Nonlinear Vibrations in the Fullerene Molecule $C_{60}$

Carlos García-Azpeitia*, Wieslaw Krawcewicz †‡
Manuel Tejada-Wriedt*, Haopin Wu ‡

May 10, 2018

Abstract

The fullerene molecule is composed of 60 carbon atoms at the vertices of a truncated icosahedron. The model for fullerene molecule, consisting of 180 equations, is built on the framework of classical mechanics, where the force field comprises bond forces between carbon atoms connected by edges, and bond bending and torsion forces. The system is equivariant under the action of the group $I \times O(3) \times O(2)$, where $I$ denotes the full icosahedral group. We prove the existence of global families of periodic solutions (nonlinear vibrational modes of oscillation) from the equilibrium configuration. We use equivariant degree to obtain the topological classification of all spatio-temporal symmetries. We find that the solutions are standing and rotating waves that propagate along the molecule with icosahedral, tetrahedral, pentagonal and triangular symmetries. We also present results of the numerical continuation of the nonlinear vibrational modes.

1 Introduction

Carbon atoms in the fullerene molecule are arranged at 60 vertices of a truncated icosahedron, where the 90 edges represent the bonds among two carbons. The fullerene molecule was discovered in 1986 by R. Smalley, R. Curl, J. Heath, S. O’Brien, and H. Kroto [19], and for this work, Smalley, Curl and Kroto were awarded the Nobel prize in chemistry in 1996. The linear vibrational modes of fullerene have been measured using IR and Raman spectroscopy, and group representation theory. Increasing attention has been given to the mathematical study of different aspects of this molecule. In particular, the determination of other vibrational modes that cannot be measured experimentally; see [13, 8, 17, 26, 27, 29, 23] and the large bibliography therein.

*Departamento de Matemáticas, Facultad de Ciencias, Universidad Nacional Autónoma de México, 04510 México, México
†Center for Applied Mathematics at Guangzhou University, Guangzhou, 510006 China.
‡Department of Mathematical Sciences University of Texas at Dallas Richardson, 75080 USA
The dynamics of the fullerene molecule are represented by Newton’s equations, where the potential is given by a force field which describes how carbon atoms interact within the molecule. Many force fields have been proposed for the fullerene in terms of bond stretching, bond bending, torsion and van der Waals forces. In [29], the authors, for the first time, designed the force field specifically for the fullerene, which implements harmonic forces. The model was improved in [27] to reflect the vibrational modes obtained experimentally.

Some force fields were optimized to duplicate the normal modes obtained using IR or Raman spectroscopy, but only few of these models reflect the nonlinear characteristics of the fullerene. In order to analyze the nonlinear effects of atomic interactions in the fullerene, we consider the force field implemented in [26] for carbon nanotubes and in [6] for the fullerene. These models consider bond deformations that exceed very small fluctuations about equilibrium states, given by Morse potentials, while other force fields, such as those proposed in [27] and [29], are designed only to consider small fluctuations.

The original work [19] has currently 15 thousand citations. To the best of our knowledge, none of these works have analyzed the real nonlinear vibrations of the fullerene molecule. Nonlinear vibrational modes of oscillation are families of periodic solutions that emerge from the equilibrium configuration with frequencies starting from the normal frequencies. These families of periodic solutions and their frequencies deviate drastically from the normal modes and frequencies for big oscillations.

In order to analyze the nonlinear vibrations of the fullerene molecule, we develop a new representation of the carbon atoms in the truncated icosahedron, which greatly simplifies the description of symmetries in the molecule. This representation uses the elements of icosahedral group as indices.
of the atoms, as illustrated in Figure 1.

To analyze the fullerene molecule we chose the force field without van der Waals forces given in [26]. Using this model, we compute the equilibrium configuration \(u_0\) and we find that the lengths of the single and double bonds are given by \(d_S = 1.438084\) and \(d_D = 1.420845\), respectively. These lengths are good approximations of the the experimental measurements presented in [13]. Moreover, we find that the normal frequencies are within the range of 100 to 1800 \(cm^{-1}\), which is well between the range obtained from the experimental and numerical data gathered in [8].

In our approach, we formulate the problem of finding periodic solutions for the fullerene as the variational problem on the Sobolev space \(H^1_{2\pi}\) (of \(2\pi\)-periodic vector-valued functions) with the functional

\[
J(u, \lambda) := \int_0^{2\pi} \left[ \frac{1}{2} |\dot{u}(t)|^2 - \lambda^2 V(u(t)) \right] dt,
\]

where \(V\) is the force field, \(\lambda^{-1}\) the frequency and \(u(t) \in H^1_{2\pi}\) the renormalized \(2\pi\)-periodic solution. The existence of periodic solutions is equivalent to the existence of critical points of \(J\). The functional \(J\) is clearly invariant under the action of the group

\[
G := I \times O(3) \times O(2),
\]

which acts as permutations of atoms, rotations in space, and translations and reflection in time, respectively.

First, we notice that the equilibrium state of the fullerene is a minimizer with icosahedral symmetries \(\tilde{I} < I \times O(3)\). We compute the normal frequencies and the irreducible representation under the action of the group \(\tilde{I}\). The number of each irreducible representation with non-zero normal frequencies is:

| Irreducible Rep. | \(V_1\) | \(V_2\) | \(V_3\) | \(V_4\) | \(V_5\) | \(V_{-1}\) | \(V_{-2}\) | \(V_{-3}\) | \(V_{-4}\) | \(V_{-5}\) |
|------------------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|
| Dimension of Rep.| 1      | 4      | 5      | 3      | 3      | 1      | 4      | 5      | 3      | 3      |
| Number of Reps.  | 2      | 6      | 8      | 4      | 4      | 1      | 6      | 7      | 5      | 5      |

Table 1: Irreducible subrepresentations in the configuration space.

This result coincides with the results in [13], [8], [17], [27], which, for different models, contains the classification of the eigenfrequencies associated to the character theory under the icosahedral symmetries.

To prove global existence of the families of periodic solutions we use the equivariant gradient degree developed in [11], see also [9] and [22] (fundamental properties of the gradient equivariant degree are collected in Appendix B). This degree satisfies all the standard properties expected from a degree theory. The values of this equivariant degree can be expressed elegantly in the form

\[
\nabla_G\text{-deg}(\nabla \varphi, \Omega) = n_1(H_1) + n_2(H_2) + \cdots + n_m(H_m), \quad n_k \in \mathbb{Z},
\]
where \((H_j)\) are the orbit types in \(\Omega\), which allows to predict the existence of various critical orbits for \(\varphi\) and their symmetries. The gradient degree is just one of many related equivariant degrees that were introduced in the last three decades, see [2], [3], [15], [18] and references therein.

The change of equivariant degree at the equilibrium configuration, \(\nabla_{G}\text{-deg}(\nabla J, \Omega)\), for \(\Omega\) a neighborhood of \(u_0\), is the invariant that topologically characterizes the existence of families of periodic solutions and their symmetries. Moreover, this procedure has the advantage that allows us to prove the global existence of families of periodic solutions. The global property means that families of periodic solutions, represented by a continuum in \(H^1_{2\pi} \times \mathbb{R}^+\), have norm or period either going to infinity, end in a collision orbit, or come back to another equilibrium. The computations of the (reduced to the Burnside ring \(A(G)\)) topological \(G\)-equivariant invariants were done with GAP programming [28].

In [10], [5], [4], equivariant degree has been applied to the problem of periodic solutions in other molecules. Other equivariant methods have been used to analyze the existence of relative equilibria in molecules, see [14], [16], [20] and references therein. Our main result can be presented as follows:

\textbf{Theorem 1.1.} For each normal frequency of the equilibrium configuration, corresponding to the irreducible representations of Table \(7\), we prove the global existence of multiple families of periodic solutions with frequency staring from the corresponding normal frequency. For the standing waves each symmetric face has the exact dynamic repeated for all times, while for the (discrete) rotating waves, there is a time shift among consecutive symmetric faces.

- \(\mathcal{V}_{\pm 1}\): Each representation has one family of standing waves with icosahedral symmetries (symmetries given by (22) and (27)).
- \(\mathcal{V}_{\pm 2}\): Each representation has a total of seven families (symmetries given by (23) and (28)). Four families are standing waves: one with tetrahedral symmetries, two with triangular symmetries and one with Klein symmetries. Three families are rotating waves: two with different pentagonal symmetries and one with triangular symmetries.
- \(\mathcal{V}_{\pm 3}\): Each representation has a total of six families (symmetries given by (24) and (29)). Three families are standing waves: one with pentagonal, one with triangular and one with Klein symmetries. Three families are rotating waves: one with pentagonal symmetries, other with different pentagonal symmetries, and one with triangular symmetries.
- \(\mathcal{V}_{\pm 4}, \mathcal{V}_{\pm 5}\): Each representation has a total of five families (symmetries given by (25)-(30) for \(n=\pm 4\), and (26)-(31) for \(n=\pm 5\)). Three families are standing waves: one with pentagonal, one with triangular and one with Klein symmetries. Two families are rotating waves: one with pentagonal and one with triangular symmetries.
The difference between the solutions of representations $\mathcal{V}_n$ and $\mathcal{V}_{-n}$ is that in the representations $\mathcal{V}_n$, the solutions are symmetric by the inversion $-I \in O(3)$, while in $\mathcal{V}_{-n}$, by the inversion $-I$ coupled with a $\pi$-phase shift in time. The families of rotating waves with pentagonal symmetries for representations $\mathcal{V}_{\pm 4}$ and $\mathcal{V}_{\pm 5}$ are different from each other because there are two conjugacy classes, $C_4$ and $C_5$, in $A_5$. Both symmetries are present in two different families in the representation $\mathcal{V}_{\pm 3}$.

Our main theorem predicts the global existence of families of periodic solutions from the fullerene minimal equilibrium configuration. Previous studies have considered only the existence of the linear modes which have constant frequency, but the non-linear system has periodic solutions where frequencies depend on the amplitudes of the oscillation. We implement a Newton’s method and pseudo-arclength procedure to numerically continue some of these nonlinear vibrational modes. The nonlinear vibrational modes and normal modes have drastic differences for big oscillations.

The study of periodic solutions in the non-linear system for the fullerene molecule is relevant to understand different non-linear phenomena. For example, it may be possible to construct devices which amplify these amplitude-frequency relations to excite or blow up the vibrational states of the fullerene molecule, with the nonlinear frequencies leading to a multitude of practical applications. Furthermore, vibrational excitation can be used to identify nonlinear effects of amplitude-frequency relations on the molecule. Furthermore, the icosahedral symmetries appear also in adenoviruses with icosahedral capsid, or other icosahedral molecules considered in [27]. The results presented here are applicable to these cases as well.

In Section 2 we present the model equations necessary to study the dynamics of the fullerene molecule. In Section 3 we prove the bifurcation of periodic solutions from the equilibrium configuration of the fullerene molecule. In Section 4 we describe the symmetries of the solutions and present some of the periodic solutions obtained by numerical continuation. In Appendix A we present the procedure used to continue the families of periodic solutions. In Appendix B we include a short review of the gradient degree, including computational algorithms, and the computations of the $I \times O(2)$-equivariant gradient degree.

