^3 + 2\lambda^4 + 2\lambda^5 + \lambda^6 + 2\lambda^7 + \lambda^8$</td>
</tr>
<tr>
<td>$E_{2g}$</td>
<td>$\lambda + 2\lambda^2 + 3\lambda^3 + 3\lambda^4 + 3\lambda^5 + 3\lambda^6 + 2\lambda^7 + \lambda^8$</td>
</tr>
<tr>
<td>$A_{1u}$</td>
<td>$\lambda^3 + \lambda^4 + 2\lambda^5 + \lambda^6 + \lambda^9$</td>
</tr>
<tr>
<td>$A_{2u}$</td>
<td>$\lambda^2 + \lambda^3 + \lambda^4 + \lambda^5 + \lambda^6 + \lambda^7$</td>
</tr>
<tr>
<td>$E_{u}$</td>
<td>$\lambda^2 + 2\lambda^3 + 3\lambda^4 + 3\lambda^5 + 2\lambda^6 + \lambda^7$</td>
</tr>
<tr>
<td>$E_{1u}$</td>
<td>$\lambda + \lambda^2 + 3\lambda^3 + 4\lambda^4 + 4\lambda^5 + 3\lambda^6 + \lambda^7 + \lambda^8$</td>
</tr>
<tr>
<td>$E_{2u}$</td>
<td>$2\lambda^2 + 3\lambda^3 + 4\lambda^4 + 4\lambda^5 + 3\lambda^6 + 2\lambda^7$</td>
</tr>
</tbody>
</table>

$\{q, p\}$ in order to represent adequately the symmetry of the system.

### 7.2.3. Symmetrized basis for the $F_2$-mode subsystem.

Generating functions for the invariants and covariants of the $O$ and $T_d$ group action on the $\mathbb{C}P^2$ are given in [84]. The generating function for the invariants has the form

\[
\frac{1 + 2\lambda^3 + 3\lambda^4 + 3\lambda^5 + 2\lambda^6 + \lambda^9}{(1 - \lambda^2)^2(1 - \lambda^3)(1 - \lambda^4)}. \tag{7.4a}
\]

$^{41}$Molien function for $\Gamma$-covariants $g(\Gamma, A_1' \oplus E'; \mu, \lambda)$ equals

\[
\frac{\text{num}(\Gamma)}{(1 - \lambda^2)(1 - \lambda^3)(1 - \mu^2)} = \text{num}(\Gamma) g(A_1', A_1' \oplus E'; \mu, \lambda).
\]

$^{42}$Formal variables $\mu$ and $\lambda$ represent $z$ and $\{x, y\}$, respectively.

$^{43}$In the case of the $E$-mode $\{z, x, y\} = \{v_1, v_2, v_3\}$.

$^{44}$Axes $z$ and $x$ correspond to symmetry axes $C_3$ and $C_2$.

$^{45}$$g$ and $u$ label $T$ symmetric and $T$ antisymmetric representations.

$^{46}$All functions have the same denominator as in (7.4b).

$^{47}$The formal variable $\lambda$ represents $z^2$, where $z$ is any of $\{z_1, z_2, z_3\}$.
The corresponding integrity basis is further simplified due to the $T$-symmetrization, which removes half of the auxiliary (numerator) invariants. The function (7.4a) becomes

\[
(7.4b) \quad \frac{1 + \lambda^3 + \lambda^4 + \lambda^5 + \lambda^6 + \lambda^9}{(1 - \lambda^2)^2(1 - \lambda^3)(1 - \lambda^4)}.
\]

Generating functions for covariants are given in Table 24.

Coefficients $c_k$ of terms $\lambda^k$ in the formal series expansion of the generating functions in Table 24 equal the number of linearly independent polynomials of the kind $z^k z^k$. Thus expansion of the function (7.4b)

\[
(7.5a) \quad 1 + 2\lambda^2 + 2\lambda^3 + 5\lambda^4 + 5\lambda^5 + \ldots
\]

suggests that there are two linearly independent $(T_d \times T)$-invariant terms $z^3 z^3$. This does not include polynomials built with powers of the scalar $n_f$ that can be taken into account if we divide (7.4b) by one more $(1 - \lambda)$. Then the corresponding formal series

\[
(7.5b) \quad 1 + \lambda + 3\lambda^2 + 5\lambda^3 + 10\lambda^4 + 15\lambda^5 + \ldots
\]

indicates five terms of degree 3, of which three should, obviously, contain $n_f$. In fact there is $n_f^3$ and two terms of the kind $n_f z^2 z^2$.

The generators of the rings of $T_d$ and $(T_d \times T)$-invariants and covariants can be constructed from the polynomials of the forms

\[
(7.6a) \quad \begin{bmatrix} abc \\ pqr \end{bmatrix} = z_1^a z_2^b z_3^c \bar{z}_1^p \bar{z}_2^q \bar{z}_3^r + \left\{ \begin{array}{c} \text{column} \\ \text{permutations} \end{array} \right\}
\]

and

\[
(7.6b) \quad \begin{bmatrix} abc \\ pqr \end{bmatrix} = \begin{bmatrix} abc \\ pqr \end{bmatrix} + \begin{bmatrix} pqr \\ abc \end{bmatrix}.
\]

In particular, $n_f = \frac{1}{100}$. The Molien functions in Table 24 characterize heuristically the structure of these rings. The denominator of the function (7.4b) tells us that there are two $z^2 \bar{z}^2$, one $z^3 \bar{z}^3$, and one $z^4 \bar{z}^4$ principal integrity basis invariants, which can enter in any degree in the expression for other invariants and covariants. The concrete choice of these four principal invariants,

\[
(7.7a) \quad \begin{bmatrix} 110 \\ 110 \end{bmatrix}, \quad \begin{bmatrix} 200 \\ 020 \end{bmatrix}, \quad \begin{bmatrix} 111 \\ 111 \end{bmatrix}, \quad \begin{bmatrix} 400 \\ 022 \end{bmatrix},
\]

and five nontrivial auxiliary (numerator) invariants,

\[
(7.7b) \quad \begin{bmatrix} 300 \\ 120 \end{bmatrix}, \quad \begin{bmatrix} 301 \\ 121 \end{bmatrix}, \quad \begin{bmatrix} 410 \\ 032 \end{bmatrix}, \quad \begin{bmatrix} 411 \\ 033 \end{bmatrix}, \quad \begin{bmatrix} 702 \\ 144 \end{bmatrix} - \begin{bmatrix} 612 \\ 054 \end{bmatrix},
\]

is suggested in [84].
7.2.4. Symmetrized basis for the complete system. Once we take all symmetries into consideration and combine the three subsystems, the integrity basis becomes very complicated. Resulting symmetrized principal polynomials and a large number of auxiliary polynomials require high powers of dynamical variables and will not be used here. Instead, we will study both the group action of $T_d \times T$ and the dynamics of the reduced system in terms of simpler dynamical invariants in Table 21. In the next section we briefly describe the tensorial basis, which we use to express the effective Hamiltonian $H_{\text{eff}}$ (normal form).

7.2.5. Tensorial bases used in molecular literature. Instead of using an integrity basis of the kind described above, spectroscopists represent their effective Hamiltonians using tensorial bases constructed by the rules of the tensorial product of the finite symmetry group of the system. For example, the $F_2$-mode Coriolis term is constructed as

$$[i \{ \bar{z} F_2 \times z F_2 \}^{F_1} \times j F_1 \}^{A_1}] = -\frac{\sqrt{2}}{\sqrt{3}}(t, j).$$

(This term is invariant with regard to a larger group $SO(3)$.) Such bases guarantee completeness but cannot exclude the possibility of linear dependence among terms of a given order. At low orders, where such dependencies are few or nonexistent, this is tolerable. Explicit construction of all linearly independent terms of a given degree using the standard coupling scheme of tensors adopted in molecular spectroscopy is often nontrivial. The difficulty increases rapidly with degree. Of course, all spectroscopic tensors can be expressed using generators in Table 21. Some of the most frequently used terms [13] are given in Tables 25 and 26.

8. Group action, fixed points, and invariant subspaces. The action of the symmetry group of our system $T_d \times T$ on the reduced phase space $\mathbb{C}P^2 \times \mathbb{C}P^1 \times \mathbb{S}^2$ is not free. Our main interest is in the fixed points of this action and in the subspaces of $\mathbb{C}P^2 \times \mathbb{C}P^1 \times \mathbb{S}^2$, which are invariant with regard to the spatial symmetry group $T_d$ and are therefore dynamically invariant.

In section 4 we analyzed the action of $T_d \times T$ using complex dynamical variables $z$ of the initial system (see section 2.2). Below we obtain the same results using the dynamical invariants in Table 21 and their symmetry properties. These invariants serve both as dynamical variables of the reduced system and as polynomial “coordinates” on the reduced phase space $\mathbb{C}P^2 \times \mathbb{C}P^1 \times \mathbb{S}^2$. We use invariants in order to remove the dynamical symmetry $G_{\text{dyn}} = T^4$ (see footnote 26 and section 6.1) and to avoid the ambiguity of the $(z, \bar{z})$ coordinates. (Indeed, the values of generators in Table 21 specify uniquely a $G_{\text{dyn}}$ orbit, which corresponds to a distinct point on $\mathbb{C}P^2 \times \mathbb{C}P^1 \times \mathbb{S}^2$.) At the same time, we cannot label orbits of the finite group $T_d \times T$ because our polynomials are not symmetrized with regard to $T_d \times T$. Instead we find concrete fixed points (and invariant subspaces) for concrete stabilizer subgroups of $T_d \times T$. Results are summarized in Tables 27 and 28.

8.1. Fixed points in the presence of spatial axial symmetry. We return to the general discussion of the axial symmetry in section 7.1.1. The action of any spatial rotation $C_k$ with $k = 2, 3, \ldots, \infty$ on the $\mathbb{C}P^1$ space and on the isomorphic 2-sphere $\mathbb{S}^2$ has two fixed points. These points lie on the symmetry axis. Thus in the $j_3$ axis example,

$$j_1 = j_2 = 0, \quad j_3 = \pm J.$$
In the complex coordinates \((z_6, z_7)\) these points can be represented as \((1,0)\) and \((0,1)\). The analysis is the same for the \(E\)-mode space.

Rotation \(C_k\) with \(k > 2\) acting on the \(CP^2\) space has three fixed points. The action of this operation on the dynamical invariants is described in section 7.1.1 for the case of rotation about \(z_3\) (take \(\varphi < \pi\) because \(k > 2\)). In this case, we find that

\[
x_3 = s_3 = s_2 = s_1 = t_1 = t_2 = 0
\]

at the fixed points. Substitution into (6.13) gives

\[
(1 - \eta)\eta = (1 - \eta)t_3 = \eta^2 - t_3^2 = 0,
\]
Table 26
Relation between low degree polynomials constructed in terms of integrity basis and spectroscopic tensorial terms. Only leading terms are taken into account (i.e., classical limit commutativity of variables is assumed).

\[
\begin{array}{c|c}
100 & 2H^0 \\
100 & 2V^A_{fff} + 4\sqrt{2}V^A_{fff} + 4\sqrt{3}V^A_{fff} \\
110 & 2\sqrt{3}V^A_{fff} \\
200 & 8V^A_{fff} - 4\sqrt{2}V^A_{fff} \\
100 & 8\sqrt{3}\left( V^{EF} + V^{A} + V^{A} \right) \\
100 & + 24\sqrt{3}V^{EF} + 8V^{A} \\
100 & 4\left( 4V^{EF} - V^{EF} + V^{EF} - V^{EF} \right) \\
100 & 0 \left( 300 \right. \\
100 & \left. 120 \right) \\
111 & 4V^{EF} + 4V^{EF} \\
111 & + 4\sqrt{3}\left( V^{EF} - V^{EF} - V^{EF} \right) \\
\end{array}
\]

where \( n_1 = n_2 = \frac{1}{2} \eta \geq 0 \) and of course \( n_3 = N_f - \eta \geq 0 \). This system has three solutions, all isolated fixed points on \( \mathbb{CP}^2 \), with \((t_3/N_f, \eta/N_f)\) equal to \((0, 0)\), \((1, 1)\), and \((1, -1)\), respectively. The first solution is invariant with regard to time reversal \( T \), while the other two constitute one \( T \) orbit. In the complex coordinates \((z_1, z_2, z_3)\) these points can be represented as \((1, 0, 0)\) and \((0, 1, \pm i)\).

