SYMMETRIES OF NONLINEAR VIBRATIONS IN TETRAHEDRAL MOLECULAR CONFIGURATIONS

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ABSTRACT. We study nonlinear vibrational modes of oscillations for tetrahedral configurations of particles. In the case of tetraphosphorus, the interaction of atoms is given by bond stretching and van der Waals forces. Using the equivariant gradient degree, we present a topological classification of the spatio-temporal symmetries of the periodic solutions with finite Weyl’s group. This procedure describes all the symmetries of the nonlinear vibrations for general force fields.

1. Introduction. Description of the dynamical motions of a collection of particles in space and time can provide a vast amounts of information, including molecular geometries, mean atomic fluctuations, and free energies. The molecular conformation is located at a local energy minimum where the net inter-particle force on each particle is close to zero and the position on the potential energy surface is stationary. Molecular motion can be modeled as vibrations around and interconversions between these stable configurations. Molecules spend most of their time in these low-lying states at a low temperature, which thus dominate the molecular properties of the system.

In this paper we study the molecular mechanics of tetrahedral molecules. Let $u(t) = (u_1(t), u_2(t), u_3(t), u_4(t))$ with $u_j(t) \in \mathbb{R}^3$ for $j = 1, 2, 3, 4$ stand for the spatial position of the system of 4-particles at time $t$. Such system satisfies the Newtonian equation

$$\ddot{u}(t) = -\nabla V(u(t)), \quad (1)$$

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where the potential energy \( V \) represents the force field given by
\[
V(u) := \sum_{1 \leq j < k \leq 4} U(|u_j - u_k|^2).
\]

When these 4-particles interact by bond stretching, van der Waals and electrostatic forces \([4, 13]\), \( U \) is given by
\[
U(x) = \left( \sqrt{x} - 1 \right)^2 + \left( \frac{B}{x^6} - \frac{A}{x^3} \right) + \frac{\sigma}{\sqrt{x}}.
\]

A local energy minimum is a stationary point \( a \in \mathbb{R}^{12} \) such that \( \nabla V(a) = 0 \). To detect possible periodic vibrations around the configuration \( a \), a natural method is to investigate the existence of periodic solutions to \((1)\) near \( a \). An important property of this molecular configuration is that it admits tetrahedral spatial symmetries, and thus the bifurcated/emerging periodic motions will have both spatial and temporal symmetry. In this case, the equation \((1)\) is equivariant under the action of the group
\[
S_4 \times O(3) \times O(2),
\]
which acts by permuting the particles, rotating and reflecting them in \( \mathbb{R}^3 \) and by temporal phase shift and reflection, respectively.

In this paper, we use the equivariant degree method to investigate the existence of periodic solution to \((1)\) around an equilibrium admitting \( S_4 \)-symmetries. The concept of equivariant gradient degree was introduced by K. Geba in \([14]\). This degree satisfies all the standard properties expected from a degree theory. In addition, it can also be generalized to settings in infinite-dimensional spaces, allowing its applications to studying critical points of invariant functionals (cf. \([2]\)). The values of the gradient equivariant degree can be expressed elegantly in the form
\[
\nabla_G \text{-deg}(\nabla \phi, \Omega) = n_1(H_1) + n_2(H_2) + \cdots + n_m(H_m), \quad n_k \in \mathbb{Z},
\]
where \((H_j)\) are the orbit types in \( \Omega \), which allow to predict the existence of various critical orbits for \( \phi \) and their symmetries. We should mention that the gradient degree is just one of many equivariant degrees (see \([2]\)) which were introduced in the last three decades: equivariant degrees with \( n \)-free parameters (primary degrees, twisted degrees), gradient and orthogonal equivariant degrees \([1, 16, 18]\). All of the above degrees are related to each other (cf. \([3, 24]\)). For multiple applications of the equivariant gradient degree to Newtonian system, we refer the reader to \([2, 8, 11, 12, 24, 25]\) and the references therein.

The local minimizer \( u_o \) of \( V \) is a regular tetrahedron located in a sphere of radius \( r_o \). Due to the fact that \( a \) is a local minimizer,
\[
\nu_0^2 := \frac{32}{3} r_o^2 U''(r_o) > 0.
\]
The 6 non-zero eigenvalues of \( D^2 V(u_o) \) are computed to be \( 4\nu_0^2 \) with multiplicity 1, \( 2\nu_0^2 \) with multiplicity 3, and \( \nu_0^2 \) with multiplicity 2. Then, the normal modes of \((1)\) are \( 2\nu_0, \sqrt{2}\nu_0, \) and \( \nu_0 \), which correspond to the irreducible representations \( A_1, T_1, \) and \( E \) (Mulliken Symbols), respectively.

Observe that the normal mode \( \nu_0 \) is \( 1 : 1 : 2 \) resonant. Due to multiplicities and resonances, the Lyapunov center theorem can be applied to prove only the local existence of a periodic solution (nonlinear normal modes) with the frequency \( 2\nu_0 \) \([19]\). On the other hand, since the equilibrium corresponds to a local minimizer of the Hamiltonian, the Weinstein-Moser theorem \([22]\) gives the existence of at least
6 periodic orbits in each (small) fixed energy level. Using the gradient equivariant degree method, we establish the global existence of branches of periodic solutions emerging from the equilibrium $u_0$, starting with the frequencies of the normal modes $2\nu_0$, $\sqrt{2}\nu_0$, and $\nu_0$. The global property means that families of periodic solutions are represented by a continuum, which has norm or period going to infinity, ends in a collision orbit, or comes back to another equilibrium.

Specifically, we prove that the tetrahedral equilibrium $u_0$ has the following global families of periodic solutions: one family with the frequency $2\nu_0$, five families with the frequency $\sqrt{2}\nu_0$, and one with the frequency $\nu_0$. If there were no resonances at $\nu_0$, the number of solutions arising from $\nu_0$ would be three. The family with the frequency $2\nu_0$ has symmetries of a brake orbits where all the particles form a regular tetrahedron at any time. The first such symmetry gives brake orbits where two pairs of particles are related by inversion, and the second symmetry where one pair of particles is related by inversion and another by a $\pi$-rotation and $\pi$-phase shift. The third symmetry, arising from the solutions with the frequency $\sqrt{2}\nu_0$, is not a brake orbit, while the particles are related by a $\pi/2$-rotoreflection and $\pi/2$-phase shift. The fourth symmetry, arising from the solutions with the frequency $\sqrt{2}\nu_0$, is a brake orbit where three particles form a triangle at all times, while another makes counterbalance movement. The fifth symmetry, arising from the solutions with the frequency $\nu_0$, has symmetries of brake orbits with two symmetries by inversion at any time. The exact description of the symmetries is given in Section 5.

The article [10] presents an extensive study of existence and stability of nonlinear modes for tetraphosphorus molecules. The authors assume the absence of resonances in the normal form of the Hamiltonian. Since in our study, we consider the nonlinear normal modes of a force field which expresses mutual interaction between the atoms, we obtain a Hamiltonian with resonances.

Methane molecule is another molecule which possesses tetrahedral symmetries. It has an equilibrium state with a carbon atom at the center and four hydrogen atoms at the vertices of a regular tetrahedron. The articles [20, 21] use a combination of geometric methods, normal forms, and Krein signature to analyze the existence of nonlinear modes and their stability. These results can be easily extrapolated to the tetraphosphorus molecule which have the same symmetries but different configuration. In this sense, the symmetries and number of solutions obtained in [20, 21] for each frequency coincide with our results. Additionally, the gradient equivariant degree allows to determine global properties of the branches and to manage resonances. Nevertheless, more precise local information can be obtained with the results of [20, 21, 10].

The paper is structured as follows. In Section 2, we analyze the isotypic decomposition of the eigenvalues of the Hessian $D^2V(u_0)$. In Section 3, we prove the global existence of families of periodic solutions from the tetrahedral equilibrium. In Section 4, we describe the symmetries of the different families of periodic solutions. In Appendix, we review preliminary notions and definitions used in group representations, along with the properties of the equivariant gradient degree and indicate the standard techniques used to compute it.