2 Fulleringe Model

2.1 Equations for Carbons

Let $A_5$ be the alternating group of permutations of five elements $\{1, 2, 3, 4, 5\}$. The five conjugacy classes in $A_5$ are listed in Table 2. The $C_{60}$ molecule is arranged in 12 unconnected pentagons of atoms. We implement the following notation for the indices of the 60 atoms (see Figure 1):

- $\tau \in C_4$ is used to denote each of the 12 pentagonal faces.
- $k \in \{1, ..., 5\} =: \mathbb{Z}[1, 5]$ is used to denote each of the 5 vertices in the 12 pentagonal faces.
Table 2: Conjugacy classes of elements in $A_5$.

| $C_1$ | $C_2$ | $C_3$ | $C_4$ | $C_5$ |
|-------|-------|-------|-------|-------|
| (1)   | (12)(34), (13)(24), (14)(23) | (123), (132) | (12345) | (12354) |
|       | (12)(35), (13)(25), (15)(23) | (124), (142) | (12453) | (12435) |
|       | (12)(45), (14)(25), (15)(24) | (125), (152) | (12534) | (12543) |
|       | (13)(45), (14)(35), (15)(34) | (134), (143) | (13254) | (13245) |
|       | (23)(45), (24)(35), (25)(34) | (135), (153) | (13542) | (13524) |

We define the set of indices as

$$\Lambda = C_4 \times \mathbb{Z}[1, 5].$$

With these notations each index $(\tau, k) \in \Lambda$ represents a face and a vertex in the face of the truncated icosahedron as it is shown on Figure 1. The vectors that represent the positions of the carbon atoms are

$$u_{\tau, k} \in \mathbb{R}^3,$$

and the vector for the 60 positions is

$$u = (u_{\tau, k})_{(\tau, k) \in \Lambda} \in (\mathbb{R}^3)^{60}.$$

The space $(\mathbb{R}^3)^{60}$ is a representation of the group $I \times O(3)$, where $I = A_5 \times \mathbb{Z}_2$ stands for the full icosahedral group. With this notation, the action of $I \times O(3)$ on $V$ has a simple definition: the action of $\sigma \in A_5$ and $-1 \in \mathbb{Z}_2$ in $u$ is defined in each component by

$$\rho(\sigma)u_{\tau, k} = u_{\sigma^{-1} \tau \sigma, \sigma^{-1}(k)} , \quad \rho(-1)u_{\tau, k} := u_{-1, k} .$$

And the action of the group $A \in O(3)$ is defined by

$$Au = (Au_{\tau, k})_{(\tau, k) \in \Lambda}.$$
2.2 Force Field

The system for the fullerene molecule is given as the following equation of motion

\[ m\ddot{u} = -\nabla V(u), \]  

(2)

where \( u(t) \) represents the positions of carbon atoms in space, \( m \) is the carbon mass and \( V(u) \) is the energy given by a force field. For simplicity, hereafter we renormalize the mass to \( m = 1 \). In order to write the force field, we define the following:

- The 60 edges in the 12 pentagonal faces represent single bonds. For these single bonds we define the function \( S : \Lambda \rightarrow \Lambda \),

\[
S(\tau, k) = (\tau, \tau(k)), \quad \tau \in \mathcal{C}_4, \ k \in \mathbb{Z}[1,5].
\]

- The 30 remaining edges in the hexagon, which connect the different pentagonal faces, represent double bounds. For these double bonds we define the function \( D : \Lambda \rightarrow \Lambda \),

\[
D(\tau, k) = (\sigma, k) \text{ with } \sigma = (k, \tau^2(k), \tau(k), \tau^4(k), \tau^3(k)).
\]

Using the above notation, the force field energy is elegantly expressed by

\[
V(u) = \sum_{(\tau, k) \in \Lambda} \left( U(|u_{\tau,k} - u_{S(\tau,k)}|) + \frac{1}{2} U(|u_{\tau,k} - u_{D(\tau,k)}|) + U_{(\tau,k)}(u) \right),
\]

where the coefficient \( \frac{1}{2} \) before the second term is to eliminate the double count bonds, and the term \( U_{(\tau,k)}(u) \) includes the bending and torsion forces.

Bond stretching is represented by potential

\[
U(x) = E_0 \left( (1 - e^{-\beta(x-r_0)})^2 - 1 \right),
\]

where \( r_0 \) is the equilibrium bond length, \( E_0 \) is the bond energy and \( \beta^{-1} \) is the width of the energy. The term \( U_{(\tau,k)}(u) \) includes bending and torsion forces given by

\[
U_{(\tau,k)}(u) = E_B(\theta_1) + E_B(\theta_2) + E_B(\theta_3) + E_T(\phi_1) + E_T(\phi_2) + E_T(\phi_3),
\]

where the bending \( E_B(\theta) \) around each atom in a molecule is governed by the hybridization of orbitals and is given by

\[
E_B(\theta) = \frac{1}{2} k_0 (\cos \theta - \cos \theta_0)^2 = \frac{1}{2} k_0 (\cos \theta + 1/2)^2, \quad \theta_0 := 2\pi/3,
\]
The torsion energy reaches a maximum value at angles \( \theta \), and the torsion energy \( E_T(\phi) \) (which describes the energy change associated with rotation around a bond with a four-atom sequence) is given by

\[
E_T(\phi) = \frac{1}{2} k_\phi (1 - \cos 2\phi) = k_\phi (1 - \cos^2 \phi).
\]

The torsion energy reaches a maximum value at angles \( \phi = \pm \pi/2 \).

Each carbon \((\tau, k) \in \Lambda\) has three angles,

\[
\cos \theta_1 = \frac{u_{\tau,k} - u_{S(\tau,k)}}{|u_{\tau,k} - u_{S(\tau,k)}|} \cdot \frac{u_{\tau,k} - u_{S^{-1}(\tau,k)}}{|u_{\tau,k} - u_{S^{-1}(\tau,k)}|},
\]

\[
\cos \theta_2 = \frac{u_{\tau,k} - u_{D(\tau,k)}}{|u_{\tau,k} - u_{D(\tau,k)}|} \cdot \frac{u_{\tau,k} - u_{S(\tau,k)}}{|u_{\tau,k} - u_{S(\tau,k)}|},
\]

\[
\cos \theta_3 = \frac{u_{\tau,k} - u_{D(\tau,k)}}{|u_{\tau,k} - u_{D(\tau,k)}|} \cdot \frac{u_{\tau,k} - u_{S^{-1}(\tau,k)}}{|u_{\tau,k} - u_{S^{-1}(\tau,k)}|}.
\]

Clearly, the bond bending at each atom \((\tau, k) \in \Lambda\) is \( E_B(\theta_1) + E_B(\theta_2) + E_B(\theta_3) \). Let

\[
n = \frac{u_{D(\tau,k)} - u_{S(\tau,k)}}{|u_{D(\tau,k)} - u_{S(\tau,k)}|} \times \frac{u_{D(\tau,k)} - u_{S^{-1}(\tau,k)}}{|u_{D(\tau,k)} - u_{S^{-1}(\tau,k)}|}
\]

be the unit normal vector to the plane passing by \( u_{D(\tau,k)} \), \( u_{S(\tau,k)} \) and \( u_{S^{-1}(\tau,k)} \). Each carbon \((\tau, k) \in \Lambda\) has three torsion energies given by

\[
\cos \phi_1 = n \cdot n_1, \quad n_1 = \frac{u_{(\tau,k)} - u_{S(\tau,k)}}{|u_{(\tau,k)} - u_{S(\tau,k)}|} \times \frac{u_{(\tau,k)} - u_{S^{-1}(\tau,k)}}{|u_{(\tau,k)} - u_{S^{-1}(\tau,k)}|},
\]

\[
\cos \phi_2 = n \cdot n_2, \quad n_2 = \frac{u_{(\tau,k)} - u_{D(\tau,k)}}{|u_{(\tau,k)} - u_{D(\tau,k)}|} \times \frac{u_{(\tau,k)} - u_{S^{-1}(\tau,k)}}{|u_{(\tau,k)} - u_{S^{-1}(\tau,k)}|},
\]

\[
\cos \phi_3 = n \cdot n_3, \quad n_3 = \frac{u_{(\tau,k)} - u_{D(\tau,k)}}{|u_{(\tau,k)} - u_{D(\tau,k)}|} \times \frac{u_{(\tau,k)} - u_{S(\tau,k)}}{|u_{(\tau,k)} - u_{S(\tau,k)}|}.
\]

Then, the bond bending at each atom \((\tau, k) \in \Lambda\) is \( E_T(\phi_1) + E_T(\phi_2) + E_T(\phi_3) \).

For this work, we use the parameters given in [6], which are \( E_0 = 6.1322 \) eV, \( \beta = 1.8502 \) A\(^{-1}\), \( r_0 = 0.14322 \) A, \( k_\theta = 10 \) eV, \( k_\phi = 0.346 \) eV. In this paper we use exactly these values.

### 2.3 Icosahedral Symmetries

By its definition, the potential energy \( V \) is invariant with respect to the action of \( c \in \mathbb{R}^3 \) in \((\mathbb{R}^3)^{60}\) by shifting, \( V(u + c) = V(u) \). Therefore, in order to make the system \([2]\) reference point-depended, we define the subspace

\[
\mathcal{Y} := \left\{ u \in (\mathbb{R}^3)^{60} : \sum_{(\sigma,k) \in \Lambda} u_{\sigma,k} = 0 \right\}
\]
\[ \Omega_o = \{ u \in V : u_{\sigma,k} \neq u_{\sigma,j} \}. \]

We have that \( \mathcal{V} \) and \( \Omega_o \) are flow-invariant for (2).

By the properties of functions \( S \) and \( D \), the potential

\[ V : \Omega_o \to \mathbb{R} \] (4)

is well defined and \( I \)-invariant. Moreover, the potential \( V \) is invariant by rotations and reflections of the group \( O(3) \) because bonding, bending and torsion forces depend only on the norm of the distances among pairs of atoms. Therefore, the potential \( V \) is \( I \times O(3) \)-invariant,

\[ V((\sigma, A)u) = V(u), \quad (\sigma, A) \in I \times O(3). \]

Let

\[
J_1 := \begin{bmatrix}
0 & 0 & 0 \\
0 & 0 & -1 \\
0 & 1 & 0
\end{bmatrix}, \quad J_2 := \begin{bmatrix}
0 & 0 & -1 \\
0 & 0 & 0 \\
1 & 0 & 0
\end{bmatrix}, \quad J_3 := \begin{bmatrix}
0 & -1 & 0 \\
1 & 0 & 0 \\
0 & 0 & 0
\end{bmatrix}
\] (5)

be the three infinitesimal generators of rotations in \( O(3) \), i.e., \( e^{\phi J_1}, e^{\theta J_2} \) and \( e^{J_3 \psi} \), where \( \phi, \theta \) and \( \psi \) are the Euler angles. The angle between two adjacent pentagons in a dodecahedron is \( \theta_0 = \arctan 2 \). Then, the rotation by \( \pi \) that fixes a pair of antipodal edges is

\[
A = e^{-(\theta_0/2)J_2} e^{\pi J_3} e^{(\theta_0/2)J_2} = \begin{bmatrix}
-\frac{1}{\sqrt{5}} & 0 & \frac{2}{\sqrt{5}} \\
0 & -1 & 0 \\
\frac{2}{\sqrt{5}} & 0 & \frac{1}{\sqrt{5}}
\end{bmatrix}.
\] (6)

The rotation by \( 2\pi/5 \) of the upper pentagonal face of a dodecahedron is

\[
B = e^{\frac{2\pi}{5}J_3} = \begin{bmatrix}
\frac{-1+\sqrt{5}}{4} & \sqrt{\frac{5+\sqrt{5}}{8}} & 0 \\
\sqrt{\frac{5+\sqrt{5}}{8}} & \frac{-1+\sqrt{5}}{4} & 0 \\
0 & 0 & 1
\end{bmatrix}.
\] (7)

The subgroup of \( O(3) \) generated by the matrices \( A \) and \( B \) is isomorphic to icosahedral group \( A_5 \). Indeed, the generators \( A \) and \( B \) satisfy the relations

\[ A^2 = B^5 = (AB)^3 = \text{Id}. \]

On the other hand, the group \( A_5 \) is generated by

\[ a = (23)(45), \quad b = (12345), \] (8)
and we have similar relations

\[ a^2 = b^5 = (ab)^3 = 1. \]

Therefore, the explicit homomorphism \( \rho : A_5 \to SO(3) \) defined on generators by \( \rho(a) := A \) and \( \rho(b) := B \) is the required isomorphism \( A_5 \simeq \rho(A_5) \subset SO(3) \). We extend

\[ \rho : A_5 \times \mathbb{Z}_2 \to O(3) \]

with \( \rho(-1) = -\text{Id} \in O(3) \), and consequently we obtain an explicit identification of the full icosahedral group \( I \) with \( \rho(I) \subset O(3) \).

### 2.4 Icosahedral Minimizer

Let \( \tilde{I} \) be the icosahedral subgroup of \( I \times O(3) \) given by

\[ \tilde{I} = \{(\sigma, \rho(\sigma)) \in I \times O(3) : \sigma \in I\}. \]

The fixed point space

\[ \Omega_{\tilde{I}}^0 = \mathcal{Y}_{\tilde{I}} \cap \Omega_o = \{(a_{\tau,k})_{(\tau,k) \in \Lambda} \in \Omega_0 : a_{\tau,k} = (\sigma, \rho(\sigma))a_{\tau,k}\}, \]

consist of all the truncated icosahedral configurations. An equilibrium of the fullerene molecule can be found as a minimizer of \( V \) on these configurations. More precisely, since \( V \) is \( I \times O(3) \)-invariant, by Palais criticality principle, the minimizer of the potential \( V \) on the fixed-point space of \( \tilde{I} \) is a critical point of \( V \).

To find the minimizer among configurations with symmetries \( \tilde{I} \), we parameterize the carbons positions by fixing the position of one of them. Let

\[ u_{b,1} = (x, 0, z), \quad x, z \in \mathbb{R}, \]

then we have

\[ u_{b,1} = (\sigma, \rho(\sigma))u_{b,1} = \rho(\sigma)u_{\sigma^{-1}b\sigma, \sigma^{-1}(1)} \]

and relations

\[ u_{\sigma^{-1}b\sigma, \sigma^{-1}(1)} = \rho(\sigma)^{-1}u_{b,1} = \rho(\sigma)^{-1}(x, 0, z)^T, \quad \sigma \in A_5, \] (9)

allow us to determine the positions of all other coordinates of the vector \( u = (u_{\tau,k}) \).

