

# Linear Hamiltonian Hopf bifurcation for point-group-invariant perturbations of the 1 : 1 : 1 resonance

BY K. EFSTATHIOU<sup>1</sup>, D. A. SADOVSKIÍ<sup>1</sup> AND R. H. CUSHMAN<sup>2</sup>

<sup>1</sup>*Université du Littoral, UMR 8101 du CNRS, 59 140 Dunkerque, France*

<sup>2</sup>*Mathematisch Instituut, Universiteit Utrecht,  
3508 TA Utrecht, The Netherlands*

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We consider  $\mathcal{G} \times \mathcal{R}$ -invariant Hamiltonians  $H$  on complex projective 2-space, where  $\mathcal{G}$  is a point group and  $\mathcal{R}$  is the time-reversal group. We find the symmetry-induced stationary points of  $H$  and classify them in terms of their linear stability. We then determine those points that can undergo a linear Hamiltonian Hopf bifurcation.

**Keywords:** Hamiltonian dynamical system with symmetry;  
Hamiltonian Hopf bifurcation; relative equilibria

## 1. Introduction

Consider a Hamiltonian system with  $s$  degrees of freedom which is defined on a smooth  $2s$ -dimensional manifold  $M$ . Let this system be invariant under the action of a symmetry group  $\mathcal{G}$  on  $M$ , that is, let the Hamiltonian  $H$  of the system be a  $\mathcal{G}$ -invariant function on  $M$ . The study of how the presence of symmetry affects the above system begins with the analysis of what restrictions this symmetry imposes on possible types, stability and bifurcations of its equilibria (Golubitsky & Stewart 1987).

We characterize the action of  $\mathcal{G}$  on  $M$  by specifying the *isotropy group* (or *stabilizer*)  $\mathcal{G}_m \subseteq \mathcal{G}$  of every  $m \in M$ , which is the maximal subgroup of  $\mathcal{G}$  that leaves  $m$  fixed,  $\mathcal{G}_m = \{g \in \mathcal{G} : g \cdot m = m\}$ . A point  $m \in M$  is called a *fixed point* of the  $\mathcal{G}$  action when  $\mathcal{G}_m = \mathcal{G}$ , that is, when it is fixed by all the elements of  $\mathcal{G}$ . The  $\mathcal{G}$ -*orbit* of  $m$  is the set  $\mathcal{G} \cdot m = \{g \cdot m : g \in \mathcal{G}\}$ . We are primarily interested in points  $m_c \in M$  such that there is a neighbourhood of  $m_c$  in which there are no points  $m$  with stabilizer  $\mathcal{G}_m$  which belongs to the same conjugacy class in  $\mathcal{G}$  as  $\mathcal{G}_{m_c}$ . We call such points  $m_c$  and the orbit  $\mathcal{G} \cdot m_c$  *isolated* or *critical*. For more details see, for example, Michel & Zhilinskií (2001). The following theorem of Michel (1971) shows why critical points are important.

**Theorem 1.1.** *Critical points of the action of a group  $\mathcal{G}$  on a smooth manifold  $M$  are stationary points of every smooth  $\mathcal{G}$ -invariant function  $H$  on  $M$ .*

Apart from the existence of special symmetric stationary points  $m_c$  of  $H$ , the symmetry analysis can derive valuable information on the stability and possible bifurcations of these points by studying the action of the isotropy group  $\mathcal{G}_{m_c}$  in the

neighbourhood of  $m_c$ . As a particularly characteristic and simple example, consider a Hamiltonian system with one degree of freedom which is invariant with regard to one of the finite groups of transformation of the plane  $\mathbf{R}^2$ , a cyclic group  $C_k$  of rotations about the origin  $0 \in \mathbf{R}^2$  by  $2\pi/k$  or a dihedral group  $D_k$ . Clearly, the origin  $0$  is a critical one-point orbit. For all  $k \geq 3$ , the corresponding stationary point of a smooth function  $H : \mathbf{R}^2 \rightarrow \mathbf{R}$  is stable. If  $(q, p)$  are standard symplectic coordinates in  $\mathbf{R}^2$  and  $H(q, p)$  is a generic smooth  $C_k$ -invariant Hamiltonian function, then  $0$  is a stable equilibrium. Furthermore, it is easy to show that, depending on  $k$ , bifurcations of this equilibrium can be of five and only five possible types. This simple theorem has important applications in a wide range of systems, including free rotations of non-rigid bodies, such as molecules (Zhilinskiĭ & Pavlichenkov 1987; Pavlichenkov & Zhilinskiĭ 1988), small vibrations of resonant systems with two degrees of freedom† and bifurcations of periodic orbits of systems with two degrees of freedom (Meyer 1970, 1971, 1986).

In the case of bifurcations of periodic orbits, the study of the periodic solution is replaced by the study of a reduced  $C_k$ -invariant system defined (locally) on the Poincaré surface of section. In the case of small vibrations, we can normalize the system globally and study its relative equilibria as stationary points of the reduced Hamiltonian. In this work, we apply the same principle in the analysis of a 1:1:1 resonant three-mode system with symmetries. Existence of relative equilibria (non-linear normal modes) of such systems has been already studied in detail by Montaldi *et al.* (1988) and in the follow-up paper (Montaldi *et al.* 1990a) on the example of tetrahedral symmetry  $\mathcal{T}_d$ . The equivalent approach, based on the reduced system defined on the  $\mathbf{CP}^2$  phase space, was suggested in Zhilinskiĭ (1989) and detailed in Sadovskii & Zhilinskiĭ (1993). In this paper, we focus on the possible types of linear stability of these relative equilibria.

The transformations in  $\mathbf{R}^3$  that leave the equilibrium configuration of a non-collinear molecule fixed form a finite point group  $\mathcal{G}$ , that is, a finite subgroup of  $O(3)$ . In the study of the small vibrations of a molecule near its equilibrium configuration, we classify these vibrations according to irreducible representations of the symmetry group  $\mathcal{G}$  of the molecule. The small vibrations  $q_i$ ,  $i = 1, \dots, n$ , which realize  $n$ -dimensional irreducible representations of  $\mathcal{G}$  form an  $n$ -fold degenerate mode, that is,  $n$  vibrations with the same frequency.

When  $\mathcal{G}$  has three-dimensional irreducible representations, the molecule can have one or more triply degenerate vibrational normal modes. Consider a molecule that has a triply degenerate vibrational mode, like  $P_4$  or  $CH_4$ , which have tetrahedral symmetry. If a potential for interatomic interactions in this molecule is known, then one can determine a model Hamiltonian for the triply degenerate mode that will be a perturbation of the harmonic oscillator

$$H_0 : T^*\mathbf{R}^3 \rightarrow \mathbf{R} : (q, p) \rightarrow H_0(q, p) = \frac{1}{2}(p_1^2 + p_2^2 + p_3^2) + \frac{1}{2}(q_1^2 + q_2^2 + q_3^2), \quad (1.1)$$

with equal frequencies. Here,  $T^*\mathbf{R}^3$  is the co-tangent bundle of  $\mathbf{R}^3$  with canonical coordinates  $(q, p) = (q_1, q_2, q_3, p_1, p_2, p_3)$ . The perturbed system will generally be of the form

$$H_\epsilon : T^*\mathbf{R}^3 \rightarrow \mathbf{R} : (q, p) \rightarrow H_\epsilon(q, p) = H_0(q, p) + \epsilon H_1(q, p) + \epsilon^2 H_2(q, p) + \dots, \quad (1.2)$$

† See, for example, Sadovskii (2001); a different but equivalent approach is discussed in Montaldi *et al.* (1990b, § 4).

where  $H_j(q, p)$  are homogeneous polynomials of degree  $j + 2$  in  $(q, p)$ .

Recall that the variables  $q$  span a three-dimensional representation  $\Gamma$  of  $\mathcal{G}$ . Since the representation  $\Gamma$  is orthogonal, the co-tangent lift of the action of  $\mathcal{G}$  from  $\mathbf{R}^3$  with variables  $(q, p)$  to  $T^*\mathbf{R}^3$  with variables  $(q, p)$  is such that the momenta  $p$  also span the same representation  $\Gamma$ . Let  $\tilde{\mathcal{G}}$  be the *image* of  $\mathcal{G}$  in the representation  $\Gamma \oplus \Gamma$  spanned by  $(q, p)$ . The Hamiltonian  $H_\epsilon$  is invariant with respect to  $\tilde{\mathcal{G}}$ . This means that, for every  $g \in \tilde{\mathcal{G}}$ ,  $H_\epsilon(g \cdot (q, p)) = H_\epsilon(q, p)$ . From now on, we will denote the group and its image in any representation by the same symbol, if there is no danger of confusion. In this paper, we consider only the three-dimensional *vector* representations  $\Gamma$  of point groups, that is, representations on which the group acts the same way as on the representation spanned by variables  $x, y, z$  of the physical space.

For free molecules, the Hamiltonian  $H_\epsilon$  is also time-reversal invariant. Here, the generator  $T$  of the time-reversal symmetry acts on  $T^*\mathbf{R}^3$  by  $T(q, p) = (q, -p)$ . The time-reversal symmetry group is  $\mathcal{R} = \{1, T\}$ . The role of the time-reversal symmetry is very important since its existence modifies the possible types of linear stability of the relative equilibria.

For small enough values of the perturbation parameter  $\epsilon$  (or, alternatively, for small enough values of the energy), we can study the main qualitative features of the system in question by normalizing it with respect to  $H_0$ . This means that we find a canonical change of coordinates so that the transformed Hamiltonian is invariant under the flow of the Hamiltonian vector field  $X_{H_0}$  of the harmonic oscillator to a sufficiently high order in  $\epsilon$ . Dropping the higher-order terms gives the normalized Hamiltonian  $\tilde{H}_\epsilon$ . Because  $\tilde{H}_\epsilon$  Poisson commutes with  $H_0$ , it induces a smooth function  $\hat{H}_\epsilon$ , called the reduced Hamiltonian, on the space of orbits of fixed energy of the harmonic oscillator. In our case, this orbit space is a complex projective 2-space  $\mathbf{C}P^2$ . Stationary points of  $\hat{H}_\epsilon$  (*relative equilibria*) correspond to periodic orbits of  $\tilde{H}_\epsilon$ . Within the limits of the validity of the normal-form approximation, they also correspond to periodic orbits of  $H_\epsilon$ .

Since the original Hamiltonian  $H_\epsilon$  is  $\mathcal{G}$ -invariant, the reduced Hamiltonian  $\hat{H}_\epsilon$  is also. Here the action of  $\mathcal{G}$  on  $\mathbf{C}P^2$  is induced from its action on  $T^*\mathbf{R}^3$  which we identify with  $\mathbf{C}^3$ . The critical points of the action of  $\mathcal{G}$  on  $\mathbf{C}P^2$  are by theorem 1.1 stationary points of  $\hat{H}_\epsilon$  and therefore also equilibria of the reduced system. In this paper we determine the possible types of linear stability of these equilibria taking into account their isotropy group. Our program is to find the fixed points of all finite subgroups of  $O(3) \times \mathcal{R}$  and then to classify them in terms of their linear stability. Since all the critical points of a group are fixed points of some of its subgroups we will have also classified all the critical points in terms of their linear stability.

An important bifurcation, which happens only in Hamiltonian systems with two or more degrees of freedom, is the Hamiltonian Hopf bifurcation (van der Meer 1985). It is a codimension-one bifurcation that occurs only if a stationary point changes stability from elliptic–elliptic to complex hyperbolic. In other words, the frequencies of the linearized system move along the imaginary axis, collide, and then move off the axis into the complex plane. This pattern of change of linear stability is called a *linear Hamiltonian Hopf bifurcation*. If we take into account the nonlinear behaviour of the system, then a nonlinear Hamiltonian Hopf bifurcation might take place, that is, a family of periodic orbits either detaches from the stationary point or it shrinks to the stationary point and disappears. The name Hamiltonian Hopf bifurcation comes from the fact that the above behaviour is reminiscent of the Hopf bifurcation for

dissipative systems. Note that the linear bifurcation is necessary but not sufficient for the nonlinear one.

