DIHEDRAL MOLECULAR CONFIGURATIONS INTERACTING BY LENNARD-JONES AND COULOMB FORCES

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Abstract. In this paper, we investigate nonlinear periodic vibrations of a group of particles with a planar dihedral configuration governed by the Lennard-Jones and Coulomb forces. Using the gradient equivariant degree, we provide a full topological classification of the periodic solutions with both temporal and spatial symmetries. In the process, we provide general formulae for the spectrum of the linearized system of equations describing the above configuration, which allows us to obtain the critical frequencies of the particles’ motions. The obtained frequencies represent the set of all critical periods for small amplitude periodic solutions emerging from a given stationary symmetric orbit of solutions.

1. Introduction. Classical forces, used in molecular mechanics and associated with bonding between the adjacent particles, electrostatic interactions, and van der Waals forces, are modeled by Lennard-Jones and Coulomb potentials. Even though in a typical molecule an atom is bonded only to a few of its neighbors, it also interacts with every other atom in the molecule. The renowned 6-12–Lennard-Jones potential was found experimentally in 1924 (cf. [15]). Since then, it is successfully used in molecular modeling. Certainly, one can expect that other types of more accurate potentials may be introduced in the future.

There are many examples of symmetric atomic molecules: octahedral compounds of sulfur hexafluoride SF₆, the molybdenum hexacarbonyl Mo(CO)₆, the tetraphosphorus P₄, a spherical fullerene molecule with the formula C₆₀ with icosahedral

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symmetry, or a dihedral molecule with 2-D interactions, etc. One can find multiple examples of symmetric molecule clusters in [22].

Let us consider \( n \) identical atoms \( u_i, j \in \{1, 2, \ldots, n-1, n\} =: X \), in the space \( \mathbb{R}^3 \). Then, a set \( \mathcal{B} \subset X \times X \), satisfying the conditions (a) \((i, j) \in \mathcal{B}\) then \((j, i) \in \mathcal{B}\) and (b) \((j, j) \notin \mathcal{B}\), can be considered as a \emph{bonding set} for a specific configuration of atoms in the molecule. Therefore, we assume that the particles \( u_i \) and \( u_j \) are bonded if \((i, j) \in \mathcal{B}\). It follows that the symmetries \( \Gamma \subset S_n \) of a molecular bonding are the permutation \( \sigma \in S_n \) such that

\[
\forall (i, j) \in \mathcal{B}, \quad (\sigma(i), \sigma(j)) \in \mathcal{B}.
\]

Then, the atomic interactions in this molecule with bondings by Lennard-Jones and Coulomb potentials can be described by the following Newtonian system

\[
\ddot{u} = -\nabla^2 \mathbf{V}(u), \quad u(t) = (u_1(t), u_2(t), \ldots, u_n(t)), \quad u_i(t) \neq u_j(t), \quad \text{for} \ i \neq j, \quad (1)
\]

where

\[
\mathbf{V}(u) := \frac{1}{2} \sum_{(i, j) \in \mathcal{B}} U(|u_i - u_j|^2) + \sum_{1 \leq i < j \leq n} W(|u_i - u_j|^2),
\]

\[
W(t) := \frac{B}{t^6} - \frac{A}{t^3} + \frac{\sigma}{t^{\sqrt{t}}}, \quad U(t) = t^2 - 2t, \quad t > 0.
\]

In this paper, we are interested in studying planar molecular interactions for (1) in a ring of \( n \) identical atoms with the dihedral \( D_n \) symmetries. Such model was studied in [10], where a similar (but not complete) classification of nonlinear vibrations was obtained using \( \mathbb{Z}_n \)-symmetries. Our methodology uses the equivariant degree to extract a topological equivariant classification of non-linear \( p \)-periodic \((p > 0)\) vibrations for a molecule in two-dimensional polygonal configuration with dihedral symmetries. The vibrational motions are characteristic of all molecules and can be detected using infrared or Raman spectroscopy. They depend on the vibrational structure of molecular electronic transitions. Such vibrations are closely connected to the related Newtonian system (see (15)), which can be reformulated as a critical point problem. As a result, a variety of variational methods can be applied, including those based on the concept of the equivariant gradient degree (see for example [2, 6, 8, 9, 10, 16, 18, 19]).

Generally, molecular vibrations admit spatial-temporal symmetries (depending on the actual molecular symmetries \( \Gamma \)), which are called \emph{modes of vibration} reflected in atomic motions of stretching, bending, rocking, wagging, and twisting. These modes and the corresponding vibrational frequencies are of great importance in molecular dynamics. It is thus desirable to distinguish periodic motions with different patterns of symmetric modes of vibrations.

The content of this paper can be described as follows. After preliminaries, in the section 3, we discuss a molecular model with Lennard-Jones and Coulomb potentials for \( n \) identical atoms bonded in a polygonal configuration. We show the existence of the symmetric equilibrium \( u^a \) and describe the dihedral isotypical decomposition of the slice to the orbit of these equilibria. Next, in the section 4, we formulate the problem of finding a periodic vibration to (7) as a bifurcation problem (15) and reformulate it as a variational bifurcation problem with \( D_n \times O(2) \)-symmetries. In the subsection 4.1, we introduce the equivariant invariant \( \omega_G(\lambda_0) \). In the subsection 4.2, we compute the spectrum of \( \mathcal{L} := \nabla^2 \mathbf{V}(u^a) \) for a general potential \( \mathbf{V} \) and, subsequently in the section 5, we formulate the main existence results based on the values of the equivariant invariants \( \omega_G(\lambda_0) \) (Theorem 5.2). In the section 5.2, we
consider an example of a particular system (15) with $D_6$-symmetries and compute several equivariant invariants to illustrate how to extract the relevant equivariant information. Finally, we confirm the obtained existence results with several computer simulations in the subsection 5.3. We also provide the Appendix A where we collect definitions and properties related to the equivariant gradient degree.

2. Preliminaries. Suppose $G$ is a compact Lie group. For a subgroup $H \subset G$ (which will always be assumed to be closed) we denote by $N (H)$ the normalizer of $H$ in $G$ and by $W (H) = N (H) / H$ the Weyl group of $H$ in $G$. If we deal with different Lie groups, to be more specific, we’ll also write $N_G (H)$ (or $W_G (H)$, respectively) instead of $N (H)$ ($W (H)$, respectively). We denote by $(H)$ the conjugacy class of $H$ in $G$ and define the following notations:

$$\Phi (G) := \{ (H) : H \text{ is a subgroup of } G \}$$

and

$$\Phi_n (G) := \{ (H) \in \Phi (G) : \dim W (H) = n \} .$$

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

$$\text{(H)} \leq \text{(K)} \iff \exists g \in G \ g H g^{-1} \subset K . \quad (2)$$

For a $G$-space $X$ and $x \in X$, we define $G_x := \{ g \in G : gx = x \}$ – the isotropy or stabilizer of $x$, $(G_x)$ – the orbit type of $x$ in $X$ and $G (x) := \{ gx : g \in G \}$ – the orbit of $x$. Moreover, for a subgroup $H \subset G$, we use the following notations:

$$X_H := \{ x \in X : G_x = H \} ; \quad X^H := \{ x \in X : G_x \supset H \} .$$

Any compact Lie group $G$ admits countably many non-equivalent (real) irreducible $G$-representations. Given a compact Lie group $G$, we assume that we have a complete list of its all (real) irreducible $G$-representations, which will be denoted $V_i$, $i = 0, 1, 2, \ldots$, starting with the trivial representation $V_0$. As an example, consider the dihedral group $D_n \leq O(2)$ of symmetries of a regular $n$-gone, which can be represented as

$$D_n = \{ 1, \gamma, \gamma^2, \ldots, \gamma^{n-1}, \kappa, \gamma \kappa, \gamma^2 \kappa, \ldots, \gamma^{n-1} \kappa \} ,$$

where $\gamma = e^{2\pi i / n}$ and $\kappa$ are te generators of $D_n$ which are identified with the matrices

$$\gamma = \begin{bmatrix} \cos \frac{2\pi}{n} & -\sin \frac{2\pi}{n} \\ \sin \frac{2\pi}{n} & \cos \frac{2\pi}{n} \end{bmatrix} , \quad \kappa = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} . \quad (3)$$

The irreducible $D_n$-representations can be easily described: $V_0$ – the one-dimensional trivial representation, $V_j$, for $0 < j \leq \lfloor \frac{n-1}{2} \rfloor$, – two-dimensional $D_n$ representation such that $V_j \simeq \mathbb{C}$, where $\gamma z = \gamma^j \cdot z$, $\kappa z = \overline{z}$, $z \in V_j$ (here ‘$\cdot$’ stands for the usual complex multiplication), and in the case $n$ is an even integer, we also have the one-dimensional irreducible $D_n$-representation $V_r$, $r = \frac{n}{2}$ (here $\gamma x = -x$, $\kappa x = x$, $x \in V_r \simeq \mathbb{R}$). There are other additional $D_n$-representations, but we won’t consider them in this paper (we refer readers to [1] for more details and other examples).