Therefore, the representation of \( u(x, z) \) given by (9) provides us with a parametrization of a connected component of \( \Omega_{\tilde{I}}^0/O(3) \) with the domain

\[ C = \{(x, z) \in \mathbb{R}^2 : 0 < z, \ x < Cz\} \]

where \( C > 0 \) is a number determined by the geometric restrictions. We define \( v : C \to \mathbb{R} \) by

\[ v(x, z) = V(u(x, z)). \]
Since \(v(x, z)\) is exactly the restriction of \(V\) to the fixed-point subspace \(\Omega_0/\text{O}(3)\), then by the
symmetric criticality condition, a critical point of \(v : \mathcal{C} \to \mathbb{R}\) is also a critical point of \(V\).

We implemented a numerical minimizing procedure to find the minimizer \((x_o, z_o)\) of \(v(x, z)\). We denote the truncated icosahedral minimizer corresponding to the fullerene \(C_{60}\) as
\[u_o = u(x_o, z_o) \in \mathcal{V}.\]

The lengths of single and double bonds for this minimizer are given by
\[d_S = |u_{b,1} - u_{S(b,1)}| = 1.438084,\]
\[d_D = |u_{b,1} - u_{D(b,1)}| = 1.420845,\]
respectively. These results are in accordance with the distances measured in the paper [13].

An advantage of the notation \(u = (u_{\tau,k})\) is that it is easy to visualize the elements associated to the rotations \(\rho(\sigma)\) in the truncated icosahedron (Figure 1). In these configurations we have \(\rho(\sigma)u_{\tau,k} = \sigma^{-1}u_{\tau,k} = u_{\sigma\tau\sigma^{-1},\sigma(k)}\), then \(\rho(\sigma)\) is identified with the rotation that sends the face \(\tau\) to \(\sigma\tau\sigma^{-1}\) and the carbon atom identified by \(k\) to \(\sigma(k)\); for example, under the \(\pi\)-rotation given by \(\rho(a) = A\), face \(b = (12345)\) goes to the face \(a_{ba}^{-1} = (13254)\), and the element \(k = 1\) to \(a(1) = 1\). In this manner, we conclude that the elements of the conjugacy classes \(C_2, C_3, C_4\) and \(C_5\) correspond to the 15 rotations by \(\pi\), the 20 rotations by \(2\pi/3\), the 12 rotations by \(2\pi/5\) and the 12 rotations by \(\pi/5\), respectively.

2.5 Isotypical Decomposition

Since the space
\[\mathcal{V} = \{u \in (\mathbb{R}^3)^{60} : u \perp (v, ...v), \ v \in \mathbb{R}^3\}\]
is \(\tilde{I}\)-invariant, then it has a \(\tilde{I}\)-isotypical decomposition. Given that the system [2] is symmetric with respect the group action of \(I \times \text{O}(3)\), the orbit of equilibria \(u_o\) is a 3-dimensional submanifold in \(\mathcal{V}\). To describe the tangent space, we define
\[J_j u = (J_j u_{\sigma,k}),\]
where \(J_j\) are the three infinitesimal generators of the rotations defined in [5]. Then, the slice \(S_o\) to the orbit of \(u_o\) is
\[S_o := \{x \in \mathcal{V} : x \cdot J_j u_0 = 0, \ j = 1, 2, 3\}.\]
Since \(u_o\) has the isotropy group \(\tilde{I}\), then \(S_o\) is an orthogonal \(\tilde{I}\) representation.

In this section we identify the \(\tilde{I}\)-isotypical components of \(S_o\). In order to simplify the notation, hereafter we identify \(\tilde{I}\) with the group \(A_5 \times \mathbb{Z}_2\),
\[\tilde{I} = A_5 \times \mathbb{Z}_2.\]
Set $\varphi = \frac{1}{2}(1 \pm \sqrt{5})$, where $\varphi_+$ is the golden ratio. Let
\[ c = (123), \]
and $a = (23)(45)$ and $b = (12345)$ as before. The character table of $A_5$ is:

| Rep. | Character | (1) | a | c | b | $b^2$ |
|------|-----------|-----|---|---|---|-------|
| $\nu_1$ | $\chi_1$ | 1   | 1 | 1 | 1 | 1   |
| $\nu_2$ | $\chi_2$ | 4   | 0 | 1 | -1| -1  |
| $\nu_3$ | $\chi_3$ | 5   | 1 | -1| 0 | 0   |
| $\nu_4$ | $\chi_4$ | 3   | -1| 0 | $\varphi_+$| $\varphi_-$ |
| $\nu_5$ | $\chi_5$ | 3   | -1| 0 | $\varphi_-$| $\varphi_+$ |

The character table of $\tilde{I} \simeq A_5 \times \mathbb{Z}_2$ is obtained from the table of $A_5$. We denote the irreducible representations of $I$ by $\nu_{\pm n}$ for $n = 1, \ldots, 5$, where the element $-1 \in \mathbb{Z}_2$ acts as $\pm \text{Id}$ in $\nu_{\pm n}$ and elements $\gamma \in A_5$ act as they act on $\nu_n$. Notice that all the representations $\nu_{\pm n}$ are absolutely irreducible. Therefore, the character table for $A_5 \times \mathbb{Z}_2$ is as follows:

| Rep. | Character | (1) | a | c | b | $b^2$ | $(-1)$ | $(a, -1)$ | $(c, -1)$ | $(b, -1)$ | $(b^2, -1)$ |
|------|-----------|-----|---|---|---|-------|---------|------------|------------|------------|-------------|
| $\chi_1$ | $\nu_1$ | 1   | 1 | 1 | 1 | 1   | 1       | 1          | 1          | 1          | 1           |
| $\chi_2$ | $\nu_2$ | 4   | 0 | 1 | -1| -1  | 4       | 0          | 1          | -1         | -1          |
| $\chi_3$ | $\nu_3$ | 5   | 1 | -1| 0 | 0   | 5       | 1          | -1         | 0          | 0           |
| $\chi_4$ | $\nu_4$ | 3   | -1| 0 | $\varphi_+$| $\varphi_-$ | 3       | -1         | 0          | $\varphi_+$| $\varphi_-$ |
| $\chi_5$ | $\nu_5$ | 3   | -1| 0 | $\varphi_-$| $\varphi_+$ | 3       | -1         | 0          | $\varphi_-$| $\varphi_+$ |
| $\chi_{-1}$ | $\nu_{-1}$ | 1   | 1 | 1 | 1 | 1   | 1       | 1          | 1          | 1          | 1           |
| $\chi_{-2}$ | $\nu_{-2}$ | 4   | 0 | 1 | -1| -1  | 4       | 0          | -1         | 1          | 1           |
| $\chi_{-3}$ | $\nu_{-3}$ | 5   | 1 | -1| 0 | -5  | 5       | -1         | 1          | 0          | 0           |
| $\chi_{-4}$ | $\nu_{-4}$ | 3   | -1| 0 | $\varphi_+$| $\varphi_-$ | -3      | 1          | 0          | $-\varphi_+$| $-\varphi_-$ |
| $\chi_{-5}$ | $\nu_{-5}$ | 3   | -1| 0 | $\varphi_-$| $\varphi_+$ | -3      | 1          | 0          | $-\varphi_-$| $-\varphi_+$ |

Table 3: Character table for $A_5 \times \mathbb{Z}_2$

Denote by
\[ \mathcal{V} = \bigoplus_{n=1}^{5} \mathcal{V}_n \oplus \mathcal{V}_{-n}, \]
the $I$-isotypical decomposition of $\mathcal{V}$, where $\mathcal{V}_{\pm n}$ is modeled on $\nu_{\pm n}$. We numerically compute the spectrum $\{ \mu_j : j = 1, 2, \ldots, 47 \}$ of the Hessian $\nabla^2 V(u_o)$ at this minimizer $u_o$. Since $\nabla^2 V(u_o) : \mathcal{V} \to \mathcal{V}$ is $I$-equivariant, by the equivariance of $\nabla^2 V(u_o)$, we have
\[ \nabla^2 V(u_o)|_{\mathcal{V}_n \cap E(\mu_j)} = \mu_j \text{Id} : \mathcal{V}_n \cap E(\mu_j) \to \mathcal{V}_n \cap E(\mu_j), \]
where $E(\mu_j)$ stands for the eigenspace corresponding to $\mu_j$.

In order to determine in which isotypical component $V_{n_j}$ the eigenspace $E(\mu_j)$ is contained for a given eigenvalue $\mu_j$, we apply the isotypical projections

$$P_n v := \frac{\dim(V_n)}{120} \sum_{g \in I} \chi_n(g) g v, \quad v \in V,$$

where $V_n, n = \pm 1, \ldots, \pm 5$, is the irreducible representation identified by the character Table 3. Then the component $V_{n_j}$ can be clearly identified by $P_n v^j = v^j$.

We found that each of the eigenspaces $E(\mu_j)$ is an irreducible subrepresentation of $V$, i.e., the isotypical multiplicity of $\mu_j$ is simple. Including the zero eigenspace, we have 47 different components. Thus we have that $\sigma(V^2(u_\omega)|_{S_0}) = \{\mu_1, \ldots, \mu_{46}\}$ with $\mu_j > 0$, so

$$S_0 = \bigoplus_{j=1}^{46} V_{n_j} \quad \text{and} \quad V^2(u_\omega)|_{V_{n_j}} = \mu_j \text{Id}. \quad (10)$$

In the following table, we show the number $n_j \in \{-5, \ldots, -1, 1, \ldots, 5\}$ that identifies the irreducible representation corresponding to the eigenvalue $\mu_j$ for $j = 1, \ldots, 46$.

**Remark 2.1.** The models in [26] and [6] consider van der Waals forces among carbon atoms, which are modeled by the potential

$$W(x) = \varepsilon \left( \frac{\sigma^{12}}{x^{12}} - 2 \frac{\sigma^6}{x^6} \right),$$

where $\sigma = 3.4681 \ A^{-1}$ is the minimum energy distance and $\varepsilon = 0.0115 \ eV$ the depth of this minimum. However, our numerical computation using van der Waals forces did not produced the acceptable bond lengths among atoms given in [13] not the spectrums given in most papers such as [8]. Actually, models in [29] and [27] do not consider van der Waals forces. Using the models [26] and [6] without van der Waals forces give us results which correctly approximate the measurements in [13] and [8] for bond lengths $d_S$ and $d_D$ and frequencies $\sqrt{\mu_j/m}$, which are within the range 100 to 1800 $\text{cm}^{-1}$.

### 3 Equivariant Bifurcation

In what follows, we are interested in finding non-trivial $T$-periodic solutions to (2), bifurcating from the orbit equilibrium points of $u_\omega$. By normalizing the period, i.e. by making the substitution $v(t) := u(\lambda t)$ in (2), we obtain the system

$$\begin{cases}
\ddot{v} = -\lambda^2 \nabla V(v), \\
v(0) = v(2\pi), \quad \dot{v}(0) = \dot{v}(2\pi),
\end{cases} \quad (11)$$

where $\lambda^{-1} = 2\pi/T$ is the frequency.
Table 4: Eigenvalues of $\nabla^2 V(u_\omega)$ according to their isotypical type.

3.1 Equivariant Gradient Map

Since $\mathcal{V}$ is an orthogonal $I \times O(3)$-representation, we can consider the first Sobolev space of $2\pi$-periodic functions from $\mathbb{R}$ to $\mathcal{V}$, i.e.,

$$H^1_{2\pi}(\mathbb{R}, \mathcal{V}) := \{ u : \mathbb{R} \to \mathcal{V} : u(0) = u(2\pi), \ u|_{[0, 2\pi]} \in H^1([0, 2\pi]; \mathcal{V}) \},$$

equipped with the inner product

$$\langle u, v \rangle := \int_0^{2\pi} (\dot{u}(t) \bullet \dot{v}(t) + u(t) \bullet v(t))dt .$$
Let $O(2) = SO(2) \cup \kappa SO(2)$ denote the group of $2 \times 2$-orthogonal matrices, where

$$\kappa = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}, \quad \begin{bmatrix} \cos \tau & -\sin \tau \\ \sin \tau & \cos \tau \end{bmatrix} \in SO(2).$$

It is convenient to identify a rotation with $e^{i\tau} \in S^1 \subset \mathbb{C}$. Notice that $\kappa e^{i\tau} = e^{-i\tau} \kappa$, i.e., $\kappa$ as a linear transformation of $\mathbb{C}$ into itself, acts as complex conjugation.