In the special case of the \( C_2 \) rotation we can only assert that

\[ s_2 = s_1 = t_1 = t_2 = 0. \]

This leaves two possibilities: an isolated fixed point

\[ n_3 = N_f, \quad n_1 = n_2 = t_3 = s_3 = 0, \]

and a 2-sphere defined as

\[ n_3 = 0, \quad t_3^2 + s_3^2 + x_3^2 = N_f^2. \]

In the original \((z_1, z_2, z_3)\) coordinates, the former is again the point \((1, 0, 0)\), while the latter is the \( \mathbb{CP}^1 \) subspace of \( \mathbb{CP}^2 \), where \( z_3 = 0 \).
Points in the critical orbits of the $T_d \times T$ group action on the reduced phase space $\mathbb{CP}^2 \times \mathbb{CP}^1 \times S^2$ characterized by values of dynamical invariants in Table 21. Points are listed without their time reversal ($T$) companions; upper and lower signs in the $\pm$ and $\mp$ notation correspond to different orbits with subscript indices 1 and 2, respectively. Matrices of stabilizers $S^v_4$, $C^{[111]}_3$, and $C^{[111]}_3$ are given in Table 4.

<table>
<thead>
<tr>
<th>Orbit</th>
<th>$x_3/N_f$</th>
<th>$s_1/N_f$</th>
<th>$s_2/N_f$</th>
<th>$s_3/N_f$</th>
<th>$t_1/N_f$</th>
<th>$t_2/N_f$</th>
<th>$t_3/N_f$</th>
<th>$v_1/N_c$</th>
<th>$v_2/N_c$</th>
<th>$v_3/N_c$</th>
<th>$j_1/J$</th>
<th>$j_2/J$</th>
<th>$j_3/J$</th>
<th>Stabilizer</th>
</tr>
</thead>
<tbody>
<tr>
<td>$A^{(2)}_{1,2}$</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>−1</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>$\mp \frac{1}{2}$</td>
<td>0</td>
<td>$\frac{1}{2}$</td>
<td>$\mp \frac{1}{2}$</td>
<td>0</td>
</tr>
<tr>
<td></td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>1</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>$\pm \frac{1}{2}$</td>
<td>0</td>
<td>$\frac{1}{2}$</td>
<td>$\pm \frac{1}{2}$</td>
<td>0</td>
</tr>
<tr>
<td></td>
<td>$\frac{1}{2}$</td>
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<td>0</td>
<td>0</td>
<td>0</td>
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<td>0</td>
<td>0</td>
<td>0</td>
<td>$\pm \frac{1}{2}$</td>
<td>$\pm \frac{1}{2}$</td>
<td></td>
<td>\text{lower sign}</td>
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<tr>
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<td>$\frac{1}{2}$</td>
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<td>0</td>
<td>0</td>
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<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>$\pm \frac{1}{2}$</td>
<td>$\pm \frac{1}{2}$</td>
<td></td>
<td>\text{upper sign}</td>
<td></td>
</tr>
<tr>
<td></td>
<td>$\frac{1}{2}$</td>
<td>−1</td>
<td>0</td>
<td>0</td>
<td>$\frac{1}{2}$</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>$\pm \frac{1}{2}$</td>
<td>$\pm \frac{1}{2}$</td>
<td></td>
<td>\text{lower sign}</td>
<td></td>
</tr>
<tr>
<td>$A^{(3)}_{1,2}$</td>
<td>0</td>
<td>$\frac{1}{2}$</td>
<td>$\frac{1}{2}$</td>
<td>$\frac{1}{2}$</td>
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<td>$B^{(3)}_{1,2}$</td>
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</table>

8.2. Fixed points of the $T_d \times T$ group action.

8.2.1. Stabilizer $S_4$. Orientation of the $S^z_4$ axis in Table 4 corresponds to the one used in section 8.1 for the general case of a $C_k$ axis; solutions for fixed points with stabilizer $C_4$ on the $F_2$-mode space $\mathbb{CP}^2$ and on the rotational space $S^2$ are already given above in section 8.1. On the $E$-mode space $\mathbb{CP}^1 \sim S^2$; the image of the $S^z_4$ operation is a rotation about axis $v_2$ by
According to the irreducible representations $A$ and $E$ reduced phase space is defined using equation 8.1. There is a fixed point and an invariant 2-sphere in the rotational sphere $S^2$ (the fixed points are the same as in the case of $S^2$). Furthermore, the whole $E$-mode space $CP^2 × CP^1 × S^2$ is invariant because operations $C_2^g$, $C_2^a$, and $C_2^y$ act trivially on this space. There is, therefore, no restriction on $(v_1, v_2, v_3)$. On the full reduced space $CP^2 × CP^1 × S^2$ we can have a point, an invariant 2-sphere, or an $S^2 × S^2$ space.

8.2.2. Stabilizer $C_2$. We can consider the $C_2$ stabilizer using directly the results in section 8.1. There is a fixed point and an invariant 2-sphere in $CP^2$ and two fixed points on the rotational sphere $S^2$ (the fixed points are the same as in the case of $S^2$). Furthermore, the whole $E$-mode space $CP^1 × S^2$ is invariant because operations $C_2^g$, $C_2^a$, and $C_2^y$ act trivially on this space. There is, therefore, no restriction on $(v_1, v_2, v_3)$. On the full reduced space $CP^2 × CP^1 × S^2$ we can have a point, an invariant 2-sphere, or an $S^2 × S^2$ space.

8.2.3. Stabilizer $C_3$. In the case of $C_3$, we also expect three fixed points on $CP^2$ and two points on $CP^1$ and $S^2$ each. We first recall that $(j_1, j_2, j_3)$ transform according to the irreducible representation $F_1$ of the $T_d$ group. Considering the matrix representation of $F_1$ for the particular operation $C_3$ in Table 4, we can see immediately that a point on the rotational sphere $S^2$ remains invariant (stable) with respect to this operation only if

$$j_1 = j_2 = j_3.$$  

Furthermore, since

$$j_1^2 + j_2^2 + j_3^2 = j^2 = J^2,$$

the two possible solutions for the fixed points on $S^2$ are

$$j_1 = j_2 = j_3 = ±J/\sqrt{3}.$$  

These two points form one $T$ orbit. There are four axes $C_3$ (four conjugate subgroups $C_{3v}$ of the $T_d$ group) and there is one orbit of the action of the full group $T_d × T$ that includes all eight points on $S^2$ with stabilizer $C_3$.

Vibrational $E$-mode polynomials $v_1$ and $(v_2, v_3)$ are chosen so that they transform according to the irreducible representations $A_2$ and $E$ of $T_d$ (see section 7). When the $E$-mode reduced phase space is defined using equation

$$v_1^2 + v_2^2 + v_3^2 = \frac{1}{4} n_c = \frac{1}{4} N_e^2,$$  

angle $\pi$. Consequently, at the two fixed points on this space, $v_1 = v_3 = 0$. 

<table>
<thead>
<tr>
<th>Stabilizer</th>
<th>Values of dynamical variables and defining equation(s)</th>
<th>Orbit size</th>
<th>Topology</th>
</tr>
</thead>
<tbody>
<tr>
<td>$C_2$</td>
<td>$0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ v_1 \ v_2 \ v_3$</td>
<td>6</td>
<td>$S_2$</td>
</tr>
<tr>
<td>$C_2^a$</td>
<td>$\xi \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ v_1 \ v_2 \ v_3$</td>
<td>6</td>
<td>$S_2 × S_2$</td>
</tr>
<tr>
<td>$C_2^y$</td>
<td>$0 \ \sigma \ \eta \ 1 - \eta \ \tau \ -\tau \ 0 \ 0 \ \frac{1}{2} \ 0 \ \frac{1}{\sqrt{2}} \ \frac{1}{\sqrt{2}} \ 0$</td>
<td>12</td>
<td>$S_2$</td>
</tr>
<tr>
<td>$0 \ \sigma \ \eta \ 1 - \eta \ \tau \ -\tau \ 0 \ 0 \ \frac{1}{2} \ 0 \ \frac{1}{\sqrt{2}} \ \frac{1}{\sqrt{2}} \ 0$</td>
<td>12</td>
<td>$S_2$</td>
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</tbody>
</table>
as a 2-sphere in the ambient 3-space with coordinates \((v_1, v_2, v_3)\), the action of the \(C_3\) operation is equivalent to the \(C_3\) rotation about axis \(v_1\). (This illustrates the abstract statement that the image of the \(T_d\) group in this case is a dihedral group \(D_3\).) The two points that are invariant with regard to this operation lie on the \(v_1\) axis (on the diametrically opposite ends),

\[
v_1 = \pm \frac{1}{2} N_e, \quad v_2 = v_3 = 0.
\]

Since \(v_1\) has the symmetry \(A_2\), these points are mapped into each other by operations \(S_4\) and \(C_s\) of \(T_d\) and, therefore, they are equivalent and form one two-point orbit. Operation \(T\) also maps these points into each other.

To find the fixed points on \(\mathbb{C}P^2\) with stabilizer \(C_3^{[111]}\), we note that polynomials \((s_1, s_2, s_3)\) and \((t_1, t_2, t_3)\) transform according to the irreducible representations \(F_2\) and \(F_1\) of the \(T_d\) group, respectively. From matrices in Table 4 we conclude that at the fixed points on \(\mathbb{C}P^2\),

\[
\begin{align*}
(8.1a) & \quad s_1 = s_2 = s_3 = \sigma N_f, \quad t_1 = t_2 = t_3 = \tau N_f, \\
\end{align*}
\]

where \(\sigma\) and \(\tau\) are dimensionless. We further note that at the same fixed point (with stabilizer \(C_3^{[111]}\)) polynomials

\[
\left(\frac{3n_3 - n_f}{\sqrt{3}}, x_3\right),
\]

which transform according to the irreducible representation \(E\), should vanish, i.e.,

\[
(8.1b) \quad 3n_3 - n_f = x_3 = n_1 - n_2 = 0,
\]

and since \(n_1 + n_2 + n_3 = N_f\) we obtain

\[
(8.1c) \quad n_1 = n_2 = n_3 = \frac{1}{3} N_f.
\]

Substituting conditions (8.1) into relations (6.13) produces equations

\[
\begin{align*}
\left\{ (1 + 3\sigma)\tau = 0, \quad \sigma^2 + \tau^2 = \frac{4}{9}, \quad \sigma^2 - \tau^2 = \frac{2}{3}\sigma \right\}
\end{align*}
\]

with two kinds of solutions:

\[
(\tau, \sigma) = \left(0, \frac{2}{3}\right) \quad \text{and} \quad \left(\pm \frac{1}{\sqrt{3}}, -\frac{1}{3}\right).
\]