Consider a finite-dimensional $G$-representation (which without loss of generality can be assumed to be orthogonal). Then $V$ admits the following decomposition into a direct sum of $G$-invariant subspaces

$$V = V_0 \oplus V_1 \oplus \cdots \oplus V_r , \quad (4)$$

which is called the $G$-isotypical (or $G$-isotypic) decomposition of $V$, such that each component $V_j$ contains all irreducible $G$-subrepresentations of $V$ equivalent to $V_j$. 
The component $\mathcal{V}_j$ is commonly called an isotypical (or isotypic) component of $V$ modeled on $\mathcal{V}_j$. One can easily show (see [1]) that the decomposition (4) is unique.

For a linear operator $A : V \to V$, we denote by $\sigma(A)$ the real spectrum of $A$ and for $\mu \in \sigma(A)$ we denote by $E(\mu) \subset V$ the generalized eigenspace associated with $\mu$. Since any $G$-equivariant linear operator $A : V \to V$ preserves the $G$-isotypical decomposition (4), i.e. $A(\mathcal{V}_j) \subset \mathcal{V}_j$, and the eigenspace $E(\mu)$ is $G$-invariant, we can introduce the integers

$$m^j(\mu) := \dim \left( E(\mu) \cap \mathcal{V}_j \right) / \dim \mathcal{V}_j, \quad j = 0, 1, 2, \ldots, r,$$

and we will call the number $m^j(\mu)$ the $\mathcal{V}_j$-isotypical multiplicity of the eigenvalue $\mu$. In the case $E(\mu)$ is $G$-equivalent to some $\mathcal{V}_j$, we will say that $\mu$ is $\mathcal{V}_j$-simple eigenvalue.

3. Model for atomic interaction with dihedral symmetries. Consider $n$ identical atoms $u_j$, $j = 0, 1, 2, \ldots, n - 1$, in the plane $\mathbb{C}$. Assume that each atom interacts with the adjacent particles $u_{j-1}$ and $u_{j+1}$, where the indices $j - 1$ and $j + 1$ are taken mod $n$. Put $u := (u_0, u_1, \ldots, u_{n-1})^T \in \mathbb{C}^n$ and define $\Omega'_o := \{u \in \mathbb{C}^n : u_k \neq u_j, \text{ if } k \neq j, \text{ with } k, j = 0, 1, 2, \ldots, n - 1\}$. The Lennard-Jones and Coulomb potential $\mathcal{V} : \Omega'_o \to \mathbb{R}$ is given by

$$\mathcal{V}(u) := \sum_{j=0}^n U(|u_{j+1} - u_j|^2) + \sum_{0 \leq j < k \leq n - 1} W(|u_j - u_k|^2),$$

where

$$U(t) = t - 2\sqrt{t}, \quad W(t) = B t^\alpha - A t^\beta + \frac{\sigma}{\sqrt{t}}, \quad t > 0.$$ 

The associated Newtonian equation for the interaction between these $n$-particles is

$$\ddot{u} = -\nabla^2 \mathcal{V}(u), \quad u \in \Omega'_o.$$ 

Notice that the function $\mathcal{V} : \Omega'_o \to \mathbb{R}$ is invariant with respect to the $\mathbb{C}$-action on $\mathbb{C}^n$ by shiftings, i.e. for all $z \in \mathbb{C}$ and $(z_0, z_1, \ldots, z_{n-1}) \in \Omega'_o$ we have $\mathcal{V}(z_0 + z, z_1 + z, \ldots, z_{n-1} + z) = \mathcal{V}(z_0, z_1, \ldots, z_n)$. In order to make system (7) independent of reference point (i.e. the choice of the origin in $\mathbb{C}^n$), we put

$$\mathcal{V}' := \{(z_0, z_1, z_2, \ldots, z_{n-1}) \in \mathbb{C}^n : z_0 + z_1 + z_2 + \cdots + z_{n-1} = 0\},$$

and $\Omega_o = \Omega'_o \cap \mathcal{V}'$, and consider (7) restricted to $u \in \Omega_o$.

The dihedral group $D_n$ (as it permutes the vertices of a regular $n$-gone) can be identified with the subgroup of the symmetric group $S_n$ of permutations of $n$-elements $\{0, 1, \ldots, n - 2, n - 1\}$ with the generators $\xi := (0, 1, 2, \ldots, n - 1)$ (the “rotation” corresponding to $\gamma = e^{2\pi i n}$ in (3)) and $\kappa := (1, n-1)(2, n-2)\ldots(m, n-m)$ (the “reflection” corresponding to complex conjugation), where $m = \left\lfloor \frac{n-1}{2} \right\rfloor$. The action of $\mathfrak{G} := D_n \times O(2)$ on $\mathbb{C}^n$ is given by

$$(\sigma, A)(z_0, z_1, \ldots, z_{n-1}) = (Az_{\sigma(0)}, Az_{\sigma(1)}, \ldots, Az_{\sigma(n-1)}),$$

where $(\sigma, A) \in D_n \times O(2)$. Notice that $\Omega_o \subset \mathcal{V}'$ is $\mathfrak{G}$-invariant and the system (7) is $\mathfrak{G}$-equivariant.
Symmetric Equilibrium for (7): Consider the point \( v^0 := (1, \gamma, \gamma^2, \ldots, \gamma^{n-1}) \in \Omega_o \), where \( \gamma := e^{i \frac{2\pi}{n}} \). Then

\[ \mathfrak{G}_{v^0} = \{(g, g) : g \in D_n\} \leq D_n \times O(2). \]

Put \( \Gamma := \mathfrak{G}_{v^0} \). Notice that \( \Gamma \) is isomorphic to \( D_n \). The \( \Gamma \)-fixed-point set \( \mathcal{V}^\Gamma \) is a one-dimensional subspace of \( \mathcal{V} \) given by

\[ \mathcal{V}^\Gamma = \text{span}_\mathbb{R} \{1, \gamma, \gamma^2, \ldots, \gamma^{n-1}\}. \]

By Symmetric Criticality Principle, a critical point of \( \mathcal{V}^\Gamma \) : \( \Omega_o \to \mathbb{R} \) is also a critical point of \( \mathcal{V} \). Since \( \mathcal{V} \) satisfies the coercivity condition, that is, \( \mathcal{V}(u) \to \infty \) as \( u \) approaches \( \partial \Omega_o \) or \( \|u\| \to \infty \), there exists a global minimum \( u^0 \) of \( \mathcal{V}^\Gamma \) in \( \Omega_o^\Gamma \) and \( \nabla \mathcal{V}^\Gamma(u^0) = 0 \). A vector \( v \in \mathcal{V}^\Gamma \) can be represented as \( v := (t, 1, \gamma, \gamma^2, \ldots, \gamma^{n-1}) \) for some \( t \in \mathbb{R} \), and we can look for the orbit of equilibria for (7) in this subspace. The restriction of \( \mathcal{V} \) to the subspace \( \{t(1, \gamma, \gamma^2, \ldots, \gamma^{n-1}) : t > 0\} \) can be written as

\[ \phi(t) = nU(\sqrt{t}) + \sum_{0 \leq j < k \leq n-1} W(a_{jk}t^2), \quad t > 0. \]

where

\[ a = 4 \sin^2 \frac{\pi}{n} \quad \text{and} \quad a_{jk} = 4 \sin^2 \frac{(k-j)\pi}{n}, \]

where \( 0 \leq j < k \leq n-1 \). Since

\[ \lim_{t \to 0^+} \phi(t) = \lim_{t \to \infty} \phi(t) = \infty, \]

there exists a minimizer \( r_o \in (0, \infty) \) of \( \phi \), i.e. the point

\[ u^0 = r_o(1, \gamma, \gamma^2, \ldots, \gamma^{n-1}) \in \Omega_o \]

which is a \( \Gamma \)-symmetric equilibrium of \( \mathcal{V} \) (see Figure 1). We put

\[ u^0 = (u^0_0, u^0_1, \ldots, u^0_{n-1}) \in \mathbb{C}^n, \]

i.e. \( u^0_k = r_o \gamma^k, k = 0, 1, 2, \ldots, n-1 \). Consequently we have the orbit of equilibria \( M = \mathfrak{G}(u^0) \). The tangent vector to \( M \) at \( u^0 \in M \) is \( v^0 = i(1, \gamma, \ldots, \gamma^{n-1}) \), thus the slice \( S_o \) to the orbit \( M \) at \( u^0 \) is \( S_o = \{z \in \mathbb{C}^n : z \cdot v^0 = 0\} \), or equivalently

\[ S_o = \left\{(z_0, z_1, \ldots, z_{n-1}) \in \mathbb{C}^n : \Re \left( \sum_{k=0}^{n-1} z_k i \gamma^{-k} \right) = 0 \right\}. \]
Define $\mu : \mathbb{C}^n \to \mathbb{R}$ and $\nu : \mathbb{C}^n \to \mathbb{C}$ by

$$\mu(z_0, z_1, \ldots, z_{n-1}) = \text{Re} \left( \sum_{k=0}^{n-1} z_k i \gamma^{-k} \right), \quad \nu(z_0, z_1, \ldots, z_{n-1}) = \sum_{k=0}^{n-1} z_k i \gamma^{-k}.$$ 

Then $\text{Ker} \mu = S_0$ and $\text{Ker} \nu \subset \text{Ker} \mu$. Notice that $\mu$ and $\nu$ are $\Gamma$-invariant so $S_0$ is a $\Gamma$-representation.