Clearly, the space $H^1_{2\pi}(\mathbb{R}, \mathcal{Y})$ is an orthogonal Hilbert representation of

$$G := I \times O(3) \times O(2).$$

Indeed, we have for $u \in H^1_{2\pi}(\mathbb{R}, \mathcal{Y})$ and $(\sigma, A) \in I \times O(3)$ (see (1))

$$(\sigma, A) u(t) = (\sigma, A)u(t), \quad e^{i\tau} u(t) = u(t + \tau), \quad \kappa u(t) = u(-t).$$

It is useful to identify a $2\pi$-periodic function $u : \mathbb{R} \to V$ with a function $\tilde{u} : S^1 \to \mathcal{Y}$ via the map $e(\tau) = e^{i\tau} : \mathbb{R} \to S^1$. Using this identification, we will write $H^1(S^1, \mathcal{Y})$ instead of $H^1_{2\pi}(\mathbb{R}, \mathcal{Y})$. Let

$$\Omega := \{ u \in H^1(S^1, \mathcal{Y}) : u(t) \in \Omega_0 \}.$$

Then, the system (11) can be written as the following variational equation

$$\nabla_u J(u, \lambda) = 0, \quad (\lambda, u) \in \mathbb{R} \times \Omega,$$

where $J : \Omega \times \mathbb{R} \to \mathbb{R}$ is defined by

$$J(u, \lambda) := \int_0^{2\pi} \left[ \frac{1}{2} |\dot{u}(t)|^2 - \lambda^2 V(u(t)) \right] dt.$$ 

Assume that $u_o \in \mathcal{Y}$ is the equilibrium point of (4) described in previous section. Then $u_o$ is a critical point of $J$. We are interested in finding non-stationary $2\pi$-periodic solutions bifurcating from $u_o$, i.e., non-constant solutions to system (13). We consider the $G$-orbit of $u_o$ in $H^1(S^1, \mathcal{Y})$. We denote by $\mathcal{S}_o$ the slice to $G(u_o)$ in $H^1(S^1, \mathcal{Y})$. We will also denote by

$$\mathcal{J} : \mathbb{R} \times (\mathcal{S}_o \cap \Omega) \to \mathbb{R},$$

the restriction of $J$ to the set $\mathcal{S}_o \cap \Omega$. Clearly, $\mathcal{J}$ is $G_{u_o}$-invariant. Then, by Slice Criticality Principle (see Theorem B.3), critical points of $\mathcal{J}$ are critical points of $J$ and consequently, they are solutions to system (13).
Consider the operator \( L : H^2(S^1; \mathcal{V}) \to L^2(S^1; \mathcal{V}) \), given by
\[
Lu = -\ddot{u} + u
\]
for \( u \in H^2(S^1, \mathcal{V}) \). Then the inverse operator \( L^{-1} \) exists and is bounded. Let \( j : H^2(S^1; \mathcal{V}) \to H^1(S^1, \mathcal{V}) \) be the natural embedding operator. Clearly, \( j \) is a compact operator. Then, one can easily verify that
\[
\nabla_u J(\lambda, u) = u - j \circ L^{-1}(\lambda^2 \nabla V(u) + u),
\]
(15)
where \( u \in H^1(S^1, \mathcal{V}) \). Consequently, the bifurcation problem (13) is equivalent to \( \nabla_u J(\lambda, u) = 0 \). Moreover, we have
\[
\nabla^2_u J(\lambda, u_o)v = v - j \circ L^{-1}(\lambda^2 \nabla^2 V(u_o)v + v),
\]
(16)
where \( v \in H^1(S^1, \mathcal{V}) \).

Consider the operator
\[
\mathcal{A}(\lambda) := \nabla^2_u J(\lambda, u_o)|_{\mathcal{S}_o} : \mathcal{S}_o \to \mathcal{S}_o.
\]
(17)
Notice that
\[
\nabla^2_u \mathcal{A}(\lambda, u_o) = \mathcal{A}(\lambda),
\]
thus, by implicit function theorem, \( G(u_o) \) is an isolated orbit of critical points, whenever \( \mathcal{A}(\lambda) \) is an isomorphism. Therefore, if a point \((\lambda_o, u_o)\) is a bifurcation point for (13), then \( \mathcal{A}(\lambda_o) \) cannot be an isomorphism. In such case we define
\[
\Lambda := \{ \lambda > 0 : \mathcal{A}(\lambda_o) \text{ is not an isomorphism} \},
\]
and call this set the critical set for the trivial solution \( u_o \).

### 3.2 Bifurcation Theorem

Consider the \( S^1 \)-action on \( H^1(S^1, \mathcal{V}) \), where \( S^1 \) acts on functions by shifting the argument (see (12)). Then, \((H^1(S^1, \mathcal{V}))^{S^1} \) is the space of constant functions, which can be identified with the space \( \mathcal{V} \), i.e.,
\[
H^1(S^1, \mathcal{V}) = \mathcal{V} \oplus \mathcal{W}, \quad \mathcal{W} := \mathcal{V}^\perp.
\]
Then, the slice \( \mathcal{S}_o \) in \( H^1(S^1, \mathcal{V}) \) to the orbit \( G(u_o) \) at \( u_o \) is exactly
\[
\mathcal{S}_o = \mathcal{S}_o \oplus \mathcal{W}.
\]

Consider the \( S^1 \)-isotypical decomposition of \( \mathcal{W} \), i.e.,
\[
\mathcal{W} = \bigoplus_{l=1}^\infty \mathcal{W}_l, \quad \mathcal{W}_l := \{ \cos(l \cdot) a + \sin(l \cdot) b : a, b \in \mathcal{V} \}.
\]
In a standard way, the space \( \mathcal{W}_l \), \( l = 1, 2, \ldots \), can be naturally identified with the complexification \( \mathcal{V}^C \) on which \( S^1 \) acts by \( l \)-folding,

\[
\mathcal{W}_l = \{ e^{il}z : z \in \mathcal{V}^C \}.
\]

Since the operator \( \mathcal{A}(\lambda) \) is \( G_{u_o} \)-equivariant with

\[
G_{u_o} = \tilde{I} \times O(2),
\]

it is also \( S^1 \)-equivariant and thus \( \mathcal{A}(\lambda)(\mathcal{W}_l) \subset \mathcal{W}_l \). Using the \( \tilde{I} \)-isotypical decomposition of \( \mathcal{V}^C \), we have the \( G_{u_o} \)-invariant decomposition

\[
\mathcal{W}_l = \bigoplus_{j=1}^{46} \mathcal{V}_{j,l}, \quad \mathcal{V}_{j,l} := \{ e^{il}z : z \in E(\mu_j)^C \},
\]

where \( \mathcal{V}_{n_j,l} = \mathcal{V}_{n_j}^C = \mathbb{C} \otimes_{\mathbb{R}} \mathcal{V}_{n_j} \) is the \( I \times O(2) \)-irreducible representation with \( O(2) \) acting on \( \mathbb{C} \) by \( l \)-folding and complex conjugation. We have

\[
\mathcal{A}(\lambda)|_{\mathcal{V}_{j,l}} = \left( 1 - \frac{\lambda^2 \mu_j + 1}{l^2 + 1} \right) \text{Id}.
\]

Thus \( A(\lambda_o)|_{\mathcal{V}_{j,l}} = 0 \) if and only if \( \lambda_o^2 = l^2/\mu_j \) for some \( l = 1, 2, 3, \ldots \) and \( j = 0, 1, 2, \ldots, 46 \).

We will write

\[
\lambda_{j,l} = \frac{l}{\sqrt{\mu_j}}
\]

to denote the critical numbers in \( \Lambda \). Then the critical set for the equilibrium \( u_o \) of system (13) is

\[
\Lambda = \{ \lambda_{j,l} : j = 0, \ldots, 46, \quad l = 1, 2, 3, \ldots \}.
\]

Consider \( \lambda_o \in \Lambda \). Since \( \mu_j \neq 0 \) for \( j = 1, 2, \ldots, 46 \), the operator \( A(\lambda_o)|_{S_o} = -\lambda_o^2 \nabla^2 V(u_o)|_{S_o} : S_o \rightarrow S_o \) is an isomorphism. Consequently, we have the following result (see Appendix B):

**Theorem 3.1.** Consider the bifurcation system (13) and assume that \( \lambda_o \in \Lambda \) is a critical number. Then \( \lambda_o \) is an isolated point in \( \Lambda \), so there exist \( \lambda_- < \lambda_o < \lambda_+ \) such that \( [\lambda_-, \lambda_+] \cap \Lambda = \{ \lambda_o \} \).

Define

\[
\omega_G(\lambda_o) := \nabla_{g_{u_o}} \text{-deg} \left( \mathcal{A}(\lambda_+), B_1(0) \right) - \nabla_{g_{u_o}} \text{-deg} \left( \mathcal{A}(\lambda_-), B_1(0) \right),
\]

where \( B_1(0) \) stands for the open unit ball in \( S_o \). If

\[
\omega_G(\lambda_o) = n_1(H_1) + n_2(H_2) + \cdots + n_m(H_m)
\]

is non-zero, i.e. \( n_j \neq 0 \) for some \( j = 1, 2, \ldots, m \), then there exists a bifurcating branch of nontrivial solutions to (13) from the orbit \( \{ \lambda_o \} \times G(u_o) \) with symmetries at least \( (H_j) \).
3.3 Conjugacy classes

In order to simplify the notation, instead of using the symbol $I$, we will write $I$ in what follows. Under this notation the isotropy group $G_{uo}$ is

$$G_{uo} = I \times O(2).$$

The notation in this section is useful to obtain the classification of all conjugacy classes ($\mathcal{H}$) of closed subgroups in $I \times O(2)$.

We have conducted the computations of the gradient $I \times O(2)$-equivariant basic degrees, where $I := A_5 \times \mathbb{Z}_2$ stands for the full icosahedral group. The representatives of the conjugacy classes of the subgroups in $A_5 \times \mathbb{Z}_2$ consisting of proper nontrivial subgroups of $A_5$ are:

$$\begin{align*}
\mathbb{Z}_2 &= \{((1), 1), ((12)(34), 1)\}, \\
\mathbb{Z}_3 &= \{((1), 1), ((123), 1), ((132), 1)\}, \\
V_4 &= \{((1), 1), ((12)(34), 1), ((13)(24), 1), ((23)(14), 1)\}, \\
\mathbb{Z}_5 &= \{((1), 1), ((12345), 1), ((13524), 1), ((14253), 1), ((15432), 1)\}, \\
D_3 &= \{((1), 1), ((123), 1), ((132), 1), ((12)(45), 1), ((13)(45), 1), ((23)(45), 1)\}, \\
A_4 &= \{((1), 1), ((12)(34), 1), ((13)(24), 1), ((14)(23), 1), ((123), 1), ((132), 1), ((124), 1), ((142), 1), ((134), 1), ((143), 1), ((234), 1), ((243), 1)\}, \\
D_5 &= \{((1), 1), ((12345), 1), ((13524), 1), ((14253), 1), ((15432), 1), ((12)(35), 1), ((13)(45), 1), ((14)(23), 1), ((15)(24), 1), ((25)(34))\}.
\end{align*}$$

The representatives of the conjugacy classes of the subgroups in $A_5 \times \mathbb{Z}_2$ will be used to describe the symmetries of nonlinear vibrations. We use the symbol $H^p$, where $H$ is a subgroup of $A_5$, to denote the product

$$H^p = H \times \mathbb{Z}_2.$$ 

In addition, the twisted subgroups $H^p$ of $A_5 \times \mathbb{Z}_2$, where $H$ is a subgroup of $A_5$, are

$$\begin{align*}
\mathbb{Z}_2^\xi &= \{((1), 1), ((12)(34), -1)\}, \\
V_4^\xi &= \{((1), 1), ((12)(34), -1), ((13)(24), -1), ((23)(14), 1)\}, \\
D_3^\xi &= \{((1), 1), ((123), 1), ((132), 1), ((12)(45), -1), ((13)(45), -1), ((23)(45), -1)\}, \\
D_5^\xi &= \{((1), 1), ((12345), 1), ((13524), 1), ((14253), 1), ((15432), 1), ((12)(35), -1), ((13)(45), -1), ((14)(23), -1), ((15)(24), -1), ((25)(34), -1)\}.
\end{align*}$$
Figure 2: Lattice of conjugacy classes of subgroups in $A_5 \times \mathbb{Z}_2$. The square boxes indicate that the related subgroup is normal in $A_5 \times \mathbb{Z}_2$.

With these definitions the subconjugacy lattice for $A_5 \times \mathbb{Z}_2$ is shown in Figure 2.

The result (see [9, 12]) provides a description of subgroups of the product group $I \times O(2)$.

Namely, for any subgroup $\mathcal{H}$ of the product group $I \times O(2)$, there exist subgroups $H \leq I$ and $K \leq O(2)$, a group $L$ and two epimorphisms $\varphi : H \to L$ and $\psi : K \to L$ such that

$$\mathcal{H} = \{(h, k) \in H \times K : \varphi(h) = \psi(k)\}.$$

In order to make this notation simpler and self-contained, we will assume that $L = K/\ker(\psi)$, so $\psi : K \to L$ is evidently the natural projection. On the other hand, the group $L$ can be naturally identified with a finite subgroup of $O(2)$ being either $D_n$ or $\mathbb{Z}_n$, $n \geq 1$. Since we are interested in describing conjugacy classes of $\mathcal{H}$, we can identify different epimorphisms $\varphi, \psi : H \to L$ by indicating

$$Z = \ker(\varphi) \quad \text{and} \quad L = K/\ker(\psi).$$

Therefore, to identify $\mathcal{H}$ we will write

$$\mathcal{H} =: H^Z \times_L K,$$

where $H$ and $Z$ are subgroups of $I$ and $m$ is a number used to identify groups in different conjugacy classes. In the case that all the epimorphisms $\varphi$ with the kernel $Z$ are conjugate, there is no need to use the number $m$ in (18), so we will simply write $\mathcal{H} = H^Z \times_L K$. In addition, in the case that
all epimorphisms $\varphi$ from $H$ to $L$ are conjugate, we can also omit the symbol $Z$, i.e. we will write $\mathcal{H} = H \times_L K$.