The Hamiltonian Hopf bifurcation in the presence of symmetry has been studied in van der Meer (1990) and Chossat *et al.* (2002). In the first paper, the author obtains results for the Hamiltonian Hopf bifurcation on the fixed-point space of a subgroup of the full symmetry group. In the second paper, the authors study the Hamiltonian Hopf bifurcation on the reduced phase space of Hamiltonian systems symmetric under the action of a compact Lie group. Since we consider the possibility of the Hamiltonian Hopf bifurcation on the phase space  $\mathbf{CP}^2$  obtained after reduction of the  $\mathbf{S}^1$  symmetry generated by the flow of  $X_{H_0}$ , this approach is partly related to ours.

Having studied the linear stability of all the fixed points, we predict which of them can go through a linear Hamiltonian Hopf bifurcation. These stationary points are then candidates for a nonlinear Hamiltonian Hopf bifurcation. The main result of our paper is the enumeration of the points and their isotropy groups that undergo linear Hamiltonian Hopf bifurcation. The method we use to determine the possible types of stability of relative equilibria is not particular to the case of point groups acting on  $\mathbf{CP}^2$ , but can be extended to cover the case of an arbitrary compact group acting on a manifold.

We now give an outline of the contents of this paper. In § 2 we describe the reduced phase space and give a coordinatization. In § 3 we discuss the action of finite point groups on  $\mathbf{CP}^2$ . In § 4 we find the fixed points of the action of the finite cyclic groups  $\mathcal{C}_k$  on  $\mathbf{CP}^2$  and determine their possible linear stability types. In § 5 we find the fixed points and the linear stability of all the other finite point groups. In § 6 we study the effect of the additional time-reversal symmetry on the above results. Table 1 summarizes the results obtained in §§ 4, 5 and 6. In § 7 we state and prove the main theorem, which characterizes those fixed points of finite-point groups extended by time reversal, which can undergo a linear Hamiltonian Hopf bifurcation. Finally, in § 8 we present the example of the action of the tetrahedral group  $\mathcal{T}_d$  on  $\mathbf{CP}^2$  extended by time reversal and show that it has only one type of critical point for which a linear Hamiltonian Hopf bifurcation can occur.

## 2. Normalization of the 1:1:1 resonance

We identify the phase space  $T^*\mathbf{R}^3$  having canonical coordinates  $(q, p)$ , with  $\mathbf{C}^3$  having coordinates  $z = (z_1, z_2, z_3)$ , where  $z_j = q_j + ip_j$ . The flow of the unperturbed harmonic oscillator Hamiltonian

$$H_0(z) = \frac{1}{2}|z|^2 = \frac{1}{2}(|z_1|^2 + |z_2|^2 + |z_3|^2)$$

induces the  $\mathbf{S}^1$  action

$$\varphi : \mathbf{S}^1 \times \mathbf{C}^3 \rightarrow \mathbf{C}^3 : (t, z) \mapsto \varphi_t(z) = \exp(it)z. \quad (2.1)$$

For  $n > 0$ , the  $n$ -level set  $H_0^{-1}(n)$  of  $H_0$  is the 5-sphere

$$\mathbf{S}_{\sqrt{2n}}^5 = \{z \in \mathbf{C}^3 : |z|^2 = 2n\} \quad (2.2)$$

of radius  $\sqrt{2n}$  (we denote by  $\mathbf{S}_r^k$  the  $k$ -sphere of radius  $r$ ). The sphere  $\mathbf{S}_{\sqrt{2n}}^5$  is invariant under  $\varphi$  (see (2.1)). The space of orbits of the  $\mathbf{S}^1$  action  $\varphi$  on the  $n$ -level

set of  $H_0$  is  $\mathbf{S}^5_{\sqrt{2n}}/\mathbf{S}^1$ . It is well known that this space of orbits is diffeomorphic to complex projective 2-space, which we denote by  $\mathbf{CP}^2_n = \mathbf{S}^5_{\sqrt{2n}}/\mathbf{S}^1$ . We will use homogeneous coordinates on  $\mathbf{CP}^2_n$ , that is, coordinates  $(z_1, z_2, z_3) \in \mathbf{C}^3$  with the restriction  $|z|^2 = 2n$  taking into account that points on  $\mathbf{S}^5_{\sqrt{2n}}$  that differ only by multiplication by a phase factor correspond to the same point on  $\mathbf{CP}^2$ . We denote the equivalence class of  $(z_1, z_2, z_3)$  as  $[z_1 : z_2 : z_3]$ .

For small energies, the perturbed Hamiltonian (1.2) has the approximate symmetry of the harmonic oscillator. In order to exploit this symmetry, we *normalize*  $H_\epsilon$ . In other words, we make a near-identity symplectic change of variables that takes  $H_\epsilon$  to  $\tilde{H}_\epsilon$ , so that  $\tilde{H}_\epsilon$  is  $\varphi$  invariant (or, equivalently,  $\{\tilde{H}_\epsilon, H_0\} = 0$ ) up to a certain order. This normalization can be carried out algorithmically using Lie series (Deprit 1969; Gröbner 1960). Since the normalization transformation is generally divergent, we normalize the Hamiltonian only up to some finite order. The result of normalization and truncation is a Hamiltonian

$$\tilde{H}_\epsilon(q, p) = H_0(q, p) + \epsilon^2 \tilde{H}_2(q, p) + \cdots + \epsilon^{2k} \tilde{H}_{2k}(q, p), \quad (2.3)$$

where  $\tilde{H}_j(q, p)$  are homogeneous polynomials of degree  $j+2$  such that  $\{\tilde{H}_j, H_0\} = 0$ . Since the value of  $\tilde{H}_\epsilon$  is constant along the orbits of  $X_{H_0}$ , we can properly define a function  $\tilde{H}_\epsilon$  on the orbit space of the flow of  $X_{H_0}$  on  $H_0^{-1}(n)$  (that is, on  $\mathbf{CP}^2_n$ ) by assigning to each orbit the value of  $\tilde{H}_\epsilon$  on a point of the orbit. The function  $\tilde{H}_\epsilon$  is called the *reduced* Hamiltonian.

### 3. The action of point groups on $\mathbf{CP}^2$ induced by their action on $\mathbf{R}^3$

Let  $\mathcal{G}$  be some point group, that is, some subgroup of  $O(3)$ , and consider its action on  $\mathbf{R}^3$ ,

$$\rho : \mathcal{G} \times \mathbf{R}^3 \rightarrow \mathbf{R}^3 : (g, q = (q_1, q_2, q_3)) \rightarrow \rho(g, q) = g \cdot q. \quad (3.1)$$

Note that we consider only three-dimensional vector representations of  $\mathcal{G}$ . Also note that point groups are defined up to conjugation in  $SO(3)$ .

Since  $\mathcal{G}$  is a subgroup of  $O(3)$ , we have  $(g^{-1})^T = g$  for every  $g \in \mathcal{G}$ . Therefore, the co-tangent lift of  $\rho$  to  $T^*\mathbf{R}^3 = \mathbf{R}^3 \times \mathbf{R}^3$  is

$$\rho^* : \mathcal{G} \times (\mathbf{R}^3 \times \mathbf{R}^3) \rightarrow \mathbf{R}^3 \times \mathbf{R}^3 : (g, (q, p)) \rightarrow (g \cdot q, g \cdot p). \quad (3.2)$$

The action of  $\mathcal{G}$  on  $\mathbf{C}^3$  with coordinates  $z = (z_1, z_2, z_3)$ , where  $z_j = q_j + ip_j$ , is then

$$\tilde{\rho} : \mathcal{G} \times \mathbf{C}^3 \rightarrow \mathbf{C}^3 : (g, z) \rightarrow g \cdot z. \quad (3.3)$$

If the Hamiltonian (1.2) is  $\mathcal{G}$  invariant, that is, for any  $g \in \mathcal{G}$ , we have

$$H_\epsilon(g \cdot (q, p)) = H_\epsilon(q, p),$$

then the normalized Hamiltonian  $\tilde{H}_\epsilon$  and the reduced Hamiltonian  $\hat{H}_\epsilon$  are also  $\mathcal{G}$  invariant. Therefore, by theorem 1.1, a critical point  $m$  of the action of the point group  $\mathcal{G}$  on  $\mathbf{CP}^2$  is also a stationary point of the  $\mathcal{G}$ -invariant reduced Hamiltonian  $\hat{H}_\epsilon$ .

Although the point groups are subgroups of  $O(3)$ , in order to study their action on  $\mathbf{CP}^2$  it is enough to consider only those point groups that are subgroups of  $SO(3)$ . This is due to the fact that the action of inversion on  $\mathbf{CP}^2$  is trivial, since

$$\iota[z_1 : z_2 : z_3] = [-z_1 : -z_2 : -z_3] = [z_1 : z_2 : z_3].$$

Define a group homomorphism

$$P : \mathrm{O}(3) \rightarrow \mathrm{SO}(3) : g \mapsto P(g) = \det(g)g. \quad (3.4)$$

Because of the triviality of the action of  $\iota$  on  $\mathbf{CP}^2$ , we obtain the following.

**Lemma 3.1.** *The action of a subgroup  $\mathcal{G}$  of  $\mathrm{O}(3)$  and the subgroup  $P(\mathcal{G})$  of  $\mathrm{SO}(3)$  on  $\mathbf{CP}^2$  are identical.*

We call a subgroup of  $\mathrm{SO}(3)$  a *proper point group*. Therefore, it is enough to study only the actions of the proper point groups instead of all the point groups. The correspondence between finite point groups and their images under  $P$  is listed below†

$$\begin{aligned} P(\mathcal{S}_{4k}) &= \mathcal{C}_{4k}, & P(\mathcal{S}_{2(2k+1)}) &= \mathcal{C}_{2k+1}, & P(\mathcal{C}_{2k,h}) &= \mathcal{C}_{2k}, \\ P(\mathcal{C}_{2k+1,h}) &= \mathcal{C}_{2(2k+1)}, & P(\mathcal{C}_{k,v}) &= \mathcal{D}_k, & P(\mathcal{D}_{2k,h}) &= \mathcal{D}_{2k}, \\ P(\mathcal{D}_{2k+1,h}) &= \mathcal{D}_{2(2k+1)}, & P(\mathcal{D}_{2k,d}) &= \mathcal{D}_{4k}, & P(\mathcal{D}_{2k+1,d}) &= \mathcal{D}_{2k+1}, \\ P(\mathcal{T}_h) &= \mathcal{T}, & P(\mathcal{T}_d) &= \mathcal{O}, & P(\mathcal{O}_h) &= \mathcal{O}, \\ P(\mathcal{Y}_h) &= \mathcal{Y}. \end{aligned}$$

The finite proper point groups are the group  $\mathcal{C}_k$  of rotations around an axis by angle  $\theta_k = 2\pi/k$ , the dihedral groups  $\mathcal{D}_k$ , the tetrahedron group  $\mathcal{T}$ , the octahedron group  $\mathcal{O}$  and the icosahedron group  $\mathcal{Y}$ . The group  $\mathcal{C}_k$  is generated by  $C_k$ . We write  $\mathcal{C}_k = \langle C_k \rangle$ . The group  $\mathcal{D}_k$  is generated by  $C_k$  and a rotation by angle  $\pi$  around an axis perpendicular to the  $C_k$ -axis. We denote this latter transformation and the corresponding axis by  $U_2$ .

In the problems that we are interested in, we also have time-reversal symmetry  $T$ . This means that the symmetry group of our Hamiltonian is  $\mathcal{G} \times \mathcal{R}$ , where  $\mathcal{G}$  is a point group and  $\mathcal{R} = \langle T \rangle$ . By lemma 3.1, we need only study the action of the group  $P(\mathcal{G})$  instead of  $\mathcal{G}$ . Thus we only have to consider the finite subgroups of  $\mathrm{SO}(3) \times \mathcal{R}$  up to conjugation in  $\mathrm{SO}(3)$ .