Combining fixed points on \(S^2\), \(\mathbb{C}P^1\), and \(\mathbb{C}P^2\) for the same stabilizer, i.e., the group generated by the \(C_3^{[111]}\) operation in Table 4, we obtain the fixed points on \(\mathbb{C}P^2 \times \mathbb{C}P^1 \times S^2\) listed in Table 27.
8.2.4. Stabilizer $C_s$. In the case of $C_s$, solution for the fixed points on the rotational sphere $S^2$ and on the $E$-mode space $CP^1 \sim S^2$ is again quite simple. Indeed, using $F_1$ and $E$ matrices of the $C_s^{xy}$ example in Table 4 we find that these fixed points are defined as

$$j_1 = -j_2, \quad j_3 = 0 \quad \text{and} \quad v_1 = 0, \quad v_3 = 0.$$  

On the $F$-mode space $CP^2$ we look for a fixed point and a $C_s$-invariant sphere (see section 8.1). In the particular case of the $C_s^{xy}$-invariant points we find that

$$t_3 = 0, \quad t_1 = -t_2 = \tau N_f, \quad s_1 = s_2 = \sigma N_f, \quad x_3 = 0.$$  

Using the notation

$$n_1 = n_2 = \frac{\eta}{2} N_f \geq 0, \quad n_3 = (1 - \eta) N_f \geq 0, \quad s_3 = s N_f,$$

we obtain from relations (6.13) that

$$\tau^2 + \sigma^2 = 2(1 - \eta)s = 2(1 - \eta)\eta,$$

$$\eta^2 - s^2 = \tau(\eta - s) = \sigma(\eta - s) = 0.$$  

These equations have two kinds of solutions: an isolated point with

$$\eta = 1, \quad s = -1, \quad \sigma = \tau = 0,$$

which is listed in Table 27, and a 2-sphere defined by

$$\eta = s, \quad 2\tau^2 + 2\sigma^2 + (2\eta - 1)^2 = 1.$$

8.3. Orbits of the $T_d \times T$ action. To find the orbits of equivalent fixed points of the $T_d \times T$ action we take the fixed points found in the previous section for concrete stabilizers in Table 4 and act on them by all symmetry operations of $T_d \times T$. We use the symmetry properties of dynamical invariants (generators in Table 21) described in section 7.1.3. These invariants are not symmetrized with regard to $T_d \times T$ and their values (which play the role of “coordinates” on $CP^2 \times CP^1 \times S^2$) differ for the points in the orbit. On the contrary, the value and behavior of any $T_d \times T$ invariant function, such as the reduced Hamiltonian $H_{eff}$, remains the same.

Table 27 presents orbits of the $T_d \times T$ action on $CP^2 \times CP^1 \times S^2$. The list of fixed points in each orbit starts with the particular point found in section 8.2. Since time reversal images of points can be easily found using (7.2), we omit them for brevity so that each orbit in Table 27 has twice the number of points listed. For example, the orbit $A_1^{(4)}$ with stabilizer $S_4 \times T$ has six equivalent fixed points, which correspond to three conjugate symmetry operations $S_4^x$, $S_4^y$, and $S_4^z$ of the $T_d$ group. The other six-point orbit $A_2^{(4)}$ differs from $A_1^{(4)}$ in the way the $F_2$- and $E$-mode coordinates are combined.

Invariant subspaces in Table 28 also are representatives of orbits of equivalent subspaces. There are six 2-spheres with stabilizer $C_2$, six $S^2 \times S^2$ spaces with the same stabilizer, and two different orbits of twelve 2-spheres with stabilizer $C_s$. Explicit coordinate representations for all these spaces can be obtained in the same way as obtained for the fixed points.
8.4. Residual group action on invariant subspaces. Invariant subspaces of the $T_d$ group action on $\mathbb{CP}^2 \times \mathbb{CP}^1 \times \mathbb{S}^2$, which are characterized in Table 28, are not homogeneous spaces with regard to the $T_d \times T$ action. This has, of course, important consequences for the dynamics, which we will analyze later.

First we can verify whether some of the fixed points of the $T_d \times T$ group action in Table 27 lie on any of the invariant subspaces. The presence of fixed points indicates that there is some nontrivial residual action of $T_d \times T$ on the subspace. Continuing the $C_2$ example in Table 28, we find that two points $A_1^{(4)}$ and $A_2^{(4)}$ lie on the $C_2$-invariant $E$-mode sphere, and four points $B_1^{(4)}$, $B_2^{(4)}$, $C_1^{(4)}$, and $C_2^{(4)}$ lie on the $C_2$-invariant space $\mathbb{S}^2 \times \mathbb{S}^2$. In the particular case of $C_2$, the residual $T_d$ action is equivalent to the rotation by $\pi$ about axes $t_3$ and $v_2$ in the respective ambient 3-spaces.

A complete study of all residual symmetries can be easily done by selecting all operations of the $T_d \times T$ group which map invariant subspaces into themselves. Such selection is, of course, greatly simplified by the fact that many invariants take definite fixed values (see Table 28). Thus when studying symmetry operations acting on the invariant space $\mathbb{S}^2 \times \mathbb{S}^2$ with stabilizer $C_2$, we consider only those operations of $T_d \times T$ which leave $j_3$ invariant (such as rotations around axis 3) or change its sign (such as reflections $C_4$ in the planes containing axis 3). In the latter case, we should add the $T$ operation to restore the sign of $j_3$. Another simplifying observation is that invariants used as coordinates on the subspaces often transform according to (rows of) different irreducible representations of the $T_d$ group. In that case the residual group can have only one-dimensional representations.

Residual group action of $T_d \times T$ on the invariant subspaces of the action of the spatial group $T_d$ on $\mathbb{CP}^2 \times \mathbb{CP}^1 \times \mathbb{S}^2$ is characterized in Table 30. We can see that the residual action on the $C_2$ and $C_3$ invariant spaces is equivalent to that of a $C_{2h}$ and a $C_h$ group, respectively. (As before we use point group analogies of groups which include reversing operations $T$, $T_s$, or $T_2$.) Due to the presence of this residual action, invariant subspaces contain lower-dimensional strata in addition to just fixed points; see Tables 29 and 30.

\begin{table}[h]
\centering
\caption{Further stratification of the invariant subspaces of $\mathbb{CP}^2 \times \mathbb{CP}^1 \times \mathbb{S}^2$ with stabilizers $C_i^{(4)}$ and $C_2$ (Table 28) due to residual group action.}
\begin{tabular}{ccc}
\hline
Stabilizer & Equations & Topology \\
\hline
$C_2 \times T_d$ & $v_1 = 0$ & $S_1$ \\
$C_2 \times T_s$ & $v_2 = 0$ & $S_1$ \\
$C_2 \times T_2$ & $v_1 = x_3 = \xi = 0$ & $T_2 = S_1 \times S_1$ \\
$C_2 \times T_s$ & $v_2 = s_3 = \sigma = 0$ & $T_2 = S_1 \times S_1$ \\
$C_i^{(4)} \times (T_2, T_s)$ & $\sigma = 0$ & $S_1$ \\
\hline
\end{tabular}
\end{table}

9. Dynamics of the reduced system. Classical equations of motion for the reduced system can, in principle, be obtained using initial dynamical variables $(z, \bar{z})$ and the Poisson bracket

$$\{z, \bar{z}\} = \{q + ip, q - ip\} = -2i$$
Table 30

Residual action of $T_d \times T$ on the dynamical invariants used to represent invariant subspaces in Table 28; note that $T_2$ and $T_s$ stand for $C_2 \circ T$ and $C_s \circ T$, respectively.

<table>
<thead>
<tr>
<th>Spaces with stabilizer $C_2^z$</th>
<th>Dynamical Classes of $T_d \times T$</th>
<th>2-sphere with stabilizer $C^2_{zy}$</th>
<th>Dynamical Classes of $T_s \times T$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$I, C_2$ $T_2$ $S_4$ $T_s$</td>
<td>$I, C_s$ $T_2$</td>
<td></td>
</tr>
<tr>
<td>$F^{(3)}_{1u}$</td>
<td>$t_3, j_3$ $1$ $1$ $1$ $1$</td>
<td>$E^{(1)}_9$ $v_2, n_3$ $1$</td>
<td></td>
</tr>
<tr>
<td>$E^{(1)}_3$</td>
<td>$v_2, n_3$ $1$ $1$ $1$ $1$</td>
<td>$F^{(1)}_{1u}$ $t_1 - t_2, j_1 - j_2$ $1$ $1$</td>
<td></td>
</tr>
<tr>
<td>$E^{(2)}_3$</td>
<td>$x_3, v_3$ $1$ $1$ $-1$ $-1$</td>
<td>$F^{(2)}_2$ $s_3 + s_2$ $\sqrt{2}$</td>
<td>$1$ $-1$</td>
</tr>
<tr>
<td>$F^{(2)}_3$</td>
<td>$s_3$ $1$ $-1$ $-1$ $1$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$A_{2u}$</td>
<td>$v_1$ $1$ $-1$ $-1$ $1$</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

if we consider the reduced Hamiltonian $H_{\text{eff}}$ as a function of $(z, \bar{z})$. These equations of motion should preserve all symplectic symmetries of $H_{\text{eff}}$, i.e., remain invariant with regard to the dynamical (oscillator) symmetry and to the action of the spatial group $T_d$ described in section 7. We can, therefore, represent them in terms of invariants in Table 21 and thus obtain equations of motion on $\mathbb{C}P^2 \times \mathbb{C}P^1 \times S^2$. A more elegant approach is to study the Poisson algebra generated by the invariants and then obtain the same equations directly.

9.1. Poisson algebra of dynamical invariants. Invariants in Table 21 generate a multiplicative ring $\mathcal{R}$ of polynomials invariant with regard to the oscillator symmetry. The Poisson bracket of any two generators in Table 21 is itself a dynamically invariant polynomial function, which is a member of $\mathcal{R}$. We say that $\mathcal{R}$ has a Poisson structure. Invariant polynomials in Table 21 generate a Poisson algebra and can be used as dynamical variables. The integrals $j$, $n_e$, and $n_f$ are Casimirs. To compute the structure of the algebra, we can return to the $(z, \bar{z})$ representation.

For the $E$-mode invariants and, of course, for the angular momentum components, we obtain the standard algebra $\text{so}(3)$,

$$
\{j_\alpha, j_\beta\} = \epsilon_{\alpha\beta\gamma} j_\gamma, \quad \{v_\alpha, v_\beta\} = \epsilon_{\alpha\beta\gamma} v_\gamma,
$$

and the Euler–Poisson equations,

$$
\frac{d}{dt} j_\alpha = \{H_{\text{eff}}, j_\alpha\} = \frac{\partial H_{\text{eff}}}{\partial j_\beta} j_\beta - \frac{\partial H_{\text{eff}}}{\partial j_\gamma} j_\gamma.
$$

Dynamics on the $\mathbb{C}P^2$ space is described by the system of equations for eight invariant polynomials, which can be considered as independent dynamical variables. Since all these polynomials are quadratic in $(z, \bar{z})$, their Poisson brackets are also quadratic and can be expressed as their linear combinations. Resulting Poisson algebra is characterized in Table 31. Given the structure matrix $\mathcal{M}$ in this table, equations of motion can be written as

$$
\dot{\theta} = \mathcal{M}^T \nabla_{\theta} H_{\text{eff}},
$$

where $\theta$ is a vector $\theta = (x_3, s_1, s_2, s_3, n_3, t_1, t_2, t_3)$ and $\mathcal{M}^T = -\mathcal{M}$. 