Then for $j = 0, 1, \ldots, n-2$, and $z_k = \gamma^{-jk}, \ k = 0, 1, 2, \ldots, n-1$

$$\sum_{k=0}^{n-1} z_k i \gamma^{-k} = i \sum_{k=0}^{n-1} \gamma^{-(j+1)k} = i \frac{1 - \gamma^{-(j+1)n}}{1 - \gamma^{-(j+1)}} = 0,$$

thus $(z, z \gamma^{-j}, z \gamma^{-2j}, \ldots, z \gamma^{-(n-1)j}) \in \text{Ker} \nu$ for $z \in \mathbb{C}$. Next, we define

$$W_j := \{(z, z \gamma^{-j}, z \gamma^{-2j}, \ldots, z \gamma^{-(n-1)j}) : z \in \mathbb{C} \} \subset \mathbb{C}^n.$$ 

The subspaces $W_j$ of $S_0$ are $\Gamma$-invariant. Using the identification of $\Gamma$ with $D_n$ (where $\gamma := (\gamma, \gamma)$ and $\kappa := (\kappa, \kappa)$) we have the following $D_n$-action on $z \in W_j$

$$(\gamma, \kappa)z = \gamma^{j+1} \cdot z, \quad (\kappa, \kappa)z = z, \quad z := (z, z \gamma^{-j}, z \gamma^{-2j}, \ldots, z \gamma^{-(n-1)j}),$$

where `.' denotes the usual complex multiplication. Therefore, $W_j$ is an irreducible $D_n$-representation which is equivalent to $\mathbb{C}$ equipped with the $D_n$-action $\gamma z = \gamma^{j+1} \cdot z, \ k \in \mathbb{Z}, \ z \in \mathbb{C}$. For $j = n-1$, the space $W_{n-1} := \{(x, x \gamma^{-(n-1)}, \ldots, x \gamma^{-1}) : x \in \mathbb{R} \}$ is a trivial subrepresentation of $S_0$.

Consequently, we obtain: Isotypical Components of $S_0$ for $n$ being an odd number: In this case, the space $S_0$ has the following isotypical components,

$$S_0 = \mathcal{Y}_0 \oplus \mathcal{Y}_1 \oplus \mathcal{Y}_2 \oplus \cdots \oplus \mathcal{Y}_j \oplus \cdots \oplus \mathcal{Y}_r,$$

with $\mathcal{Y}_0 = W_{n-1}$, that is,

$$\mathcal{Y}_0 = \text{span}_\mathbb{R}\{(1, \gamma^{-(n-1)}, \gamma^{-2(n-1)}, \ldots, \gamma^{-(n-1)(n-1)}\} = \text{span}_\mathbb{R}\{(1, \gamma, \gamma^2, \ldots, \gamma^{n-1})\}. $$

$$\mathcal{Y}_1 = W_{n-2} \text{ and for } \left\lfloor \frac{n}{2} \right\rfloor \geq j > 1,$$

$$\mathcal{Y}_j = W_{j-1} \oplus W_{n-j-1}.$$ 

Put

$$\mathbf{u}^j = (1, \gamma^{-(j-1)}, \gamma^{-2(j-1)}, \ldots, \gamma^{-(n-1)(j-1)}),$$

$$\mathbf{v}^j = (1, \gamma^{j+1}, \gamma^{2(j+1)}, \ldots, \gamma^{(n-1)(j+1)}),$$

Then for $j = 1, 2, \ldots, r$, $\mathcal{Y}_j$ is a complex subspace of $\mathbb{C}^n$ such that

$$\mathcal{Y}_j = \text{span}_\mathbb{C}\{\mathbf{u}^j\} \oplus \text{span}_\mathbb{C}\{\mathbf{v}^j\}. $$

Isotypical Components of $S_0$ for $n$ being an even number: In this case, the space $S_0$ has the following isotypical components,

$$S_0 = \mathcal{Y}_0 \oplus \mathcal{Y}_1 \oplus \mathcal{Y}_2 \oplus \cdots \oplus \mathcal{Y}_j \oplus \cdots \oplus \mathcal{Y}_r,$$

with the same components $\mathcal{Y}_j$ in (13) for $j < \frac{n}{2} = r$, and an additional isotypical component $\mathcal{Y}_r$, given by

$$\mathcal{Y}_r := W_{r-1} = \text{span}_\mathbb{C}\{(1, \gamma^{-(r-1)}, \gamma^{-2(r-1)}, \ldots, \gamma^{-(n-1)(r-1)}\}$$

$$= \text{span}_\mathbb{C}\{(1, -\gamma, \gamma^2, \ldots, (-1)^k \gamma^k, \ldots, -\gamma^{n-1})\}. $$
4. Variational reformulation. We are interested in finding non-trivial $p$-periodic solutions to (7), bifurcating from the orbit equilibrium points $\Theta(u^c)$. By normalizing the period in (7) (i.e. by making the substitution $v(t) = u\left(\frac{t}{p}\right)$) we obtain the following system,

$$\begin{align*}
\dot{v} &= -\lambda^2 \nabla V(v), \\
v(0) &= v(2\pi), \quad \dot{v}(0) = \dot{v}(2\pi),
\end{align*}$$

where $\lambda = \frac{p}{2}$. The problem (15) can be reformulated as a variational problem.

We consider the first Sobolev space of $2\pi$-periodic functions from $\mathbb{R}$ to $\mathcal{V}$, that is,

$$H^1_{2\pi}(\mathbb{R}, \mathcal{V}) = \{z : \mathbb{R} \to \mathcal{V} : z(0) = z(2\pi), \quad z|_{[0, 2\pi]} \in H^1([0, 2\pi]; \mathcal{V})\},$$
equipped with the inner product

$$\langle z, w \rangle = \int_0^{2\pi} (\dot{z}(t) \cdot \dot{w}(t) + z(t) \cdot w(t)) dt, \quad z, w \in H^1_{2\pi}(\mathbb{R}, \mathcal{V}).$$

The space $H^1_{2\pi}(\mathbb{R}, \mathcal{V})$ is an orthogonal Hilbert representation of $G := D_n \times O(2) \times O(2)$ with the $G$-action given by (see (9))

$$\begin{align*}
\left(\xi, A, e^{i\tau}\right) x(t) &= (\xi, A)x(t + \tau), \\
\left(\xi, A, e^{i\tau} \kappa\right) x(t) &= (\xi, A)x(-t + \tau),
\end{align*}$$

where $z \in H^1_{2\pi}(\mathbb{R}, \mathcal{V})$, $(\xi, A) \in D_n \times O(2)$ and $e^{i\tau}, \kappa \in O(2)$.

By identifying a $\mathbb{R}/2\pi\mathbb{Z}$ with $S^1$, any $2\pi$-periodic function $x : \mathbb{R} \to \mathcal{V}$ can be identified with $\bar{x} : S^1 \to \mathcal{V}$, we can write, for simplicity, $H^1(S^1, \mathcal{V})$ instead of $H^1_{2\pi}(\mathbb{R}, \mathcal{V})$. Put

$$\Omega = \{u \in H^1(S^1, \mathcal{V}) : u(t) \in \Omega_o, \quad \text{for all } t \in \mathbb{R}\}.$$

Then system (15) is equivalent to the following variational equation

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

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

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

Clearly, the equilibrium point $u^c = r_o(1, \gamma, \gamma^2, \gamma^{n-1}) \in \mathbb{C}^n$ of (7) (described in subsection 3) is a critical point of $J$. We consider the $G$-orbit $G(u^c)$ in the space $H^1(S^1, \mathcal{V})$. We are interested in finding non-stationary $2\pi$-periodic solutions bifurcating from $G(u^c)$, that is, non-constant solutions to system (18).