**Lemma 3.2.** *The finite subgroups of  $\mathrm{SO}(3) \times \mathcal{R}$  (up to conjugation in  $\mathrm{SO}(3)$ ) are as follows.*

- (1) *The cyclic and dihedral groups are*
  - (a)  $\mathcal{C}_k = \langle C_k \rangle$ ;
  - (b)  $\mathcal{D}_k = \langle C_k, U_2 \rangle$ .
- (2) *The time-reversal extended cyclic and dihedral groups are*
  - (c)  $\mathcal{C}_k \times \mathcal{R} = \langle C_k, T \rangle$ ;
  - (d)  $\mathcal{C}_k \wedge C_{2k}T = \langle C_k, C_{2k}T \rangle$ ;
  - (e)  $\mathcal{C}_k \wedge U_2T = \langle C_k, U_2T \rangle$ ;

† We are using here the standard physics and chemistry notation for finite point groups. The definitions and descriptions of these groups can be found in many textbooks (see, for example, Landau & Lifshitz (1958) or Hammermesh (1962)). Note that some of these groups are isomorphic to each other, but we consider them to be different because their actions on the physical space are different.

- (f)  $\mathcal{D}_k \times \mathcal{R} = \langle C_k, U_2, T \rangle;$   
 (g)  $\mathcal{D}_k \wedge C_{2k}T = \langle C_k, U_2, C_{2k}T \rangle.$

(3) The cubic groups are

- (h)  $\mathcal{T}, \mathcal{T} \times \mathcal{R}, \mathcal{T} \wedge U_2T, \mathcal{O}, \mathcal{O} \times \mathcal{R}, \mathcal{Y}, \mathcal{Y} \times \mathcal{R}.$

*Proof.*  $SO(3) \times \mathcal{R}$  and  $SO(3) \times \mathcal{C}_i$ , which is isomorphic to  $O(3)$ , where  $\mathcal{C}_i = \langle \iota \rangle$ , are isomorphic. The isomorphism is given by the map  $\tau : O(3) \rightarrow SO(3) \times \mathcal{R}$  that is the identity on  $SO(3)$  and maps  $\iota$  to  $T$ . This means that the finite subgroups of  $SO(3) \times \mathcal{R}$ , up to conjugation in  $SO(3)$ , are the images under  $\tau$  of the finite subgroups of  $O(3)$  up to conjugation in  $SO(3)$ , that is, the finite point groups.

Let  $\mathcal{G} \wedge g$  denote the group generated by  $\mathcal{G}$  and an element  $g \notin \mathcal{G}$ . Then the finite point groups can be written as follows:†

- (a)  $\mathcal{C}_k = \langle C_k \rangle;$   
 (b)  $\mathcal{D}_k = \langle C_k, U_2 \rangle;$   
 (c)  $\mathcal{C}_k \times \mathcal{C}_i = \langle C_k, \iota \rangle$ , which is  $\mathcal{S}_{2k}$  for  $k$  odd and  $\mathcal{C}_{kh}$  for  $k$  even;  
 (d)  $\mathcal{C}_k \wedge C_{2k}\iota = \langle C_k, C_{2k}\iota \rangle$ , which is  $\mathcal{S}_{2k}$  for  $k$  even and  $\mathcal{C}_{kh}$  for  $k$  odd;  
 (e)  $\mathcal{C}_k \wedge U_2\iota = \langle C_k, U_2\iota \rangle$ , which is  $\mathcal{C}_{kv}$ ;  
 (f)  $\mathcal{D}_k \times \mathcal{C}_i = \langle C_k, U_2, \iota \rangle$ , which is  $\mathcal{D}_{kh}$  for  $k$  even and  $\mathcal{D}_{kd}$  for  $k$  odd;  
 (g)  $\mathcal{D}_k \wedge C_{2k}\iota = \langle C_k, U_2, C_{2k}\iota \rangle$ , which is  $\mathcal{D}_{kh}$  for  $k$  odd and  $\mathcal{D}_{kd}$  for  $k$  even;  
 (h)  $\mathcal{T}, \mathcal{T} \times \mathcal{C}_i, \mathcal{T}_d = \mathcal{T} \wedge U_2\iota, \mathcal{O}, \mathcal{O} \times \mathcal{C}_i, \mathcal{Y}, \mathcal{Y} \times \mathcal{C}_i.$

In the list above,  $C_k$  and  $C_{2k}$  represent rotations around the same axis, while  $U_2$  represents rotations by  $\pi$  around an axis perpendicular to the first one. Substituting  $\iota$  in the above list by  $T$ , we obtain the lemma. ■

#### 4. Fixed points of the $\mathcal{C}_k$ action

In this section we determine the fixed points of the point group  $\mathcal{C}_k$  on  $CP^2$  and their linear stability type.

##### (a) Position of fixed points

Positions of fixed points on  $CP^2$  for many point groups that are interesting for molecular applications are given in Zhilinskiĭ (1989). Time reversal is not considered in that reference.

Rotations  $C_k$  by angle  $\theta_k = 2\pi/k$  around an axis form a cyclic group of order  $k$ , denoted  $\mathcal{C}_k$ . Thus

$$\mathcal{C}_k = \{1, C_k, C_k^2, \dots, C_k^{k-1}\}. \quad (4.1)$$

† Our notation is somewhat different from that usually used in the description of point groups in order to make more apparent the role of inversion in each group.

Geometrically, the axis of rotation of  $C_k$  in  $\mathbf{R}^3$  is given by an arbitrary vector  $v = (v_1, v_2, v_3)$ . In order to simplify our study, we perform a rotation by  $Q = Q(v) \in \text{SO}(3)$ , so that  $Qv = (0, 0, 1)$ . We denote the rotated coordinates again by  $(q_1, q_2, q_3)$ . The representation of  $C_k$  in the rotated coordinates is

$$C_k = \begin{pmatrix} \cos \theta_k & \sin \theta_k & 0 \\ -\sin \theta_k & \cos \theta_k & 0 \\ 0 & 0 & 1 \end{pmatrix}. \quad (4.2)$$

From (3.3), we see that the action of  $C_k$  on  $\mathbf{C}^3$  is

$$\tilde{\rho} : C_k \times \mathbf{C}^3 \rightarrow \mathbf{C}^3 : (C_k^j, z) \rightarrow C_k^j z. \quad (4.3)$$

The following result is adapted from Zhilinskiĭ (1989).

**Lemma 4.1 (cf. Zhilinskiĭ).** *The set of fixed points of the  $C_2$  action on  $\mathbf{CP}^2$  is a disjoint union of the critical point  $Z_3 = [0 : 0 : 1]$  and a 2-sphere  $\mathbf{S}^2$  of non-critical fixed points. The fixed points of  $C_k$  for  $k \geq 3$  are  $Z_3 = [0 : 0 : 1]$  and  $Z_{\pm} = [1 : \pm i : 0]$ .*

*Proof.* In order to find the fixed points of the  $C_k$  action on  $\mathbf{CP}^2$ , we define new coordinates  $u = (u_1, u_2, u_3)$ , where  $u_1 = z_1 + iz_2$ ,  $u_2 = z_1 - iz_2$ ,  $u_3 = z_3$ . In these coordinates, the action becomes diagonal, namely,

$$\hat{\rho} : C_k \times \mathbf{C}^3 \rightarrow \mathbf{C}^3 : (C_k^j, u) \mapsto (\exp(-ij\theta_k)u_1, \exp(ij\theta_k)u_2, u_3). \quad (4.4)$$

The  $\mathbf{S}^1$  action  $\varphi$  on the  $u$  coordinates becomes

$$\hat{\varphi} : \mathbf{S}^1 \times \mathbf{C}^3 \rightarrow \mathbf{C}^3 : (t, u) \mapsto \exp(it)u. \quad (4.5)$$

The fixed points of the action of  $C_k$  on  $\mathbf{CP}^2$  are the solutions of the equation  $C_k u = \exp(it)u$  for some  $t \in \mathbf{S}^1 \simeq \mathbf{R}/2\pi\mathbf{Z}$ . Specifically, the system of equations that we need to solve is

$$\left. \begin{aligned} \exp(-i\theta_k)u_1 &= \exp(it)u_1, \\ \exp(i\theta_k)u_2 &= \exp(it)u_2, \\ u_3 &= \exp(it)u_3. \end{aligned} \right\} \quad (4.6)$$

For  $k \geq 3$ , the solutions of (4.6) are the points  $u^{(1)} = [1 : 0 : 0]$ ,  $u^{(2)} = [0 : 1 : 0]$  and  $u^{(3)} = [0 : 0 : 1]$ ; while, for  $k = 2$ , we have two types of solutions. When  $u_3 \neq 0$ , we obtain the isolated point  $u^{(3)} = [0 : 0 : 1]$ ; while, when  $u_3 = 0$ , we find that  $|u_1|^2 + |u_2|^2 = 1$ . The last equation defines a 3-sphere  $\mathbf{S}^3$  in  $\mathbf{C}^2$ . Points on this 3-sphere that lie on the same orbit of the  $\mathbf{S}^1$  action  $\hat{\varphi}$  (see (4.5)) represent the same point. Therefore, the solutions of (4.6) lie on a manifold  $\mathbf{S}^3_{\sqrt{2n}}/\mathbf{S}^1$ , which is diffeomorphic to  $\mathbf{CP}^1$ , that is, the 2-sphere  $\mathbf{S}^2$ . This manifold is dynamically invariant for every  $C_2$ -invariant Hamiltonian.

In the original complex variables  $[z_1 : z_2 : z_3]$ , we find that, for  $k \geq 3$ , the fixed points are  $Z_+ = [1 : i : 0]$ ,  $Z_- = [1 : -i : 0]$  and  $Z_3 = [0 : 0 : 1]$ . For  $k = 2$ , the fixed point is  $Z_3 = [0 : 0 : 1]$  and the invariant sphere as  $|z_1|^2 + |z_2|^2 = 1$ . Note that although all the points of the sphere are fixed under the  $C_2$  action, they are not, in general, stationary points of the reduced Hamiltonian, because they are not isolated and therefore they are not critical. ■

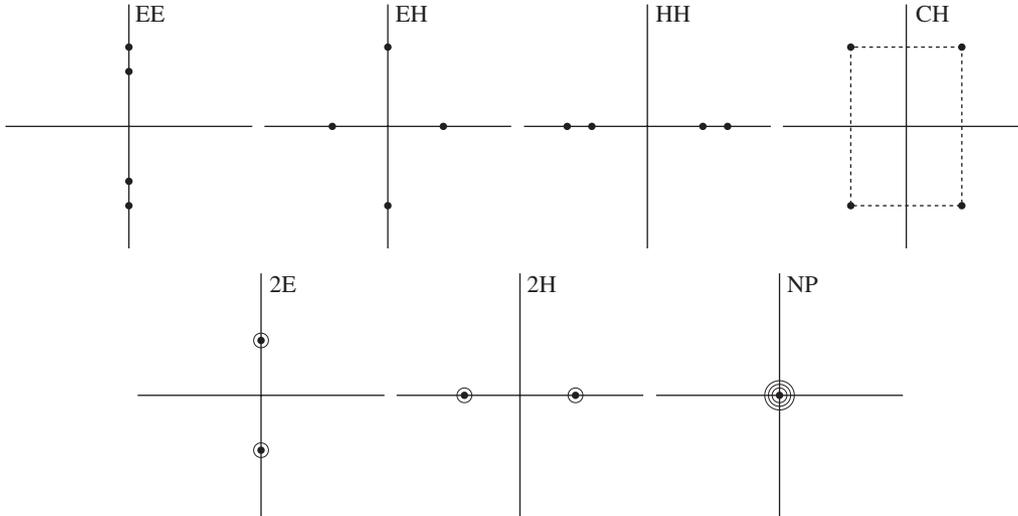


Figure 1. Types of linear stability for an equilibrium of a two-degree-of-freedom Hamiltonian. Starting at the upper left: EE, EH, HH, CH, 2E, 2H and NP.