2. Model for atomic interaction. Consider 4 identical particles $u_j$ in the space $\mathbb{R}^3$, for $j = 1, 2, 3, 4$. Assume that each particle $u_j$ interacts with all other particles
\( u_k \) for \( k \neq j \). Put \( u := (u_1, u_2, u_3, u_4)^T \in \mathbb{R}^{12} \) and
\[
\hat{\Omega}_o := \{u \in \mathbb{R}^{12} : \forall_{k \neq j} \ u_k \neq u_j \}.
\]
The Newtonian equation that describes the interaction between these 4-particles is
\[
\ddot{u} = -\nabla V(u), \quad u \in \hat{\Omega}_o.
\]
(2)

The potential energy \( V : \hat{\Omega}_o \to \mathbb{R} \),
\[
V(u) := \sum_{1 \leq j < k \leq 4} U(|u_j - u_k|^2),
\]
is well defined, and when \( U \in C^2(\mathbb{R}^+) \), \( U \) satisfies
\[
\lim_{x^+ \to 0} U(x) = \infty, \quad \lim_{x \to \infty} U(x) = \infty.
\]
(4)

Classical forces used in molecular mechanics are associated with bending between adjacent particles, electrostatic interactions, and van der Walls forces. The condition (4) holds when \( U \) is determined by these force fields.

2.1. The tetrahedral equilibrium. One can easily notice that the space \( \mathbb{R}^{12} \) is a representation of the group
\[
\mathfrak{G} := S_4 \times O(3),
\]
where \( S_4 \) stands for the symmetric group of four elements. More precisely \( S_4 \) is the group of permutations of four elements \( \{1, 2, 3, 4\} \). Then the action of \( \mathfrak{G} \) on \( \mathbb{R}^{12} \) is given by
\[
(\sigma, A)(u_1, u_2, u_3, u_4)^T = (Au_{\sigma(1)}, Au_{\sigma(2)}, Au_{\sigma(3)}, Au_{\sigma(4)})^T,
\]
where \( A \in O(3) \) and \( \sigma \in S_4 \).

Notice that \( S_4 \) can be considered as a subgroup of \( O(3) \), representing the actual symmetries of a tetrahedron \( T \subset \mathbb{R}^3 \). More precisely, consider the regular tetrahedron given by
\[
T := \{\gamma_1, \gamma_2, \gamma_3, \gamma_4\},
\]
where
\[
\gamma_1 = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}, \quad \gamma_2 = \begin{pmatrix} \frac{2}{3} \sqrt{2} \\ 0 \\ -\frac{1}{3} \end{pmatrix}, \quad \gamma_3 = \begin{pmatrix} -\frac{1}{3} \sqrt{2} \\ \frac{\sqrt{3}}{3} \sqrt{6} \\ -\frac{1}{3} \end{pmatrix}, \quad \gamma_4 = \begin{pmatrix} -\frac{1}{3} \sqrt{2} \\ -\frac{\sqrt{3}}{3} \sqrt{6} \\ -\frac{1}{3} \end{pmatrix}.
\]
The tetrahedral group \( \{A \in O(3) : A(T) = T\} \) can be identified with the group \( S_4 \). Indeed, any \( A \) such that \( A(T) = T \) permutes the vertices of \( T \), i.e.
\[
A\gamma_j = \gamma_{\sigma(j)}
\]
for \( j = 1, 2, 3, 4 \). Thus, we can identify \( A_{\sigma} \) with the permutation \( \sigma \in S_4 \) by these relations. Explicitly, for the permutations \((1, 2)\) and \((2, 3, 4)\), which are generators of \( S_4 \), we have the following identification
\[
A_{(1,2)} = \begin{bmatrix} \frac{1}{3} & 0 & \frac{2}{3} \\ 0 & 1 & 0 \\ \frac{2}{3} & 0 & 1 \end{bmatrix} \quad \text{and} \quad A_{(2,3,4)} = \begin{bmatrix} -\frac{1}{3} & -\frac{\sqrt{2}}{2} & 0 \\ \frac{\sqrt{2}}{2} & 1 & 0 \\ -\frac{1}{3} & -\frac{\sqrt{2}}{2} & 0 \end{bmatrix}.
\]
These generators define an explicit isomorphism \( A_{\sigma} : S_4 \to O(3) \).
Notice that the function \( V : \tilde{\Omega}_o \to \mathbb{R} \) is invariant with respect to the action of \( c \in \mathbb{R}^3 \) on \((\mathbb{R}^3)^4\) by shifting, \( V(u + c) = V(u) \). Therefore in order to fix the center of mass at the origin in the system (2), we define the subspace
\[
\mathcal{V} := \{(u_1, u_2, u_3, u_4)^T \in (\mathbb{R}^3)^4 : u_1 + u_2 + u_3 + u_4 = 0\}
\]
and \( \Omega_o = \tilde{\Omega}_o \cap \mathcal{V} \). Then, one can easily notice that \( \mathcal{V} \) and \( \Omega_o \) are invariant under the nonlinear dynamics of (2), and, in addition, \( \Omega_o \) is \( G \)-invariant.

Consider the point \( v_0 := (\gamma_1, \gamma_2, \gamma_3, \gamma_4) \in \Omega_o \). The isotropy group \( \Phi_{v_0} \) is given by
\[
\tilde{S}_4 := \{(\sigma, A_\sigma) \in S_4 \times O(3) : \sigma \in S_4\},
\]
where \( S_4 \) is considered as a subgroup of \( O(3) \), using the above identification for \( A_\sigma \). Since \( \tilde{S}_4 \) is a finite group, \( \mathcal{V}^{\tilde{S}_4} \) is a one-dimensional subspace of \( \mathcal{V} \), and we have that
\[
\mathcal{V}^{\tilde{S}_4} = \text{span}_{\mathbb{R}}\{(\gamma_1, \gamma_2, \gamma_3, \gamma_4)^T\}.
\]
Then, by Symmetric Criticality Condition, a critical point of \( V^{\tilde{S}_4} : \Omega^{\tilde{S}_4}_o \to \mathbb{R} \) is also a critical point of \( V \). Since \( \mathcal{V}^{\tilde{S}_4} \) is one-dimensional, we denote its vectors by \( rv_0 \in \mathbb{R}^{12} \) for \( r \in \mathbb{R} \). Notice that
\[
\phi(r) := \sum_{1 \leq j < k \leq 4} U\left(\frac{8}{3} r^2\right), \quad r > 0.
\]
is exactly the restriction of \( V \) to the fixed-point subspace \( \mathcal{V}^{\tilde{S}_4} \cap \Omega_o \). Thus in order to find an equilibrium for (2), by Symmetric Criticality Principle, it is sufficient to identify a critical point \( r_o \) of \( \phi(r) \). Clearly by (4),
\[
\lim_{r \to 0^+} \phi(r) = \lim_{r \to \infty} \phi(r) = \infty.
\]
Then, there exists a minimizer \( r_o \in (0, \infty) \), which is clearly a critical point of \( \varphi \). Consequently,
\[
u_o := r_o v_0 \in \Omega_o
\]
is the \( \tilde{S}_4 \)-symmetric equilibrium of \( V \). The components of \( u_o \), which are \( r_o \gamma_j \) for \( j = 1, 2, 3, 4 \), give us the configuration of the stationary solution of (2), see Figure 1.