### 3.4 Topological invariants

Let us point out that in a general case, if there are resonances, the critical numbers may not be uniquely identified by indices $(j,l)$. The first and last critical numbers for $l = 1$ are $\lambda_{1,1} = 0.075263$ and $\lambda_{46,1} = 0.57318$, respectively. We computed numerically (with precision $10^{-5}$) all the different values $\lambda_{j,l}$ from $\lambda_{1,1}$ to $\lambda_{46,1}$ and obtained that there is no-resonance with harmonic critical values from $\lambda_{1,1}$ to $\lambda_{46,1}$, i.e.,

$$\lambda_{1,1} < \lambda_{2,1} < \lambda_{3,1} < \lambda_{4,1} < \lambda_{5,1} < \ldots < \lambda_{5,7} < \lambda_{26,3} < \lambda_{21,4} < \lambda_{27,3} < \lambda_{46,1}. \quad (19)$$

By applying the computational formula (44) with the group $G_{u_0}$, we obtain for $\lambda \not\in \Lambda$ that

$$\nabla_{G_{u_0}}-\text{deg}(\mathcal{A}(\lambda), B_1(0)) = \prod\left\{ (j,l) \in \mathbb{N}^2: \lambda_{j,l} < \lambda \right\} \nabla-\text{deg}_{V_{n,j,l}}. \quad (20)$$

For each critical number $\lambda_{j_0,1}$ we choose two numbers $\lambda_- < \lambda_{j_0,1} < \lambda_+$ such that $[\lambda_-, \lambda_+] \cap \Lambda = \{\lambda_{j_0,1}\}$. Given that the eigenvalues $\lambda_{j,1}$ are non-resonant for $j = 1, \ldots, 46$, we have

$$\omega_G(\lambda_{j_0,1}) := \left((I \times O(2)) - \nabla-\text{deg}_{V_{n,j_0,1}}\right) \prod\left\{ (j,l) \in \mathbb{N}^2: \lambda_{j,l} < \lambda_{j_0,1} \right\} \nabla-\text{deg}_{V_{n,j,l}}. \quad (21)$$

The exact values of $\omega_G(\lambda_{j_0,1})$ can be effectively computed using the eigenvalues listed in Table 4 and the order of $\lambda_{j,1}$ in (19). For example, the first equivariant invariants are given by

$$\omega_G(\lambda_{1,1}) = (I \times O(2)) - \nabla-\text{deg}_{V_{3,1}}$$
$$\omega_G(\lambda_{2,1}) = \nabla-\text{deg}_{V_{3,1}} * \left((I \times O(2)) - \nabla-\text{deg}_{V_{-3,1}}\right)$$
$$\omega_G(\lambda_{3,1}) = \nabla-\text{deg}_{V_{3,1}} * \nabla-\text{deg}_{V_{-3,1}} * \left((I \times O(2)) - \nabla-\text{deg}_{V_{2,1}}\right).$$

Since $\lambda_{j,1}$ are non-resonant, the existence of families of periodic solutions from $\lambda_{j,1}$, with limit frequency $\sqrt{\mu_j}$, are determined by the maximal isotropy groups (in the first Fourier mode) in the topological invariant $\omega_G(\lambda_{j,1})$ for $j = 1, \ldots, 46$. Therefore, by (21), the existence of families of periodic solutions from $\lambda_{j,1}$ are determined by the maximal isotropy groups in

$$(I \times O(2)) - \nabla-\text{deg}_{V_{n,j,1}}.$$ 

The basic degrees $\nabla-\text{deg}_{V_{n,j}}$ for $j = \pm 1, \ldots, \pm 5$ are computed in Appendix B. We deduce the existence of a periodic solution from frequency $\sqrt{\mu_j}$ with the maximal orbit types according to the
irreducible representation $\mathcal{V}_{n_j}$. For the representations $\mathcal{V}_{n}$ with positive $n$ the maximal groups in the topological invariants (see Appendix B) are

$$\mathcal{V}_1 : (A_5^p \times D_1).$$

$$\mathcal{V}_2 : (D_3^p Z_2 \times D_2), (V_4^p Z_2 \times D_2), (A_4^p \times D_1), (D_3^p D_3 \times D_3 D_3),$$

$$\mathcal{V}_3 : (D_3^p Z_2 \times D_2), (D_3^p D_3 \times D_2), (V_4^p Z_2 \times D_2), (D_3^p D_3 \times D_3 D_3) .$$

$$\mathcal{V}_4 : (D_3^p Z_2 \times D_2), (D_3^p D_3 \times D_2), (V_4^p Z_2 \times D_2), (D_3^p Z_2 \times D_3 D_3).$$

$$\mathcal{V}_5 : (D_3^p Z_2 \times D_2), (D_3^p D_3 \times D_2), (V_4^p Z_2 \times D_2), (D_3^p Z_2 \times D_3 D_3).$$

And for the representations with negative $n$,

$$\mathcal{V}_{-1} : (A_5^p A_5 \times Z_2 D_2).$$

$$\mathcal{V}_{-2} : (A_5^p A_4 \times Z_2 D_2), (D_3^p D_3 \times Z_2 D_2), (V_4^p V_4 \times Z_2 D_2), (D_3^p Z_2 \times Z_2 D_2),$$

$$\mathcal{V}_{-3} : (D_3^p D_3 \times Z_2 D_2), (V_4^p V_4 \times Z_2 D_2), (A_4^p A_4 \times Z_2 D_2),$$

$$\mathcal{V}_{-4} : (D_3^p D_3 \times Z_2 D_2), (V_4^p V_4 \times Z_2 D_2), (D_3^p Z_2 \times Z_2 D_2),$$

$$\mathcal{V}_{-5} : (D_3^p D_3 \times Z_2 D_2), (V_4^p V_4 \times Z_2 D_2), (D_3^p Z_2 \times Z_2 D_2).$$

This concludes the proof of our main theorem.

4 Description of Symmetries and Numerical results

The symmetries in the representations $\mathcal{V}_{-n}$ are exactly as $\mathcal{V}_{n}$ for $n = 1, \ldots, 5$, except that instead of the element $-1 \in \mathbb{Z}_2 < I$ which gives a symmetry by inversion

$$u_{\tau,k}(t) = -u_{\tau-1,k}(t),$$

the representations $\mathcal{V}_{-n}$ have the element $(-1, -1) \in \mathbb{Z}_2 \times S^1$ in the maximal groups, which gives the symmetry

$$u_{\tau,k}(t) = -u_{\tau-1,k}(t + \pi).$$

Therefore, we only describe the symmetries of the maximal groups for representation $\mathcal{V}_{n}$.

The existence of the symmetry $\kappa \in O(2)$ in the maximal groups implies that the solutions are brake orbits,

$$u_{\tau,k}(t) = u_{\tau,k}(-t),$$
i.e., the velocity \( \dot{u} \) of all the molecules are zero at times \( t = 0, \pi \), i.e., \( \dot{u}(0) = \dot{u}(\pi) = 0 \). We classify the maximal groups in two classes: the groups that have the element \( \kappa \in O(2) \) and the groups that have the element \( \kappa \) coupled with a rotation of \( I \). That is, there is an element \( \gamma \in C_2 \) such that \( (\gamma, \kappa) \) is in the second class of groups, i.e., their solutions have the symmetry

\[
    u_{\tau,k}(t) = \rho(\gamma)u_{\gamma^\tau\gamma^{-1},\gamma^{-1}(k)}(-t).
\]

The only group that does not have a symmetry \( (\gamma, \kappa) \) is \((A_4^p V_4 \times Z_6 Z_6^2)\) which is the only maximal group with Weyl group of dimension one.

### 4.1 Standing Waves (Brake Orbits)

In this category we consider the groups that have the element \( \kappa \in O(2) \), which generate the group \( D_1 < O(2) \).

For groups

\[
(A_5^p \times D_1), (A_4^p \times D_1), (D_5^p \times D_1), (D_3^p \times D_1)
\]

the solutions have icosahedral symmetries at all times for group \( A_5 \), tetrahedral symmetries for group \( A_4 \), pentagonal symmetries for group \( D_5 \) and triangular symmetries for group \( D_3 \).

For the group

\[
(D_3^p \times Z_3 \times Z_2 D_2)
\]

the solutions are symmetric by the \( 2\pi/3 \)-rotations of \( Z_3 < D_3 < I \), while the reflection of \( D_3 < I \) is coupled with the \( \pi \)-time shift of \(-1 \in Z_2 < S^1 \). Therefore, the solutions in three faces have the exact dynamics, but these faces are not symmetric by reflection such as in the symmetries of \((D_3^p \times D_1)\).

For the group

\[
(V_4^p \times Z_2 \times Z_2 \times D_2),
\]

the solutions are symmetric by the \( \pi \)-rotations of \( V_4 < I \), while the other \( \pi \)-rotation of \( Z_2 < V_4 \) is coupled with the \( \pi \)-time shift of \(-1 \in D_2 < S^1 \).

These seven symmetries give solutions which are standing waves in the sense that each symmetric face have the exact dynamic repeated for all times.

### 4.2 Discrete Rotating Waves

In groups

\[
(D_5^p \times D_5^p \times D_5^p \times D_5^p \times D_5^p), (D_5^p \times Z_3 \times D_5^p \times D_5^p)
\]

the spatial dihedral group \( D_5 < I \) is coupled with the temporal group \( D_5 < O(2) \). Therefore, in these solutions we have 5 faces with the same dynamics, but there is a \( 2\pi/5 \)-time shift in time between consecutive faces. In addition, \( \kappa \) is coupled with a \( \pi \)-rotation, i.e., there is an axis of
symmetry in each face. In this sense, the solutions have the appearance of a discrete rotating wave with a $2\pi/5$ delay along consecutive faces. There are two groups because there are two different conjugacy classes, $C_4$ and $C_5$, of $A_5$.

Similarly, in the solutions of the group

$$(D_3^p \mathbb{Z}_p \times D_3)$$

we have 3 faces with the same dynamics, but with a $2\pi/3$-time shift, i.e., the solutions have the appearance of a discrete rotating wave in 3 faces with a $2\pi/3$-time shift and each face has an axis of symmetry.

For the solutions of the group

$$(A_4^p V_4 \times \mathbb{Z}_6 \mathbb{Z}_6)$$

we have 3 faces with the same dynamics with a $2\pi/3$-time shift. Moreover, in these solutions the inversion is coupled with a $\pi$-time shift in time. Therefore, there are a total of 6 faces (3 faces and their inversions) that have the same dynamics but with $2\pi/6$-time shift. In these solutions the faces do not have an axis of symmetry, instead there are two symmetries by a $\pi$-rotation.

### 4.3 Numerical results

We have implemented a pseudo-arc length procedure to numerically continue some families of periodic solutions, which we describe in Appendix A. We present the results of our numerical computations in Figures 3 and 4. The position of the atoms in space are in the right columns. The atoms with the same color have oscillations related by a rotation or inversion in $O(3)$. In addition, atoms with the same color but different texture describe oscillations that are related by the inversion coupled with a $\pi$-phase shift in time, $u_{\tau,k}(t) = -u_{\tau-1,k}(t + \pi)$. In the left columns of Figures 3 and 4 we illustrate the norm of the atoms oscillating in time.
Figure 3: Top: Solutions from eigenvalue $j = 2$ with symmetries ($D_5^p \times D_1$). Middle: Solution from eigenvalue $j = 3$ with symmetries ($D_3^p \times Z_2 \times D_2$). Bottom: Solutions from eigenvalue $j = 4$ with symmetries ($V_4^p V_4^i \times Z_2 \times D_2$).
Figure 4: Top: Solutions from eigenvalue $j = 5$ with symmetries ($D_3^p \mathbb{Z}_1 \times D_6^p D_6$). Middle: Solution from eigenvalue $j = 6$ with symmetries ($V_4^p \mathbb{Z}_2^p \times \mathbb{Z}_2^p D_2$). Bottom: Solutions from eigenvalue $j = 9$ with symmetries ($A_5^p \times D_1$).
Appendices

A Numerical Continuation

In order to compute numerically the families of periodic solutions, we use the Hamiltonian equation,

$$\dot{x} = J \nabla H(x), \quad x = (q, p),$$

(32)

where $H(q, p) = |p|^2/2 - V(q)$ is the Hamiltonian and $J$ is the symplectic matrix

$$J = \begin{pmatrix} 0 & -I \\ I & 0 \end{pmatrix}.$$ 

Since the Hamiltonian is invariant by the action of the group $\mathbb{R}^3$ that acts by translation, $O(3)$ by rotations and $\varphi \in S^1$ by time shift, then the Hamiltonian satisfies the orthogonal relations

$$\langle H(x), A_j(x) \rangle = 0,$$

for $j = 1, ..., 7$, where $A_j$ are the generators of the groups,

$$A_j(q, p) = \partial_{\tau}|_{\tau=0}(q + \tau \mathcal{E}_j, p) = (\mathcal{E}_j, 0), \quad \mathcal{E}_j = (e_j, ..., e_j)$$

$$A_{j+3}(q, p) = \partial_{\theta}|_{\theta=0}(e^{\theta \mathcal{J}_j} q, e^{\theta \mathcal{J}_j} p) = (\mathcal{J}_j q, \mathcal{J}_j p), \quad \mathcal{J}_j = \text{diag}(J_j, ..., J_j)$$

for $j = 1, 2, 3$, and

$$A_7(q, p) = \partial_{\varphi}|_{\varphi=0}(q, p)(t + \varphi) = J \nabla H.$$

Remark A.1. Actually, the conserved quantities $G_j$ are related to the generator fields $A_j$ by

$$A_j = J \nabla G_j.$$ 

Using the Poisson bracket, the orthogonality relations are equivalent to

$$\{H, G_j\} = \langle \nabla H, J \nabla G_j \rangle = \langle \nabla H, A_j \rangle = 0.$$

The explicit conserved quantities are $G_j = -p \cdot \mathcal{E}_j$, $G_{j+3} = p^T \mathcal{J}_j q$, for $j = 1, 2, 3$, and $G_7 = H$.