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. Then $j$ is a compact operator and we have

$$\nabla_u J(\lambda, u) = u - j \circ L^{-1}(\lambda^2 N_{\nabla \mathcal{V}}(u) + u), \quad u \in H^1(S^1, \mathcal{V}),$$

where

$$N_{\nabla \mathcal{V}}(u)(t) = \nabla \mathcal{V}(u(t)), \quad t \in \mathbb{R}.$$ 

Consequently, the bifurcation problem (18) can be written as

$$\mathcal{F}(\lambda, u) := u - j \circ L^{-1}(\lambda^2 N_{\nabla \mathcal{V}}(u) + u) = 0.$$
Notice that $\mathcal{F}$ is a completely continuous gradient field. Moreover, we have
\[ D_u \mathcal{F}(\lambda, u^o) = \nabla^2 u J(\lambda, u^o) = \text{Id} - j \circ L^{-1}(\lambda^2 \nabla^2 \mathcal{V}(u^o) + \text{Id}), \tag{21} \]
where
\[ (N \nabla \mathcal{V}(u^o)v)(t) = \nabla^2 \mathcal{V}(u^o)v(t), \quad v \in H^1(S^1, \mathcal{V}); \quad t \in \mathbb{R}. \]
In what follows we put
\[ \mathcal{L} := \nabla^2 \mathcal{V}(u^o) : \mathcal{V} \rightarrow \mathcal{V} \quad \text{and} \quad \mathcal{L}_o : P \circ \mathcal{L}|_{S_o} : S_o \rightarrow S_o. \tag{22} \]
Put $G := G_{u^o} = \Gamma \times O(2) \cong D_n \times O(2)$ and denote by $\mathcal{I}_o$ the slice to $G(u^o) = \mathcal{G}(u^o)$ in $H^1(S^1, \mathcal{V})$. We will also denote by $\mathcal{J} : \mathbb{R} \times \tilde{\Omega} \rightarrow \mathbb{R}$ the restriction of $J$ to the set $\mathbb{R} \times \tilde{\Omega}$, where $\tilde{\Omega} = \mathcal{I}_o \cap \Omega$ and $\mathcal{J}(\lambda, u) = J(\lambda, u^o + u), \; u \in \tilde{\Omega}$. Notice that $\mathcal{J}$ is $G$-invariant. Consider the operator $\mathcal{A}(\lambda) : \mathcal{I}_o \rightarrow \mathcal{I}_o$, given by
\[ \mathcal{A}(\lambda) := P(\nabla^2 u J(\lambda, u^o)). \tag{23} \]
Notice that
\[ \nabla^2 u \mathcal{J}(\lambda, u^o) = \mathcal{A}(\lambda), \]
thus, by implicit function theorem, $G(u^o)$ is an isolated orbit of critical points of $J$, whenever $\mathcal{A}(\lambda)$ is an isomorphism. Therefore, if a point $(\lambda_0, u^o)$ is a bifurcation point for (18), then $\mathcal{A}(\lambda_0)$ is not an isomorphism. Based on this observation we define $\Lambda = \{ \lambda > 0 : \mathcal{A}(\lambda_0) \text{ is not an isomorphism} \}$. We will call the set $\Lambda$ the critical set for the trivial solution $u^o$.

Consider the restricted $S^1$-action on $H^1(S^1, \mathcal{V})$ (see (16)). The fixed-point space $(H^1(S^1, \mathcal{V}))^{S^1}$, by identifying it with the subspace of constant functions, is the space $\mathcal{V}$. Thus we have
\[ H^1(S^1, \mathcal{V}) = \mathcal{V} \oplus \mathcal{W}, \quad \mathcal{W} := \mathcal{V}^\perp, \]
so the slice $\mathcal{I}_o$ in $H^1(S^1, \mathcal{V})$ to the orbit $\mathcal{G}(u^o)$ at $u^o$ is exactly
\[ \mathcal{I}_o = S_o \oplus \mathcal{W}. \]

4.1. Application of the equivariant gradient degree. Assume that $\lambda_0 \in \Lambda$ is an isolated point in the critical set $\Lambda$, i.e. there exists $\lambda_- < \lambda_0 < \lambda_+$ such that $[\lambda_-, \lambda_+] \cap \Lambda = \{ \lambda_0 \}$. Recall $G := D_n \times O(2)$ and $G := D_n \times O(2) \times O(2)$. For the basic properties of the equivariant gradient degree we refer to the Appendix A.

Define the following equivariant invariants (cf. [12]):
\[ \omega_G(\lambda_0) := \nabla_G \text{deg}\left( \mathcal{A}(\lambda_-), B_1(0) \right) - \nabla_G \text{deg}\left( \mathcal{A}(\lambda_+), B_1(0) \right), \tag{24} \]
\[ \omega_G(\lambda_0) := \Theta(\omega_G(\lambda_0)), \tag{25} \]
where $B_1(0)$ stands for the open unit ball in $\mathcal{I}_o$ and $\Theta : U(G) \rightarrow U(\mathcal{G})$ is given by $\Theta(H) = (H)$ for all $(H) \in \Phi(G)$. By the homotopy and existence property of the gradient degree, by applying standard arguments, one can easily show using the Slice Principle (see Theorem A.5) that if
\[ \omega_G(\lambda_0) = n_1(H_1) + n_2(H_2) + \cdots + n_m(H_m), \]
is non-zero, i.e. $n_j \neq 0$ for some $j = 1, 2, \ldots, m$, then $\omega_G(\lambda_0) = n_1(H_1) + n_2(H_2) + \cdots + n_m(H_m)$ also has non-zero coefficient $n_j$, and there exists a bifurcating branch of nontrivial solutions to (18) from the orbit $\{ \lambda_0 \} \times G(u^o)$ with symmetries at least $(H_j)$ (with respect to the $G$-action).
Consider the $S^1$-isotypical decomposition of $\mathcal{W}$, that is,

$$
\mathcal{W} = \bigoplus_{l=1}^{\infty} \mathcal{W}_l, \quad \mathcal{W}_l := \{ \cos(l) \alpha + \sin(l) \beta : \alpha, \beta \in \mathcal{V} \}.
$$

In a standard way, the space $\mathcal{W}_l$, $l = 1, 2, \ldots$, can be naturally identified with the space $\mathcal{V}^c$ on which $S^1$ acts by $l$-folding, i.e. $\mathcal{W}_l = \{ e^{ilz} : z \in \mathcal{V} \}$. Notice that, since the operator $\mathcal{A}(\lambda)$ is $G$-equivariant, it is also $S^1$-equivariant and thus $\mathcal{A}(\lambda)(\mathcal{W}_l) \subset \mathcal{W}_l$. On the other hand, we have

$$
\sigma(\mathcal{A}(\lambda)|_{\mathcal{W}_l}) = \left\{ 1 - \frac{\lambda^2 \mu + 1}{\mu^2 + 1} : \mu \in \sigma(\mathcal{L}_o) \right\}, \quad (26)
$$

which under the assumption that $0 \notin \sigma(\mathcal{L}_o)$, implies that $\lambda_o \in \Lambda$ if and only if $\lambda_o^2 = \frac{\mu^2}{\mu}$ for some $l = 1, 2, 3, \ldots$ and $\mu \in \sigma(\mathcal{L}_o)$. Therefore, in order to apply the formula (47) (see Appendix A), it is essential to know the spectrum $\sigma(\mathcal{L}_o)$.

4.2. Computation of the spectrum $\sigma(\mathcal{L})$. Since the potential $\mathcal{V}$ is given by (6), we can write that $\mathcal{V}(u) = \Phi(u) + \Psi(u)$, $u \in \Omega$, where

$$
\Phi(u) = \sum_{j=0}^{n} U(|u_{j+1} - u_j|^2), \quad \Psi(u) = \sum_{0 \leq j < k \leq n-1} W(|u_j - u_k|^2).
$$

Then

$$
\nabla \Phi(u) = 2 \begin{bmatrix}
U'(|u_0 - u_{n-1}|^2)(u_0 - u_{n-1}) + U'(|u_0 - u_1|^2)(u_0 - u_1) \\
U'(|u_1 - u_2|^2)(u_1 - u_2) + U'(|u_1 - u_0|^2)(u_1 - u_0) \\
\vdots \\
U'(|u_{n-1} - u_0|^2)(u_{n-1} - u_0) + U'(|u_{n-1} - u_{n-2}|^2)(u_{n-1} - u_{n-2})
\end{bmatrix},
$$

and

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

Matrix Representation of $\mathcal{L}$: For a given complex number $z = x + iy$, which we write in a vector form $z = (x, y)^T$, we define the matrix $m_z := zz^T$, i.e.

$$
m_z := \begin{bmatrix} x \\ y \end{bmatrix}, \quad [x, y] = \begin{bmatrix} x^2 & xy \\ xy & y^2 \end{bmatrix}.
$$

We will also apply the following notation $z_{jk} := \gamma^j - \gamma^k$, $\gamma := e^{\frac{2\pi i}{n}}$, $j, k \in \mathbb{Z}$ and we put $m_{jk} := m_{z_{jk}}$. Notice that

$$
\text{Re}(\gamma^j - \gamma^k) = 2 \sin \left( \frac{(k-j)\pi}{n} \right) \sin \left( \frac{(k+j)\pi}{n} \right),
$$