![Figure 1](image-url)

**Figure 1.** Stationary solution to equation (2) with tetrahedral symmetries.
2.2. Isotypic decomposition. Since the system (2) is symmetric with respect to the group action $\mathcal{G} := S_4 \times O(3)$, we have that the orbit of equilibria $\mathcal{G}(u_o)$ is a 3-dimensional submanifold in $\mathcal{Y}$. The slice $S_o$ to the orbit $\mathcal{G}(u_o)$ at $u_o$ is

$$ S_o := \{ x \in \mathcal{Y} : x \cdot T_{u_o} \mathcal{G}(u_o) = 0 \} . $$

The tangent space $T_{u_o} \mathcal{G}(u_o)$ is described as

$$ T_{u_o} \mathcal{G}(u_o) = \text{span}\{(J_j \gamma_1, J_j \gamma_2, J_j \gamma_3, J_j \gamma_4)^T \in \mathcal{Y} : j = 1, 2, 3\} , $$

where $J_j$ are the three infinitesimal generators of the rotations:

$$ J_1 := \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{bmatrix} , \quad J_2 := \begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \end{bmatrix} , \quad J_3 := \begin{bmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} . $$

Since the $\mathcal{G}$-isotropy group of $u_o$ is $\tilde{S}_4$, $S_o$ is an orthogonal $\tilde{S}_4$ representation. To identify the $\tilde{S}_4$-isotypic components, we consider first the $\tilde{S}_4$-representation $V = \mathbb{R}^{12}$ on which $\tilde{S}_4$-acts by (5). We have the following table of characters $\chi_j$, $j = 0, 1, 2, 3, 4$, for all irreducible $\tilde{S}_4$-representations $V_j$ (all of them of real type) and the character $\chi_V$ of the representation $V$:

| Rep. | Character | $(1)$ | $(1, 2)$ | $(1, 2)(3, 4)$ | $(1, 2, 3)$ | $(1, 2, 3, 4)$ |
|------|-----------|-------|----------|---------------|-------------|---------------|
| $V_0$ | $\chi^0$ | 1 | 1 | 1 | 1 | 1 |
| $V_1$ | $\chi^1$ | 3 | 1 | -1 | 0 | -1 |
| $V_2$ | $\chi^2$ | 2 | 0 | 2 | -1 | 0 |
| $V_3$ | $\chi^3$ | 3 | -1 | -1 | 0 | 1 |
| $V_4$ | $\chi^4$ | 1 | -1 | 1 | 1 | -1 |
| $V$ | $\chi_V$ | 12 | 2 | 0 | 0 | 0 |

One can easily conclude that we have the following $\tilde{S}_4$-isotypic decomposition:

$$ V = V_0 \oplus (V_1 \oplus V_1) \oplus V_2 \oplus V_3 . $$

Since the subspace $V$ is obtained by fixing the center of mass at the origin, and $\{ (v, v, v, v) \in \mathbb{R}^{12} : v \in \mathbb{R}^3 \}$ is equivalent to the irreducible $\tilde{S}_4$-representation $V_1$, we have the the $\tilde{S}_4$-isotypic decomposition

$$ \mathcal{Y} = V_0 \oplus V_1 \oplus V_2 \oplus V_3 , \quad V_j = V_j . \quad (8) $$

In order to determine the $\tilde{S}_4$-isotypic type of the tangent space $T_{u_o} \mathcal{G}(u_o)$ (which has to be an irreducible $\tilde{S}_4$-representation of dimension 3), we apply the isotypic projections $P_j : V \rightarrow V_j$, $j = 1$ and 3, given by

$$ P_j v := \frac{\dim(V_j)}{72} \sum_{g \in \tilde{S}_4} \chi_j(g) g v , \quad v \in V , $$

to conclude that $T_{u_o} \mathcal{G}(u_o) \simeq V_3$. Therefore, the $\tilde{S}_4$-isotypic decomposition of the slice $S_o$ is

$$ S_o = V_0 \oplus V_1 \oplus V_2 . \quad (9) $$
2.3. Computation of the spectrum $\sigma(\nabla^2 V(u_0))$. Since the potential $V$ is given by (3), we have

$$\nabla V(u) = 2 \begin{bmatrix} \sum_{k \neq 0} U'(|u_0 - u_k|^2)(u_0 - u_k) \\ \sum_{k \neq 1} U'(|u_1 - u_k|^2)(u_1 - u_k) \\ \vdots \\ \sum_{k \neq n-1} U'(u_{n-1} - u_k)(u_{n-1} - u_k) \end{bmatrix}.$$ 

Notice that we have $\nabla V(u_o) = 0$ when $U'(r_o) = 0$.

For a given vector $v = (x, y, z)^T \in \mathbb{R}^3$, we define the matrix $m_v := vv^T$, i.e.

$$m_v := \begin{bmatrix} x \\ y \\ z \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} x^2 & xy & xz \\ xy & y^2 & yz \\ xz & yz & z^2 \end{bmatrix}.$$ 

Then one can easily see that the matrix $m_v$ represents the linear operator $\|v\|^2 P_v : \mathbb{R}^3 \to \mathbb{R}^3$, where $P_v$ is the orthogonal projection onto the subspace generated by $v \in \mathbb{R}^3$. Put

$$m_{j,k} := m_{(\gamma_j - \gamma_k)}.$$ 

Clearly, $m_{j,k} = m_{k,j}$. Notice that

$$m_{j,k} (\gamma_j) = \frac{4}{3}(\gamma_j - \gamma_k).$$

By direct computations, one can derive the following matrix form of $\nabla^2 V(u_o)$

$$M := \nabla^2 V(u_o) = 4r_o^2 U''(r_o)$$

$$M := \begin{bmatrix} \sum_{j \neq 1} m_{1j} & -m_{12} & -m_{13} & -m_{14} \\ -m_{21} & \sum_{j \neq 2} m_{2j} & -m_{23} & -m_{24} \\ -m_{31} & -m_{32} & \sum_{j \neq 3} m_{3j} & -m_{34} \\ -m_{41} & -m_{42} & -m_{43} & \sum_{j \neq 4} m_{4j} \end{bmatrix}.$$ 

Since $M : \mathcal{V} \to \mathcal{V}$ is $\tilde{S}_4$-equivariant, it follows that

$$M_j := M|_{V_j} : V_j \to V_j, \quad j = 0, 1, 2.$$ 

Since the sub-representations $V_j = V_j$ are absolutely irreducible, we have that

$$M_j = \mu_j \text{Id} : V_j \to V_j, \quad j = 0, 1, 2,$$

which implies $\sigma(M|_{S_n}) = \{\mu_0, \mu_1, \mu_2\}$.

To find explicit formulae for the eigenvalues $\mu_j$, we notice that

$$v_0 := \begin{bmatrix} \gamma_1 \\ \gamma_2 \\ \gamma_3 \\ \gamma_4 \end{bmatrix} \in V_0, \quad v_1 := \begin{bmatrix} -2\gamma_1 \\ \gamma_1 + \gamma_2 \\ \gamma_1 + \gamma_3 \\ \gamma_1 + \gamma_4 \end{bmatrix} \in V_1, \quad v_2 := \begin{bmatrix} \gamma_2 - \gamma_3 \\ \gamma_1 - \gamma_4 \\ \gamma_1 - \gamma_1 \\ \gamma_3 - \gamma_2 \end{bmatrix} \in V_2.$$
By direct application of the matrix $\mathcal{L}$ on the vectors $\mathbf{v}_j$, $j = 0, 1, 2$, we obtain that

\[
\begin{align*}
\mu_0 &= \frac{128}{3} r_o^2 U''(r_o) = 4\nu_0^2, \\
\mu_1 &= \frac{64}{3} r_o^2 U''(r_o) = 2\nu_0^2, \\
\mu_2 &= \frac{32}{3} r_o^2 U''(r_o) = \nu_0^2.
\end{align*}
\]

Notice that $0 < \mu_2 < \mu_1 < \mu_0$.

3. **Equivariant bifurcation.** In what follows, we are interested in finding non-trivial $T$-periodic solutions to (2), bifurcating from the orbit of equilibrium points $\mathfrak{O}(u_0)$. By normalizing the period, i.e. by making the substitution $v(t) := u \left(\frac{t}{\mu T}\right)$ in (2), we obtain the following system

\[
\begin{align*}
\ddot{v} &= -\lambda^2 \nabla V(v), \\
v(0) &= v(2\pi), \quad \dot{v}(0) = \dot{v}(2\pi),
\end{align*}
\tag{10}
\]

where $\lambda^{-1} = 2\pi/T$ is the frequency.