We introduce a more convenient parametrization of the 2-sphere  $\mathbf{S}^2$ , which will be useful in what follows. Note that the 2-sphere  $\mathbf{S}^2$  can be defined as the set of points  $(z_1, z_2) \in \mathbf{C}^2$  with  $|z_1|^2 + |z_2|^2 = 1$  that are equivalent under the  $\mathbf{S}^1$  action  $(t, (z_1, z_2)) \rightarrow \exp(it)(z_1, z_2)$ . We can parametrize the orbit space of this action using the invariants

$$s_1 = z_1 \bar{z}_1 - z_2 \bar{z}_2, \quad s_2 = z_1 \bar{z}_2 + \bar{z}_1 z_2 \quad \text{and} \quad s_3 = i(z_1 \bar{z}_2 - \bar{z}_1 z_2),$$

which are subject to the relation

$$s_1^2 + s_2^2 + s_3^2 = (|z_1|^2 + |z_2|^2)^2 = 1.$$

A computation shows that, for  $k \geq 3$ , the induced action of  $C_k$  on  $\mathbf{R}^3$  with coordinates  $(s_1, s_2, s_3)$  is

$$C_k(s_1, s_2, s_3) = (\cos(2\theta_k)s_1 + \sin(2\theta_k)s_2, -\sin(2\theta_k)s_1 + \cos(2\theta_k)s_2, s_3).$$

When  $k = 2$ , we find again that  $2\theta_k = 2\pi$ . Therefore, all the points on the 2-sphere  $\mathbf{S}^2$  remain fixed.

### (b) Stability of fixed points

In order to determine the possible types of linear stability of the fixed points of the action of  $C_k$  on  $\mathbf{C}P^2$  under the flow of the reduced  $C_k$ -invariant Hamiltonian  $\hat{H}_\epsilon$ , we need to compute the eigenvalues of the corresponding linearized vector field (the frequencies) at the fixed point. If one of the frequencies is  $\lambda \in \mathbf{C}$ , then  $-\lambda$ ,  $\bar{\lambda}$  and  $-\bar{\lambda}$  are also frequencies. Therefore, there are generically four types of linear stability depending on the arrangement of the frequencies on the complex plane (see figure 1).

- (a) Elliptic–elliptic (EE) when all the frequencies are on the imaginary axis.
- (b) Elliptic–hyperbolic (EH) when two of the frequencies are real and two are imaginary.

- (c) Hyperbolic–hyperbolic (HH) when all frequencies are real.
- (d) Complex hyperbolic (CH) when  $\lambda$  is neither real nor imaginary and the frequencies form a quadruplet  $\lambda, -\lambda, \bar{\lambda}, -\bar{\lambda}$ .

There are also three non-generic cases in the space of all possible quadratic Hamiltonians.

- (e) Two pairs of equal frequencies on the imaginary axis  $\pm i\lambda$  (twice) with  $\lambda \in \mathbf{R}$ . We denote this case by 2E.
- (f) Two pairs of equal frequencies on the real axis  $\pm\lambda$  (twice) with  $\lambda \in \mathbf{R}$ . We denote this case by 2H.
- (g) All frequencies are zero. We denote this case by NP (nilpotent).

As we will see later, some of these non-generic cases become generic in the presence of particular symmetries.

Since the procedure that we use in order to determine the possible types of linear stability of a fixed point can be applied to point groups other than  $\mathcal{C}_k$ , we describe it in some generality. Consider a  $\mathcal{G}$ -invariant reduced Hamiltonian  $\tilde{H}$  and let  $m \in \mathbf{C}\mathbf{P}^2$  be a critical point with non-trivial isotropy group  $\mathcal{G}_m$ . Define a local chart  $\chi : \mathbf{C}\mathbf{P}^2 \rightarrow \mathbf{R}^4 : \ell \rightarrow (x_1, x_2, y_1, y_2)$  near  $m$  so that  $\chi(m) = 0$  and the constant part of the symplectic form is  $\omega = dx_1 \wedge dy_1 + dx_2 \wedge dy_2$ . The linear action of  $\mathcal{G}_m$  in this chart can be determined from its action on  $\mathbf{C}^3$ . Let  $H^{\text{loc}}$  be the reduced Hamiltonian expressed in the local chart. The *crucial fact* is that  $H^{\text{loc}}$  is  $\mathcal{G}_m$  invariant. The frequencies of the vector field at  $m$  are the eigenvalues of  $Y = DX_{H^{\text{loc}}}(0)$ . Let

$$H^{\text{loc}}(x, y) = H_0^{\text{loc}}(x, y) + H_1^{\text{loc}}(x, y) + H_2^{\text{loc}}(x, y) + H_3^{\text{loc}}(x, y) + \dots$$

be the Taylor expansion of  $H^{\text{loc}}$  around 0, where each  $H_j^{\text{loc}}(x, y)$  is a homogeneous polynomial of degree  $j$  in  $(x, y)$ . Notice that  $dH^{\text{loc}}(0) = 0$ , since 0 is a stationary point for  $H^{\text{loc}}$ . Similarly, let  $\omega(x, y) = \omega_0(x, y) + \omega_1(x, y) + \dots$  be the Taylor expansion of the symplectic form, where each  $\omega_j(x, y)$  has coefficients that are homogeneous polynomials of degree  $j$ .

**Lemma 4.2.**  $Y$  is determined by  $H_2^{\text{loc}}(x, y)$  and  $\omega_0(x, y) = \omega(0)$ .

*Proof.* In this proof, we write  $H$  instead of  $H^{\text{loc}}$ . Notice that  $dH_j(0) = 0$  for  $j \geq 2$ , and hence  $dH(0) = dH_1(0) = 0$ . This means that  $H_1(x, y) = 0$ . The vector field  $X_H$  is determined by  $\mathbf{i}_{X_H}\omega = dH$ . Taylor expand (the yet unknown)  $X_H(x, y)$  around 0:  $X_H(x, y) = X_0(x, y) + X_1(x, y) + \dots$ , where each  $X_j(x, y)$  has coefficients that are homogeneous polynomials of order  $j$  in  $(x, y)$ . Then, equating terms of the same order, we obtain the system of equations

$$\begin{aligned} \mathbf{i}_{X_0}\omega_0 &= dH_1 = 0, \\ \mathbf{i}_{X_0}\omega_1 + \mathbf{i}_{X_1}\omega_0 &= dH_2, \\ &\vdots \end{aligned}$$

From the first equation, we find  $X_0 = 0$ . From the second equation, we can determine  $X_1$ . Note that

$$Y = DX_H(0) = DX_0(0) + DX_1(0) + DX_2(0) + \dots$$

Since  $X_0 = 0$  and the coefficients of  $X_j(x, y)$  for  $j \geq 2$  are homogeneous polynomials of degree 2, we have

$$Y = DX_H(0) = DX_1(0).$$

This means that  $X_1$  and therefore  $Y$  can be determined from  $H_2(x, y)$  and  $\omega_0(x, y)$  solving the equation  $i_{X_1}\omega_0 = dH_2$ . ■

Since we know the action of  $\mathcal{G}_m$  on the local chart, we can write the most general  $\mathcal{G}_m$ -invariant quadratic Hamiltonian  $H_2^{\text{loc}}$  in the local chart. From  $H_2^{\text{loc}}$ , we can compute  $Y = DX_{H^{\text{loc}}}(0)$ .

We can now study the linear stability of the fixed points of  $C_k$ .

**Lemma 4.3.** *The fixed point  $Z_3 = [0 : 0 : 1]$  of the action of  $C_k$  can have any type of linear stability.*

*Proof.* For the fixed point  $Z_3 = [0 : 0 : 1]$ , we define local coordinates  $(x, y)$  on  $\mathbf{CP}^2$  by  $w_1 = z_1/z_3 = x_1 + iy_1$ ,  $w_2 = z_2/z_3 = x_2 + iy_2$  satisfying the constraints  $z_3 = 1/(1 + |w_1|^2 + |w_2|^2)^{1/2}$  and  $\text{Im}(z_3) = 0$ . The constant term of the symplectic form on  $\mathbf{CP}^2$  in these coordinates is  $\omega = dx_1 \wedge dy_1 + dx_2 \wedge dy_2$ .

The action of  $C_k$  on  $w_1, w_2$  can be easily computed as

$$C_k w_1 = \frac{C_k z_1}{C_k z_3} = \frac{\cos \theta_k z_1 + \sin \theta_k z_2}{z_3} = \cos \theta_k w_1 + \sin \theta_k w_2$$

and

$$C_k w_2 = \frac{C_k z_2}{C_k z_3} = \frac{-\sin \theta_k z_1 + \cos \theta_k z_2}{z_3} = -\sin \theta_k w_1 + \cos \theta_k w_2.$$

We now diagonalize this action. Introduce coordinates  $v_1 = x_1 + ix_2$ ,  $v_2 = y_1 + iy_2$ . Then the action of  $C_k$  on  $(v_1, v_2) \in \mathbf{C}^2$  is

$$C_k(v_1, v_2) = (\exp(i\theta_k)v_1, \exp(i\theta_k)v_2).$$

For  $k \geq 3$ , the quadratic invariants of the  $C_k$  action are spanned by

$$v_1 \bar{v}_1, \quad v_2 \bar{v}_2, \quad v_1 \bar{v}_2 \quad \text{and} \quad \bar{v}_1 v_2.$$

If we express these invariants in terms of real variables  $(x, y)$ , we find that the real quadratic invariants of  $C_k$  are spanned by

$$x_1^2 + x_2^2, \quad y_1^2 + y_2^2, \quad x_1 y_1 + x_2 y_2 \quad \text{and} \quad x_1 y_2 - x_2 y_1.$$

For  $k \geq 3$ , the most general quadratic  $C_k$ -invariant Hamiltonian is

$$H_2^{\text{loc}}(x, y) = \frac{1}{2}a(x_1^2 + x_2^2) + \frac{1}{2}b(y_1^2 + y_2^2) + c(x_1 y_1 + x_2 y_2) + d(x_1 y_2 - x_2 y_1), \quad (4.7)$$

where  $a, b, c, d \in \mathbf{R}$ . The frequencies in this case are  $\pm i(d \pm \sqrt{ab - c^2})$ .

For  $k = 2$ , all quadratic monomials of  $v_1, v_2, \bar{v}_1$  and  $\bar{v}_2$  are invariant under  $C_2$ . This means that there are no restrictions on the quadratic local Hamiltonian or on the frequencies at  $Z_3$ . ■

When  $k \geq 3$  for the fixed points  $Z_{\pm} = [1 : \pm i : 0]$ , we have the following.

**Lemma 4.4.** *The fixed points  $Z_{\pm}$  of the action of  $C_k$ ,  $k \geq 5$ , have linear stability type  $EE$ . For  $k = 4$ , the fixed points can have stability type either  $EE$  or  $EH$  and, for  $k = 3$ , they can have any type of stability.*

*Proof.* It is enough to study the fixed point  $Z_+ = [1 : i : 0]$ . We define a local chart on  $\mathbf{CP}^2$  by

$$i + x_1 + iy_1 = i + w_1 = \frac{z_2}{z_1} \quad \text{and} \quad x_2 + iy_2 = w_2 = \frac{z_3}{z_1},$$

with the constraints  $z_1 = 1/(1 + |i + w_1|^2 + |w_2|^2)^{1/2}$  and  $\text{Im}(z_1) = 0$ . In the  $(x, y)$  coordinates, the constant term of the symplectic form is  $\omega = dx_1 \wedge dy_1 + dx_2 \wedge dy_2$ .