The $2 \times 2$ matrix $m_{jk}$ can be described using the complex operators as

$$
m_{jk} = \frac{|z_{jk}|^2}{2} \left[ 1 - \gamma^{j+k} \right] = 2 \sin^2 \frac{\pi(j-k)}{n} \left[ 1 - \gamma^{j+k} \right].$$
Put

\[ v_{jk} := U'(a_{jk}r_o^2), \quad v_{jj} := 0 \]
\[ u_{jk} := 2U''(a_{jk}r_o^2) \sin^2 \frac{\pi(j - k)}{n}, \quad u_{jj} := 0 \]
\[ v_{jk} := W'(a_{jk}r_o^2), \quad v_{jj} := 0 \]
\[ u_{jk} := 2W''(a_{jk}r_o^2) \sin^2 \frac{\pi(j - k)}{n}, \quad u_{jj} := 0 \]

Clearly, \( v_{j+k+l} = v_{jk} \) and \( u_{j+k+l} = u_{jk} \). Then, by direct computations, we have

\[ \nabla^2 \Phi(u^o) = 2U'(ar_o^2)A + 4r_o^2 U''(ar_o^2)B, \]

where

\[ A := \begin{bmatrix}
2 & -1 & 0 & \ldots & -1 \\
-1 & 2 & -1 & \ldots & 0 \\
\vdots & \vdots & \ddots & \ddots & \vdots \\
-1 & 0 & 0 & \ldots & 2
\end{bmatrix}, \]

and

\[ B := \begin{bmatrix}
m_{0,0} & -m_{0,1} & 0 & \ldots & -m_{0,n-1} \\
-m_{1,0} & m_{1,0} + m_{1,2} & -m_{1,2} & \ldots & 0 \\
\vdots & \vdots & \ddots & \ddots & \vdots \\
-m_{n-1,0} & 0 & 0 & \ldots & m_{n-1,n-2} + m_{n-1,n-1}
\end{bmatrix} \]

\[ = 2 \sin^2 \frac{\pi}{n} \begin{bmatrix}
2 - (\gamma^{-1} + \gamma)\kappa & -1 + \gamma\kappa & 0 & \ldots & -1 + \gamma^{-1}\kappa \\
-1 + \gamma\kappa & 2 - (\gamma^3 + \gamma^3)\kappa & -1 + \gamma^3\kappa & \ldots & 0 \\
\vdots & \vdots & \ddots & \ddots & \vdots \\
-1 + \gamma^{-1}\kappa & 0 & 0 & \ldots & 2 - (\gamma^3 + \gamma^{-1})
\end{bmatrix}, \]

Next, by direct computations one can derive the following matrix form of

\[ \nabla^2 \Psi(u^o) = 2C + 4r_o^2 D, \]

where

\[ C := \begin{bmatrix}
\sum_{j \neq 0} W'(a_{0j}r_o^2) & -W'(a_{01}r_o^2) & \ldots & -W'(a_{0,n-1}r_o^2) \\
-W'(a_{10}r_o^2) & \sum_{j \neq 1} W'(a_{1j}r_o^2) & \ldots & -W'(a_{2,n-1}r_o^2) \\
\vdots & \vdots & \ddots & \vdots \\
-W'(a_{n-1,0}r_o^2) & -W'(a_{n-1,1}r_o^2) & \ldots & \sum_{j \neq n-1} W'(a_{n-1,j}r_o^2)
\end{bmatrix} \]
Using the above decompositions, we have the following matrix representations of $A_j$:

$$
\begin{align*}
&= \left[
\begin{array}{cccc}
\sum_j v_{0j} & -v_{01} & -v_{02} & \cdots & -v_{0,n-1} \\
-v_{10} & \sum_j v_{1j} & -v_{12} & \cdots & -v_{1,n-1} \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
-v_{n-1,0} & -v_{n-1,1} & -v_{n-1,2} & \cdots & \sum_j v_{n-1,j}
\end{array}
\right]
\end{align*}
\] 

and

$$
\begin{align*} 
\mathcal{D} :=& \left[
\begin{array}{cccc}
\sum_{j \neq 0} W''(a_0 r_n^2)m_{0j} & -W''(a_0 r_n^2)m_{01} & -W''(a_0 r_n^2)m_{02} & \cdots & -W''(a_0 r_n^2)m_{0,n-1} \\
-W''(a_1 r_n^2)m_{10} & \sum_{j \neq 1} W''(a_1 r_n^2)m_{1j} & -W''(a_1 r_n^2)m_{12} & \cdots & -W''(a_1 r_n^2)m_{1,n-1} \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
-W''(a_{n-1} r_n^2)m_{n-1,0} & -W''(a_{n-1} r_n^2)m_{n-1,1} & \cdots & \sum_{j \neq n-1} W''(a_{n-1} r_n^2)m_{n-1,j}
\end{array}
\right] \\
&= \tilde{C} - \mathcal{F}_n K,
\end{align*}
\] 

with

$$
\begin{align*}
\tilde{C} :=& \left[
\begin{array}{cccc}
\sum_j u_{0j} & -u_{01} & -u_{02} & \cdots & -u_{0,n-1} \\
-u_{10} & \sum_j u_{1j} & -u_{12} & \cdots & -u_{1,n-1} \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
-u_{n-1,0} & -u_{n-1,1} & -u_{n-1,2} & \cdots & \sum_j u_{n-1,j}
\end{array}
\right]
\end{align*}
\] 

and

$$
\mathcal{F}_n := \left[
\begin{array}{cccc}
\sum_j u_{0j} \gamma^j & -u_{01} \gamma & -u_{02} \gamma & \cdots & -u_{0,n-1} \gamma^{-1} \\
-u_{10} \gamma & \sum_j u_{1j} \gamma^{j+1} & -u_{12} \gamma & \cdots & -u_{1,n-1} \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
-u_{n-1,0} \gamma^{-1} & -u_{n-1,1} \gamma & \cdots & \sum_j u_{n-1,j} \gamma^{-j-1}
\end{array}
\right].
\] 

Using the above decompositions, we have the following matrix representations of $A_k := A|_{\gamma_k}, B_k := B|_{\gamma_k}, C_k := C|_{\gamma_k}, \tilde{C}_k := \tilde{C}|_{\gamma_k},$ and $A_k := A|_{\gamma_k}$:

**Case 1 ($n$ being an odd number).** We have the following matrices:

$$
A_0 = [2 - 2\text{Re} (\gamma)] = \left[ 4\sin^2 \frac{\pi}{n} \right], \quad A_1 = [2 - 2\text{Re} (\gamma^2)] = \left[ 4\sin^2 \frac{2\pi}{n} \right]
$$