3.1. **Equivariant gradient map.** Since $\mathcal{V}$ is an orthogonal $\mathfrak{G}$-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

$$\langle u, v \rangle := \int_0^{2\pi} (\dot{u}(t) \cdot \dot{v}(t) + u(t) \cdot v(t)) dt.$$  

Let $O(2) = SO(2) \cup \kappa \cdot SO(2)$ 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 $H^1_{2\pi}(\mathbb{R}, \mathcal{V})$ is an orthogonal Hilbert representation of

$$G := \mathfrak{G} \times O(2), \quad \mathfrak{G} = S_4 \times O(3).$$

Indeed, for $u \in H^1_{2\pi}(\mathbb{R}, \mathcal{V})$ and $(\sigma, A) \in \mathfrak{G}$ (see (5)), we have

\[
\begin{align*}
(\sigma, A) u(t) &= (\sigma, A) u(t), \\
e^{i\tau} u(t) &= u(t + \tau), \\
\kappa u(t) &= u(-t).
\end{align*}
\tag{11}
\]

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

Put

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

Then, the system (10) can be written as the following variational equation

$$\nabla_u J(\lambda, u) = 0, \quad (\lambda, u) \in \mathbb{R} \times \Omega, \tag{12}$$
where $J : \mathbb{R} \times \Omega \to \mathbb{R}$ is defined by
\[
J(\lambda, u) := \int_0^{2\pi} \left[ \frac{1}{2} \dot{u}(t)^2 - \lambda^2 V(u(t)) \right] dt. \tag{13}
\]
Assume that $u_0 \in \mathbb{R}^{12}$ is the equilibrium point of (2) described in subsection 2.1. Then, clearly, $u_0$ is a critical point of $J$. We are interested in finding non-stationary $2\pi$-periodic solutions bifurcating from $u_0$, i.e. non-constant solutions to system (12).

We consider the $G$-orbit of $u_0$ in the space $H^1(S^1, \mathcal{V})$. By $\mathcal{S}_o$, we denote the slice to $G(u_0)$ in $H^1(S^1, \mathcal{V})$. By
\[
\mathcal{J} : \mathbb{R} \times (\mathcal{S}_o \cap \Omega) \to \mathbb{R}
\]
we will also denote the restriction of $J$ to the set $\mathcal{S}_o \cap \Omega$. Clearly, $\mathcal{J}$ is $G_{u_0}$-invariant. Then, the orbit $G(u_0)$ is orthogonal to the slice $\mathcal{S}_o$, critical points of $\mathcal{J}$ are critical points of $J$ in a small tubular neighborhood of the orbit $G(u_0)$. Consequently, these critical points are solutions to system (12). This property allows to establish the Slice Criticality Principle (see Theorem 5.4) for computing the $G$-equivariant gradient degree of $J$ on this small tubular neighborhood. This computation, in its turn, will provide us the full equivariant topological classification of all non-constant periodic orbits, bifurcating from the equilibrium $u_o$.

Consider the operator $L : H^2(S^1; \mathcal{V}) \to L^2(S^1; \mathcal{V})$, given by $Lu = -\ddot{u} + u$, $u \in H^2(S^1, \mathcal{V})$. 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
\[
\nabla_u J(\lambda, u) = u - j \circ L^{-1} (\lambda^2 \nabla V(u) + u), \tag{14}
\]
where $u \in H^1(S^1, \mathcal{V})$. Consequently, the bifurcation problem (12) can be written as $u - j \circ L^{-1} (\lambda^2 \nabla V(u) + u) = 0$. Moreover, we have
\[
\nabla_u^2 J(\lambda, u_0)v = v - j \circ L^{-1} (\lambda^2 \nabla^2 V(u_0)v + v), \tag{15}
\]
where $v \in H^1(S^1, \mathcal{V})$.

Consider the operator
\[
\mathcal{A}(\lambda) := \nabla_u^2 J(\lambda, u_0) |_{\mathcal{S}_o} : \mathcal{S}_o \to \mathcal{S}_o. \tag{16}
\]
Notice that
\[
\nabla_u^2 \mathcal{J}(\lambda, u_0) = \mathcal{A}(\lambda).
\]
Thus, by implicit function theorem, $G(u_0)$ is an isolated orbit of critical points of $J$, whenever $\mathcal{A}(\lambda)$ is an isomorphism. Therefore, if a point $(\lambda_o, u_0)$ is a bifurcation point for (12), then $\mathcal{A}(\lambda_o)$ cannot be an isomorphism. In such a case we put
\[
\Lambda := \{ \lambda > 0 : \mathcal{A}(\lambda) \text{ is not an isomorphism} \},
\]
and we call the set $\Lambda$ 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 (11)). 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.
\[
H^1(S^1, \mathcal{V}) = \mathcal{V} \oplus \mathcal{W}, \quad \mathcal{W} := \mathcal{V}^{S^1}.
\]
Then, the slice $\mathcal{S}_o$ in $H^1(S^1, \mathcal{V})$ to the orbit $G(u_0)$ at $u_0$ is exactly
\[
\mathcal{S}_o = \mathcal{S}_o \oplus \mathcal{W}.
\]
Since the eigenvalues are $\mu_j \neq 0$ for $j = 0, 1, 2$, any $\lambda_0 \in \Lambda$ satisfying the condition $\mathcal{A}(\lambda_0)|_{S_o} : S_o \to S_o$ is an isomorphism. This, in its turn, leads to the following theorem:

**Theorem 3.1.** Consider the bifurcation system (12) and assume that $\lambda_0 \in \Lambda$ is isolated in the critical set $\Lambda$, i.e. there exists $\lambda_- < \lambda_0 < \lambda_+$ such that $[\lambda_-, \lambda_+] \cap \Lambda = \{\lambda_0\}$. Define
\[ \omega_G(\lambda_o) := \nabla_{G_{u_o}} \text{deg}(\mathcal{A}(\lambda_+), B_1(0)) - \nabla_{G_{u_o}} \text{deg}(\mathcal{A}(\lambda_-), B_1(0)), \]
where $B_1(0)$ stands for the open unit ball in $\mathcal{H}$. 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 (12) from the orbit $\{\lambda_o\} \times G(u_o)$ with symmetries at least $(H_j)$.

Consider the $S^1$-isotypic decomposition of $\mathcal{H}$, i.e.
\[ \mathcal{H} = \bigoplus_{l=1}^{\infty} \mathcal{H}_l, \quad \mathcal{H}_l := \{\cos(l \cdot) a + \sin(l \cdot) b : a, b \in \mathcal{V}\}. \]
In a standard way, the space $\mathcal{H}_l$, $l = 1, 2, \ldots$, can be naturally identified with the space $\mathcal{V}^C$ on which $S^1$ acts by $l$-folding,
\[ \mathcal{H}_l = \{e^{l \cdot z} : z \in \mathcal{V}^C\}. \]
Since the operator $\mathcal{A}(\lambda)$ is $G_{u_o}$-equivariant with
\[ G_{u_o} = \tilde{S}_4 \times O(2), \]
it is also $S^1$-equivariant, and thus $\mathcal{A}(\lambda)(\mathcal{H}_l) \subset \mathcal{H}_l$. Using the $\tilde{S}_4$-isotypic decomposition of $\mathcal{V}^C$, we have the $G_{u_o}$-isotypic decomposition
\[ \mathcal{H}_l = W_{0,l} \oplus W_{1,l} \oplus W_{2,l} \oplus W_{3,l}, \quad W_{j,l} = W_{j,l}. \]
Moreover, we have
\[ \mathcal{A}(\lambda)|_{W_{j,l}} = \left(1 - \frac{l^2 \mu_j + 1}{l^2 + 1}\right) \text{Id}, \]
which implies that $\lambda_o \in \Lambda$ if and only if $\lambda_o^2 = l^2 / \mu_j$ for some $l = 1, 2, 3, \ldots$ and $j = 0, 1, 2$.