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Table 31

Poisson algebra of the invariants describing dynamics on \(\mathbb{C}P^2 \times \mathbb{C}P^1 \times S^2\) (\(F_2\)- and E-mode polyads and rotational subsystem). Here \(x_1 = n_2 - n_3, x_3 = n_1 - n_2, x_2 = n_3 - n_1,\) and \(x_1 + x_2 + x_3 = 0.\)

<table>
<thead>
<tr>
<th>(x_3)</th>
<th>(s_1)</th>
<th>(s_2)</th>
<th>(s_3)</th>
<th>(n_3)</th>
<th>(t_1)</th>
<th>(t_2)</th>
<th>(t_3)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(-t_1)</td>
<td>(-t_2)</td>
<td>(2t_3)</td>
<td>(0)</td>
<td>(s_1)</td>
<td>(s_2)</td>
<td>(-2s_3)</td>
<td>(j_2)</td>
</tr>
<tr>
<td>(s_1)</td>
<td>(-t_3)</td>
<td>(t_2)</td>
<td>(t_1)</td>
<td>(2x_1)</td>
<td>(-s_3)</td>
<td>(s_2)</td>
<td>(j_3)</td>
</tr>
<tr>
<td>(s_2)</td>
<td>(-t_1)</td>
<td>(-t_2)</td>
<td>(s_3)</td>
<td>(2x_2)</td>
<td>(-s_1)</td>
<td>(t_3)</td>
<td>(-t_2)</td>
</tr>
<tr>
<td>(n_3)</td>
<td>(0)</td>
<td>(-s_2)</td>
<td>(s_1)</td>
<td>(2x_3)</td>
<td>(t_1)</td>
<td>(t_3)</td>
<td>(-t_2)</td>
</tr>
<tr>
<td>(t_1)</td>
<td>(s_1)</td>
<td>(-s_2)</td>
<td>(0)</td>
<td>(t_3)</td>
<td>(-t_2)</td>
<td>(t_1)</td>
<td>(t_3)</td>
</tr>
<tr>
<td>(t_2)</td>
<td>(0)</td>
<td>(-s_2)</td>
<td>(s_1)</td>
<td>(2x_3)</td>
<td>(t_1)</td>
<td>(t_3)</td>
<td>(-t_2)</td>
</tr>
</tbody>
</table>

### 9.2. Canonical variables in the limit of linearization.

In section 8.2 we found RE, or equilibria of the reduced system, as isolated fixed points (critical orbits) of the \(T_k \times T\) action. To study dynamics near these RE, and in particular to determine their stability, we should linearize \(H_{eff}\) near them. Linearization in terms of \((z, \bar{z})\) variables was already introduced in section 5.1.4.

Similarly to finding coordinates of RE in section 8.2, linearizing near an RE can be understood on the example of a \(C_k\) symmetric RE whose symmetry axis is oriented as in section 7.1.1. Axis \(S_k\) (or \(C_1\)) has such an orientation, and coordinates of the RE \(A_{1,2}^4\) and \(B_{1,2}^4\) on the \(\mathbb{C}P^2\) space and rotational sphere \(S^2\) (see Table 27) define, in fact, fixed points and RE for any \(C_k^2\) action on these spaces with \(k = 3, 4, \ldots, \infty.\)

Consider first the familiar simple case of the rotational sphere \(S^2\) described by \((j_1, j_2, j_3)\) or by scaled variables

\[
\tilde{j}_i = \frac{j_i}{\sqrt{j}}, \quad i = 1, 2, 3.
\]

At the fixed point \(j_3 = J\), the only nonzero Poisson bracket is \(\{j_1, j_2\} = j_3\) (Table 31), and consequently the scaled variables \((\tilde{j}_1, \tilde{j}_2)\) become the standard canonical coordinate–momentum pair in the limit of linearization near the relative equilibrium with \(j_3 = J\). Near the second fixed point on \(S^2\) with \(j_3 = -J\) (which is the time reversal image of the first point) canonical variables will be \((\tilde{j}_2, \tilde{j}_1)\); i.e., \(\tilde{j}_2\) will play the role of coordinate and \(\tilde{j}_1\) the role of conjugate momentum.

The \(E\)-mode space \(\mathbb{C}P^1\) is isomorphic to a sphere \(S^2\) defined in the ambient 3-space with coordinates \((v_1, v_2, v_3)\). We should scale these coordinates as follows:

\[
\tilde{v}_i = \frac{v_i\sqrt{2}}{\sqrt{N_e}}, \quad i = 1, 2, 3.
\]

The \(S_k^1\) operation acts on the \(E\)-mode sphere as rotation by \(\pi\) about axis \(v_2\); the two fixed points with \(v_2 = \pm N_e/2\) lie on this axis. In the limit of linearization near these points we use canonical coordinates \((\tilde{v}_1, \tilde{v}_3)\) and \((\tilde{v}_3, \tilde{v}_1)\).

On the \(F_2\)-mode space \(\mathbb{C}P^2\) we proceed in a similar fashion [97]. We compute the Poisson structure in Table 31 at each relative equilibrium and then find canonical variables of the
Notice that near the RE we can express all the invariants in terms of the displacements we use is selected from among the invariants

\[ \zeta \]

\[ (9.5) \]

\[ F \]

\[ \text{implicit function theorem are satisfied. Specifically, let} \]

\[ \text{of the syzygy relations (6.13) and} \]

\[ \zeta \]

\[ \text{express the remaining invariants} \]

\[ \text{that these coordinates be canonical. The set of coordinate invariants} \]

\[ \zeta \]

\[ \text{are} \]

\[ \text{that the solution takes a simple form.} \]

\[ \text{This can be done only by inspecting the solutions in each case.} \]

\[ \text{For example, for the} \]

\[ \text{point} \]

\[ \text{with stabilizer} \]

\[ \text{are} \]

\[ \text{that the 10} \]

\[ \times \]

\[ 5 \]

matrix \[ a \]

\[ \equiv \]

\[ \sqrt{2} \]

\[ N_f \]

\[ a = s, t, n, x, \quad i = 1, 2, 3, \]

we obtain the results in Table 32.

Another way to proceed is to find coordinates near each RE on \( \mathbb{C}P^2 \) without demanding that these coordinates be canonical. The set of coordinate invariants \( \zeta_{i}^{(c)} \) \( (i = 1, \ldots, 4) \) that we use is selected from among the invariants \( n_{i}, s_{i}, \) and \( t_{i} \) \( (i = 1, 2, 3) \) such that the syzygy relations (6.13), together with the constraint \( n_{1} + n_{2} + n_{3} = N_{f} \), can be solved in order to express the remaining invariants \( \zeta_{i}^{(r)} \) \( (i = 1, \ldots, 5) \) in terms of \( \zeta_{i}^{(c)} \) and \( N_{f} \).

We find a set of invariants with the above property by checking that the conditions of the implicit function theorem are satisfied. Specifically, let \( F_{i} \) \( (i = 1, \ldots, 9) \) be the left-hand sides of the syzygy relations (6.13) and \( F_{10} = n_{1} + n_{2} + n_{3} - N_{f} \). The invariants \( \zeta_{i}^{(r)} \) are selected in such a way that the 10 \( \times \) 5 matrix

\[ (9.5) \]

\[ \frac{\partial (F_{i})}{\partial (\zeta_{j}^{(r)})} \]

has rank 5. Then \( \zeta_{i}^{(r)} \) can be expressed in terms of \( \zeta_{i}^{(c)} \) and \( N_{f} \). There is usually more than one choice for \( \zeta_{i}^{(c)} \), but not all choices are equally acceptable. Since we need to actually solve the equations \( F_{i} = 0 \), we must try to find a set \( \zeta_{i}^{(c)} \) such that the solution takes a simple form. This can be done only by inspecting the solutions in each case.

For example, for the \( A_{4}^{(4)} \) point \( (1, 0, 0) \) with stabilizer \( D_{2d}^{(x)} \times T \), we find that \( \zeta^{(c)} = (s_{2}, s_{3}, t_{2}, t_{3}) \) is a suitable set of invariants. The values of these invariants on the specific RE are \( \zeta^{(c)*} = (0, 0, 0, 0) \). We define the displacement vector

\[ d_{i}^{A_{4}^{(4)}} = \zeta_{i} = \zeta_{i}^{(c)} - \zeta_{i}^{(c)*}, \quad i = 1, \ldots, 4. \]

Notice that near the RE we can express all the invariants in terms of the displacements \( \zeta_{i} \).

An important difference with regard to the previous discussion is that the displacements here are not necessarily canonically conjugate variables. It is therefore important to calculate the linearized Poisson structure near each RE. In order to do this we calculate each Poisson bracket \( \{ \zeta_{i}, \zeta_{j} \} \) using the invariants, and then we express the result as a function of the

\[ 48 \text{Notation as in Table 21 with} \ n \equiv N_{f}. \]
Table 33

Dynamically invariant local coordinates at the RE on the $F^2$-mode space $\mathbb{CP}^2$.

<table>
<thead>
<tr>
<th>Type of RE</th>
<th>Poisson algebra$^{40}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$A^{(4)}$</td>
<td>$D^{(2)}_{2\theta} \times T$</td>
</tr>
<tr>
<td></td>
<td>$s_2 = \zeta_1$ 0 $-2n$ 0</td>
</tr>
<tr>
<td></td>
<td>$s_3 = \zeta_2$ 0 $2n$ 0</td>
</tr>
<tr>
<td></td>
<td>$t_2 = \zeta_3$ 0 $0$</td>
</tr>
<tr>
<td></td>
<td>$t_3 = \zeta_4$</td>
</tr>
<tr>
<td>$A^{(2)}$</td>
<td>$C^{(x)}_{2\theta} \times T$</td>
</tr>
<tr>
<td></td>
<td>$n_2 - \frac{1}{2}n = \zeta_1$ 0 0 $n$</td>
</tr>
<tr>
<td></td>
<td>$s_1 = \zeta_2$ 0 $0$</td>
</tr>
<tr>
<td></td>
<td>$t_1 = \zeta_3$ 0 $0$</td>
</tr>
<tr>
<td></td>
<td>$t_3 = \zeta_4$</td>
</tr>
<tr>
<td>$A^{(3)}$</td>
<td>$C^{(x)}_{2\theta} \times T$</td>
</tr>
<tr>
<td></td>
<td>$s_2 - 2n/3 = \zeta_1$ 0 0 $-2n/3$</td>
</tr>
<tr>
<td></td>
<td>$s_3 - 2n/3 = \zeta_2$ 0 $2n/3$ 0</td>
</tr>
<tr>
<td></td>
<td>$t_2 = \zeta_3$ 0 $0$</td>
</tr>
<tr>
<td></td>
<td>$t_3 = \zeta_4$</td>
</tr>
<tr>
<td>$B^{(3)}$</td>
<td>$C_{3}^{[111]} \wedge T_{3}^{</td>
</tr>
<tr>
<td></td>
<td>$s_2 + n/3 = \zeta_1$ $-n/\sqrt{3}$ 0 $n/3$</td>
</tr>
<tr>
<td></td>
<td>$s_3 + n/3 = \zeta_2$ $-n/\sqrt{3}$ 0 $n/\sqrt{3}$</td>
</tr>
<tr>
<td></td>
<td>$t_2 - n/\sqrt{3} = \zeta_3$ $n/\sqrt{3}$</td>
</tr>
<tr>
<td></td>
<td>$t_3 - n/\sqrt{3} = \zeta_4$</td>
</tr>
<tr>
<td>$B^{(4)}$</td>
<td>$S_{4}^{(x)} \wedge T_{2}^{(9)}$</td>
</tr>
<tr>
<td></td>
<td>$n_3 - \frac{1}{2}n = \zeta_1$ $-n$ 0 0</td>
</tr>
<tr>
<td></td>
<td>$s_1 = \zeta_2$ 0 $0$</td>
</tr>
<tr>
<td></td>
<td>$s_2 = \zeta_3$ 0 $0$</td>
</tr>
<tr>
<td></td>
<td>$t_2 = \zeta_4$</td>
</tr>
</tbody>
</table>

Displacements $\zeta_i$, keeping terms only up to first order. We can follow the above program for all the RE. The results are summarized in Table 33. Observe that for most cases in this table it is immediately obvious how to define standard canonically conjugate variables. Thus in the case of the $A^{(3)}$ point, we can define canonically conjugate variables $(\xi, \eta)$,

$$\xi_1 = \alpha \zeta_2, \eta_1 = \alpha \zeta_3, \xi_2 = \alpha \zeta_4, \eta_2 = \alpha \zeta_1, \quad \alpha = \sqrt[3]{\frac{3}{2N_f}},$$

such that the local 2-form is $d\xi_1 \wedge d\eta_1 + d\xi_2 \wedge d\eta_2$. The only case where the proper definition of the canonical variables is not obvious is the case of the $B^{(3)}$ point.