$$
A_k = \left[
\begin{array}{cc}
2 - 2\text{Re}(\gamma^{k-1}) & 0 \\
0 & 2 - 2\text{Re}(\gamma^k)
\end{array}
\right] = \left[
\begin{array}{cc}
4\sin^2 \frac{\pi(k-1)}{n} & 0 \\
0 & 4\sin^2 \frac{\pi(k+1)}{n}
\end{array}
\right],
\]
for $1 < k < \left[ \frac{\pi}{2} \right]$. Since
\[ E_k u^k = 2 \text{Re} (\gamma - \gamma^k) v^k = -4 \sin \frac{(1 + k)}{n} \sin \frac{(1 - k)}{n} v^k, \]
\[ E_k v^k = 2 \text{Re} (\gamma - \gamma^k) u^k = -4 \sin \frac{(1 + k)}{n} \sin \frac{(1 - k)}{n} u^k, \]
we get
\[ B_0 = \left[ \begin{array}{c} 8 \sin^4 \frac{\pi}{n} \end{array} \right], \quad B_1 = \left[ \begin{array}{c} 8 \sin^2 \frac{\pi}{n} \sin^2 \frac{2\pi}{n} \end{array} \right], \]
\[ B_k = \left[ \begin{array}{c} 8 \sin^2 \frac{\pi}{n} \sin^2 \frac{(k+1)}{n} \sin \frac{(1-k)}{n} \sin \frac{(1-k)}{n} \sin \frac{(1-k)}{n} \sin \frac{(1-k)}{n} \end{array} \right], \]
for $1 < k < \left[ \frac{\pi}{2} \right]$. Put
\[ a_k := \sum_j v_{0j} - \sum_j v_{0j} \gamma^{(1-k)j} = \sum_{j=1}^{n-1} 4v_{0j} \sin^2 \frac{(1-k)j}{n}, \]
\[ b_k := \sum_j v_{0j} - \sum_j v_{0j} \gamma^{(1+k)j} = \sum_{j=1}^{n-1} 4v_{0j} \sin^2 \frac{(1+k)j}{n}, \]
\[ a_k := \sum_j u_{0j} - \sum_j u_{0j} \gamma^{(1-k)j} = \sum_{j=1}^{n-1} 4u_{0j} \sin^2 \frac{(1-k)j}{n}, \]
\[ b_k := \sum_j u_{0j} - \sum_j u_{0j} \gamma^{(1+k)j} = \sum_{j=1}^{n-1} 4u_{0j} \sin^2 \frac{(1+k)j}{n}. \]
Since
\[ C u^k = \left( \sum_j v_{0j} - \sum_j v_{0j} \gamma^{(1-k)j} \right) u^k, \quad C v^k = \left( \sum_j v_{0j} - \sum_j v_{0j} \gamma^{(1+k)j} \right) v^k, \]
thus we obtain
\[ C_0 = [a_0], \quad C_1 = 0, \quad \tilde{C}_0 = [a_0], \quad \tilde{C}_1 = 0, \]
\[ C_k = \begin{bmatrix} a_k & 0 \\ 0 & b_k \end{bmatrix}, \quad \tilde{C}_k = \begin{bmatrix} a_k & 0 \\ 0 & b_k \end{bmatrix}, \]
for $1 < k < \left[ \frac{\pi}{2} \right]$. Next, put
\[ c_k = \sum_j u_{0j} \gamma^j - \sum_j u_{0j} \gamma^j \gamma^{j(k-1)} = 4 \sum_{j=1}^{n-1} u_{0j} \sin \frac{\pi j}{n} \sin \frac{\pi j}{n} \sin \frac{\pi j}{n}. \]
Since
\[ F_\gamma u^k = \left( \sum_j u_{0j} \gamma^j - \sum_j u_{0j} \gamma^j \gamma^{j(k-1)} \right) v^k, \]
\[ F_\gamma v^k = \left( \sum_j u_{0j} \gamma^j - \sum_j u_{0j} \gamma^j \gamma^{j(k-1)} \right) u^k. \]
we obtain
\[ D_0 = [a_0], \quad D_1 = [c_1] = [0], \]
\[ D_k = \begin{bmatrix} a_k & -c_k \\ -c_k & b_k \end{bmatrix}, \quad \text{for } 1 < k < \left\lfloor \frac{n}{2} \right\rfloor \]

Finally, we get the following matrix representations of \( L_k \)
\[ L_0 = [\alpha_0], \quad L_1 = [\alpha_1], \quad (27) \]

where
\[ \alpha_0 = 8 \left( U'(a_o^2) + 4r_o^2U''(a_o^2) \sin^2 \frac{\pi}{n} \right) \sin^2 \frac{\pi}{n} + \sum_{j=1}^{\left\lfloor \frac{n-1}{2} \right\rfloor} (8v_{0j} + 16r_o^2u_{0j}) \sin^2 \frac{\pi j}{n} \] (28)
\[ \alpha_1 = 8 \left( U'(a_o^2) + 4r_o^2U''(a_o^2) \sin^2 \frac{2\pi}{n} \right) \sin^2 \frac{2\pi}{n} \quad (29) \]
and
\[ L_k = \begin{bmatrix} 2\alpha_k & \delta_k \\ \delta_k & 2\beta_k \end{bmatrix}, \quad 1 < k \leq \left\lfloor \frac{n-1}{2} \right\rfloor \quad (30) \]

where
\[ \alpha_k := 4U'(a_o^2) \sin^2 \frac{\pi(k-1)}{n} + 16r_o^2U''(a_o^2) \sin^2 \frac{\pi}{n} \sin^2 \frac{\pi(1-k)}{n} \]
\[ + \sum_{j=1}^{\left\lfloor \frac{n-1}{2} \right\rfloor} (4v_{0j} + 8r_o^2u_{0j}) \sin^2 \frac{\pi(1-k)j}{n}, \] (31)
\[ \beta_k := 4U'(a_o^2) \sin^2 \frac{\pi(k+1)}{n} + 16r_o^2U''(a_o^2) \sin^2 \frac{\pi}{n} \sin^2 \frac{\pi(1+k)}{n} \]
\[ + \sum_{j=1}^{\left\lfloor \frac{n-1}{2} \right\rfloor} (4v_{0j} + 8r_o^2u_{0j}) \sin^2 \frac{\pi(1+k)j}{n}, \] (32)
\[ \delta_k := 32r_o^2U''(a_o^2) \sin^2 \frac{\pi}{n} \sin \frac{\pi(1+k)}{n} \sin \frac{\pi(1-k)}{n} \]
\[ - 32r_o^2 \sum_{j=1}^{\left\lfloor \frac{n-1}{2} \right\rfloor} u_{0j} \sin \frac{\pi j(k-1)}{n} \sin \frac{\pi j(k+1)}{n}. \] (33)

**Case 2 (n being an even number).** In this case we have an additional isotypical component \( r, \quad r = \frac{n}{2}. \) The entries of the matrix \( L_k, \) for \( 0 \leq k < \frac{n}{2}, \) given by formulae (27) and (30), are slightly different, i.e.
\[ \alpha_0 = 8 \left( U'(a_o^2) + 4r_o^2U''(a_o^2) \sin^2 \frac{\pi}{n} \right) \sin^2 \frac{\pi}{n} + \sum_{j=1}^{\left\lfloor \frac{n-1}{2} \right\rfloor} (8v_{0j} + 16r_o^2u_{0j}) \sin^2 \frac{\pi j}{n} \]
\[ + 4v_{0r} + 8u_{0r}r_o^2, \] (34)
\[ \alpha_1 = 8 \left( U'(a_o^2) + 4r_o^2U''(a_o^2) \sin^2 \frac{2\pi}{n} \right) \sin^2 \frac{2\pi}{n}, \] (35)
Moreover, all the eigenvalues where

\begin{align}
\alpha_k &:= 4U'(ar_o^2)\sin^2 \frac{\pi(k-1)}{n} + 16r_o^2a''(ar_o)\sin^2 \frac{\pi(1-k)}{n} \\
+ \sum_{j=1}^{\lfloor n/2 \rfloor} (4v_{oj} + 8r_o^2u_{oij})\sin^2 \frac{\pi(k-j)}{n} + \delta(k) (2v_{o0r} + 4r_o^2u_{0or}), \\
\beta_k &:= 4U'(ar_o^2)\sin^2 \frac{\pi(k+1)}{n} + 16r_o^2a''(ar_o)\sin^2 \frac{\pi(1+k)}{n} \\
+ \sum_{j=1}^{\lfloor n/2 \rfloor} (4v_{oj} + 8r_o^2u_{oij})\sin^2 \frac{\pi(k+j)}{n} + \delta(k) (2v_{o0r} + 4r_o^2u_{0or}), \\
\delta_k &:= 32r_o^2a''(ar_o)\sin^2 \frac{\pi}{n} \sin \frac{\pi(1-k)}{n} \\
- 32r_o^2 \sum_{j=1}^{\lfloor n/2 \rfloor} u_{oij} \sin \left( \frac{\pi(k-1)}{n} \right) \sin \left( \frac{\pi(k+j)}{n} \right) + 16\delta(k)r_o^2u_{0or},
\end{align}

for $1 < k \leq r - 1$. In addition we have $\mathcal{L}_k = [\alpha_r]$, where

\begin{align}
\alpha_r &:= 8U'(ar_o^2)\cos^2 \frac{\pi}{n} + 32r_o^2a''(ar_o)\sin^2 \frac{\pi}{n} \cos^2 \frac{\pi}{n} \\
+ \sum_{j=1}^{\lfloor n/2 \rfloor} (8v_{oj} + 16r_o^2u_{oij})\sin^2 \left( \frac{\pi(1-r)}{n} \right)j + (4v_{o0r} + 8r_o^2u_{0or}).
\end{align}

Spectrum of the Matrix $\mathcal{L}':$ Consequently, we obtain the following results:

**Proposition 4.1.** For $n$ being an odd number we have the following explicit formulae for the spectrum of the operator $\mathcal{L}$

$$
\sigma(\mathcal{L}) = \left\{ \mu_0, \mu_1, \mu_k^\pm, \ 1 < k \leq \left\lfloor \frac{n-1}{2} \right\rfloor \right\},
$$

where

$$
\mu_0 := \alpha_0, \quad \mu_1 := \alpha_1,
$$

$$
\mu_k^\pm := \alpha_k + \beta_k \pm \sqrt{(\alpha_k - \beta_k)^2 + \delta_k^2}, \quad 1 < k \leq \left\lfloor \frac{n-1}{2} \right\rfloor.
$$

and the coefficients $\alpha_j, \beta_j, \delta_j$ are given by (28), (29), (31), (32) and (33). Moreover, all the eigenvalues $\mu_j, j = 0, 1$ or $\mu_j^\pm, 1 < j \leq \left\lfloor \frac{n-1}{2} \right\rfloor$, are $V_j$-simple.