To numerically continue the solutions it is necessary to augment the differential equation with Lagrange multipliers $\lambda_j \in \mathbb{R}$ for $j = 1, ..., 7$,

$$\dot{x} = J \nabla H(x) + \sum_{j=1}^{7} \lambda_j J A_j(x).$$

(33)
The solutions of equation (33) are solutions of the original equations of motion when the values of the seven parameters are zero. If \( A_j(x) \) are linearly independent, a solution \( x \) to the equation (33) is a solution to the equation (32) because

\[
0 = \langle \dot{x}, JA_i(x) \rangle = \sum_{j=1}^{7} \lambda_j \langle A_j, A_i \rangle
\]

implies that \( \lambda_j = 0 \) for \( j = 1, ..., 7 \).

The period \( T = 2\pi\lambda \) can be obtained as parameter in equation (33) by rescaling time,

\[
\dot{x} = TJ\nabla H + \sum_{j=1}^{7} \lambda_j JA_j.
\]

Let \( \varphi_t(x) \) be the flow of this equation. We can define the time one map (for the rescaled time) as

\[
\varphi_1(x; \lambda_1, ..., \lambda_7, T) : V \times \mathbb{R}^7 \times \mathbb{R} \to V,
\]

where the period \( T \) is a parameter. Therefore, a fixed point of \( \varphi_1(x) \) corresponds to a \( T \)-periodic solutions of the Hamiltonian system.

To numerically continue the fixed points of \( \varphi_1(x) \) it is necessary to implement Poincaré sections. For this we define the augmented map

\[
F(q, p, \lambda_1, ..., \lambda_7; T) : V \times \mathbb{R}^7 \times \mathbb{R} \to V \times \mathbb{R}^7
\]

\[
F = (x - \varphi_1(x), A_j(\tilde{x}) \cdot (x - \tilde{x})).
\]

Then a solution of \( F = 0 \) is a \( T \)-periodic solution of the Hamiltonian system. The restrictions \( A_j(\tilde{x}) \cdot (x - \tilde{x}) = 0 \) for \( j = 1, ..., 7 \) represent the Poincaré sections, where \( \tilde{x} \) is a previously computed solutions on the family of solutions of \( F = 0 \). This map is a local submersion except for bifurcation points, see [21].

The map \( \varphi_1(x) \) is computed numerically using a Runge-Kutta integrator. A first solution of \( F = 0 \) is obtained by applying a Newton method in the approximating solution obtained by solving the linearized Hamiltonian system. The family of periodic solutions is computed numerically using a pseudo-arclength procedure to continue the solutions of \( F = 0 \).

### B Equivariant Gradient Degree

In what follows \( G \) always stands for a compact Lie group and all subgroups of \( G \) are assumed to be closed. For a subgroup \( H \subset G \), \( N(H) \) stands for the normalizer of \( H \) in \( G \), and \( W(H) = N(H) / H \).
denotes the Weyl group of $H$ in $G$. We denote by $(H)$ the conjugacy class of $H$ in $G$ and use the notations $\Phi(G) := \{(H) : H$ is a subgroup of $G\}$ and $\Phi_n(G) := \{(H) \in \Phi(G) : \dim W(H) = n\}$. The set $\Phi(G)$ has a natural partial order given by: $(H) \leq (K) \iff \exists g \in G$ $gHg^{-1} \subset K$.

For a $G$-space $X$ and $x \in X$, we put $G_x := \{g \in G : gx = x\}$ to denote the isotropy group of $x$, $G(x) := \{gx : g \in G\}$ to denote the orbit of $x$, and the conjugacy class $(G_x) := \{H \subset G : \exists g \in G$ $G_x = g^{-1}Hg\}$ will be called the orbit type of $x$, and $\Phi(G; X) := \{(G_x) : x \in X\}$ will stand for the set of all the orbit types in $X$. We also put $\Phi_n(G; X) := \Phi(G; X) \cap \Phi_n(G)$.

For a subgroup $H \subset G$, we write $X^H := \{x \in X : G_x \supset H\}$ to denote the $H$-fixed point space of $H$. The orbit space for a $G$-space $X$ will be denoted by $X/G$.

As any compact Lie group admits only countably many non-equivalent real irreducible representations, given a compact Lie group $G$, we will assume that we have a complete list of all real irreducible representations, denoted $\nu_i, i = 0, 1, \ldots$, which could also be identified by the character list $\{\chi_i\}$. We refer to [3] for examples of such lists and the related notation.

Let $V$ be a finite-dimensional real $\Gamma$-representation (without loss of generality, $V$ can be assumed to be orthogonal). Then, $V$ decomposes into the direct sum of $G$-invariant subspaces

$$V = V_0 \oplus V_1 \oplus \cdots \oplus V_r,$$  \hspace{1cm} (34)

called the $G$-isotypical decomposition of $V$, where each isotypical component $V_i$ is modeled on the irreducible $G$-representation $\nu_i, i = 0, 1, \ldots, r$, i.e., $V_i$ contains all the irreducible subrepresentations of $V$ which are equivalent to $\nu_i$.

Let $V$ be a $G$-representation, $\Omega \subset V$ an open $G$-invariant bounded set and $f : V \rightarrow V$ a continuous $G$-equivariant map such that for all $x \in \partial \Omega$ we have $f(x) \neq 0$. Then we say that $f$ is an $\Omega$-admissible $G$-map and we call $(f, \Omega)$ an admissible $G$-pair. The set of all admissible $G$-pairs in $V$ will be denoted by $\mathcal{M}^G(V)$. We also put $\mathcal{M}^G := \bigcup_V \mathcal{M}^G(V)$ (here $V$ denotes all possible $G$-representations) to denote the set of all admissible $G$-pairs. A map $f : V \rightarrow V$ is called a gradient map if there exists a continuously differentiable $\varphi : V \rightarrow \mathbb{R}$ such that $f = \nabla \varphi$. We denote by $\mathcal{M}_\nabla(V)$ the subset of $\mathcal{M}^G(V)$ consisting of all gradient maps and we define $\mathcal{M}^G := \bigcup_V \mathcal{M}^G(V)$. In the set $\mathcal{M}^G(V)$ (resp. $\mathcal{M}_\nabla(V)$) we have the so-called admissible homotopy (resp. admissible gradient homotopy) relation between $(f_0, \Omega)$ and $(f_1, \Omega)$, i.e., if $f_1$ and $f_2$ are homotopic by an homotopy $h : [0, 1] \times V \rightarrow V$, such that $h_t$ belongs to $\mathcal{M}^G(V)$ (resp. $\mathcal{M}_\nabla(V)$) for every $t \in [0, 1]$.

Finally, we denote by $B(V)$ the open unit ball in $V$, and for $x, y \in V := \mathbb{R}^n$ we will denote by $x \cdot y$ the standard inner product in the Euclidian space $\mathbb{R}^n$.

**B.1 Euler and Burnside Rings**

The concept of Euler ring, which was introduced by T. tom Dieck in [25], due to its topological definition, is rather complicated for a general compact Lie group. However, in our case of interest,
when \( G := \Gamma \times O(2) \), where \( \Gamma \) is a finite group, the computations of the Euler ring can be effectively done using other techniques based on the properties of the Euler ring homomorphisms (see [9] for more details).

We put \( U(G) := \mathbb{Z}[\Phi(G)] \), i.e., \( U(G) \) is the free \( \mathbb{Z} \)-module generated by \( \Phi(G) \). Next, we define a ring multiplication on generators \((H), (K) \in \Phi(G)\) as follows:

\[
(H) \ast (K) = \sum_{(L) \in \Phi(G)} n_L(L),
\]

where

\[
n_L := \chi_c\left(\left(G/H \times G/K\right)_L/N(L)\right)
\]

with \( \chi_c \) the Euler characteristic taken in Alexander-Spanier cohomology with compact support (cf. [24]). The \( \mathbb{Z} \)-module \( U(G) \) equipped with the multiplication (35) and (36) is a ring called the Euler ring of the group \( G \) (cf. [7]).

The \( \mathbb{Z} \)-module \( A(G) := \mathbb{Z}[\Phi_0(G)] \) equipped with a similar multiplication as in \( U(G) \) but restricted to generators from \( \Phi_0(G) \) is called Burnside ring, i.e.,

\[
(H) \cdot (K) = \sum_{(L)} n_L(L), \quad (H), (K), (L) \in \Phi_0(G),
\]

where \( n_L := \left|\left(G/H \times G/K\right)_L/N(L)\right| \) (here \( |X| \) stands for the number of elements in the set \( X \)). In this case, we have

\[
n_L = \frac{n(L, K) |W(K)| n(L, H) |W(H)| - \sum_{(L)} n(L, \tilde{L}) n_{\tilde{L}} |W(\tilde{L})|}{|W(L)|},
\]

where

\[
n(L, K) = \left|\frac{N(L, K)}{N(K)}\right|, \quad N(L, K) := \{g \in G : gLg^{-1} \subset K\},
\]

and \((H), (K), (L), (\tilde{L})\) are taken from \( \Phi_0(G) \).

The structure of the Burnside ring \( A(G) \) is significantly simpler and can be effectively computed for a large class of classical compact Lie groups. It is also possible to implement the G.A.P. routines in computer programs evaluating Burnside rings products. Notice that \( A(G) \) is a \( \mathbb{Z} \)-submodule of \( U(G) \), but not a subring. Define \( \pi_0 : U(G) \rightarrow A(G) \) on generators \((H) \in \Phi(G)\) by

\[
\pi_0((H)) = \begin{cases} (H) & \text{if } (H) \in \Phi_0(G), \\ 0 & \text{otherwise}. \end{cases}
\]

Then we have:
Lemma B.1. (cf. [1]) The map \( \pi_0 \) defined by (38) is a ring homomorphism, i.e.,
\[
\pi_0 ((H) \ast (K)) = \pi_0 ((H)) \cdot \pi_0 ((K)), \quad (H), (K) \in \Phi (G),
\]
where ‘\( \cdot \)’ denotes the multiplication in the Burnside ring \( A(G) \).

Lemma B.1 allows us to use Burnside ring multiplication structure in \( A(G) \) to partially compute the Euler ring multiplication structure in \( U(G) \). The additional algorithms allowing the full computation of the Euler ring structure for \( G = \Gamma \times O(2) \) (without using topological computations) are described in [9].

B.2 Equivariant Gradient Degree

The existence and properties of the so-called \( G \)-equivariant gradient degree are presented in the following result from [11]:

Theorem B.2. There exists a unique map \( \nabla_{G} \text{-deg} : \mathcal{M}_{G} \rightarrow U(G) \), which assigns to every \( (\nabla \varphi, \Omega) \in \mathcal{M}_{G} \) an element \( \nabla_{G} \text{-deg} (\nabla \varphi, \Omega) \in U(G) \), called the \( G \)-gradient degree of \( \nabla \varphi \) on \( \Omega \),
\[
\nabla_{G} \text{-deg} (\nabla \varphi, \Omega) = \sum_{(H_i) \in \Phi (\Gamma)} n_{H_i} (H_i) = n_{H_1} (H_1) + \cdots + n_{H_m} (H_m),
\]
(39)
satisfying the following properties:

(Existence) If \( \nabla_{G} \text{-deg} (\nabla \varphi, \Omega) \neq 0 \), i.e., there is in (39) a non-zero coefficient \( n_{H_i} \), then exists \( u_0 \in \Omega \) such that \( \nabla \varphi (u_0) = 0 \) and \( (G_{u_0}) \geq (H_i) \).