Then, the critical set $\Lambda$ for the equilibrium $u_o$ of the system (2) is
\[ \Lambda := \left\{ \frac{l}{\sqrt{\mu_j}} : j = 0, 1, 2, \quad l = 1, 2, 3, \ldots \right\}, \]
and we can identify the critical numbers $\lambda \in \Lambda$ as
\[ \lambda_{j,l} = \frac{l}{\sqrt{\mu_j}}. \]
Due to the resonances, the critical numbers are not uniquely identified by the indices $(j, l)$. Indeed, let us list the first critical numbers from $\Lambda$
\[ \lambda_{0,1} < \lambda_{1,1} < \lambda_{2,1} = \lambda_{0,2} < \lambda_{1,2} < \lambda_{2,2} = \lambda_{0,4}. \]

**Definition 3.2.** For simplicity, hereafter, we denote by $S_4$ the isotropy group $G_{u_o} = \tilde{S}_4$, i.e. with this notation we write
\[ G_{u_o} = \mathcal{G}_{u_o} \times O(2) = S_4 \times O(2). \]
From the computation of the gradient degree in (32) with $G_{u_0}$, we obtain

$$
\nabla_{G_{u_0}} \text{deg} \left( \varphi(\lambda_0), B_1(0) \right) = \prod_{\{(j,i) \in \mathbb{N}^2 : \lambda_j < \lambda_i \}} \nabla \text{deg}_{W_{j,i}} \quad (17)
$$

for $\lambda \notin \Lambda$.

For each critical number $\lambda_{j,i}$, we choose two numbers $\lambda_- < \lambda_{j,i} < \lambda_+$ such that $[\lambda_- , \lambda_+] \cap \Lambda = \{ \lambda_{j,i} \}$. Calculating the difference of the gradient degree at $\lambda_+$ and $\lambda_-$ using (17), we obtain that the equivariant invariants are given by

$$
\omega_G(\lambda_0, 1) = \nabla \text{deg}_{W_{0,1}} - (S_4 \times O(2))
$$

$$
\omega_G(\lambda_{1,1}) = \nabla \text{deg}_{W_{1,1}} \ast \left( \nabla \text{deg}_{W_{1,1}} - (S_4 \times O(2)) \right)
$$

$$
\omega_G(\lambda_{2,1}) = \nabla \text{deg}_{W_{0,1}} \ast \nabla \text{deg}_{W_{1,1}} \ast \left( \nabla \text{deg}_{W_{2,1}} \ast \nabla \text{deg}_{W_{0,2}} - (S_4 \times O(2)) \right)
$$

3.3. Computation of the gradient degree. Given two groups $G_1$ and $G_2$, we consider the product group $G_1 \times G_2$. The well-known result (see \cite{8,15}) provides a description of the product group $G_1 \times G_2$. Namely, for any subgroup $\mathcal{H}$ of the product group $G_1 \times G_2$, there exist subgroups $H \leq G_1$ and $K \leq G_2$, a group $L$, and two epimorphisms $\varphi : H \to L$ and $\psi : K \to L$ such that

$$
\mathcal{H} = \{(h,k) \in H \times K : \varphi(h) = \psi(k)\}. \quad (18)
$$

In this case, we will use the notation

$$
\mathcal{H} =: H^\varphi \times_L^\psi K
$$

and the group $H^\varphi \times_L^\psi K$ will be called an amalgamated subgroup of $G_1 \times G_2$.

Therefore, any closed subgroup $\mathcal{H}$ of $S_4 \times O(2)$ is an amalgamated subgroup $H^\varphi \times_L^\psi K$, where $H \leq S_4$ and $K \leq O(2)$. To make the amalgamated subgroup notation simpler and self-contained we will assume that

$$
L = K/\ker(\psi).
$$

Therefore, $\psi : K \to L$ is evidently the natural projection, and there is no need to indicate it. On the other hand, the group $L$ can be naturally identified with a finite subgroup of $O(2)$ being either $D_n$ or $Z_n$, $n \geq 1$. Since we are interested in describing conjugacy classes of $\mathcal{H}$, we can identify the epimorphism $\varphi : H \to L$ by indicating

$$
Z = \ker(\varphi) \quad \text{and} \quad R = \varphi^{-1}(\langle r \rangle),
$$

where $r$ is the rotation generator in $L$ and $\langle r \rangle$ is the cyclic subgroup generated by $r$. Then, instead of using the notation $H^\varphi \times_L^\psi K$, we will write

$$
\mathcal{H} =: H^Z \times_L^R K, \quad (19)
$$

where $H$, $Z$, and $R$ are subgroups of $S_4$ identified by

$$
\begin{align*}
V_4 &= \{(1), (12)(34), (13)(24), (14)(23)\}, \\
D_4 &= \{(1), (1324), (12)(34), (1423), (34), (14)(23), (12), (13)(24)\}, \\
Z_4 &= \{(1), (1324), (12)(34), (1423)\}, \\
D_3 &= \{(1), (123), (132), (12), (23), (13)\}, \\
D_2 &= \{(1), (12)(34), (12), (34)\}, \\
D_1 &= \{(1), (12)\}.
\end{align*}
$$
If all the epimorphisms $\varphi$ with the kernel $Z$ are conjugate, there is no need to use the symbol $R$ in (19). Therefore, we will simply write $\mathcal{H} = H^2 \times L K$. In addition, if all epimorphisms $\varphi$ from $H$ to $L$ are conjugate, we can also omit the symbol $Z$, i.e. we will write $\mathcal{H} = H \times L K$.

The notation above is useful to obtain the classification of the all conjugacy classes ($\mathcal{H}$) of closed subgroups in $S_4 \times O(2)$.

Let us point out that to obtain a complete equivariant classification of the bifurcating branches of nontrivial solutions, the full topological invariants $\omega_G(\lambda_{j_{r,1}}) \in U(I \times O(2))$ should be considered. In particular, although it is not the case here, the invariant $\omega_G(\lambda_{j_{r,1}})$ may contain maximal orbit types $(H)$ with infinite Weyl’s group $W(H)$. Therefore, we consider the truncation to $A(I \times O(2))$ given by

$$\tilde{\omega}_G(\lambda_{j_{r,1}}) := \pi_0\left(\omega_G(\lambda_{j_{r,1}})\right),$$

where $\pi_0 : U(G) \rightarrow A(G)$ is a ring homomorphism. Other more complex molecular structures may require the full value of the invariant $\omega_G(\lambda_{j_r})$ in the Euler ring $U(G)$. We should keep in mind that it is necessary to use the full $G$-equivariant gradient degree for its analysis.

We use GAP programming (see [23]) to compute the basic degrees truncated to $A(G)$:

\begin{align*}
\text{Deg}_{W_0,1} &= - (S_4 \times D_1) + (S_4 \times O(2)), \\
\text{Deg}_{W_1,1} &= - (D_4 \times D_2 \times Z_2 D_2) - (D_2 \times D_1 \times Z_2 D_2) - (D_4 \times Z_1 \times D_1 D_4) - (D_4 \times D_1) \\
&\quad - (D_3 \times Z_2 \times D_4) + 2(D_1 \times D_1) - (Z_4 \times D_4) + (Z_2 \times Z_2 D_2) \\
&\quad + (D_2 \times Z_2 \times D_2) + (V_4 \times D_1 \times D_2) + (D_2 \times D_1 \times D_1) - (Z_2 \times D_2) + (S_4 \times O(2)), \\
\text{Deg}_{W_2,1} &= - (S_4 \times D_4) - (D_4 \times D_1) + (V_4 \times D_1) - (D_4 \times V_2 \times Z_2 D_2) \\
&\quad + 2(D_4 \times D_1, D_1) + (S_4 \times O(2)), \\
\text{Deg}_{W_3,1} &= - (D_4 \times Z_2 \times D_2) - (D_4 \times Z_1 \times D_4) - (D_2 \times D_1 \times D_2) + 2(D_1 \times Z_1 \times D_2) \\
&\quad + (Z_2 \times D_1 \times D_2) - (Z_4 \times D_1) - (D_3 \times Z_2 \times D_3 D_4) + (Z_2 \times D_1 \times D_2) + (V_4 \times D_1 \times D_2) - (Z_2 \times Z_2 \times D_1) \\
&\quad + (S_4 \times O(2)), \\
\text{Deg}_{W_4,1} &= - (S_4 \times D_4 \times Z_2 D_2) + (S_4 \times O(2)),
\end{align*}