And

**Proposition 4.2.** For $n$ being an even number we have the following explicit formulae for the spectrum of the operator $\mathcal{L}$

$$
\sigma(\mathcal{L}) = \left\{ \mu_0, \mu_1, \mu_r, \mu_k^\pm, \ 1 < k \leq \frac{n}{2} \right\},
$$

where

$$
\mu_0 := \alpha_0, \quad \mu_1 := \alpha_1, \quad \mu_r := \alpha_r,
$$

$$
\mu_k^\pm := \alpha_k + \beta_k \pm \sqrt{(\alpha_k - \beta_k)^2 + \delta_k^2}, \quad 1 < k \leq \left\lfloor \frac{n-1}{2} \right\rfloor.
$$

and the coefficients $\alpha_j, \beta_j, \delta_j$ are given by (34), (35), (36), (32), (38) and (39). Moreover, all the eigenvalues $\mu_j, j = 0, 1, r$, or $\mu_j^\pm, 1 < j \leq \left\lfloor \frac{n-1}{2} \right\rfloor$, are $V_j$-simple.
5. Existence result and examples.

5.1. Computation of the equivariant bifurcation invariants. In order to describe the $G$-isotypical decomposition of the slice $S_n$ (recall $G := D_n \times O(2)$), first, we identify the irreducible $G$-representations related to the isotypical decomposition of $\mathcal{W}$. These representations are $\mathcal{W}_{jl} := \mathcal{V}_j \otimes \mathcal{U}_l$, where $\mathcal{U}_l$ is the $l$-th irreducible $O(2)$-representation (listed according to the convention introduced in [1]), $j = 0, 1, \ldots, \lfloor \frac{n-1}{2} \rfloor$, $l = 1, 2, 3, \ldots$. The corresponding to $\mathcal{W}_{jl}$ isotypical components of $\mathcal{W}$ are

$$\mathcal{W}'_{jl} := \{ \cos(l) a + \sin(l) b : a, b \in \mathcal{V}_j \}.$$ 

These irreducible $G$-representations can be easily described. For example, if $j = 1, \ldots, \lfloor \frac{n-1}{2} \rfloor$, the representation $\mathcal{W}_{jl} = \mathbb{C} \oplus \mathbb{C}$ is a 4-dimensional (real) representation of real type with the action of $G$ given by the formulae

$$\gamma(z_1, z_2) := (\gamma^j \cdot z_1, \gamma^{-j} \cdot z_2),$$
$$\kappa(z_1, z_2) := (z_2, z_1),$$
$$\xi(z_1, z_1) := (\xi^j \cdot z_1, \xi^{-j} \cdot z_2),$$
$$\kappa(z_1, z_2) := (\xi_1, \xi_2),$$

where $\xi \in SO(2)$, $O(2) = SO(2) \cup SO(2) \kappa$ and

$$D_n := \{ 1, \gamma, \ldots, \gamma^{n-1}, \kappa, \kappa \gamma, \ldots, \gamma^{n-1} \kappa \}.$$

For positive eigenvalue $\mu_j^+ \in \sigma(\mathcal{L})$, $1 < j \leq \lfloor \frac{n-1}{2} \rfloor$, we put $\lambda_{j,l}^+ := \frac{\mu_j^+}{\mu_j}$, and for other positive eigenvalues $\mu_j$, $j = 0, 1$ or $j = r$ (when $n$ is even), we put $\lambda_{j,l}^+ := \frac{\mu_j}{\mu_j}$, $l \in \mathbb{N}$. Then

$$\Lambda = \left\{ \lambda_{j,l}^+ : 1 < j \leq \left\lfloor \frac{n-1}{2} \right\rfloor, l \in \mathbb{N} \right\} \cup \{ \lambda_{k,l} : k = 0, 1 \text{ or } r \text{ if } n \text{ is even} \}.$$ 

Since each of the eigenvalues $\mu_j^+ \in \sigma(\mathcal{L})$ or $\mu_j \in \sigma(\mathcal{L})$ (otherwise) has $\mathcal{V}_j$-isotypical multiplicity one, it follows that for $\lambda_0 < \lambda_0 := \lambda_{j,l}^+ < \lambda_0^+$ (respectively $\lambda_0 < \lambda_0 := \lambda_{j,l}^+ < \lambda_0^+$), where $[\lambda_-, \lambda_+] \cap \Lambda = \{ \lambda_0 \}$, we have $\sigma_-(\mathcal{L}_-) = \sigma_-(\mathcal{L}_+) \cup \{ \lambda_0 \}$.

Consequently, for $\lambda_0 = \lambda_{j,d}^+$ or $\lambda_0 = \lambda_{j,l}$, by applying formula (47), we obtain that

$$\omega_G(\lambda_0) = \nabla_G \text{deg} \left( \mathcal{L}_-, B_1(0) \right) - \nabla_G \text{deg} \left( \mathcal{L}_+, B_1(0) \right) = \prod_{\xi \in \sigma_-(\mathcal{L}_-) \cup \{ \lambda_0 \}} (\text{Deg}_{W_{ik}}^{m_{ik}(\xi)}) - \prod_{\xi \in \sigma_-(\mathcal{L}_+) \cup \{ \lambda_0 \}} (\text{Deg}_{W_{ik}}^{m_{ik}(\xi)})$$

$$= \prod_{\xi \in \sigma_-(\mathcal{L}_+) \cup \{ \lambda_0 \}} (\text{Deg}_{W_{ik}}^{m_{ik}(\xi)}) \ast \left( \text{Deg}_{W_{jl}} - (G) \right). \quad (40)$$

**Example 5.1.** In the case of the group $G = D_6 \times O(2)$, we have the following basic degrees\(^1\) $\text{Deg}_{W_{jk}}$ (which were obtained in [21] using GAP programming)

$$\text{Deg}_{W_{jk}} = (D_6 \times O(2)) - (D_6 \times D_1),$$

\(^1\)Let us point out that for practical applications of the gradient $D_n \times O(2)$-degree, it is fully justified (see [6]) to use is values truncated to the Burnside ring $A(D_n \times O(2))$.}
Under the assumptions formulated in section 3, i.e. we list the maximal orbit types in maximal orbit types

\[ \text{Deg}_{W_1} = (D_6 \times O(2)) - (D_6^{Z_1} \times D_6 D_{40}) - (D_2^{D_1} \times Z_2 D_{21}) -(D_2^{D_1} \times Z_2 D_{21}) + 2(D_2^{Z_1} \times D_6 D_{40}) + (Z_2^{Z_1} \times Z_2 D_{21}), \]

\[ \text{Deg}_{W_2} = (D_6 \times O(2)) - (D_6^{Z_2} \times D_3 D_{31}) - (D_2^{Z_2} \times Z_2 D_{21}) - (D_2 \times D_1) + 2(D_2^{Z_2} \times D_3 D_{31}) + (Z_2 \times D_1), \]

\[ \text{Deg}_{W_3} = (D_6 \times O(2)) - (D_6^{D_3} \times Z_2 D_{21}). \]

In this way we are in a position to formulate the following existence result:

**Theorem 5.2.** Under the assumptions formulated in section 3, i.e. \( \mathcal{V} : \Omega_{\rho} \rightarrow \mathbb{R} \) is given by (6) and the \( \Gamma \)-symmetric equilibrium \( u^* \) of \( \mathcal{V} \) is given (12), for every \( \lambda_0 = \lambda_{j,1}, \) \( 0 < j \leq \left\lfloor \frac{2}{3} \right\rfloor, \) and \( \lambda_0 = \lambda_{0,1}, \lambda_{1,1} \) or \( \lambda_{r,1} \) there exists an orbit of bifurcating branches of nontrivial periodic solutions to (18) from the orbit \( \{ \lambda_{j,1} \} \times \mathcal{G}(u^*). \) More precisely, for every orbit type \( (H_{j,1}) \) in \( D_{j,1} \) there exists an orbit of periodic solutions with symmetries at least \( H_{j,1}. \)

**Proof.** This result is a direct consequence of the Existence Property (P1) of the gradient equivariant degree formulated in Theorem A.2.