To conclude this section, we should add one important remark. The above canonical (or noncanonical) variables can only be used to study linear Hamiltonian equations of the reduced system near the RE. This limitation is due to the fact that the symplectic form near the RE has a standard matrix ($\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$) only to the first order (in the limit of linearization). When nonlinear equations of motion near the RE are sought (e.g., when bifurcations of the RE are studied) this form should be further “flattened” in higher orders; see section V.8.2 of [11].

9.3. Dynamics on invariant subspaces of $\mathbb{CP}^2 \times \mathbb{CP}^1 \times \mathbb{S}^2$. In section 8.4 and Table 28 we describe three possible types of subspaces of the reduced phase space $\mathbb{CP}^2 \times \mathbb{CP}^1 \times \mathbb{S}^2$ that

$^{40}$Notation as in Table 21 with $n \equiv N_f$. 

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are invariant with regard to the (symplectic) action of the spatial group $T_d$ and are therefore dynamically invariant subspaces of the reduced system. These subspaces are either 2-spheres $S^2 \sim \mathbb{C}P^1$ or a product of 2-spheres $S^2 \times S^2$. Dynamics on each $S^2$ can be described by Euler–Poisson equations. The corresponding “angular momentum” algebras $so(3)$ are constructed below.

The construction is most straightforward in the case of the $C_2$-invariant $S^2$ subspace of $\mathbb{C}P^2$ (which can be represented using complex coordinates $(z_1, z_2)$ and $z_3 = 0$). We can see from Tables 21 and 28 that the three $so(3)$ components can be chosen as

\[(Y_1, Y_2, Y_3) = \left( \frac{s_3}{2}, \frac{t_3}{2}, \frac{x_3}{2} \right).\]

Restricting the Poisson algebra in Table 31 to the $C_2^Z$-invariant sphere defined in Table 28 shows that this is indeed $so(3)$,

\[\{Y_\alpha, Y_\beta\} = \epsilon_{\alpha\beta\gamma} Y_\gamma,\]

with Casimir

\[Y_1^2 + Y_2^2 + Y_3^2 = \left( \frac{N_f}{2} \right)^2.\]

Dynamics on the $S^2 \times S^2$ invariant subspace in Table 28 is described using an $so(3) \times so(3)$ algebra. The second $so(3)$ is generated by $(v_1, v_2, v_3)$, commutes with $(Y_1, Y_2, Y_3)$, and has the Casimir

\[v_1^2 + v_2^2 + v_3^2 = \left( \frac{N_e}{2} \right)^2.\]

Dynamical variables for the $C_4^{xy}$-invariant sphere in Table 28 are obtained analogously. Restricting the Poisson algebra in Table 31, we find polynomials

\[(X_1, X_2, X_3) = \left( \frac{t_1 - t_2}{2\sqrt{2}}, \frac{s_1 + s_2}{2\sqrt{2}}, \frac{2s_3 - N_f}{2} \right) = \left( \frac{\tau}{\sqrt{2}}, \frac{\sigma}{\sqrt{2}}, \frac{2\eta - 1}{2} \right) N_f,\]

which form the $so(3)$ algebra, such that

\[X_1^2 + X_2^2 + X_3^2 = \left( \frac{N_f}{2} \right)^2, \quad \{X_i, X_j\} = \epsilon_{ijk} X_k.\]

10. Existence and stability of RE. RE are special stationary solutions of the equations of motion (9.1), which in many cases are defined entirely by symmetry and exist for any generic small symmetry-preserving perturbation. Isolated fixed points of the $T_d \times T$ group action on the reduced phase space $\mathbb{C}P^2 \times \mathbb{C}P^1 \times S^2$ found in section 8 are necessarily stationary solutions of (9.1) and are therefore representing RE. We show how to determine the stability of these RE using the reduced Hamiltonian $H_{\text{eff}}$ defined as a function on $\mathbb{C}P^2 \times \mathbb{C}P^1 \times S^2$. Subsequently, we search for other RE, which are not fixed by the action of the finite symmetry group.
10.1. Linear stability of fixed RE. Fixed RE of our system correspond to fixed points of the group action found in sections 8.1 and 8.2 (see Table 10, 15, and 27). Stability of these RE was already analyzed in section 5.1.4, where we studied analytical Poincaré surfaces of section using initial phase space variables \((z, \bar{z})\). Here we use invariants in Table 21 to study RE stability directly on \(CP^2 \times CP^1 \times S^2\), i.e., without lifting back to the initial phase space. As before, we can explain our approach in the example of axial symmetry with axis \(C_k\) oriented as \(C_k^1\) (see sections 8.1 and 9.2).

Analysis on \(CP^2\) is the most difficult [97]. Using canonical variables of the linearization limit found in section 9.2 and Table 32, we come to the problem of determining linear stability of a stationary point in different canonical planes. Each such plane has its origin at the relative \(\zeta\) found in section 9.2 and Table 32, we come to the problem of determining linear stability of these RE in section 9.2. All stationary points found should satisfy Morse conditions for the respective subspace.

As explained in section 5, we should study the \(C_s\)-invariant subspace, which is a 2-sphere with no critical orbits of the symmetry group action (no RE fixed by symmetry). This sphere
Table 34
Action of stabilizers on dynamically invariant local coordinates on $\mathbb{CP}^2$ defined in Table 33.

Action of $D_{2d}^{(x)} \times T$ on $E_y \oplus E_u$ for the $A_1^{(4)}$ RE

<table>
<thead>
<tr>
<th>$R$</th>
<th>$R\zeta_1$</th>
<th>$R\zeta_2$</th>
<th>$R\zeta_3$</th>
<th>$R\zeta_4$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E$</td>
<td>$\zeta_1$</td>
<td>$\zeta_2$</td>
<td>$\zeta_3$</td>
<td>$\zeta_4$</td>
</tr>
<tr>
<td>$C_2^x$</td>
<td>$-\zeta_1$</td>
<td>$-\zeta_2$</td>
<td>$\zeta_3$</td>
<td>$-\zeta_4$</td>
</tr>
<tr>
<td>$C_2^y$</td>
<td>$\zeta_1$</td>
<td>$-\zeta_2$</td>
<td>$\zeta_3$</td>
<td>$-\zeta_4$</td>
</tr>
<tr>
<td>$C_2^z$</td>
<td>$-\zeta_1$</td>
<td>$\zeta_2$</td>
<td>$-\zeta_3$</td>
<td>$\zeta_4$</td>
</tr>
<tr>
<td>$\sigma^{yz}$</td>
<td>$\zeta_2$</td>
<td>$\zeta_1$</td>
<td>$-\zeta_4$</td>
<td>$-\zeta_3$</td>
</tr>
<tr>
<td>$\sigma^{yx}$</td>
<td>$-\zeta_2$</td>
<td>$-\zeta_1$</td>
<td>$\zeta_4$</td>
<td>$\zeta_3$</td>
</tr>
<tr>
<td>$(S_1^4)^{-1}$</td>
<td>$\zeta_2$</td>
<td>$-\zeta_1$</td>
<td>$-\zeta_4$</td>
<td>$\zeta_3$</td>
</tr>
</tbody>
</table>

Action of $S_4^{(x)} \wedge T_2^{(y)}$ on $B_1 \oplus B_2 \oplus E$ for the $B_1^{(4)}$ RE

<table>
<thead>
<tr>
<th>$R$</th>
<th>$R\zeta_1$</th>
<th>$R\zeta_2$</th>
<th>$R\zeta_3$</th>
<th>$R\zeta_4$</th>
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</thead>
<tbody>
<tr>
<td>$E$</td>
<td>$\zeta_1$</td>
<td>$\zeta_2$</td>
<td>$\zeta_3$</td>
<td>$\zeta_4$</td>
</tr>
<tr>
<td>$C_2^x$</td>
<td>$\zeta_1$</td>
<td>$\zeta_2$</td>
<td>$-\zeta_3$</td>
<td>$-\zeta_4$</td>
</tr>
<tr>
<td>$S_4^x$</td>
<td>$-\zeta_1$</td>
<td>$-\zeta_2$</td>
<td>$\zeta_4$</td>
<td>$\zeta_3$</td>
</tr>
<tr>
<td>$(S_1^4)^{-1}$</td>
<td>$-\zeta_2$</td>
<td>$-\zeta_1$</td>
<td>$\zeta_4$</td>
<td>$\zeta_3$</td>
</tr>
</tbody>
</table>

Action of $C_{2v}^{(x)} \times T$ on $A_{2g} \oplus A_{2u} \oplus B_{1g} \oplus B_{1u}$ for the $A_1^{(2)}$ RE

<table>
<thead>
<tr>
<th>$R$</th>
<th>$R\zeta_1$</th>
<th>$R\zeta_2$</th>
<th>$R\zeta_3$</th>
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</tr>
</thead>
<tbody>
<tr>
<td>$E$</td>
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<td>$\zeta_2$</td>
<td>$\zeta_3$</td>
<td>$\zeta_4$</td>
</tr>
<tr>
<td>$C_2^x$</td>
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<td>$-\zeta_2$</td>
<td>$\zeta_3$</td>
<td>$\zeta_4$</td>
</tr>
<tr>
<td>$\sigma^{yz}$</td>
<td>$-\zeta_1$</td>
<td>$\zeta_2$</td>
<td>$-\zeta_3$</td>
<td>$\zeta_4$</td>
</tr>
<tr>
<td>$\sigma^{yx}$</td>
<td>$\zeta_1$</td>
<td>$-\zeta_2$</td>
<td>$-\zeta_3$</td>
<td>$\zeta_4$</td>
</tr>
<tr>
<td>$T$</td>
<td>$\zeta_1$</td>
<td>$-\zeta_2$</td>
<td>$\zeta_3$</td>
<td>$\zeta_4$</td>
</tr>
<tr>
<td>$C_{3}^{[111]}$</td>
<td>$-\zeta_1$</td>
<td>$-\zeta_2$</td>
<td>$\zeta_3$</td>
<td>$\zeta_4$</td>
</tr>
<tr>
<td>$(C_{3}^{[111]})^2$</td>
<td>$\zeta_1$</td>
<td>$\zeta_2$</td>
<td>$\zeta_3$</td>
<td>$\zeta_4$</td>
</tr>
<tr>
<td>$\sigma^{yz}$</td>
<td>$\zeta_1$</td>
<td>$-\zeta_2$</td>
<td>$\zeta_3$</td>
<td>$\zeta_4$</td>
</tr>
<tr>
<td>$\sigma^{yx}$</td>
<td>$-\zeta_1$</td>
<td>$\zeta_2$</td>
<td>$-\zeta_3$</td>
<td>$\zeta_4$</td>
</tr>
<tr>
<td>$T$</td>
<td>$\zeta_1$</td>
<td>$-\zeta_2$</td>
<td>$\zeta_3$</td>
<td>$\zeta_4$</td>
</tr>
<tr>
<td>$(C_{3}^{[111]})^2$</td>
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<td>$-\zeta_2$</td>
<td>$\zeta_3$</td>
<td>$\zeta_4$</td>
</tr>
<tr>
<td>$\sigma^{yz}$</td>
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<td>$-\zeta_2$</td>
<td>$\zeta_3$</td>
<td>$\zeta_4$</td>
</tr>
<tr>
<td>$\sigma^{yx}$</td>
<td>$-\zeta_1$</td>
<td>$\zeta_2$</td>
<td>$-\zeta_3$</td>
<td>$\zeta_4$</td>
</tr>
</tbody>
</table>