Next, we again use GAP programming (see [23]) and the product $*$ of the Euler ring $U(\Gamma)$ to compute the full equivariant invariants $A(I \times O(2))$, where the maximal
isotropy classes are colored red:
\[
\overline{\omega}_G(\lambda_{0,1}) = -(S_4 \times D_1),
\]
\[
\overline{\omega}_G(\lambda_{1,1}) = -(D_4^{D_2 \times Z_2 D_2} - (D_2^{D_1 \times Z_2 D_2} - (D_4^{Z_4 \times D_1 D_4} + (D_3 \times D_1)
\]
\[
- (D_3^{Z_4 \times Z_3 D_3}) + (D_2 \times D_1) - (D_1 \times D_1) + (Z_2^{Z_4 \times Z_2 D_2})
\]
\[
+ (D_2^{Z_4 \times D_2 D_2} + (V_4^{Z_4 \times D_2 D_2}) + (D_4^{D_2 \times D_1 D_1} + (D_1^{Z_1 \times D_1 D_1})
\]
\[
- (Z_2^{Z_1 \times D_1 D_1}),
\]
\[
\overline{\omega}_G(\lambda_{2,1}) = -(S_4^{V_4 \times D_3 D_3} - (S_4 \times D_2) + (D_4^{V_4 \times Z_2 D_2}) - (Z_4^{Z_2 \times Z_2 D_2})
\]
\[
+ 2(D_2^{D_1 \times Z_2 D_2} - (D_1^{Z_4 \times Z_2 D_2}) - 2(Z_2^{Z_4 \times Z_2 D_2}) + 2(S_4 \times D_1)
\]
\[
- (D_4 \times D_1) - 2(D_3 \times D_1) - (D_2 \times D_1) + (D_1 \times D_1)
\]
\[
+ (Z_4 \times D_1) + 2(D_4^{D_2 \times Z_2 D_2}) + 2(D_3^{Z_4 \times D_1 D_3}) - (D_4^{Z_4 \times D_4 D_2})
\]
\[
- (D_2^{Z_4 \times D_2 D_2} - (D_2^{Z_4 \times D_2 D_2}) - (V_4^{Z_4 \times D_2 D_2}) - (D_4^{D_2 \times D_1 D_1})
\]
\[
+ (D_4^{V_4 \times D_1 D_1}) - (D_2^{D_1 \times D_1 D_1}) + 3(Z_2^{Z_1 \times D_1 D_1}).
\]

4. Description of the symmetries. The invariants \(\overline{\omega}_G(\lambda_{j,1})\) give the bifurcation of periodic solutions for each of five maximal groups. However, we only know that a group is maximal if it is maximal in a certain isotypic component of a Fourier mode. Since the bifurcation from \(\lambda_{3,1} = \lambda_{0,2}\) with maximal group \(S_4^{S_4 \times Z_2 D_2}\) is not independent of minimal period bifurcation from \(\lambda_{0,1}\) with maximal group \(S_4^{S_4 \times Z_1 D_1}\), we cannot conclude that these two bifurcations are different from each other.

We can conclude that the other 7 maximal groups in the invariants \(\overline{\omega}_G(\lambda_{j,1})\) for \(j = 0, 1, 2\) give different global families of periodic solutions with period \(T = 2\pi \lambda_{j,1} l_o\) (for some \(l_o \in \mathbb{N}\), where \((\lambda_{j,1} l_o)^{-1}\) is the limit frequency. Next we describe the symmetries of the solutions for these maximal isotropy groups. Notice that we have identified the elements of \(S_4\) with \(S_4\), i.e. in a maximal group, an element \(\sigma \in S_4\) acts as
\[
\sigma u_j = A_\sigma u_{\sigma(j)}.
\]

4.1. Families with frequency \(\sqrt{\mu_0}\). The tetrahedron configuration has one global family of periodic solutions, which starts with the frequency \(\lambda_{0,1}^{-1} = \sqrt{\mu_0}\). This family has symmetries of the group
\[
S_4^{S_4 \times Z_1 D_1}.
\]

This group is generated by \(S_4\) and \(\kappa \in D_1\). The symmetry \(S_4\) implies that the configurations is a regular tetrahedron at any time. Moreover, the group \(D_1\) implies that
\[
u(t) = \kappa u(t) = u(-t),
\]
i.e. the periodic solution is a brake orbit. This, in its turn, means that the velocity \(\dot{u}\) of all the molecules are zero at the times \(t = 0, \pi\),
\[
\dot{u}(0) = \dot{u}(\pi) = 0.
\]

Therefore, these solutions consist of a regular tetrahedron that expands and contracts in periodic motion in an orbit which is similar to a line.
4.2. **Families with frequency** $\sqrt{\mu_1}$. The tetrahedron configuration has five different families of periodic solutions which start with the frequency $\lambda_{1,1}^{-1} = \sqrt{\mu_1}$. Each family has a different group of symmetries.

The group

$$D_4D_2 \times Z_2D_2$$

is generated by the elements $\kappa \in O(2)$, $(12), (34) \in S_4$ and $((13)(24), e^{i\pi}) \in S_4 \times O(2)$. As described above, the element $\kappa$ implies that the periodic solution is a brake orbit. Thus, $A_{(12)}$ is the inversion over the plane, containing the points $\gamma_3$, $\gamma_4$, and the middle point of $\gamma_1$ and $\gamma_2$, which interchanges $\gamma_1$ with $\gamma_2$. Then, the symmetry $(12)$ implies that $u_1$ is the inversion of $u_2$, and similarly, the symmetry $(34)$ implies that $u_3$ is the inversion of $u_4$. The element $A_{(13)(24)}$ is a rotation by $\pi$ that interchanges $\gamma_1$ with $\gamma_3$ and $\gamma_2$ with $\gamma_4$. Therefore $u_1$ is the $\pi$-rotation and $\pi$-phase shift of $u_3(t)$. In these symmetries all the orbits are determined by the positions of only one of the particles, i.e. $u_1$.

The group

$$D_2O_1 \times Z_2D_2$$

is generated by the elements $\kappa \in O(2)$, $(12) \in S_4$ and $((34), e^{i\pi}) \in S_4 \times O(2)$. The symmetry $\kappa$ implies that the solutions is a brake orbit; the symmetry $(12)$ implies that $u_1$ is the inversion of $u_2$; and the symmetry $((34), e^{i\pi})$ implies that $u_3$ is the $\pi$-rotation and $\pi$-phase shift of $u_4(t)$. In this case, the orbit of $u_1$ determines $u_2$, and $u_4$ determines $u_3$. Nevertheless, there is no relation among these two pairs of particles.

The group

$$D_4 \cong D_1 \rtimes D_4$$

is generated by $((12), \kappa)$ and $((1324), e^{i\pi/2})$ in $S_4 \times O(2)$. The element $((12), \kappa)$ implies that $u_1(t)$ is the inversion of $u_2(-t)$. In this case, the orbit is not brake, which means it is similar to a circle. The matrix $A_{(1324)}$ is a rotor reflection by $\pi/2$. Then, the symmetry $((1324), e^{i\pi/2})$ implies that the particles are related by applying a $\pi/2$-rotoreflection and, at the same, a temporal phase shift by $\pi/2$.