(Additivity) Let \( \Omega_1 \) and \( \Omega_2 \) be two disjoint open \( G \)-invariant subsets of \( \Omega \) such that \( (\nabla \varphi)^{-1} (0) \cap \Omega \subset \Omega_1 \cup \Omega_2 \). Then, \( \nabla_{G} \text{-deg} (\nabla \varphi, \Omega) = \nabla_{G} \text{-deg} (\nabla \varphi, \Omega_1) + \nabla_{G} \text{-deg} (\nabla \varphi, \Omega_2) \).

(Homotopy) If \( \nabla_2 \Psi : [0, 1] \times V \rightarrow V \) is a \( G \)-gradient \( \Omega \)-admissible homotopy, then
\[
\nabla_{G} \text{-deg} (\nabla_v \Psi (t, v), \Omega) = \text{constant}.
\]

(Normalization) Let \( \varphi \in C^2_C (V, \mathbb{R}) \) be a special \( \Omega \)-Morse function such that \( (\nabla \varphi)^{-1} (0) \cap \Omega = G (u_0) \) and \( G_{u_0} = H \). Then,
\[
\nabla_{G} \text{-deg} (\nabla \varphi, \Omega) = (-1)^{m^- (\nabla^2 \varphi (u_0))} \cdot (H),
\]
where “\( m^- (\cdot) \)” stands for the total dimension of eigenspaces for negative eigenvalues of a (symmetric) matrix.
(Multiplicativity) For all \((\nabla \varphi_1, \Omega_1), (\nabla \varphi_2, \Omega_2) \in M^G\),

\[
\nabla_G\text{-deg}(\nabla \varphi_1 \times \nabla \varphi_2, \Omega_1 \times \Omega_2) = \nabla_G\text{-deg}(\nabla \varphi_1, \Omega_1) \ast \nabla_G\text{-deg}(\nabla \varphi_2, \Omega_2)
\]

where the multiplication ‘\(\ast\)’ is taken in the Euler ring \(U(G)\).

(Functoriality) [cf. [9]] Suppose \(G_0 \leq G\) is a subgroup of a compact Lie group \(G\) such that \(\dim G_0 = \dim G\). Then any gradient admissible \(G\)-pair \((\nabla \varphi, \Omega)\) is also an admissible \(G_0\)-pair and we have

\[
\Psi[\nabla_G\text{-deg}(\nabla \varphi, \Omega)] = \nabla_{G_0}\text{-deg}(\nabla \varphi, \Omega),
\]

where \(\Psi : U(G) \to U(G_0)\) is the Euler ring homomorphism induced by the inclusion \(\psi : G_0 \hookrightarrow G\) (see [9]).

Using a standard finite-dimensional approximation technique, the \(G\)-equivariant gradient degree can be extended to admissible \(G\)-pairs in Hilbert \(G\)-representation for the class of \(G\)-equivariant completely continuous gradient fields with the same properties as in Theorem B.2 (cf. [2, 9]).

One of the most important properties of \(G\)-equivariant gradient degree \(\nabla_G\text{-deg}(f, \Omega)\) is that it provides a full equivariant topological classification of the solution set for \(f(x) = 0\) and \(x \in \Omega\). More precisely, in addition to the properties listed in Theorem B.2 the equivariant gradient degree has also the so-called Universality Property, which says that two \(B(V)\)-admissible \(G\)-equivariant gradient maps \(f_1, f_2 : V \to V\) have the same gradient degrees if and only if they are \(B(V)\)-admissibly gradient homotopic.

Suppose that

\[
\nabla_G\text{-deg}(f, \Omega) = n_1(H_1) + n_2(H_2) + \cdots + n_k(H_k) + \cdots + n_m(H_m),
\]

and \(n_k \neq 0\). Then, by the existence property, there exists a solution \(x_0 \in \Omega\) of \(f(x) = 0\), such that \(H := G_{x_0}\). In addition, if \((H_k)\) is a maximal orbit type in \(\Omega\), then for any \(\Omega\)-admissible continuous deformation \(\{f_t\}_{t \in [0,1]}\) (in the class of gradient maps) we obtain a continuum of solutions in \(\Omega\) to \(f_t(x) = 0\) that starts at \(x_0\) for \(t = 0\) and ends at \(x_1\) for \(t = 1\), and \(G_{x_1} = H\). This property is called Continuation Property.

B.3 Degree on the Slice

Let \(\mathcal{H}\) be a Hilbert \(G\)-representation. Suppose that the orbit \(G(u_o)\) of \(u_o \in \mathcal{H}\) is contained in a finite-dimensional \(G\)-invariant subspace, so the \(G\)-action on that subspace is smooth and \(G(u_o)\) is a smooth submanifold of \(\mathcal{H}\). Denote by \(S_o \subset \mathcal{H}\) the slice to the orbit \(G(u_o)\) at \(u_o\). Denote by \(V_o := \tau_{u_o} G(u_o)\) the tangent space to \(G(u_o)\) at \(u_o\). Then \(S_o = V_o^\perp\) and \(S_o\) is a smooth Hilbert \(G_{u_o}\)-representation.

Then we have (cf. [5])
**Theorem B.3. (Slice Principle)** Let \( \mathcal{H} \) be a Hilbert \( G \)-representation, and \( \varphi : \mathcal{H} \to \mathbb{R} \) a continuously differentiable \( G \)-invariant functional such that \( \nabla \varphi \) is a completely continuous field. Let \( u_o \in \mathcal{H} \) and assume that \( G(u_o) \) is an isolated critical orbit of \( \varphi \). Let \( S_o \) be the slice to the orbit \( G(u_o) \) and \( U \) an isolated tubular neighborhood of \( G(u_o) \). Put \( \varphi_o : S_o \to \mathbb{R} \) by \( \varphi_o(v) := \varphi(u_o + v), \quad v \in S_o \). Then

\[
\nabla_{G_o}\deg (\nabla \varphi, U) = \Theta(\nabla_{G_{u_o}}\deg (\nabla \varphi_o, U \cap S_o)),
\]

where \( \Theta : U(G_{u_o}) \to U(G) \) is defined on generators \( \Theta(H) = (H), (H) \in \Phi(G_{u_o}) \).

**B.4 Computation of the \( G \)-Equivariant Gradient Degree**

Let us establish a computational formula to evaluate the \( G \)-equivariant degree \( \nabla_{G_o}\deg (A, B(V)) \), where \( A : V \to V \) is a symmetric \( G \)-equivariant linear isomorphism and \( V \) is an orthogonal \( G \)-representation, i.e., \( A = \nabla \varphi \) for \( \varphi(v) = \frac{1}{2}(\mathcal{A} v \cdot v), \quad v \in V \). Consider the \( G \)-isotypical decomposition (34) of \( V \) and put \( A_i := A|_{V_i} : V_i \to V_i \), \( i = 0, 1, \ldots, r \).

Then, by the multiplicativity property,

\[
\nabla_{G_o}\deg(A, B(V)) = \prod_{i} \nabla_{G_o}\deg(A_i, B(V_i))
\]

Take \( \xi \in \sigma_-(\mathcal{A}) \), where \( \sigma_-(\mathcal{A}) \) stands for the negative spectrum of \( \mathcal{A} \), and consider the corresponding eigenspace \( E(\xi) := \ker(\mathcal{A} - \xi \text{Id}) \). Define the numbers \( m_i(\xi) \) by

\[
m_i(\xi) := \dim (E(\xi) \cap V_i) / \dim V_i,
\]

and the so-called gradient \( G \)-equivariant basic degrees by

\[
\nabla_{G_o}\deg_{V_i} := \nabla_{G_o}\deg(-\text{Id}, B(V_i)), \quad i = 0, 1, 2, \ldots
\]

Then

\[
\nabla_{G_o}\deg(A, B(V)) = \prod_{\xi \in \sigma_-(\mathcal{A})} \prod_{i=0}^{r} (\nabla_{G_o}\deg_{V_i})^{m_i(\xi)}. \tag{44}
\]

**B.5 Computation of the \( \Gamma \times O(2) \)-Equivariant Basic Degrees**

In order to be able to effectively use the formula (44), it is important to establish the exact values of the gradient \( G \)-equivariant basic degrees. A direct usage of topological definition (see [11]) of the gradient \( G \)-equivariant degree to compute the basic degrees \( \nabla_{G_o}\deg_{V_i} \) may be very complicated for infinite compact Lie groups \( G \). However, in the case of the group \( G := \Gamma \times O(2) \) (\( \Gamma \) being a...
finite group) there were developed effective reduction techniques (see [9]) based on the usage of the homomorphism $\pi_0$ and the Euler ring homomorphism $\Psi : U(\Gamma \times O(2)) \to U(\Gamma \times S^1)$, allowing to establish the exact values of the gradient $\Gamma \times O(2)$-equivariant basic degrees.

The $G$-equivariant Brouwer degree $G\text{-deg}(f, \Omega) \in A(G)$ is defined for admissible $G$-pairs $(f, \Omega) \in \mathcal{M}^G(V)$ and has similar existence, additivity, homotopy and multiplicativity properties as the gradient degree. Moreover, it can effectively be computed applying the following recurrence formula to the usual Brouwer degrees of maps $f^H : V^H \to V^{H'}$, $(H) \in \Phi_0(G; V)$, i.e.,

$$G\text{-deg}(f, \Omega) = \sum_{(H) \in \Phi_0(G; V)} n_H(H),$$

and

$$n_H = \frac{\text{deg}(f^H, \Omega^H) - \sum_{(L) > (H)} n_L n(H, L) |W(L)|}{|W(H)|}.$$  \hspace{1cm} (45)

The formula (45) allows the usage of computational programs based on G.A.P. platform to obtain exact symbolic evaluation of the $G$-equivariant Brouwer degree of linear isomorphisms for a large class of classical groups and their products (see [28]).

In addition, for any gradient admissible $G$-pair $(f, \Omega)$, the $G$-equivariant Brouwer degree $G\text{-deg}(f, \Omega) \in A(G)$ is well-defined and we have the following relation (see [9])

$$\pi_0 (\nabla G\text{-deg}(f, \Omega)) = G\text{-deg}(f, \Omega).$$ \hspace{1cm} (46)

One can define the Brouwer $G$-equivariant basic degrees

$$\text{deg}_{\mathcal{V}_i} := G\text{-deg}(-\text{Id} , B(\mathcal{V}_i)) , \quad i = 0, 1, 2, 3, \ldots$$

Then we have

$$\text{deg}_{\mathcal{V}_i} = \pi_0 \nabla \text{deg}_{\mathcal{V}_i} , \quad i = 0, 1, 2, 3 \ldots$$ \hspace{1cm} (47)

Therefore, by (47),

$$\nabla \text{deg}_{\mathcal{V}_i} = \text{deg}_{\mathcal{V}_i} + \sum_{(H) \in \Phi_1(G; \mathcal{V}_i)} x_H(H),$$

where the integers $x_H$ are to be determined.

Since the gradient basic degrees $\text{deg}_{\mathcal{V}_i}$ for the group $\Gamma \times S^1$ are well-known, one can apply the Euler ring homomorphism $\Psi : U(\Gamma \times O(2)) \to U(\Gamma \times S^1)$ to determine these coefficients (see [9]) by using the relation

$$\widetilde{\text{deg}}_{\mathcal{V}_i} = \Psi \text{deg}_{\mathcal{V}_i} + \sum_{(H) \in \Phi_1(G; \mathcal{V}_i)} x_H \Psi(H),$$
The Euler ring homomorphism $\Psi : U(\Gamma \times O(2)) \to U(\Gamma \times S^1)$ is defined on the generators by

\[
\Psi(H) = \begin{cases} 
2(K) & \text{if } K = H \text{ and } K \sim K' \text{ in } \Gamma \times SO(2), \\
(K) + (K') & \text{if } K = H \text{ and } K \not\sim K' \text{ in } \Gamma \times SO(2), \\
(K) & \text{if } K \neq H,
\end{cases}
\]

where $K := H \cap \Gamma \times SO(2)$, $K' := \kappa H \kappa \cap \Gamma \times SO(2)$.