Action of $C_{3}^{[111]} \times T$ on $E_y \oplus E_u$ for the $A_1^{(3)}$ RE

<table>
<thead>
<tr>
<th>$R$</th>
<th>$R\zeta_1$</th>
<th>$R\zeta_2$</th>
<th>$R\zeta_3$</th>
<th>$R\zeta_4$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E$</td>
<td>$\zeta_1$</td>
<td>$\zeta_2$</td>
<td>$\zeta_3$</td>
<td>$\zeta_4$</td>
</tr>
<tr>
<td>$C_{3}^{[111]}$</td>
<td>$-\zeta_1$</td>
<td>$-\zeta_2$</td>
<td>$\zeta_3$</td>
<td>$\zeta_4$</td>
</tr>
<tr>
<td>$(C_{3}^{[111]})^2$</td>
<td>$\zeta_1$</td>
<td>$\zeta_2$</td>
<td>$\zeta_3$</td>
<td>$\zeta_4$</td>
</tr>
<tr>
<td>$\sigma^{yz}$</td>
<td>$\zeta_1$</td>
<td>$-\zeta_2$</td>
<td>$\zeta_3$</td>
<td>$\zeta_4$</td>
</tr>
<tr>
<td>$\sigma^{yx}$</td>
<td>$-\zeta_1$</td>
<td>$\zeta_2$</td>
<td>$-\zeta_3$</td>
<td>$\zeta_4$</td>
</tr>
<tr>
<td>$T$</td>
<td>$\zeta_1$</td>
<td>$-\zeta_2$</td>
<td>$\zeta_3$</td>
<td>$\zeta_4$</td>
</tr>
</tbody>
</table>

Action of $C_{3}^{[111]} \wedge T_3$ on $E \oplus E$ for the $B_1^{(3)}$ RE

<table>
<thead>
<tr>
<th>$R$</th>
<th>$R\zeta_1$</th>
<th>$R\zeta_2$</th>
<th>$R\zeta_3$</th>
<th>$R\zeta_4$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E$</td>
<td>$\zeta_1$</td>
<td>$\zeta_2$</td>
<td>$\zeta_3$</td>
<td>$\zeta_4$</td>
</tr>
<tr>
<td>$C_{3}^{[111]}$</td>
<td>$-\zeta_1$</td>
<td>$-\zeta_2$</td>
<td>$\zeta_3$</td>
<td>$\zeta_4$</td>
</tr>
<tr>
<td>$(C_{3}^{[111]})^2$</td>
<td>$\zeta_1$</td>
<td>$\zeta_2$</td>
<td>$\zeta_3$</td>
<td>$\zeta_4$</td>
</tr>
<tr>
<td>$\sigma^{yz}$</td>
<td>$\zeta_1$</td>
<td>$-\zeta_2$</td>
<td>$\zeta_3$</td>
<td>$\zeta_4$</td>
</tr>
<tr>
<td>$\sigma^{yx}$</td>
<td>$-\zeta_1$</td>
<td>$\zeta_2$</td>
<td>$-\zeta_3$</td>
<td>$\zeta_4$</td>
</tr>
<tr>
<td>$T$</td>
<td>$\zeta_1$</td>
<td>$-\zeta_2$</td>
<td>$\zeta_3$</td>
<td>$\zeta_4$</td>
</tr>
</tbody>
</table>
\(S^2\) has an invariant circle \(S^1\) with stabilizer \(T_2\), which is defined by \(X_2 = 0\) (or equivalently \(s_1 = s_2 = \sigma = 0\). The Morse requirements of two stationary points, a minimum and a maximum, for both the sphere \(S^2\) and its invariant subspace \(S^1\) can be satisfied if the two points lie on \(S^1\). To find these points we first restrict \(H_{\text{eff}}\) to the \(C_8\) sphere using Table 28 and reexpress it as a function of dynamical variables \((X_1, X_2, X_3)\). If \(H_{\text{eff}}(X)\) is a Morse function, we will always find at least two stationary points of \(H_{\text{eff}}(X)\) on the \(T_2\)-invariant circle \(S^1\). Such points are particular solutions to the Euler–Poisson equations

\[
(10.1) \quad \dot{X} = \begin{pmatrix} 0 & X_1 & -X_2 \\ -X_3 & 0 & X_1 \\ X_2 & -X_1 & 0 \end{pmatrix}^T \nabla_X H_{\text{eff}}(X) = 0,
\]

where we should set \(X_2 = 0\).

11. Examples.

11.1. Vibrational structure of the \(F_2\)-mode polyads. Possible configurations and different types of stability of the RE of the \(F_2\)-mode subsystem were studied in section 5.3.2. In section 5.2.3 we emphasized the difference between simplest and nonsimplest Hamiltonians on \(\mathbb{C}P^2\) and described the system of RE in each case. Below we study this system in more detail on a model example, which is discussed in more detail in [98].

The Hamiltonian of a molecule, which has the \(F_2\) mode, can be written as \(\omega H_{\text{vib}}^{F_2} + H'\), where to order \(\epsilon^2\)

\[
H_{\text{vib}}^{F_2} = \frac{1}{2}(q_1^2 + p_1^2) + \frac{1}{2}(q_2^2 + p_2^2) + \frac{1}{2}(q_3^2 + p_3^2) + \epsilon K_3q_1q_2q_3 + \epsilon^2 K_4 \frac{1}{2}(q_1^4 + q_2^4 + q_3^4)
\]

\[
+ \epsilon^2 K_5 \frac{1}{2}(q_1^2 + q_2^2 + q_3^2)^2 + \epsilon^2 K_6 \frac{1}{2} [p \times q]^2,
\]

and \(H'\) represents other degrees of freedom and interaction of these degrees with the \(F_2\)-mode subsystem (cf. section 5.3.2). In order to study this subsystem, we should consider \(H'\) explicitly, normalize the Hamiltonian \(\omega H_{\text{vib}}^{F_2} + H'\), and then restrict the obtained normal form on \(\mathbb{C}P^2\) by setting to zero all dynamical variables of other subsystems. This approach was used in [13] for the case of the \(A_4\) molecule, where we set to zero integrals \(j\), \(N_e\), and \(N_a\), angular momenta \((j_1, j_2, j_3)\), and \(E\)-mode vibrational variables \((v_1, v_2, v_3)\); see Table 21. Furthermore, the simple atom–atom bond model of \(A_4\) used in [13] gives

\[
(11.1b) \quad \begin{array}{cccccc}
\text{Constant} & \omega & K_3 & K_4 & K_6 & K_7 \\
\text{Value} & \sqrt{2} & 3/2^{5/4} & 2^{-5/2} & -5/2^{9/2} & 7/2^{-9/2} \\
\end{array}
\]

Here the parameter \(\lambda\) is introduced so that the value of \(K_7\) obtained in [13] corresponds to \(\lambda = 1\). In the present study we focus on the \(F_2\)-mode subsystem without taking interactions with other subsystems into account. To this end we use a simplified model, where \(H'\) is neglected before normalization. This model turns out to be sufficient for studying the transition from the simplest to the nonsimplest Hamiltonian on \(\mathbb{C}P^2\).

The normal form of (11.1a) \(H_{\text{eff}}^{F_2} = n + \epsilon^2 H_{\text{vib}}^{F_2} + \cdots\) can be expressed using invariants in Table 21. In the second order \(H_{\text{vib}}^{F_2}\) we obtain
Taking the $T_d \times T$ symmetry into account (Table 25), we can verify that $\mathcal{H}_{2}^{\nu_3}$ has indeed only three independent terms:

<table>
<thead>
<tr>
<th>Term</th>
<th>Coefficient</th>
</tr>
</thead>
<tbody>
<tr>
<td>$e^2 n^2$</td>
<td>$\frac{1}{2}(K_1^2/24 + K_1 + K_s + 3K_1/4)$</td>
</tr>
<tr>
<td>$e^2 (s_1^2 + s_2^2 + s_3^2)$</td>
<td>$\frac{1}{2}(-K_3^2/4 - K_1 + K_s/2)$</td>
</tr>
<tr>
<td>$e^2 (2mn_3 - 3n_3^2 - x_3^2)$</td>
<td>$\frac{1}{2}(K_1^2/24 + K_1 - K_s/2 - 3K_1/4)$</td>
</tr>
</tbody>
</table>

In fact, the Hamiltonian $\mathcal{H}_{2}^{\nu_3}$ has been long suggested by Hecht [95] as a model Hamiltonian for describing the internal structure of the $F_2$-mode polyads. Hecht expressed his model $\mathcal{H}_{2}^{\nu_3}$ in terms of

\begin{align}
(11.2a) & \quad n^2 = V_{ffff}^{A_1} + \sqrt{2}V_{ffff}^{E} + \sqrt{3}V_{ffff}^{F_2}, \\
(11.2b) & \quad t^2 = t_1^2 + t_2^2 + t_3^2 = [p \times q]^2 = n^2 - 3V_{ffff}^{A_1}, \\
(11.2c) & \quad m = n_1^2 + n_2^2 + n_3^2 = V_{ffff}^{A_1} + \sqrt{2}V_{ffff}^{E},
\end{align}

where the “vibrational angular momentum” $t^2$ is often denoted as $l^2$ [95, 96]. Considering relations (6.13), we note an alternative to $m$ or $t$,

\begin{equation}
(11.2d) \quad s^2 = s_1^2 + s_2^2 + s_3^2 = 2n^2 - 2m - t^2.
\end{equation}

Hecht’s representation

\begin{equation}
(11.3) \quad \mathcal{H}_{2}^{\nu_3} = c_0 n^2 + c_t t^2 + c_m m,
\end{equation}

or, alternatively,

\begin{equation}
(11.3') \quad \mathcal{H}_{2}^{\nu_3} = c'_0 n^2 + c'_t t^2 + c_s s^2
\end{equation}

is particularly convenient for the order $e^2$ classification of qualitatively different normal forms $H_{eff}^{\nu_3}$ on $\mathbb{C}P^2_n$. We remark that the term $n^2$ is just an additive (“scalar”) energy constant (for the reduced system on $\mathbb{C}P^2_n$, i.e., within one $n$ polyad). Neglecting this term, the energies of RE of the $F_2$-mode system with Hamiltonian (11.3) or (11.3’) are given below:

<table>
<thead>
<tr>
<th>Type of RE</th>
<th>$\mathcal{H}_{2}n^2 - c_0'$</th>
<th>$\mathcal{H}_{2}n^2 - c_0$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$C_{2v} \times T$</td>
<td>$c_s$</td>
<td>$\frac{1}{2}c_m$</td>
</tr>
<tr>
<td>$C_{3v} \times T$</td>
<td>$\frac{1}{2}c_s$</td>
<td>$\frac{1}{3}c_m$</td>
</tr>
<tr>
<td>$C_3 \times T$</td>
<td>$\frac{1}{2}c_s$</td>
<td>$\frac{1}{3}c_m$</td>
</tr>
<tr>
<td>$D_{2d} \times T$</td>
<td>$c_t + \frac{1}{3}c_s$</td>
<td>$c_t + \frac{1}{3}c_m$</td>
</tr>
<tr>
<td>$S_4 \times T$</td>
<td>$c_t$</td>
<td>$c_t + \frac{1}{3}c_m$</td>
</tr>
<tr>
<td>$C_s \times T$</td>
<td>$(c_t')^2(c_t' - \frac{1}{3}c_s)^{-1}$</td>
<td></td>
</tr>
</tbody>
</table>

It follows that reciprocal energies of RE of such system and, therefore, the structure of the vibrational polyads of the $F_2$ mode, are described (to the lowest order) by one parameter, the
ratio of \( c_l \) and \( c_m \) or \( c_l' \) and \( c_s \). To study all possibilities we set \( c_l' \) and \( c_s \) in \((11.3')\) to \( \cos(\alpha \pi) \) and \( \sin(\alpha \pi) \), respectively. Resulting RE energies \( \mathcal{H}_{2n} n^{-2} - c_0' \) are shown in Figure 17.