We compute the action of  $C_k$  on  $w_1$  up to first-order terms as follows,

$$\begin{aligned} i + C_k w_1 &= \frac{C_k z_2}{C_k z_1} \\ &= \frac{-\sin \theta_k z_1 + \cos \theta_k z_2}{\cos \theta_k z_1 + \sin \theta_k z_2} \\ &= \frac{-\sin \theta_k + \cos \theta_k (i + w_1)}{\cos \theta_k z_1 + \sin \theta_k (i + w_1)} \\ &= \frac{i \exp(i\theta_k) + \cos \theta_k w_1}{\exp(i\theta_k) + \sin \theta_k w_1} \\ &= \frac{i + \exp(-i\theta_k) \cos \theta_k w_1}{1 + \exp(-i\theta_k) \sin \theta_k w_1} \\ &= i + \exp(-2i\theta_k) w_1 + O(|w_1|^2) \end{aligned} \tag{4.8}$$

and on  $w_2$  as follows,

$$\begin{aligned} C_k w_2 &= \frac{C_k z_3}{C_k z_1} \\ &= \frac{z_3}{\cos \theta_k z_1 + \sin \theta_k z_2} \\ &= \frac{w_2}{\cos \theta_k + \sin \theta_k (i + w_1)} \\ &= \frac{w_2}{\exp(i\theta_k) + \sin \theta_k w_1} \\ &= \frac{\exp(-i\theta_k) w_2}{1 + \exp(-i\theta_k) \sin \theta_k w_1} \\ &= \exp(-i\theta_k) w_2 + O(|w_1| |w_2|). \end{aligned} \tag{4.9}$$

We now find the invariants of this action for  $k \geq 3$ , since the only isolated fixed point of the action of  $C_2$  on  $\mathbf{CP}^2$  is  $Z_3$ .

For  $k \geq 5$ , the quadratic invariants are spanned by  $w_1 \bar{w}_1$  and  $w_2 \bar{w}_2$ . Therefore, the most general quadratic local Hamiltonian is

$$H_2^{\text{loc}}(w_1, w_2) = \frac{1}{2} a w_1 \bar{w}_1 + \frac{1}{2} b w_2 \bar{w}_2, \tag{4.10}$$

with  $a, b \in \mathbf{R}$ . In real coordinates,

$$H_2^{\text{loc}}(x, y) = \frac{1}{2} a (x_1^2 + y_1^2) + \frac{1}{2} b (x_2^2 + y_2^2). \tag{4.11}$$

The frequencies are  $\pm ia$  and  $\pm ib$ . Therefore, the fixed point is always EE.

For  $k = 4$ , the quadratic invariants are spanned by  $w_1\bar{w}_1$ ,  $w_2\bar{w}_2$ ,  $w_1^2$  and  $\bar{w}_1^2$ . Consequently, the real quadratic invariants are spanned by  $x_1^2$ ,  $y_1^2$ ,  $x_1y_1$  and  $x_2^2 + y_2^2$ . Therefore, the most general quadratic Hamiltonian is

$$H_2^{\text{loc}}(x, y) = \frac{1}{2}ax_1^2 + \frac{1}{2}by_1^2 + cx_1y_1 + \frac{1}{2}d(x_2^2 + y_2^2). \quad (4.12)$$

The frequencies are  $\pm(c^2 - ab)^{1/2}$  and  $\pm id$ . Therefore, the stationary point can be either EE or EH.

For  $k = 3$ , the quadratic invariants are spanned by  $w_1\bar{w}_1$ ,  $w_2\bar{w}_2$ ,  $w_1w_2$  and  $\bar{w}_1\bar{w}_2$ . In real coordinates, they are spanned by

$$x_1^2 + y_1^2, \quad x_2^2 + y_2^2, \quad x_1x_2 - y_1y_2 \quad \text{and} \quad x_1y_2 + x_2y_1.$$

Hence we have

$$H_2^{\text{loc}}(x, y) = \frac{1}{2}a(x_1^2 + y_1^2) + \frac{1}{2}b(x_2^2 + y_2^2) + c(x_1x_2 - y_1y_2) + d(x_1y_2 + x_2y_1). \quad (4.13)$$

The frequencies in this case are  $\pm \frac{1}{2}i(a - b \pm \sqrt{(a + b)^2 - 4(c^2 + d^2)})$ . ■

## 5. Fixed points of other finite proper point groups

We use the results of the preceding section in order to find the fixed points of the rest of the finite proper point groups, namely,  $\mathcal{D}_k$ ,  $\mathcal{T}$ ,  $\mathcal{O}$  and  $\mathcal{Y}$ .

Note that although we are interested in the linear stability type of the critical points of each finite point group, it is enough to study only the linear stability type of the *fixed* points of finite point groups, since each critical point  $m$  of a point group  $\mathcal{G}$  is a fixed point of its isotropy group  $\mathcal{G}_m$ , which is a subgroup of  $\mathcal{G}$ .

The group  $\mathcal{D}_k$  can be obtained from  $\mathcal{C}_k$  if we add a  $U_2$ -axis perpendicular to the  $\mathcal{C}_k$ -axis. This induces the appearance of  $k - 1$  more  $U_2$ -axes perpendicular to the  $\mathcal{C}_k$ -axis.

**Lemma 5.1.** *The fixed points of  $\mathcal{D}_2$  on  $\mathbf{CP}^2$  are  $Z_1 = [1 : 0 : 0]$ ,  $Z_2 = [0 : 1 : 0]$  and  $Z_3 = [0 : 0 : 1]$ . They can have either EE, EH or HH linear stability type.*

*Proof.* The group  $\mathcal{D}_2$  has three mutually perpendicular  $C_2$ -axes. By choosing a suitable system of coordinates, we can identify these axes with the coordinate axes.  $C_2$  denotes rotations around the axis  $(0, 0, 1)$  and  $U_2$  denotes rotations around the axis  $(1, 0, 0)$ . These rotations generate  $\mathcal{D}_2$ . The fixed points of  $C_2$  on  $\mathbf{CP}_n^2$  are  $Z_3 = [0 : 0 : 1]$  and the 2-sphere  $\mathbf{S}^2$ , which we described in § 3 using the variables  $(s_1, s_2, s_3)$  as  $s_1^2 + s_2^2 + s_3^2 = 1$ . The action of  $U_2$  on  $\mathbf{CP}^2$  is  $U_2[z_1 : z_2 : z_3] = [z_1 : -z_2 : -z_3]$ .  $Z_3$  is a fixed point of  $U_2$ , since  $U_2[0 : 0 : 1] = [0 : 0 : -1] = [0 : 0 : 1]$ . The action of  $U_2$  on  $\mathbf{S}^2$  is  $U_2(s_1, s_2, s_3) = (s_1, -s_2, -s_3)$ . It leaves invariant only the points  $(\pm 1, 0, 0)$ , which correspond to the points  $Z_1 = [1 : 0 : 0]$  and  $Z_2 = [0 : 1 : 0]$  on  $\mathbf{CP}^2$ , respectively. We deduce that the fixed points of  $\mathcal{D}_2$  are  $Z_1 = [1 : 0 : 0]$ ,  $Z_2 = [0 : 1 : 0]$  and  $Z_3 = [0 : 0 : 1]$ . It is enough to study the types of linear stability for any one of them, since they belong to the same  $\mathcal{D}_2$  orbit. In § 4 we defined coordinates  $v_1 = x_1 + ix_2$  and  $v_2 = y_1 + iy_2$  near  $[0 : 0 : 1]$  and found that the action of  $C_2$  is  $C_2v_1 = -v_1$  and  $C_2v_2 = -v_2$ . The action of  $U_2$  is  $U_2v_1 = -\bar{v}_1$  and  $U_2v_2 = -\bar{v}_2$ . Therefore, the quadratic invariants of the  $\mathcal{D}_2$  action on the local chart are spanned by

$$v_1\bar{v}_1, \quad v_2\bar{v}_2, \quad v_1^2 + \bar{v}_1^2, \quad v_2^2 + \bar{v}_2^2, \quad v_1\bar{v}_2 + \bar{v}_1v_2 \quad \text{and} \quad v_1v_2 + \bar{v}_1\bar{v}_2.$$

The corresponding real quadratic invariants are spanned by

$$x_1^2, \quad x_2^2, \quad y_1^2, \quad y_2^2, \quad x_1y_1 \quad \text{and} \quad x_2y_2.$$

Therefore, the most general quadratic local Hamiltonian is

$$H_2^{\text{loc}}(x, y) = \frac{1}{2}ax_1^2 + \frac{1}{2}bx_2^2 + \frac{1}{2}cy_1^2 + \frac{1}{2}dy_2^2 + ex_1y_1 + fx_2y_2. \quad (5.1)$$

The frequencies in this case are  $\pm(e^2 - ac)^{1/2}$  and  $\pm(f^2 - bd)^{1/2}$ . Therefore, the linear stability type of the fixed point can be either EE, EH or HH. ■

For higher-order groups  $\mathcal{D}_k$ , we have the following.

**Lemma 5.2.**  $\mathcal{D}_k$ , for  $k \geq 3$ , has one fixed point on  $\mathbf{CP}^2$  with coordinates  $Z_3 = [0 : 0 : 1]$ . It can have linear stability type either 2E or 2H.

*Proof.* Since the group  $\mathcal{D}_k$  contains  $\mathcal{C}_k$  as a subgroup, we check to see which of the fixed points of  $\mathcal{C}_k$  remain fixed points for the larger group and whether the larger symmetry has any effect on the linear stability.

The fixed point of  $\mathcal{C}_k$  with coordinates  $Z_3 = [0 : 0 : 1]$  is also a fixed point for every  $U_2$  rotation around an axis perpendicular to the  $\mathcal{C}_k$ -axis, since  $U_2Z_3 = [0 : 0 : -1] = [0 : 0 : 1]$ . We choose coordinates so that one  $U_2$ -axis passes through  $(1, 0, 0)$  in configuration space, while the  $\mathcal{C}_k$ -axis still passes through  $(0, 0, 1)$ . From now on, we will always denote by  $U_2$  the axis that passes through  $(1, 0, 0)$ . The action of  $U_2$  on the  $[z_1 : z_2 : z_3]$  is  $U_2[z_1 : z_2 : z_3] = [z_1 : -z_2 : -z_3]$ . Its action on the local variables  $(x, y)$  is therefore  $U_2(x_1, x_2, y_1, y_2) = (-x_1, x_2, -y_1, y_2)$ . We have found that the quadratic real invariants for the  $\mathcal{C}_k$  action are spanned by

$$x_1^2 + x_2^2, \quad y_1^2 + y_2^2, \quad x_1y_1 + x_2y_2 \quad \text{and} \quad x_1y_2 - x_2y_1.$$

Only the first three of the above are invariant under the  $U_2$  action. Therefore, the most general quadratic  $\mathcal{D}_k$ -invariant Hamiltonian for  $k \geq 3$  is

$$H_2^{\text{loc}}(x, y) = \frac{1}{2}a(x_1^2 + x_2^2) + \frac{1}{2}b(y_1^2 + y_2^2) + c(x_1y_1 + x_2y_2). \quad (5.2)$$

The frequencies in this case are  $\pm(c^2 - ab)^{1/2}$  (twice). Therefore, the fixed point can have either 2E or 2H as linear stability type.

Now consider the fixed points of  $\mathcal{C}_k$  with coordinates  $Z_{\pm} = [1 : \pm i : 0]$ . We have  $U_2[1 : \pm i : 0] = [1 : \mp i : 0]$ . This means that  $Z_{\pm}$  are not fixed points of  $\mathcal{D}_k$  for  $k \geq 3$ . ■

Finally, for the tetrahedron, octahedron and icosahedron groups, we obtain the following.

**Lemma 5.3.** The actions of  $\mathcal{T}$ ,  $\mathcal{O}$  and  $\mathcal{Y}$  on  $\mathbf{CP}^2$  do not have any fixed points.

*Proof.* These groups have intersecting  $\mathcal{C}_3$ -axes. ■

Note that this lemma does not say that the action of these groups does not have any critical points on  $\mathbf{CP}^2$ , but that there are no critical points of any group action with these isotropy groups.