### B.6 Computations of the $I \times O(2)$-Equivariant Basic Degrees

We use GAP programming (see [28]) to classify all the conjugacy classes of closed subgroups in $G := I \times O(2)$. In this way, we compute the following basic gradient degrees (corresponding to the irreducible $G$-representations associated to the characters listed in Table 3, where we use red color to indicate the maximal orbit types (in the class of $2\pi$-periodic functions $x : \mathbb{R} \to V$ with Furrier mode 1).

\[
\begin{align*}
\nabla \text{-deg}_{V_{1,1}} &= -(A_6^p \times D_1) + (A_5^p \times O(2)), \\
\nabla \text{-deg}_{V_{2,1}} &= -(D_3^p \times \mathbb{Z}_2 \times D_2) - (V_4^p \times \mathbb{Z}_2 \times D_2) - 2(\mathbb{Z}_2^p \times \mathbb{Z}_2 D_2) - (A_4^p \times D_1) \\
&\quad - (D_5^p \times D_1) + 2(\mathbb{Z}_3^p \times D_1) + 2(\mathbb{Z}_2^p \times D_1) - 2(\mathbb{Z}_1^p \times D_1) \\
&\quad - (D_5^p \times D_1) - (D_5^p \times D_5) - (D_5^p \times D_3) + (V_4^p \times D_2 D_2) \\
&\quad + (D_3^p \times D_1) + (V_4^p \times D_1) + (A_4^p \times O(2)) \\
&\quad - (\mathbb{Z}_2^p \times \mathbb{Z}_1) - (\mathbb{Z}_2^p \times \mathbb{Z}_1), \\
\nabla \text{-deg}_{V_{4,1}} &= -(D_3^p \times \mathbb{Z}_2 \times D_2) - (D_5^p \times D_1) - (D_3^p \times D_1) \\
&\quad + 2(\mathbb{Z}_2^p \times D_1) - (\mathbb{Z}_1^p \times D_1) - (D_5^p \times D_5) - (D_5^p \times D_3) \\
&\quad + (V_4^p \times D_2 D_2) + (\mathbb{Z}_2^p \times D_1) + (A_4^p \times O(2)) \\
&\quad - (A_4^p \times \mathbb{Z}_3^p \times \mathbb{Z}_2) - (\mathbb{Z}_2^p \times \mathbb{Z}_2 \times \mathbb{Z}_2), \\
\nabla \text{-deg}_{V_{5,1}} &= -(D_3^p \times \mathbb{Z}_2 \times D_2) - (D_5^p \times \mathbb{Z}_2 \times D_2) - (V_4^p \times \mathbb{Z}_2 \times D_2) + 3(\mathbb{Z}_2^p \times \mathbb{Z}_2 D_2) \\
&\quad - (\mathbb{Z}_1^p \times D_1) - (D_5^p \times D_5) - (D_3^p \times D_3) + (V_4^p \times D_2 D_2) \\
&\quad + (\mathbb{Z}_2^p \times D_1) + (A_5^p \times O(2)) - (\mathbb{Z}_2^p \times \mathbb{Z}_2 \times \mathbb{Z}_2), \\
\nabla \text{-deg}_{V_{6,1}} &= -(D_3^p \times \mathbb{Z}_2 \times D_2) - (D_5^p \times \mathbb{Z}_2 \times D_2) - (V_4^p \times \mathbb{Z}_2 \times D_2) + 3(\mathbb{Z}_2^p \times \mathbb{Z}_2 D_2) \\
&\quad - (\mathbb{Z}_1^p \times D_1) - (D_5^p \times D_5) - (D_3^p \times D_3) + (V_4^p \times D_2 D_2) \\
&\quad + (\mathbb{Z}_2^p \times D_1) + (A_5^p \times O(2)) - (\mathbb{Z}_2^p \times \mathbb{Z}_2 \times \mathbb{Z}_2).
\end{align*}
\]
\[ \nabla \cdot \text{deg}_{V_{-1,1}} = -\left( A_5^p A_5 \times_{Z_2} D_2 \right) + \left( A_5^p \times O(2) \right), \]
\[ \nabla \cdot \text{deg}_{V_{-2,1}} = -\left( A_4^p A_4 \times_{Z_2} D_2 \right) - \left( D_3^p D_3 \times_{Z_2} D_2 \right) - \left( D_3^p D_3 \times_{Z_2} D_2 \right) - \left( V_4^p V_4 \times_{Z_2} D_2 \right) + 2\left( \mathbb{Z}_3^p Z_3 \times_{Z_2} D_2 \right) + 2\left( \mathbb{Z}_2^p Z_2 \times_{Z_2} D_2 \right) + 2\left( \mathbb{Z}_2^p Z_2 \times_{Z_2} D_2 \right) - 2\left( \mathbb{Z}_1^p Z_1 \times_{Z_2} D_2 \right) - \left( D_5^p Z_5 \times_{D_{10}} D_{10} \right) - \left( D_5^p Z_5 \times_{D_{10}} D_{10} \right) - \left( D_5^p Z_5 \times_{D_{10}} D_{10} \right) - \left( D_5^p Z_5 \times_{D_{10}} D_{10} \right) - \left( V_4^p Z_4 \times_{D_2} D_2 \right) + \left( V_4^p Z_4 \times_{D_2} D_2 \right) + \left( A_5^p \times O(2) \right) + \left( \mathbb{Z}_1^p Z_1 \times_{Z_2} Z_2 \right), \]
\[ \nabla \cdot \text{deg}_{V_{-3,1}} = -\left( D_5^p D_5 \times_{Z_2} D_2 \right) - \left( D_3^p D_3 \times_{Z_2} D_2 \right) - \left( V_4^p V_4 \times_{Z_2} D_2 \right) + 3\left( \mathbb{Z}_2^p Z_2 \times_{Z_2} D_2 \right) - \left( \mathbb{Z}_1^p Z_1 \times_{Z_2} D_2 \right) - \left( D_5^p Z_5 \times_{D_{10}} D_{10} \right) - \left( D_5^p Z_5 \times_{D_{10}} D_{10} \right) + \left( A_5^p \times O(2) \right) - \left( \mathbb{Z}_2^p Z_2 \times_{Z_2} Z_2 \right), \]
\[ \nabla \cdot \text{deg}_{V_{-4,1}} = -\left( D_5^p D_5 \times_{Z_2} D_2 \right) - \left( D_3^p D_3 \times_{Z_2} D_2 \right) - \left( V_4^p V_4 \times_{Z_2} D_2 \right) + 3\left( \mathbb{Z}_2^p Z_2 \times_{Z_2} D_2 \right) - \left( \mathbb{Z}_1^p Z_1 \times_{Z_2} D_2 \right) - \left( D_5^p Z_5 \times_{D_{10}} D_{10} \right) + \left( V_4^p Z_4 \times_{D_2} D_2 \right) + \left( A_5^p \times O(2) \right) - \left( \mathbb{Z}_2^p Z_2 \times_{Z_2} Z_2 \right). \]

Let us point out that the computational algorithms for the basic degrees truncated to $A(I \times O(2))$ where established in [9], and are now being effectively implemented into a computer software for equivariant gradient degree. Most of the maximal orbit types of periodic vibrations have finite Weyl groups, i.e., they are in the basic gradient degrees truncated to $A(I \times O(2))$. Nevertheless, we have detected in the basic gradient degree of the representations $V_{\pm 3,1}$ a maximal group with Weyl group of dimension one.

**Acknowledgement.** C. García was partially supported by PAPIIT-UNAM through grant IA105217. W. Krawcewicz acknowledge partial support from National Science Foundation through grant DMS-1413223.

**Acknowledgement.** C. García was partially supported by PAPIIT-UNAM through grant IA105217. W. Krawcewicz acknowledge partial support from National Science Foundation through grant DMS-1413223.
References

[1] Z. Balanov, W. Krawcewicz, and H. Ruan. Periodic solutions to O(2)-symmetric variational problems: $O(2) \times S^1$-equivariant gradient degree approach. In Nonlinear analysis and optimization II. Optimization, volume 514 of Contemp. Math., pages 45–84. Amer. Math. Soc., Providence, RI, 2010.

[2] Z. Balanov, W. Krawcewicz, S. a. Rybicki, and H. Steinlein. A short treatise on the equivariant degree theory and its applications. J. Fixed Point Theory Appl., 8(1):1–74, 2010.

[3] Z. Balanov, W. Krawcewicz, and H. Steinlein. Applied equivariant degree, volume 1 of AIMS Series on Differential Equations & Dynamical Systems. American Institute of Mathematical Sciences (AIMS), Springfield, MO, 2006.

[4] I. Berezovik, C. García-Azpeitia, and W. Krawcewicz. Symmetries of nonlinear vibrations in tetrahedral molecular configurations. ArXiv e-prints, 2017.

[5] I. Berezovik, Q. Hu, and W. Krawcewicz. Dihedral molecular configurations interacting by Lennard-Jones and Coulomb forces. ArXiv e-prints, 2017.

[6] Z. Berkai, M. Daoudi, N. Mendil, and A. Belghachi. Theoretical study of fullerene (C60) force field at room temperature. Energy Procedia, 74:59–64, 2015. The International Conference on Technologies and Materials for Renewable Energy, Environment and Sustainability TMREES15.

[7] T. Bröcker and T. tom Dieck. Representations of compact Lie groups, volume 98 of Graduate Texts in Mathematics. Springer-Verlag, New York, 1985.

[8] C. H. Choi, M. Kertesz, and L. Mihaly. Vibrational assignment of all 46 fundamentals of C60 and C606−: scaled quantum mechanical results performed in redundant internal coordinates and compared to experiments. Journal of Physical Chemistry A, 104:102–112, 2000.

[9] M. Dabkowski, W. Krawcewicz, Y. Lv, and H.-P. Wu. Multiple periodic solutions for Γ-symmetric Newtonian systems. J. Differential Equations, 263(10):6684–6730, 2017.

[10] C. García-Azpeitia and M. Tejada-Wriedt. Molecular chains interacting by Lennard-Jones and Coulomb forces. Qual. Theory Dyn. Syst., 16(3):591–608, 2017.

[11] K. Gęba. Degree for gradient equivariant maps and equivariant Conley index. In Topological nonlinear analysis, II (Frascati, 1995), volume 27 of Progr. Nonlinear Differential Equations Appl., pages 247–272. Birkhäuser Boston, Boston, MA, 1997.
[12] E. Goursat. Sur les substitutions orthogonales et les divisions régulières de l’espace. *Ann. Sci. École Norm. Sup. (3)*, 6:9–102, 1889.

[13] K. Hedberg, L. Hedberg, D. S. Bethune, C. A. Brown, H. C. Dorn, R. D. Johnson, and M. De Vries. Bond lengths in free molecules of buckminsterfullerene, C60, from gas-phase electron diffraction. *Science*, 254(5030):410–412, 1991.

[14] R. B. Hoyle. Shapes and cycles arising at the steady bifurcation with icosahedral symmetry. *Physica D: Nonlinear Phenomena*, 191(3):261 – 281, 2004.

[15] J. Ize and A. Vignoli. *Equivariant degree theory*, volume 8 of *De Gruyter Series in Nonlinear Analysis and Applications*. Walter de Gruyter & Co., Berlin, 2003.

[16] I. S. J. Montaldi, M. Roberts. Periodic solutions near equilibria of symmetric hamiltonian systems. *Philosophical Transactions of the Royal Society of London A: Mathematical, Physical and Engineering Sciences*, 325(1584):237–293, 1988.

[17] D. Jing and Z. Pan. Molecular vibrational modes of C60 and C70 via finite element method. *European Journal of Mechanics - A/Solids*, 28(5):948 – 954, 2009.

[18] W. Krawcewicz and J. Wu. *Theory of degrees with applications to bifurcations and differential equations*. Canadian Mathematical Society Series of Monographs and Advanced Texts. John Wiley & Sons, Inc., New York, 1997. A Wiley-Interscience Publication.

[19] H. W. Kroto, J. R. Heath, S. C. Obrien, R. F. Curl, and R. E. Smalley. C(60): Buckminsterfullerene. *Nature*, 318:162, 1985.

[20] J. A. Montaldi and R. M. Roberts. Relative equilibria of molecules. *Journal of Nonlinear Science*, 9(1):53–88, Feb 1999.

[21] F. Muoz-Almaraz, E. Freire, J. Galn, E. Doedel, and A. Vanderbauwhede. Continuation of periodic orbits in conservative and hamiltonian systems. *Physica D: Nonlinear Phenomena*, 181(1):1 – 38, 2003.

[22] S. a. Rybicki. Applications of degree for $S^1$-equivariant gradient maps to variational nonlinear problems with $S^1$-symmetries. *Topol. Methods Nonlinear Anal.*, 9(2):383–417, 1997.

[23] P. Schwerdtfeger, L. N. Wirz, and J. Avery. The topology of fullerenes. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, 5(1):96–145, 2015.

[24] E. H. Spanier. *Algebraic topology*. McGraw-Hill Book Co., New York-Toronto, Ont.-London, 1966.
[25] T. tom Dieck. Transformation groups, volume 8 of De Gruyter Studies in Mathematics. Walter de Gruyter & Co., Berlin, 1987.

[26] J. H. Walther, R. Jaffe, T. Halicioglu, and P. Koumoutsakos. Molecular dynamics simulations of carbon nanotubes in water. In Studying Turbulence Using Numerical Simulation Databases - VIII, pages 5–20. Center for Turbulence Research, 2000. Proceedings of the 2000 Summer Program.

[27] D. E. Weeks and W. G. Harter. Rotationvibration spectra of icosahedral molecules. II. icosahedral symmetry, vibrational eigenfrequencies, and normal modes of buckminsterfullerene. The Journal of Chemical Physics, 90(9):4744–4771, 1989.

[28] H.-P. Wu. A program for the computations of Burnside ring $A(\Gamma \times O(2))$. [http://bitbucket.org/psistwu/gammao2](http://bitbucket.org/psistwu/gammao2), 2016. Developed at University of Texas at Dallas.

[29] Z. C. Wu, D. A. Jelski, and T. F. George. Vibrational motions of buckminsterfullerene. Chemical Physics Letters, 137:291–294, 1987.