We call the three principal limiting cases of the \( F_2 \)-mode system with \( \alpha = 0, \frac{1}{4}, \text{ and } 1 \) the \( t^2 \), \( m \), and \( (-t^2) \) limits, respectively (see Figure 17). All these limits have continuous symmetries and the system is integrable. The \( s^2 \) limit shown in Figure 17 is indicated primarily for convenience. It has no simple integrals and, probably, is not integrable.

The symmetry group of the \( t^2 \) limit contains the spatial group SO(3). The energy in this limit is a function of the vibrational angular momentum \( t^2 = l^2 \), which is zero for the \( A \)-type RE and maximum \( l = n \) for the \( B \)-type RE. The corresponding quantum polyad is split into multiplets with \( l = n, n-2, \ldots \). The \( (-t^2) \) limit is the same as the \( t^2 \) limit, albeit for the opposite sign of energies.

The spatial symmetry of the \( m \) limit is cubic, so this limit better represents the symmetry of the system. However, this limit has continuous dynamical symmetry \( T^3 = S^1 \times S^1 \times S^1 \). The energy can be represented as a function of three integrals in involution \( (n_1, n_2, n_3) \), i.e., actions of individual oscillators, such that \( n_1 + n_2 + n_3 = n \). The quantum states can be labeled with the three corresponding quantum numbers. The number of degenerate states is normally given by the number of permutations of the set of the three integers \( [N_1, N_2, N_3] \). In the \( n = 10 \) example in Figure 17, it is either 3 or 6 (maximum).

Transition between the \( t^2 \) and \( m \) limits has been studied by Patterson [96], who remarked that \( F_2 \)-mode polyads of certain molecules, such as SiF\(_4\), SF\(_6\), and UF\(_6\), belong to the interval of \( \alpha = [0, \frac{1}{4}] \). On the other hand, our prediction for P\(_4\) suggests that the \( \nu_3 \) polyads of this molecule fall into the \( \alpha \geq \frac{1}{2} \) category. A complimentary approach to classifying \( \nu_3 \)-mode systems is by specifying the intervals of \( \alpha \)-values, where the second order normalized
Hamiltonian (11.3') represents particular classes of \((T_d \times T)\)-invariant Morse functions on \(\mathbb{C}P^2\) introduced in section 5.2.3. We can see in Figure 17 that there are at least three such regions. Furthermore, we notice that the \(H_{eff}^{\nu_3}\) Hamiltonian is of the simplest Morse type only on the interval \(\alpha = (\pi^{-1} \tan^{-1} 2, \frac{\pi}{2})\), where the additional nonfixed RE of symmetry \(C_s \wedge T_2\) does not exist.

In this paper we would like to uncover the precise role of the vibrational angular momentum term \((p \times q)^2\) in the transition between the simplest and nonsimplest RE structures. To this end we detail our example in section 5.3.2. Note that even though \((p \times q)^2\) enters in both the initial Hamiltonian (11.1a) and the normalized (i.e., \(n\)-polyad) Hamiltonian (11.3'), the actual vibrational angular momentum of the system is measured by the parameter \(K_1\) of (11.1a) and not by the effective parameter \(c_t\) or \(c_t'\). Therefore, we should take the vibrational Hamiltonian (11.1a), replace \(K_1\) with \(\lambda K_1\), use constants (11.1b) obtained in [13], and make \(\lambda\) vary between, for example, 0 and 2. Normalizing and using the \((s^2, t^2, n)\) representation (11.3') with parameters (11.1b) gives

\[
\frac{c_s}{c_t'} = \frac{5K_3^2 + 18K_t}{18K_t + 12K_s - K_3^2 - 24\lambda K_t} = \frac{51}{5 - 16\lambda}.
\]

It follows that we study the \(F_2\)-mode system near the \(s^2\) limit in the range \(\alpha \approx [0.469, 0.655]\); see Figure 17.

The stability analysis of RE for \(\lambda = 0\), i.e., without the vibrational angular momentum term \((p \times q)^2\) in (11.1a), shows that the corresponding normal form \(H_{eff}^{\nu_3}\) is a Morse function on \(\mathbb{C}P^2\) of the simplest kind. In the \(A_4\) molecule model of [13] (with \(\lambda = 1\) and \(\alpha \approx 0.567\), \(H_{eff}^{\nu_3}\) is of the nonsimplest kind. The transition from the simplest to the nonsimplest case is clearly related to the \((p \times q)^2\) term. The RE energy computed using the normal form of the Hamiltonian (11.1) as a function of the parameter \(\lambda\) is shown in Figure 18, where we also indicate the Morse signatures and stability types of the RE. As can be seen in this figure, the \(B\)-type RE, which are shaped as loops in the configuration space (see Figure 16) and thus induce the maximum vibrational angular momentum, respond largely to the change of \(\lambda\), while the energy of the \(A\)-type RE remains unchanged. As a consequence, the RE structure as a whole has to change qualitatively. This change involves two bifurcations.

The first bifurcation happens at \(\lambda = 5/16\) (\(\alpha = 0\)). The \(B^{(4)}\) relative equilibrium, which was unstable with Morse index 1 (Poincaré index +2) for \(\lambda < 5/16\), becomes stable with index 0 (+4) for \(\lambda > 5/16\). At the moment of bifurcation the energies of the \(B^{(4)}\) and \(A^{(4)}\) RE are equal, then as \(\lambda\) increases, the energy of \(B^{(4)}\) becomes greater. At the same time, the \(A^{(4)}\) relative equilibrium, which was stable with Morse index 0 (+4), becomes doubly unstable with Morse index 2 (0). In order for the Morse conditions to be satisfied globally, a new relative equilibrium bifurcates from \(A^{(4)}\). This is the \(C_s \wedge T_2\) symmetric RE described in section 5.2.3. The new relative equilibrium is unstable with Morse index 2 (0). Part of the described bifurcation can be regarded as a so-called “pitchfork bifurcation,” or a bifurcation with broken symmetry \(Z_2\). Indeed, the system restricted to the \(C_s\) sphere (see section 5.2.3) undergoes such bifurcation. Taken to the whole four-dimensional space, this phenomenon is more complex because it involves the \(B^{(4)}\) relative equilibrium.

The second bifurcation happens at \(\lambda = 11/8\) (\(\alpha \approx 0.1\)). The moment of bifurcation is easy to notice because the second normal form energies of the \(B^{(3)}\) and \(A^{(4)}\) RE (i.e., values of the
Hamiltonian \((11.3')\) shown in Figures 18 and 17) become equal. The \(B^{(3)}\) relative equilibrium undergoes a Hamiltonian Hopf bifurcation \([97, 98]\), and from a focus–focus (complex unstable) relative equilibrium at \(\lambda < 11/8\) it becomes elliptic (linearly stable) at \(\lambda > 11/8\). The Morse index does not change. Unlike the previous case, the Morse requirements remain satisfied globally and there is no need for changing the number and/or stability of other RE.

Information on the RE of the system with Hamiltonian \((11.1)\) can be used to characterize the spectrum of the corresponding quantum system as proposed in section 5.4.3. We consider the RE energies as functions of the action \(n\) and compare them to the quantum energy levels (see Figure 19). Levels with the same quantum number \(N_f\) form a polyad whose structure can be related to the reciprocal RE energies for corresponding classical action \(n = N_f + \frac{3}{2}\). Like RE, polyads are described using the normalized Hamiltonian \(H_{\text{eff}}^{\nu_3}\), where we can distinguish between “scalar” and “splitting” terms. The former depend only on \(n\) and describe an average increase in energy; the latter describe the internal structure of polyads. In the simplest approximation given by the second order normal form \((11.3')\), or the Hecht Hamiltonian, the internal structure of polyads is described by one-parameter \(\alpha\); see Figure 18.

Provided that the model potential of the \(P_4\) molecule \([13]\) is qualitatively correct, the \(\nu_3\) polyads of \(P_4\) should correspond to the value of \(\alpha \approx 0.6\) near the so-called \(s^2\) limit. The most characteristic feature of the \(\nu_3\) polyads with such \(\alpha\) is the presence of level clusters at the \(A^{(3)}\) end (maximum in Figure 17 and minimum in Figures 18 and 19). The limiting \(A^{(3)}\) cluster has four levels and in the case of \(N_f = 10\) decomposes into symmetry components \(A + F\) (Figure 18). At higher \(N_f = 15\) (Figure 19) we can even see the second cluster of eight
levels with components \( F + F + E \). As can be seen in Figures 18 and 19, the \( A^{(3)} \) clusters remain insensitive to large variations of the structure parameter \( \alpha \) or \( \lambda \). The situation is more unclear at the opposite energy end of the \( \nu_3 \) polyads. If, as predicted, \( \alpha > \frac{1}{2} \), then the \( B^{(4)} \) clusters of six levels should appear as shown in Figure 18 (top right) and 19 (topmost level of the \( N_f = 10, \ldots, 15 \) polyads). They decompose as \( A + F + E \) for \( N_f = 10 \) and \( F + F \) for \( N_f = 15 \). If, however, \( \alpha \) for \( P_4 \) turns out to be sufficiently smaller than \( \frac{1}{2} \), then we should expect \( A^{(4)} \) clusters of three levels (such as the lowest energy levels of the \( N_f = 10 \) polyad for \( \alpha = 0.4 \) in Figure 17). Furthermore, if the \( B^{(3)} \) relative equilibrium becomes sufficiently stable, a corresponding eight-fold cluster might also show up.

Several aspects should be taken into account in order to continue our analysis of the \( \nu_3 \) polyad structure presented in this paper. A simple analysis based on energy separation fails as different systems of localized states overlap, and complimentary information on expectation values of characteristic dynamical invariants should be used. Degeneracy of quantum states caused by symmetry can either enhance or obscure the presence of level clusters. The position of the limiting localized state and the corresponding RE depends on the stability of the RE and the relation between \( n \) and \( N_f \).

### 11.2. Rotational structure of the \( F_2 \)-mode polyads

Consider an effective Hamiltonian \( H_{\text{eff}} \) commonly used to describe rotational structure of low excited \( F_2 \)-mode vibrations. In the spectroscopic notation of Table 25, this Hamiltonian can be written as

\[
H_{\text{eff}} = \omega_f n_f + Bj^2 - D j^4 - h_{ff}^{2(0,A_1)} \frac{4}{3} n_f j^2 + h_{ff}^{1(F_1)} H_{ff}^{1(F_1)} + \sum_{\Gamma=E,F_2} h_{ff}^{2(2,\Gamma)} H_{ff}^{2(2,\Gamma)}
\]

Figure 19. Spectrum of quantum levels and energies of the RE of the \( F_2 \)-mode system with Hamiltonian (11.1) with \( \epsilon = 1 \) and \( \lambda = 0 \) (left), \( \lambda = 1 \) (right). Circles mark \( N_f = 15 \) level clusters discussed in the text, and classical RE energy is plotted for \( n = N_f + \frac{3}{2} \).
where $\omega_f$ is harmonic frequency of the $F_2$ mode, $B$ is the rotational constant of the molecule (for a tetrahedral molecule $A_4$ with four atoms of mass $m$ whose equilibrium positions lie at a distance $R$ from the center of mass, the constant $B$ equals $1/(2mR^2)$), and $h_{ff}, D$, and $D_t$ are parameters of higher order terms in the reduced Hamiltonian. We can omit the terms (11.4a), which have constant value in the reduced system. The energies of fixed RE can be found straightforwardly as values of the $H_{\text{eff}}$ in (11.4) at the points listed in Table 27.