## 6. The fixed points of time-reversal extended groups

We have found the fixed points and their linear stability types of stability for all non-trivial finite proper point groups  $\mathcal{G}$ . If the original  $\mathcal{G}$ -invariant Hamiltonian has time-reversal symmetry  $T$ , which is the case for Hamiltonians in molecular systems, then its symmetry group is the extended group  $\mathcal{G} \times \mathcal{R}$ . The isotropy group of a critical point can then be one of the  $T$  extended finite subgroups of  $\text{SO}(3) \times \mathcal{R}$  that we listed in §3. In this section we study the linear stability type of the fixed points of these groups.

**Lemma 6.1.** *For  $k \geq 3$ , the groups  $\mathcal{C}_k \times \mathcal{R}$  and  $\mathcal{D}_k \times \mathcal{R}$  have only one fixed point, with coordinates  $Z_3 = [0 : 0 : 1]$ , which has linear stability type either 2E or 2H. The group  $\mathcal{C}_2 \times \mathcal{R}$  has one isolated fixed point  $Z_3 = [0 : 0 : 1]$  that can have any stability type and a circle of fixed points that are not critical. The group  $\mathcal{D}_2 \times \mathcal{R}$  has three isolated fixed points with coordinates  $Z_1 = [1 : 0 : 0]$ ,  $Z_2 = [0 : 1 : 0]$  and  $Z_3 = [0 : 0 : 1]$ . They have linear stability type either EE, EH or HH.*

*Proof.* Note that the action of  $T$  on the local chart near  $Z_3$  is diagonal, since  $T(x, y) = (x, -y)$ . In particular, it is diagonal on the space of quadratic monomials in  $x$  and  $y$ . In order to find the most general  $\mathcal{G} \times \mathcal{R}$ -invariant quadratic local Hamiltonian, we need to consider only the local quadratic Hamiltonians that we found previously for the different groups  $\mathcal{G}$  and keep only those monomials that are invariant under  $T$ .

For  $\mathcal{C}_2 \times \mathcal{R}$ , we find

$$H_2^{\text{loc}}(x, y) = \frac{1}{2}ax_1^2 + \frac{1}{2}bx_2^2 + \frac{1}{2}cy_1^2 + \frac{1}{2}dy_2^2 + ex_1x_2 + fy_1y_2. \quad (6.1)$$

In this case, the frequencies are  $\pm \frac{1}{\sqrt{2}}(-\alpha \pm (\alpha^2 - 4\beta\gamma)^{1/2})^{1/2}$ , where there are four choices of plus or minus signs and  $\alpha = ac + bd + 2ef$ ,  $\beta = e^2 - ab$  and  $\gamma = f^2 - cd$ . The fixed point can have any linear stability type.

The action of  $T$  on the sphere  $\mathcal{S}^2$  of fixed points is  $T(s_1, s_2, s_3) = (s_1, s_2, -s_3)$ . It leaves invariant the circle  $\{s_3 = 0\}$  on  $\mathcal{S}^2$ .

For  $\mathcal{C}_k \times \mathcal{R}$ ,  $\mathcal{D}_k \times \mathcal{R}$ , and  $k \geq 3$  from equations (4.7) and (5.2), we find that

$$H_2^{\text{loc}}(x, y) = \frac{1}{2}a(x_1^2 + x_2^2) + \frac{1}{2}b(y_1^2 + y_2^2). \quad (6.2)$$

In this case, the frequencies are  $\pm i\sqrt{ab}$  (twice) and therefore the fixed point can have linear stability type either 2E or 2H.

For  $\mathcal{D}_2 \times \mathcal{R}$ , from equation (5.1), we find that

$$H_2^{\text{loc}}(x, y) = \frac{1}{2}ax_1^2 + \frac{1}{2}bx_2^2 + \frac{1}{2}cy_1^2 + \frac{1}{2}dy_2^2. \quad (6.3)$$

The frequencies in this case are  $\pm i\sqrt{ac}$  and  $\pm i\sqrt{bd}$ . Therefore, the fixed point can have linear stability type either EE, EH or HH. ■

**Lemma 6.2.** *The groups  $\mathcal{C}_k \wedge C_{2k}T$  and  $\mathcal{D}_k \wedge C_{2k}T$  for  $k \geq 2$  have a unique fixed point  $Z_3 = [0 : 0 : 1]$ , which has linear stability type either 2E or 2H.*

*Proof.* We have found that  $\mathcal{C}_k$  for  $k \geq 3$  has the fixed points  $Z_3$  and  $Z_{\pm}$ . Only  $Z_3$  is fixed under the action of  $C_{2k}T$ . Therefore, it is the only fixed point of  $\mathcal{C}_k \wedge C_{2k}T$ . The quadratic invariants near  $Z_3$  for  $\mathcal{C}_k$  are spanned by

$$v_1\bar{v}_1, \quad v_2\bar{v}_2, \quad v_1\bar{v}_2 \quad \text{and} \quad \bar{v}_1v_2.$$

Therefore, the quadratic invariants of the action  $C_{2k}T(v_1, v_2) = \exp(i\theta_{2k})(v_1, -v_2)$  are spanned by  $v_1\bar{v}_1$  and  $v_2\bar{v}_2$ . Consequently,

$$H_2^{\text{loc}} = \frac{1}{2}a(x_1^2 + x_2^2) + \frac{1}{2}b(y_1^2 + y_2^2). \quad (6.4)$$

The frequencies are  $\pm i\sqrt{ab}$  (twice).

For  $k = 2$ , the group  $C_2$  has the isolated fixed point  $Z_3$  and a 2-sphere  $\mathbf{S}^2$  of fixed points. The action of  $C_4T$  on  $\mathbf{S}^2$  is  $C_4T(s_1, s_2, s_3) = (-s_1, -s_2, -s_3)$ , which does not have any fixed points on  $\mathbf{S}^2$ . Therefore, the only fixed point of  $C_2 \wedge C_4T$  is  $Z_3$ . The quadratic invariants in this case are spanned by

$$v_1\bar{v}_1, \quad v_2\bar{v}_2, \quad v_1v_2 \quad \text{and} \quad \bar{v}_1\bar{v}_2.$$

The most general quadratic invariant Hamiltonian is

$$H_2^{\text{loc}} = \frac{1}{2}a(x_1^2 + x_2^2) + \frac{1}{2}b(y_1^2 + y_2^2) + c(x_1y_1 - x_2y_2) + d(x_1y_2 + x_2y_1). \quad (6.5)$$

The frequencies are  $\pm\sqrt{c^2 + d^2 - ab}$  (twice).

The only fixed point of the group  $\mathcal{D}_k$  for  $k \geq 3$  is  $Z_3$ . It also remains fixed under  $C_{2k}T$ . The quadratic invariants for  $\mathcal{D}_k$  are spanned by

$$v_1\bar{v}_2, \quad v_2\bar{v}_2 \quad \text{and} \quad v_1\bar{v}_2 + \bar{v}_1v_2.$$

Because of the action of  $C_{2k}T$ , only the first two remain invariant under  $\mathcal{D}_k \wedge C_{2k}T$ . Therefore, we have

$$H_2^{\text{loc}} = \frac{1}{2}a(x_1^2 + x_2^2) + \frac{1}{2}b(y_1^2 + y_2^2). \quad (6.6)$$

The frequencies are  $\pm i\sqrt{ab}$  (twice).

Finally, for  $k = 2$ , the group  $\mathcal{D}_2$  has the fixed points  $Z_1, Z_2$  and  $Z_3$ . The action of  $C_4T$  is  $C_4T[z_1 : z_2 : z_3] = [\bar{z}_2 : -\bar{z}_1 : \bar{z}_3]$ . Therefore,  $C_4T(Z_1) = Z_2$  and  $C_4T(Z_2) = Z_1$ . The only fixed point of  $\mathcal{D}_2 \wedge C_4T$  is therefore  $Z_3$ . Because of the action of  $C_4T$ , the quadratic invariants of  $\mathcal{D}_2 \wedge C_4T$  near  $Z_3$  are spanned by

$$v_1\bar{v}_1, \quad v_2\bar{v}_2 \quad \text{and} \quad v_1v_2 + \bar{v}_1\bar{v}_2.$$

We have

$$H_2^{\text{loc}} = \frac{1}{2}a(x_1^2 + x_2^2) + \frac{1}{2}b(y_1^2 + y_2^2) + c(x_1y_1 - x_2y_2). \quad (6.7)$$

The frequencies are  $\pm\sqrt{c^2 - ab}$  (twice). ■

**Lemma 6.3.** *The groups  $\mathcal{C}_k \wedge U_2T$  for  $k \geq 3$  have fixed points  $Z_3 = [0 : 0 : 1]$  and  $Z_{\pm} = [1 : \pm i : 0]$ .  $Z_3$  can have any type of linear stability.  $Z_{\pm}$  can have any type of linear stability for  $k = 3$ . It can be either *EE* or *EH* for  $k = 4$ ; while, for  $k \geq 5$ , it can only be *EE*. The group  $\mathcal{C}_2 \wedge U_2T$  has a unique isolated fixed point  $Z_3$ , which can have any linear stability type.*

*Proof.* We have found that  $\mathcal{C}_k$  for  $k \geq 3$  has the fixed points  $Z_3 = [0 : 0 : 1]$  and  $Z_{\pm} = [1 : \pm i : 0]$ . Since these points are fixed under  $U_2T$  and  $\mathcal{C}_k$  is a subgroup of  $\mathcal{C}_k \wedge U_2T$ , they are fixed points of  $\mathcal{C}_k \wedge U_2T$ . The quadratic invariants of  $\mathcal{C}_k$  near  $Z_3$  are spanned by

$$v_1\bar{v}_1, \quad v_2\bar{v}_2, \quad v_1\bar{v}_2 \quad \text{and} \quad \bar{v}_1v_2.$$

The quadratic invariants of the action  $U_2T(v_1, v_2) = (-\bar{v}_1, \bar{v}_2)$  are therefore spanned by

$$v_1\bar{v}_1, \quad v_2\bar{v}_2 \quad \text{and} \quad v_1\bar{v}_2 - \bar{v}_1v_2.$$

In real coordinates  $(x, y)$ , these quadratic invariants are spanned by

$$x_1^2 + x_2^2, \quad y_1^2 + y_2^2 \quad \text{and} \quad x_2y_1 - x_1y_2.$$

The most general quadratic local Hamiltonian is therefore

$$H_2^{\text{loc}}(x, y) = \frac{1}{2}a(x_1^2 + x_2^2) + \frac{1}{2}b(y_1^2 + y_2^2) + c(x_1y_2 - x_2y_1). \quad (6.8)$$

The frequencies in this case are  $\pm i(c \pm \sqrt{ab})$ .

The action of  $U_2T$  is given by  $U_2T[z_1 : z_2 : z_3] = [\bar{z}_1 : -\bar{z}_2 : -\bar{z}_3]$ . Therefore,  $U_2T(Z_+) = Z_+$  and  $U_2T(Z_-) = Z_-$ . Its action in the local chart near  $Z_+$  is  $U_2T(w_1, w_2) = -(\bar{w}_1, \bar{w}_2)$ . For  $k = 3$ , we know the quadratic invariants. Taking into account the  $U_2T$  action, the quadratic invariants are spanned by

$$w_1\bar{w}_1, \quad w_2\bar{w}_2 \quad \text{and} \quad w_1w_2 + \bar{w}_1\bar{w}_2.$$

Thus the most general quadratic invariant local Hamiltonian is

$$H_2^{\text{loc}}(x, y) = \frac{1}{2}a(x_1^2 + y_1^2) + \frac{1}{2}b(x_2^2 + y_2^2) + c(x_1x_2 - y_1y_2). \quad (6.9)$$

The frequencies in this case are  $\pm \frac{1}{2}i(a - b \pm ((a + b)^2 - 4c^2)^{1/2})$ . All choices of sign are possible.

For  $k = 4$ , we find that

$$H_2^{\text{loc}}(x, y) = \frac{1}{2}ax_1^2 + \frac{1}{2}a'y_1^2 + \frac{1}{2}b(x_2^2 + y_2^2), \quad (6.10)$$

and the frequencies are  $\pm ib$  and  $\pm i\sqrt{aa'}$ .