The group

$$D_3 \times D_1$$

is generated by $\kappa$, which implies that the solution is a brake orbit, and the group $D_3$, which implies that the positions $u_1$, $u_2$, and $u_3$ always form a triangle. In this case, $u_4$ follows a trajectory that counterbalances the triangle formed by these elements.

The group

$$-D_3 \cong D_1 \rtimes D_3$$

is generated by the elements $((123), e^{i2\pi/3})$ and $(12), \kappa)$. The element $((123), e^{i2\pi/3})$ implies that $u_1(t) = u_2(t + 2\pi/3) = u_3(t + 4\pi/3)$. Therefore, the movement in these three elements is a (discrete) rotating wave. In addition, the element $(12), \kappa)$ implies that this rotating wave is invariant by an inversion in time: $u_1(t) = A_{(1,2)}u_2(-t) = A_{(1,2)}u_1(-t - 2\pi/3)$.

4.3. **Families with frequency** $\sqrt{\mu_2}$. The tetrahedron configuration has one family of periodic solutions which starts with the frequency $\lambda_{1,1}^{-1} = \sqrt{\mu_2}$. It possesses the symmetries of $S_4 \times D_3$. This group is generated by $V_4$ and $((123), 2\pi/3), ((12), \kappa) \in S_4 \times O(2)$. The symmetries $V_4$ place coordinates $u(t)$ in the shape of a non-regular tetrahedron figure with two axes of symmetry at any time. The element
((123), 2\pi/3) implies that \(u_1, u_2, \text{and } u_3\) are related by a rotation of \(2\pi/3\) and a phase shift of \(2\pi/3\).

5. Appendix: Equivariant gradient degree.

5.1. Group actions. In what follows, \(G\) always stands for a compact Lie group, and all subgroups of \(G\) are assumed to be closed \([5, 17]\). For a subgroup \(H \subset G\), denote by \(N(H)\) the normalizer of \(H\) in \(G\), and by \(W(H) = N(H)/H\) the Weyl group of \(H\) in \(G\). In the case when we are dealing with different Lie groups, we also write \(N_G(H)\) (resp. \(W_G(H)\)) instead of \(N(H)\) (resp. \(W(H)\)). We denote by \((H)\) the conjugacy class of \(H\) in \(G\) and use the notations:

\[
\Phi(G) := \{(H) : H \text{ is a subgroup of } G\},
\]
\[
\Phi_n(G) := \{(H) \in \Phi(G) : \dim W(H) = n\}.
\]

The set \(\Phi(G)\) has a natural partial order defined by

\[
(H) \leq (K) \iff \exists g \in G \text{ s.t. } gHg^{-1} \subset K. \tag{20}
\]

For a \(G\)-space \(X\) and \(x \in X\), the subgroup \(G_x := \{g \in G : gx = x\}\) is called the isotropy of \(x\). \(G(x) := \{gx : g \in G\}\) is called the orbit of \(x\), and the conjugacy class \((G_x)\) is the orbit type of \(x\). Also, for a subgroup \(H \subset G\), we use

\[
X^H := \{x \in X : G_x \supset H\}
\]

for the fixed point space of \(H\). The orbit space for a \(G\)-space \(X\) will be denoted by \(X/G\).

Any compact Lie group admits only countably many non-equivalent real (resp. complex) irreducible representations. Given a compact Lie group \(G\), we will assume that we know a complete list of all its real (resp. complex) irreducible representations, denoted \(V_i, i = 0, 1, \ldots\) (resp. \(W_j, j = 0, 1, \ldots\)). We refer to [1] for examples of such lists and the related notation.

Let \(V\) (resp. \(W\)) be a finite-dimensional real (resp. complex) \(G\)-representation. Without loss of generality, \(V\) (resp. \(W\)) can be assumed to be orthogonal (resp. unitary). Then, \(V\) (resp. \(W\)) decomposes into the direct sum of \(G\)-invariant subspaces

\[
V = V_0 \oplus V_1 \oplus \cdots \oplus V_r, \tag{21}
\]

(resp. \(W = W_0 \oplus W_1 \oplus \cdots \oplus W_s\)), called the \(G\)-isotypic decomposition of \(V\) (resp. \(W\)). Each isotypic component \(V_i\) (resp. \(W_j\)) is modeled on the irreducible \(G\)-representation \(V_i, i = 0, 1, \ldots, r\) (resp. \(W_j, j = 0, 1, \ldots, s\)), i.e., \(V_i\) (resp. \(W_j\)) contains all the irreducible subrepresentations of \(V\) (resp. \(W\)) which are equivalent to \(V_i\) (resp. \(W_j\)).

5.2. Euler ring. Let

\[
U(G) := \mathbb{Z}[\Phi(G)]
\]

denote the free \(\mathbb{Z}\)-module generated by \(\Phi(G)\).

**Definition 5.1.** (cf. [9]) Define a ring multiplication on generators \((H), (K) \in \Phi(G)\) as follows:

\[
(H) \ast (K) = \sum_{(L) \in \Phi(G)} n_L(L), \tag{22}
\]

where

\[
n_L := \chi_c((G/H \times G/K)_L/N(L)) \tag{23}
\]
with \( \chi_c \) the Euler characteristic taken in Alexander-Spanier cohomology with compact support (cf. [26]). The \( \mathbb{Z} \)-module \( U(G) \) equipped with the multiplication (22), (23) is a ring called the \textit{Euler ring} of the group \( G \) (cf. [6]).

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 a \textit{Burnside ring}, i.e.

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

where \( n_L := ((G/H \times G/K)_L/N(L)) = [(G/H \times G/K)_L/N(L)] \) (here \( \chi \) stands for the usual Euler characteristic). In this case, we have

\[
n_L = \frac{n(L,K) |W(K)| n(L,H) |W(H)| - \sum_{(I) > (L)} n(L,I) n_I |W(I)|}{|W(L)|},
\]

where

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

and \( (H), (K), (L), (I) \) are taken from \( \Phi_0(G) \).

Notice that \( A(G) \) is a \( \mathbb{Z} \)-submodule of \( U(G) \) but not a subring. Define \( \pi_0 : U(G) \to A(G) \) 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 5.2.** (cf. [3]) The map \( \pi_0 \) defined by (25) is a ring homomorphism, i.e.

\[
\pi_0((H) * (K)) = \pi_0((H)) \cdot \pi_0((K)), \quad (H), (K) \in \Phi(G).
\]

Let us point out that although the computations of the Euler ring structure \( U(G) \) are quite challenging in general, in the case \( G = \Gamma \times O(2) \) (here \( \Gamma \) is a finite group) the process becomes simpler. Using the Burnside ring multiplication structure in \( A(G) \), Lemma 5.2 allows us to partially describe the Euler ring multiplication structure in \( U(G) \).

### 5.3. Equivariant gradient degree.

Let \( G \) be a compact Lie group and \( V \) be a \( G \)-representation. Let \( \varphi : V \to \mathbb{R} \) be a continuously differentiable \( G \)-invariant functional. Define \( \mathcal{M}^G_\varphi \) as the set of pairs \( (\nabla \varphi, \Omega) \) with \( \nabla \varphi \) a \( G \)-equivariant field \( \nabla \varphi : V \to V \) such that

\[
\nabla \varphi(v) \neq 0 \text{ for } v \in \partial \Omega.
\]

**Theorem 5.3.** There exists a unique map \( \nabla_{G,-}\text{deg} : \mathcal{M}^G_\varphi \to U(G) \), which assigns to every \( (\nabla \varphi, \Omega) \in \mathcal{M}^G_\varphi \) an element \( \nabla_{G,-}\text{deg} (\nabla \varphi, \Omega) \in U(G) \), called the \textit{G-gradient degree} of \( \nabla \varphi \) on \( \Omega \),

\[
\nabla_{G,-}\text{deg} (\nabla \varphi, \Omega) = \sum_{(H_i) \in \Phi(\Gamma)} n_{H_i}(H_i) = n_{H_1}(H_1) + \cdots + n_{H_m}(H_m),
\]

satisfying the following properties:

1. **(Existence)** If \( \nabla_{G,-}\text{deg} (\nabla \varphi, \Omega) \neq 0 \), i.e. there is in (26) a non-zero coefficient \( n_{H_i} \), then exists \( u_0 \in \Omega \) such that \( \nabla \varphi(u_0) = 0 \) and \( (G_{u_0}) \geq (H_i) \).