To find the two remaining RE, we restrict $H_{\text{eff}}$ in (11.4) to the $C_s$-invariant sphere using the definition of this sphere in Table 28 and express the result as a function of dynamical variables $X$ of the $C_s$ restricted system,

\begin{equation}
H_{\text{eff}}^{C_s} = b(J)X_1 - a(J)X_3 + c(J,N_f),
\end{equation}

where

\begin{align*}
a &= \sqrt{2} h_{ff}^{2(2,E)} J^2 - \frac{2}{\sqrt{3}} h_{ff}^{2(2,F_2)} J^2, \\
b &= -\frac{2\sqrt{2}}{\sqrt{3}} h_{ff}^{1(F_1)} J + \left[ \frac{8\sqrt{2}}{\sqrt{3}} h_{ff}^{3(F_1)} + \frac{4}{\sqrt{5}} h_{ff}^{3(F_1)} \right]^{3/2}, \\
c &= D_t J^4 + \frac{\sqrt{2}}{6} h_{ff}^{2(2,E)} N_f J^2 + \frac{1}{\sqrt{3}} h_{ff}^{2(F_2)} N_f J^2.
\end{align*}

Note that $H_{\text{eff}}^{C_s}$ is linear in $X$ and that it is invariant with regard to $T_d \times T$ and to its subgroup $T_2$ and therefore cannot depend linearly on $X_2$. Equations of motion (10.1) for this Hamiltonian are very simple:

\begin{equation}
\dot{X} = (-aX_2, bX_3 + aX_1, -bX_2).
\end{equation}

Setting $X_2 = 0$ in these equations gives the condition for an equilibrium point of $H_{\text{eff}}^{C_s}$ on the $T_2$-invariant circle,

\begin{equation}
bX_3 + aX_1 = 0,
\end{equation}

which should be satisfied together with the defining equation of the circle

\begin{equation}
X_1^2 + X_3^2 = \frac{1}{4} N_f^2.
\end{equation}

Since $a(J)$ and $b(J)$ depend differently on $J$; the two solutions

\begin{equation}
(X_1, X_2, X_3) = \pm \frac{N_f}{2\sqrt{b^2 + a^2}} (b, 0, -a)
\end{equation}

move along the circle when $J$ changes: when $J$ is small and $b \gg a$ they are close to the point where $X_3 = 0$; at large $J$ they approach $X_1 = 0$. The energies of these RE are

\begin{equation}
\pm \frac{N_f}{2} \sqrt{b(J)^2 + a(J)^2} + c(J,N_f).
\end{equation}
Table 35
Energy of rotation–vibration RE in the case of low excited \( F_2 \)-mode vibrations of a tetrahedral molecule \( \Lambda_4 \).

<table>
<thead>
<tr>
<th>Point(^50)</th>
<th>Energy of RE (values of ( H_{\text{eff}} ))</th>
</tr>
</thead>
<tbody>
<tr>
<td>( A^{(2)} )</td>
<td>(-\frac{\sqrt{2}}{3} h_{ff}^{2(2,E)} N_f J^2 - \frac{2}{\sqrt{3}} h_{ff}^{2(2,F_2)} N_f J^2 + D_t J^4 )</td>
</tr>
<tr>
<td>( A^{(3)} )</td>
<td>(-8\frac{\sqrt{3}}{9} h_{ff}^{2(2,F_2)} N_f J^2 + \frac{8}{3} D_t J^4 )</td>
</tr>
<tr>
<td>( A^{(4)} )</td>
<td>(-4\frac{\sqrt{7}}{3} h_{ff}^{2(2,E)} N_f J^2 - 4D_t J^4 )</td>
</tr>
<tr>
<td>( B,C^{(3)} )</td>
<td>( \mp \frac{\sqrt{2}}{\sqrt{3}} h_{ff}^{2(1,F_1)} N_f J + \frac{4\sqrt{3}}{9} h_{ff}^{2(2,F_2)} N_f J^2 )</td>
</tr>
<tr>
<td></td>
<td>( \pm \frac{4\sqrt{2}}{3} \left( h_{ff}^{3(1,F_1)} + \frac{2\sqrt{2}}{\sqrt{15}} h_{ff}^{3(3,F_1)} \right) N_f J + \frac{8}{3} D_t J^4 )</td>
</tr>
<tr>
<td>( B,C^{(4)} )</td>
<td>( \mp \frac{\sqrt{2}}{\sqrt{3}} h_{ff}^{2(1,F_1)} N_f J + \frac{4\sqrt{2}}{3} h_{ff}^{2(2,E)} N_f J^2 )</td>
</tr>
<tr>
<td></td>
<td>( \pm \frac{4\sqrt{2}}{3} \left( h_{ff}^{3(1,F_1)} - \frac{\sqrt{2}}{\sqrt{15}} h_{ff}^{3(3,F_1)} \right) N_f J^3 - 4D_t J^4 )</td>
</tr>
</tbody>
</table>

The simplest way to compare the energies of RE in Table 35 and (11.6) to molecular energy levels is to plot all of them in a form of an energy-momentum diagram for fixed vibrational integral \( N_f \). In the lowest excited vibrational quantum state of the \( \nu_3 \) mode, also called the fundamental or harmonic state, the quantum number \( \tilde{N}_f \), equals 1 which corresponds to the classical value \( N_f = 1 + \frac{3}{2} \).

We illustrate our results using the Hamiltonian \( H_{\text{eff}} \) (without the scalar part (11.4a)), which describes the \( \nu_3 \) vibration of the CH\(_4\) molecule. Parameters of this Hamiltonian can be taken from [92].

\[
\begin{align*}
h_{ff}^{1(1,F_1)} & = -0.706007 & D_t & = 4.42516 \times 10^{-6} \\
h_{ff}^{2(2,E)} & = 1.5760 \times 10^{-2} & h_{ff}^{2(2,F_2)} & = -0.7220 \times 10^{-2} \\
h_{ff}^{3(1,F_1)} & = -0.635 \times 10^{-4} & h_{ff}^{3(3,F_1)} & = -0.187 \times 10^{-4}
\end{align*}
\]

The quantum energy level spectrum of the \( \nu_3 = 1 \) state is shown schematically by the shaded area. This spectrum exhibits three characteristic branches formed due to the first order Coriolis interaction [81]. As shown in section 7.2.5 and Table 25, the term describing this interaction in the reduced system is the scalar product \( (t, j) \), which has spherical symmetry, i.e., to the first order; the energy depends on the angle between the 3-vectors \( t \) and \( j \). Assuming \( H_1 \propto (t, j) \), as in the case of CH\(_4\), the energy is maximal, minimal, or zero when \( t \) and \( j \) are parallel (RE of type \( B \)), antiparallel (RE of type \( C \)), or orthogonal (RE of type \( A \)), respectively. Since the quantity \( (t, j) \) is (approximately) conserved, we can introduce another angular momentum \( r = j - t \) and represent the first order energy as function of \( r^2 \), \( t^2 \), and \( j^2 \) called “rotational,” “vibrational,” and total angular momenta, respectively. In the quantum

\(^{50}\)Fixed points of the \( T_d \times T \) group action on \( \mathbb{C}P^2 \times \mathbb{C}P^3 \times S^2 \) defined in Table 27; signs + and − in the notation ± (equivalently, − and + in \( \mp \)) correspond to points \( B \) and \( C \), respectively.
Figure 20. Energies of rotation–vibration RE for the \( \nu_3 \) mode of the \( \text{CH}_4 \) molecule. Colored lines show classical energies (see Table 35 and equation (11.6)) with \( N_f \) set to \( \frac{5}{2} \); indices \( (2, 3, 4) \) on the right give the symmetry of the corresponding RE. Thin black lines show the same energies with \( N_f = 1 \); shaded area represents quantum multiplets.

state with \( \hat{N}_f = 1 \), the quantum number \( \hat{t} \) equals 1 and the quantum number \( \hat{r} \) takes the values of \( \hat{j} - 1 \), \( \hat{j} \), and \( \hat{j} + 1 \). These values label the three Coriolis branches of the \( \nu_3 = 1 \) state.

Bold lines in Figure 20 represent energies of the nine RE (two noncritical orbits are given in (11.6) and seven critical orbits in Table 35) with \( N_f \) set to its classical value \( 1 + \frac{3}{2} \). The same energies—but with \( N_f = 1 \)—are shown by thin lines, which border exactly the three rotational branches of quantum levels. This suggests a straightforward semiclassical interpretation. The RE energy with \( N_f = \frac{5}{2} \) gives classical limit (classical extremum) energy for rotation–vibration levels; with \( N_f = 1 \) we approximate vibrational quantum energy of the state localized near the corresponding RE and obtain classical limit energy for the rotational structure only. In the case of the Hamiltonian (11.4) whose vibrational part is quadratic, this approximation matches exactly the extrema of the so-called “rotational energy surfaces” [32, 36, 35], which are obtained when all rotational operators in \( H_{\text{eff}} \) are replaced by their quantum analogues. Further examples can be found in [58, 13, 12].

12. Discussion of the results. This paper, together with [13], reports on the first substantial attempt to extend the analysis of molecular energy levels based on RE (also known as nonlinear normal modes and, in some cases, local modes, principal periodic orbits, stationary axes of rotation, etc.) from simple, often model systems to complex rotation–vibration Hamiltonians of real molecules. Our predecessors (see section 1) studied classical vibrational systems with two or three degrees of freedom [14, 15, 16, 77, 70], notably a great number of triatomic molecules [19, 22, 23, 24, 25, 26, 27, 99, 100, 101, 102, 103, 104, 105, 106], and rotational systems [31, 32, 33, 34, 37, 38, 55, 28, 29, 12]. Generalization of these studies to combined systems led to “hybrid” quantum classical systems [36, 35, 41, 42, 43, 56, 107, 108, 109]. We take the next step by studying the whole of the combined system classically and using the results for
the interpretation and prediction of the corresponding quantum system. We consider the example of the rotating tetrahedral molecule $A_4$ with six internal vibrational degrees of freedom, a system which is, arguably, at the limit of molecular systems whose rotation–vibration energy levels have already been studied in detail.

Our principal molecular result is the relation of rotation–vibration RE and the structure of the rotation–vibration energy level spectrum. Thus, we show how extremal quantum states in the rotation–vibration multiplet are associated with particular periodic rotation–vibration motion of the molecule. We took advantage of the simplicity of the classical RE description in order to analyze the structure of highly excited energy levels in different limits. In particular, we compared the structure of rotationally excited polyads to that in the case of high purely vibrational excitation. We found that when the interaction of the rotational and vibrational subsystems is significant, RE become qualitatively different from what can be expected for (or deduced from) the separable system. We predicted qualitative modifications of the system of RE and then followed it with a concrete example. This is our main mathematical result.

We also took advantage of the rich topological structure and high symmetry of our example system in order to predict and explain many important basic qualitative features of this complex system. Subsequently, we confirmed our predictions quantitatively. In particular we analyzed existence and stability of rotation–vibration RE. We extend this study to different parametric limits of molecular potential and corresponding limiting cases of the normalized system (polyads). Our more specialized mathematical results concern group-theoretical aspects of combining two subsystems, in particular the analysis of the group action on the combined phase space on the basis of the action on individual subspaces. The last, but not least, is the dynamically invariant formulation of the theory in section 9, which is the weapon of choice for further analysis of the hidden regular structures of seemingly irregular highly excited molecular states.

REFERENCES