Finally, for  $k \geq 5$ , the most general quadratic Hamiltonian is

$$H_2^{\text{loc}}(x, y) = \frac{1}{2}a(x_1^2 + y_1^2) + \frac{1}{2}b(x_2^2 + y_2^2), \quad (6.11)$$

with frequencies  $\pm ia$  and  $\pm ib$ .

For  $k = 2$ , the action of  $\mathcal{C}_2$  has an isolated fixed point  $Z_3 = [0 : 0 : 1]$  and a 2-sphere  $S$  of fixed points. The action of  $U_2T$  on  $S$  is  $U_2T(s_1, s_2, s_3) = (s_1, -s_2, s_3)$ . It leaves fixed the points on the circle  $\{s_2 = 0\}$ . Therefore, the only isolated fixed point of  $\mathcal{C}_2 \wedge U_2T$  is  $Z_3$ . In local coordinates, the quadratic invariants are spanned by

$$v_1\bar{v}_1, \quad v_2\bar{v}_2, \quad v_1\bar{v}_2 - \bar{v}_1v_2, \quad v_1v_2 - \bar{v}_1\bar{v}_2, \quad v_1^2 + \bar{v}_1^2 \quad \text{and} \quad v_2^2 + \bar{v}_2^2.$$

In real coordinates, the quadratic invariants are spanned by

$$x_1^2, \quad x_2^2, \quad y_1^2, \quad y_2^2, \quad x_1y_2 \quad \text{and} \quad x_2y_1.$$

The most general quadratic local Hamiltonian is

$$H_2^{\text{loc}}(x, y) = \frac{1}{2}ax_1^2 + \frac{1}{2}a'x_2^2 + \frac{1}{2}by_1^2 + \frac{1}{2}b'y_2^2 + cx_1y_2 - c'x_2y_1. \quad (6.12)$$

In this case, the fixed point can have any linear stability type. ■

**Lemma 6.4.** *The  $T$  extended cubic groups  $\mathcal{T} \times \mathcal{R}$ ,  $\mathcal{T} \wedge C_4T$ ,  $\mathcal{O} \times \mathcal{R}$  and  $\mathcal{Y} \times \mathcal{R}$  do not have any fixed points.*

Table 1. Possible types of stability for fixed points of finite subgroups of  $\text{SO}(3) \times \mathcal{R}$ 

(Notation follows lemma 4.1; indices 1, 2 and 3 refer to the coordinate axes in  $\mathbf{R}^3$ , axis 3 corresponds to the symmetry axis of the groups  $\mathcal{C}_k$ . In the fourth column, we give the decomposition of the representation spanned by  $(x_1, x_2, y_1, y_2)$  into irreducible representations. Representations are denoted by  $B$ ,  $E$  and  $E^C$  if they are one-dimensional, two-dimensional real and two-dimensional complex, respectively. Different subscripts 1, 2, 3, 4 are used to distinguish between non-isomorphic representations of the same type.)

group	fixed point	stability	decomposition
$\mathcal{C}_2$	$Z_3$	any	$B(x_1) \oplus B(x_2) \oplus B(y_1) \oplus B(y_2)$
$\mathcal{C}_k, k \geq 3$	$Z_3$	any	$E^C(x_1, x_2) \oplus E^C(y_1, y_2)$
$\mathcal{C}_3$	$Z_{\pm}$	any	$E^C(x_1, y_1) \oplus E^C(x_2, -y_2)$
$\mathcal{C}_4$	$Z_{\pm}$	EE, EH	$B(x_1) \oplus B(y_1) \oplus E^C(x_2, y_2)$
$\mathcal{C}_k, k \geq 5$	$Z_{\pm}$	EE	$E_1^C(x_1, y_1) \oplus E_2^C(x_2, y_2)$
$\mathcal{D}_2$	$Z_1, Z_2, Z_3$	EE, EH, HH	$B_1(x_1) \oplus B_2(x_2) \oplus B_1(y_1) \oplus B_2(y_2)$
$\mathcal{D}_k, k \geq 3$	$Z_3$	2E, 2H	$E(x_1, x_2) \oplus E(y_1, y_2)$
$\mathcal{C}_2 \times \mathcal{R}$	$Z_3$	any	$B_1(x_1) \oplus B_1(x_2) \oplus B_2(y_1) \oplus B_2(y_2)$
$\mathcal{C}_k \times \mathcal{R}, k \geq 3$	$Z_3$	2E, 2H	$E_1^C(x_1, x_2) \oplus E_2^C(y_1, y_2)$
$\mathcal{D}_2 \times \mathcal{R}$	$Z_1, Z_2, Z_3$	EE, EH, HH	$B_1(x_1) \oplus B_2(x_2) \oplus B_3(y_1) \oplus B_4(y_2)$
$\mathcal{D}_k \times \mathcal{R}, k \geq 3$	$Z_3$	2E, 2H	$E_1(x_1, x_2) \oplus E_2(y_1, y_2)$
$\mathcal{C}_2 \wedge C_4T$	$Z_3$	2E, 2H	$E^C(x_1, x_2) \oplus E^C(y_2, y_1)$
$\mathcal{C}_k \wedge C_{2k}T, k \geq 3$	$Z_3$	2E, 2H	$E_1^C(x_1, x_2) \oplus E_2^C(y_1, y_2)$
$\mathcal{D}_2 \wedge C_4T$	$Z_3$	2E, 2H	$E(x_1, x_2) \oplus E(-y_1, y_2)$
$\mathcal{D}_k \wedge C_{2k}T, k \geq 3$	$Z_3$	2E, 2H	$E_1(x_1, x_2) \oplus E_2(y_1, y_2)$
$\mathcal{C}_2 \wedge U_2T$	$Z_3$	any	$B_1(x_1) \oplus B_2(x_2) \oplus B_2(y_1) \oplus B_1(y_2)$
$\mathcal{C}_k \wedge U_2T, k \geq 3$	$Z_3$	any	$E(x_1, x_2) \oplus E(-y_2, y_1)$
$\mathcal{C}_3 \wedge U_2T$	$Z_{\pm}$	any	$E(x_1, y_1) \oplus E(x_2, -y_2)$
$\mathcal{C}_4 \wedge U_2T$	$Z_{\pm}$	EE, EH	$B_1(x_1) \oplus B_2(y_1) \oplus E(x_2, y_2)$
$\mathcal{C}_k \wedge U_2T, k \geq 5$	$Z_{\pm}$	EE	$E_1(x_1, y_1) \oplus E_2(x_2, y_2)$

*Proof.* Each one of these groups has one of the proper cubic groups as a subgroup. Since the proper cubic groups do not have any fixed points, neither do the  $T$  extended groups. ■

The results of the three previous sections about the linear stability type of the relative equilibria are summarized in table 1.

Notice that we have not taken into account the cases for  $k = 1$ . One can easily see that either these groups are identical to one of the groups we already studied or they do not have any isolated fixed points.

Besides the finite subgroups of  $\text{SO}(3) \times \mathcal{R}$ , there are also continuous subgroups that are interesting in applications. For these groups we have the following result.

**Lemma 6.5.** *The fixed points and their linear stability types are as in table 2.*

The method for finding the fixed points and their type of linear stability for the continuous subgroups of  $\text{SO}(3) \times \mathcal{R}$  is the same as that used in this and previous sections for the finite groups. Notice, in particular, that the quadratic invariants for

Table 2. Possible types of stability for fixed points of continuous subgroups of  $\text{SO}(3) \times \mathcal{R}$   
(Notation in last column is as in table 1.)

group	alt. notation	fixed point	stability	decomposition
$\text{SO}(2)$	$\mathcal{C}_\infty$	$Z_3$	any	$E^{\mathcal{C}}(x_1, x_2) \oplus E^{\mathcal{C}}(y_1, y_2)$
$\text{SO}(2)$	$\mathcal{C}_\infty$	$Z_\pm$	EE	$E_1^{\mathcal{C}}(x_1, y_1) \oplus E_2^{\mathcal{C}}(x_2, y_2)$
$\text{SO}(2) \wedge U_2$	$\mathcal{D}_\infty$	$Z_3$	2E, 2H	$E(x_1, x_2) \oplus E(y_1, y_2)$
$\text{SO}(2) \times \mathcal{R}$	$\mathcal{C}_\infty \times \mathcal{R}$	$Z_3$	2E, 2H	$E_1^{\mathcal{C}}(x_1, x_2) \oplus E_2^{\mathcal{C}}(y_1, y_2)$
$(\text{SO}(2) \wedge U_2) \times \mathcal{R}$	$\mathcal{D}_\infty \times \mathcal{R}$	$Z_3$	2E, 2H	$E_1(x_1, x_2) \oplus E_2(y_1, y_2)$
$\text{SO}(2) \wedge U_2T$	$\mathcal{C}_\infty \wedge U_2T$	$Z_3$	any	$E(x_1, x_2) \oplus E(-y_2, y_1)$
$\text{SO}(2) \wedge U_2T$	$\mathcal{C}_\infty \wedge U_2T$	$Z_\pm$	EE	$E_1(x_1, y_1) \oplus E_2(x_2, y_2)$

each continuous subgroup of  $\text{SO}(3) \times \mathcal{R}$  are spanned by the same invariants as the quadratic invariants of some finite group for large enough  $k$ .

## 7. Linear Hamiltonian Hopf bifurcation

We have studied the fixed points of all the finite subgroups of  $\text{SO}(3) \times \mathcal{R}$  and, because of lemma 3.1, also of all the finite subgroups of  $\text{O}(3) \times \mathcal{R}$ . Note that, in each case, we have expressed the fixed points in a system of coordinates in which the  $C_k$ -axis of the group is at the direction  $(0, 0, 1)$  in  $\mathbf{R}^3$ . In general, the  $C_k$ -axis can be in any direction. We still use the notation  $Z_{1,2,3,\pm}$  for the fixed points of groups, but we note that the coordinate representation of these points depends on the direction of the axis. Recall that, by  $\mathcal{G}_{m_c}$ , we denote the isotropy group of a critical point  $m_c$ . Let  $\tilde{P} : \text{O}(3) \times \mathcal{R} \rightarrow \text{SO}(3) \times \mathcal{R}$  be the extension of the homomorphism  $P : \text{O}(3) \rightarrow \text{SO}(3)$  in (3.4) defined by  $\tilde{P}(T) = T$ . We can now state and prove the main theorem of this paper.

**Theorem 7.1.** Consider a  $\mathcal{G} \times \mathcal{R}$ -invariant Hamiltonian defined on  $\mathbf{CP}^2$ , where  $\mathcal{G}$  is a finite point group and the action of  $\mathcal{G}$  on  $\mathbf{CP}^2$  is induced by its action on the vector representation spanned by  $q_1, q_2, q_3$ . A critical point  $m \in \mathbf{CP}^2$  of the  $\mathcal{G} \times \mathcal{R}$  action can go through a linear Hamiltonian Hopf bifurcation only if

- (a)  $\tilde{P}(\mathcal{G}_m) = \mathcal{C}_2 \times \mathcal{R}$  and  $m$  is the point  $Z_3$  of  $\mathcal{G}_m$ , or
- (b)  $\tilde{P}(\mathcal{G}_m) = \mathcal{C}_3$  or  $\tilde{P}(\mathcal{G}_m) = \mathcal{C}_3 \wedge U_2T$  and  $m$  is one of the points  $Z_\pm$  of  $\mathcal{G}_m$ .