2. **(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, \( \nabla_{G,-}\text{deg} (\nabla \varphi, \Omega) = \nabla_{G,-}\text{deg} (\nabla \varphi, \Omega_1) + \nabla_{G,-}\text{deg} (\nabla \varphi, \Omega_2) \).
3. **(Homotopy)** If $\nabla_x \Psi : [0, 1] \times V \to V$ is a $G$-gradient $\Omega$-admissible homotopy, then
$$\nabla_G\text{-deg} (\nabla_x \Psi(t, v), \Omega) = \text{constant}.$$  

4. **(Normalization)** Let $\varphi \in C^2_0(V, \mathbb{R})$ 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 “$m^-$” stands for the total dimension of eigenspaces for negative eigenvalues of a (symmetric) matrix.

5. **(Multiplicativity)** For all $(\nabla \varphi_1, \Omega_1), (\nabla \varphi_2, \Omega_2) \in \mathcal{M}_G^2$,
$$\nabla_G\text{-deg} (\nabla \varphi_1 \times \nabla \varphi_2, \Omega_1 \times \Omega_2) = \nabla_G\text{-deg} (\nabla \varphi_1, \Omega_1) \ast \nabla_G\text{-deg} (\nabla \varphi_2, \Omega_2)$$
where the multiplication ‘$\ast$’ is taken in the Euler ring $U(G)$.

6. **(Suspension)** If $W$ is an orthogonal $G$-representation and $B$ an open bounded invariant neighborhood of $0 \in W$, then
$$\nabla_G\text{-deg} (\nabla \varphi \times \text{Id}_W, \Omega \times B) = \nabla_G\text{-deg} (\nabla \varphi, \Omega).$$

7. **(Hopf Property)** Assume $B(V)$ is the unit ball of an orthogonal $G$-representation $V$ and for $(\nabla \varphi_1, B(V)), (\nabla \varphi_2, B(V)) \in \mathcal{M}_G^2$, one has
$$\nabla_G\text{-deg} (\nabla \varphi_1, B(V)) = \nabla_G\text{-deg} (\nabla \varphi_2, B(V)).$$
Then, $\nabla \varphi_1$ and $\nabla \varphi_2$ are $G$-gradient $B(V)$-admissible homotopic.

5.4. **Equivariant gradient degree in Hilbert Spaces.** Let $\mathcal{H}$ be a Hilbert $G$-representation and $\Omega \subset \mathcal{H}$ an open bounded $G$-invariant set. A $C^1$-differentiable $G$-invariant functional $f : \mathcal{H} \to \mathbb{R}$ given by $f(x) = \frac{1}{2} \|x\|^2 - \varphi(x), x \in \mathcal{H}$, is called $\Omega$-admissible if $\nabla \varphi : \mathcal{H} \to \mathcal{H}$ is a completely continuous map and
$$\forall x \in \partial \Omega \quad \nabla f(x) = x - \nabla \varphi(x) \neq 0.$$
By a $G$-equivariant approximation scheme $\{P_n\}_{n=1}^\infty$ in $\mathcal{H}$, we mean a sequence of $G$-equivariant orthogonal projections $P_n : \mathcal{H} \to \mathcal{H}$, $n = 1, 2, \ldots$, such that:

(a) the subspaces $\mathcal{H}^n := P_n(\mathcal{H}), n = 1, 2, \ldots$, are finite-dimensional;

(b) $\mathcal{H}^n \subset \mathcal{H}^{n+1}, n = 0, 1, 2, \ldots$;

(c) $\lim_{n \to \infty} P_n x = x$ for all $x \in \mathcal{H}$.

Then for an $\Omega$-admissible $G$-map $f : \mathcal{H} \to \mathbb{R}$, one can define a sequence $f_n : \mathcal{H}^n \to \mathbb{R}$ by $f_n(x) := \frac{1}{2} \|x\|^2 - \varphi(x), x \in \mathcal{H}^n$. By a standard argument, for sufficiently large $n \in \mathbb{N}$, the maps $\nabla f_n(x) := x - P_n \nabla \varphi(x), x \in \mathcal{H}$, are $\Omega_n$-admissible, where $\Omega_n := \Omega \cap \mathcal{H}^n$. Moreover, the gradient equivariant degrees $\nabla_G\text{-deg} (\nabla f_n, \Omega_n)$ are well defined and are the same, i.e. for $n$ sufficiently large
$$\nabla_G\text{-deg} (\nabla f_n, \Omega_n) = \nabla_G\text{-deg} (\nabla f_{n+1}, \Omega_{n+1}).$$
This, by Suspension Property of the $G$-equivariant gradient degree, implies that we can put
$$\nabla_G\text{-deg} (\nabla f, \Omega) := \nabla_G\text{-deg} (\nabla f_n, \Omega_n), \quad (27)$$
where $n$ is sufficiently large. One can verify that this construction doesn’t depend on the choice of a $G$-approximation scheme in the space $\mathcal{H}$, for instance see [8]. We should mention that the ideas behind the usage of the approximation methods to define topological degree can be rooted to [7].
5.5. Degree on the slice. Suppose that the orbit $G(u_o)$ of $u_o \in \mathcal{K}$ is contained in a finite-dimensional $G$-invariant subspace. Therefore, the $G$-action on that subspace is smooth, and $G(u_o)$ is a smooth submanifold of $\mathcal{K}$. Denote by $S_o \subset \mathcal{K}$ the slice to the orbit $G(u_o)$ at $u_o$. Denote by $V_o := T_{u_o}G(u_o)$ the tangent space to $G(u_o)$ at $u_o$. Then clearly, $S_o = V_o^\perp$ and $S_o$ is a smooth Hilbert $G_{u_o}$-representation.

Then we have (cf. [4]).

**Theorem 5.4.** (Slice Principle) Let $\mathcal{E}$ be an orthogonal $G$-representation, $\varphi : \mathcal{K} \to \mathbb{R}$ be a continuously differentiable $G$-invariant functional such that $\nabla \varphi$ is a completely continuous field, and let $u_o \in \mathcal{K}$, $G(u_o)$ an isolated critical orbit of $\varphi$ contained in a finite-dimensional $G$-invariant subspace of $\mathcal{K}$. 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 $\varphi_o(v) := \varphi(u_o + v)$, $v \in S_o$. 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 $\Theta(H) = (H), (H) \in \Phi(G_{u_o})$.

We show how to compute $\nabla_{G}\deg(\mathcal{A}, B(V))$, where $\mathcal{A} : V \to V$ is a symmetric $G$-equivariant linear isomorphism and $V$ is an orthogonal $G$-representation, i.e. $\mathcal{A} = \nabla \varphi$ for $\varphi(v) = \frac{1}{2}(\mathcal{A} \cdot v)$, $v \in V$, where “$\cdot$” stands for the inner product. Consider the $G$-isotypic decomposition (21) of $V$ and put

$$\mathcal{A}_i := \mathcal{A}|_{V_i} : V_i \to V_i, \quad i = 0, 1, \ldots, r.$$

Then, by the multiplicativity property,

$$\nabla_{G}\deg(\mathcal{A}, B(V)) = \prod_i \nabla_{G_i}\deg(\mathcal{A}_i, B(V_i)).$$

(29)

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

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

(30)

and the so-called basic gradient degrees by

$$\deg_{V_i} := \nabla_{G}\deg(-\text{Id}, B(V_i)).$$

(31)

Then, have that

$$\nabla_{G}\deg(\mathcal{A}, B(V)) = \prod_{\xi \in \sigma_-(\mathcal{A})} \prod_i (\deg_{V_i})^{m_i(\xi)}.$$

(32)

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