*Proof.* Instead of studying the action of  $\mathcal{G} \times \mathcal{R}$  on  $\mathbf{CP}^2$ , by lemma 3.1, we can study the equivalent action of  $\tilde{P}(\mathcal{G} \times \mathcal{R}) = P(\mathcal{G}) \times \mathcal{R}$ . A point  $m \in \mathbf{CP}^2$  is a critical point of  $P(\mathcal{G}) \times \mathcal{R}$  if and only if it is an isolated fixed point of some subgroup of  $P(\mathcal{G}) \times \mathcal{R}$ . In our situation, all subgroups of  $P(\mathcal{G}) \times \mathcal{R}$  are finite subgroups of  $\text{SO}(3) \times \mathcal{R}$ . The points that can go through a linear Hamiltonian Hopf bifurcation are  $Z_3$  with isotropy groups  $\mathcal{C}_k$  ( $k \geq 2$ ),  $\mathcal{D}_2$ ,  $\mathcal{C}_2 \times \mathcal{R}$ ,  $\mathcal{C}_k \wedge U_2T$  ( $k \geq 2$ ) and  $\mathcal{C}_2 \wedge C_4T$  and  $Z_\pm$  with isotropy groups  $\mathcal{C}_3$  and  $\mathcal{C}_3 \wedge U_2T$ . Note that, since the original symmetry is of the form  $\mathcal{G} \times \mathcal{R}$  and since  $TZ_3 = Z_3$ , the isotropy group of  $Z_3$  always contains  $T$ . Therefore,  $\mathcal{C}_k$ ,  $\mathcal{D}_2$ ,  $\mathcal{C}_k \wedge U_2T$  and  $\mathcal{C}_2 \wedge C_4T$  cannot be isotropy groups of  $Z_3$ . We are now left only with the cases described in the theorem. ■

**Remark 7.2.** A more general definition of the linear Hamiltonian Hopf bifurcation is given in Hanßmann & van der Meer (2002). What is described in that paper is the bifurcation of short periodic orbits that happens when the fixed point  $Z_3$  of the  $\text{SO}(2) \times \mathcal{R}$  group changes linear stability type from 2E to 2H. Note that our results predict this change of linear stability (see table 2). What we describe in this paper as a linear Hamiltonian Hopf bifurcation is a *standard* linear Hamiltonian Hopf bifurcation in Hanßmann & van der Meer (2002).

The main technical problem when studying the bifurcation from 2E to 2H is that, exactly at the bifurcation, the Hamiltonian vector field is nilpotent. In general, it would be impossible to normalize with respect to the  $\text{SO}(2)$  symmetry, as it is usually done when studying the nonlinear Hamiltonian Hopf bifurcation. Since the Hamiltonian in Hanßmann & van der Meer (2002) is already  $\text{SO}(2)$  invariant, this normalization is not necessary. This permits the authors to study the bifurcation and to find that the nonlinear behaviour of the system is the same as that for a standard nonlinear Hamiltonian Hopf bifurcation.

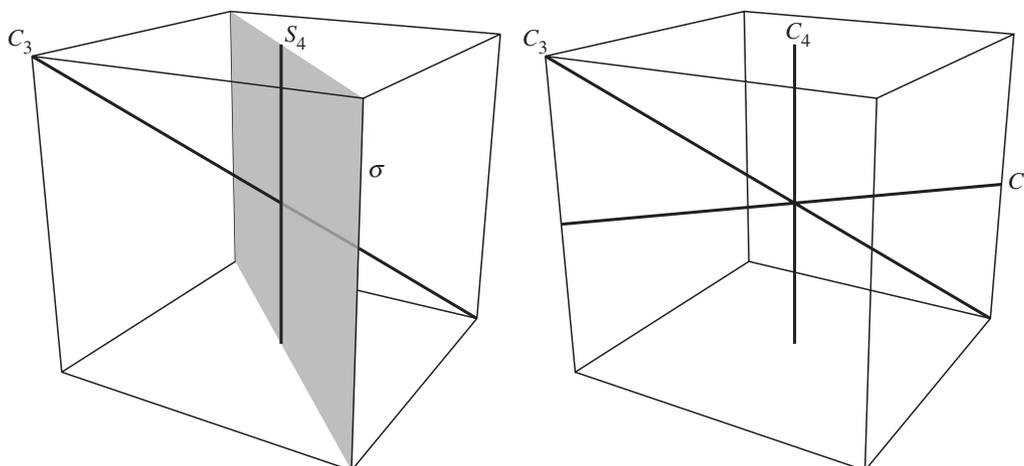
It is possible that this generalized notion of the linear Hamiltonian Hopf bifurcation that demands the existence of  $\text{SO}(2)$  symmetry can be extended to the case of a finite group symmetry  $\mathcal{C}_k$ , at least in specific examples. For example, for  $k \geq 5$ , the real invariants of the  $\mathcal{C}_k$  action on the local chart near  $Z_3$  are spanned up to fourth order by the same invariants as for the  $\text{SO}(2)$  action. This means that the Hamiltonian is already normalized up to fourth order with respect to the  $\text{SO}(2)$  symmetry. Provided that the normal form for the Hamiltonian Hopf bifurcation is not degenerate at this order, we can deduce that a generalized nonlinear Hamiltonian Hopf bifurcation is taking place.

**Remark 7.3.** Van der Meer (1990) considers some general conditions that a group  $G$  should satisfy in order to be a symmetry group of a Hamiltonian Hopf bifurcation. In our case, we know all possible groups of interest and we check explicitly whether this type of bifurcation can happen.

Melbourne & Dellnitz (1993) consider normal forms of linear Hamiltonian vector fields that commute with the action of a compact Lie group  $G$ . Dellnitz *et al.* (1992) find under what conditions the imaginary eigenvalues of a Hamiltonian matrix that meet, move off to the complex plane (split) or go through each other (pass). The main tool in these papers is the decomposition of the eigenspace of the Hamiltonian matrix into irreducible representations of  $G$ . In a sense, this approach is complementary to ours.

The authors in the latter paper begin with a specific arrangement of eigenvalues of the Hamiltonian matrix. We begin with a particular group action and, without making any assumption on the eigenvalues, we use invariant theory to find the most general quadratic  $G$  invariant Hamiltonian  $H_2$  and then we compute the corresponding eigenvalues of the linear Hamiltonian vector field corresponding to  $H_2$ .

We can also obtain our results in a slightly different way. First we decompose the vector space spanned by the variables  $(x_1, x_2, y_1, y_2)$  in irreducible representations of the group  $G$  under consideration and then we find all the quadratic invariants by coupling these representations in an appropriate manner. In tables 1 and 2, we give this decomposition for the groups that we have studied. Notice that, in some cases (for example, the fixed point  $Z_3$  of the group  $\text{SO}(2) \wedge U_2T$ ), the decomposition does not belong to any of the cases that are described in the aforementioned papers as

Figure 2. The tetrahedral group  $\mathcal{T}_d$  and the octahedron group  $\mathcal{O}$ .

generic for compact Lie groups when we have resonant eigenvalues on the imaginary axes.

### 8. Example: the action of $\mathcal{T}_d \times \mathcal{R}$ on $CP^2$

Here, we study in detail the case of  $\mathcal{T}_d \times \mathcal{R}$ -invariant Hamiltonians. The example of tetrahedral molecules was first studied by Montaldi *et al.* (1988), where they found the relative equilibria. The method that we use here for finding the relative equilibria is due to Zhilinskii (1989). In this section, we find all critical points of the action of  $\mathcal{T}_d$  on  $CP^2$  and then apply the results in the previous sections to determine their linear stability type. An application of our techniques in the more complex problem of coupled rotational-vibrational motions of a tetrahedral molecule can be found in Efstathiou *et al.* (2003).

The  $\mathcal{T}_d$  group contains six reflection planes  $\sigma$ , three  $S_4$  rotation–reflection axes and four  $C_3$ -axes (figure 2). Note that  $\mathcal{T}_d$  (the group of all the symmetries of the tetrahedron) is not a proper point group, since it contains reflections and rotation–reflections. The image of  $\mathcal{T}_d$  under the homomorphism  $P$  in (3.4) is the octahedral group  $\mathcal{O}$ . Therefore, it is sufficient to study the action of  $\mathcal{O}$  on  $CP^2$  instead of that of  $\mathcal{T}_d$ .

The octahedron group contains six  $C_2$ -axes, three  $C_4$ -axes and four  $C_3$ -axes (figure 2). In order to find critical points of  $\mathcal{O}$ , we have to find fixed points of each one of these axes. If some axis  $C_k$  has  $C_2$ -axes perpendicular to it, then the isotropy group of the fixed points of  $C_k$  might be larger. Therefore, we have to take into account the existence of perpendicular  $C_2$ -axes in order to determine the isotropy group of a fixed point.

Note that each  $C_2$ -axis always has two other  $C_2$ -axes perpendicular to it. They form the group  $\mathcal{D}_2$ . From lemma 5.1,  $\mathcal{D}_2$  has three fixed points. Because of the time-reversal symmetry and lemma 6.1, they can have linear stability type EE, EH or HH.

Each  $C_3$ -axis has three  $C_2$ -axes perpendicular to it. Therefore, to each one of the four  $C_3$ -axes correspond three critical points. In a system of coordinates where the

$C_3$ -axis lies along the direction  $(0, 0, 1)$ , they have coordinates  $Z_{\pm} = [1 : \pm i : 0]$  and  $Z_3 = [0 : 0 : 1]$ . Because of the perpendicular  $C_2$ -axes,  $Z_3$  is also fixed under  $\mathcal{D}_3$ . Also taking into account the  $T$  symmetry, we conclude that  $Z_3$  is fixed under  $\mathcal{D}_3 \times \mathcal{R}$ . From lemma 6.1,  $Z_3$  for the  $C_3$ -axis can have linear stability type either 2E or 2H. The isotropy group of  $Z_{\pm}$  is  $\mathcal{C}_3 \wedge U_2T$ . Therefore, these points can have any linear stability type. In particular, they can be CH.

Finally, the three  $C_4$ -axes have critical points  $Z_3 = [0 : 0 : 1]$  and  $Z_{\pm} = [1 : \pm i : 0]$  in a system of coordinates where the  $C_4$ -axis points in the direction  $(0, 0, 1)$ . Each  $C_4$ -axis has two  $C_2$ - and two  $C_4$ -axes perpendicular to it. Since  $C_4$ -axes are also  $C_2$ -axes (because  $C_4^2 = C_2$ ), there are four  $C_2$ -axes perpendicular to it. Therefore,  $Z_3$  is fixed under  $\mathcal{D}_4 \times \mathcal{R}$  and, by lemma 6.1, it can have linear stability type either 2E or 2H. Just as in the case of the  $C_3$ -axes,  $Z_{\pm}$  is fixed under the action of  $\mathcal{C}_4 \wedge U_2T$ . By lemma 4.4, the fixed points  $Z_{\pm}$  of  $\mathcal{C}_4 \wedge U_2T$  can have linear stability type EE or EH.

In summary, we have found that the action of  $\mathcal{T}_d \times \mathcal{R}$  on  $\mathbf{CP}^2$  has 27 critical points (six for the  $C_2$ -axes, 12 for the  $C_3$ -axes and nine for the  $C_4$ -axes), among which there are eight with isotropy group  $\mathcal{C}_3 \wedge U_2T$ . Only these latter can undergo a linear Hamiltonian Hopf bifurcation.

We can do the same analysis for all the cubic groups  $\mathcal{T}$ ,  $\mathcal{T}_d$ ,  $\mathcal{T}_h$ ,  $\mathcal{O}$ ,  $\mathcal{O}_h$ ,  $\mathcal{Y}$  and  $\mathcal{Y}_h$ . In all these cases, we can easily prove that the only points that can go through a linear Hamiltonian Hopf bifurcation are the  $Z_{\pm}$  points of the  $C_3$ -axes. Thus we have proved the following.

**Theorem 8.1.** *Let  $H$  be  $\mathcal{G} \times \mathcal{R}$ -invariant Hamiltonian on  $\mathbf{CP}^2$ , where the action of  $\mathcal{G}$  on  $\mathbf{CP}^2$  is induced by its action on the vector representation spanned by  $q_1, q_2, q_3$ . The only critical points of the action of  $\mathcal{G} \times \mathcal{R}$  (and thus of  $H$ ) that can go through a linear Hamiltonian Hopf bifurcation are the points  $Z_{\pm}$  of the  $C_3$ -axes of the image of  $\mathcal{G}$  under the homomorphism  $P$  (see (3.4)).*

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