5.2 Computational example. In this section we consider a dihedral configuration of molecules composed of \( n = 6 \) particles. When it comes to the function \( W \) in (6), we put \( A = 0.002205918750, B = 0.000004055064608 \) and \( \sigma = 0.35. \) Therefore, we obtain that \( \phi \) defined at (10) assumes its minimum at \( r_0 = 1.214894009. \) The distinct eigenvalues of the Hessian matrix \( \nabla^2 \mathcal{V}(u^*) \) are \( \mu_0 = 10.10496819, \) \( \mu_1 = 8.469351217, \) \( \mu_2 = 3.854423919, \) \( \mu_3 = 6.442637681 \) and \( \mu_4 = -0.007288929. \) Several values of the critical set \( \Lambda, \) particularly for \( l = 1, 2, 3, 4 \) are listed in Table 1.

| \( j \)   | \( \mu_j \) | \( \lambda_{j,1} \) | \( \lambda_{j,2} \) | \( \lambda_{j,3} \) | \( \lambda_{j,4} \) |
|---------|--------------|-----------------|----------------|----------------|----------------|
| 0       | 10.10496819  | 0.31458103      | 0.62916205     | 0.94374308     | 1.25832410     |
| 1       | 8.469351217  | 0.34361723      | 0.68723445     | 1.03805168     | 1.37446891     |
| 2       | 3.854423919  | 0.50935463      | 1.01870927     | 1.52806390     | 2.03741854     |
| 2\*     | 6.442637681  | 0.62767390      | 1.25534781     | 1.88320217     | 2.51069561     |
| 2\-     | 0.007288929  | 11.7130006      | 23.4260011     | 35.1390017     | 46.8520023     |

**Table 1.** The values \( \lambda_{j,1} \) in the critical set \( \Lambda \)

One can notice that we have the following inequalities:

\[ \lambda_{0,1} < \lambda_{1,1} < \lambda_{3,1} < \lambda_{4,1} < \lambda_{0,2} < \lambda_{1,2} < \lambda_{0,3} < \lambda_{3,2} < \lambda_{1,3} < \lambda_{2,3} < \lambda_{0,4} < \lambda_{1,4} < \lambda_{3,3} < \ldots \]

**Topological Invariants \( \omega(\lambda_0):** In Table 5.2 we list the maximal orbit types in \( \mathcal{W}_{j,l} \setminus \{ 0 \}, \) \( l \geq 1 \):

| \( \mathcal{W}_{j,l} \setminus \{ 0 \} \) | maximal orbit types |
|-----------------|-----------------|
| \( \mathcal{W}_{0,l} \) | \( D_6 \times D_1 \) |
| \( \mathcal{W}_{1,l} \) | \( D_6^{Z_1} \times D_6 D_{40}, \) \( D_2^{D_1} \times Z_2 D_{21}, \) \( D_2^{D_1} \times Z_2 D_{21} \) |
| \( \mathcal{W}_{2,l} \) | \( D_6^{Z_2} \times D_3 D_{31}, \) \( D_2^{Z_2} \times Z_2 D_{21}, \) \( D_2 \times D_1 \) |
| \( \mathcal{W}_{3,l} \) | \( D_6^{D_3} \times Z_2 D_{21} \) |

**Table 2.** Maximal orbit types in \( \mathcal{W}_{j,l} \)
Next, we list the values of the equivariant invariants \(\omega(\lambda_{j,l})\) (given by (40)):

\[
\omega_G(\lambda_{0,1}) = \text{Deg}_{\omega_{0,1}} - (G)
\]
\[
\omega_G(\lambda_{1,1}) = \text{Deg}_{\omega_{1,1}} * (\text{Deg}_{\omega_{1,1}} - (G))
\]
\[
\omega_G(\lambda_{3,1}) = \text{Deg}_{\omega_{0,1}} * \text{Deg}_{\omega_{1,1}} * (\text{Deg}_{\omega_{2,1}} - (G))
\]
\[
\omega_G(\lambda_{2,1}^+) = \text{Deg}_{\omega_{0,1}} * \text{Deg}_{\omega_{1,1}} * \text{Deg}_{\omega_{2,1}} * (\text{Deg}_{\omega_{2,1}} - (G))
\]

These sequences of equivariant invariants \(\omega(\lambda_{j,l})\) can be continued indefinitely due to the theorem that any \(p\)-periodic solution is also \(2p\), \(3p\), \(4p\), etc. periodic as well. However, in order to get a clear picture of the emerging from the symmetric equilibrium vibrations, it is sufficient to exhaust all the critical values \(\lambda_{j,1}\). In our case the last critical value in mode one will be \(\lambda_{2,1}\), which will occur as 112th element in \(\Lambda\). Therefore, \(\omega(\lambda_{2,1})\) is a product of 113 factors (basic degrees), indicating quite complex nature of emerging branches near that critical point. Let us point out that although the computation of \(\lambda_{2,1}\) may be elaborated, it is still just a technicality that can be easily achieved using computer software that was developed for this purpose (see [21]). Let us also point out that the exact value of the equivariant invariants \(\omega(\lambda_{j,l})\) can be symbolically computed either in its truncated to the Burnside ring \(A(D_n \times O(2))\) form (such programs are already available) or in \(U(D_n \times O(2))\) (we have all the needed algorithms so the appropriate computer programs were being presently created). Notice that each equivariant invariant \(\omega_G(\lambda_{j,l})\) carries the full equivariant topological information about the bifurcating from the equilibrium \(u^0\) periodic vibrations corresponding to the limit period \(p = 2\pi\lambda_{j,l} m\) (for some \(m \in \mathbb{N}\)). Below, as an example, we present the equivariant invariant \(\omega_G(\lambda_{2,1}^+)\) (truncated to the Burnside ring \(A(D_n \times O(2))\))

\[
\omega_G(\lambda_{2,1}^+) = \text{Deg}_{\omega_{0,1}} * \text{Deg}_{\omega_{1,1}} * \text{Deg}_{\omega_{2,1}} * (\text{Deg}_{\omega_{2,1}} - (D_6 \times O(2)))
\]
\[
= - (D_2 \times_{Z_2} Z_2 D_2) + (\tilde{D}_1 \times_{Z_1} Z_2 D_2) + (D_2 \times D_1)
\]
\[
- (D_1 \times D_1) - (D_6 \times_{Z_2} Z_2 D_3) + (\tilde{D}_3 \times_{Z_1} Z_1 D_3)
\]
\[
+ (D_3 \times_{D_1} D_3) + (D_2 \times_{D_1} D_2) + (D_2 \times_{Z_2} Z_1 D_1)
\]
\[
- (D_2 \times_{D_1} D_1) - (\tilde{D}_1 \times_{Z_1} Z_1 D_1) - (D_1 \times_{Z_1} D_1).
\]

In order to make predictions about the emerging periodic vibrations with a particular limit period \(p = 2\pi\lambda_{j,l} m\), one can look in \(\omega_G(\lambda_{j,l})\) for maximal orbit types listed in Table 5.2. In such a way, we can list some types of the branches of periodic vibrations emerging from the equilibrium \(u^0\):

\(\lambda_{0,1}\): For the limit period 1.9765709 \(m\) there exist at least one orbit of \(p\)-periodic vibrations with spatio-temporal symmetries at least \((D_6 \times D_1)\):

\(\lambda_{1,1}\): For the limit period 2.15901073 \(m\) there exist at least the following three orbits of \(p\)-periodic vibrations with spatio-temporal symmetries at least \((D_6 \times_{Z_1} Z_2 D_2), (D_2 \times_{Z_1} D_2), (D_2 \times D_1)\).

\(\lambda_{3,1}\): For the limit period 3.20036952 \(m\) there exists at least the following orbit of \(p\)-periodic vibrations with spatio-temporal symmetries at least \((D_6 \times_{Z_1} Z_2 D_2)\).

\(\lambda_{2,1}^+\): For the limit period 3.94379143 \(m\) there exist at least the following three orbits of \(p\)-periodic vibrations with spatio-temporal symmetries at least \((D_6 \times_{Z_2} D_3), (D_2 \times_{Z_2} Z_2 D_2), (D_2 \times D_1)\).
\( \lambda_{1,2} \): For the limit period 1.91622311 there exist at least the following three orbits of \( p \)-periodic vibrations with spatio-temporal symmetries at least \((D_6 \mathbb{Z}_l \times D_6 D_{12}), (D_2 D_1 \times \mathbb{Z}_l D_4), (D_2 D_1 \times \mathbb{Z}_l D_4)\).

\( \lambda_{2,1}^- \): For the limit period 73.59495327 there exist at least the following three orbits of \( p \)-periodic vibrations with spatio-temporal symmetries at least \((D_6 \mathbb{Z}_l \times D_3 D_4), (D_2 \mathbb{Z}_l \times D_2 D_4), (D_2 \times D_1)\).

The equivariant invariant can also be used to provide some information about the global behavior of the bifurcation branches, for instance, the non-existence of bounded branches.

5.3. Numerical simulations. In this subsection, we present some simulations of the periodic solutions predicted by our theory. On Figures 2–5, we show the periodic solutions which were found for \( \lambda_0^2 = \frac{1}{p}, l = 1 \) and \( \mu \) near the eigenvalue \( \mu_0 = 10.10496819 \) of \( \nabla^2 V(u^0) \).

5.4. Concluding remarks. In this paper, we analyzed a system (7) with \( n \) particles in the plane \( \mathbb{R}^2 \) admitting dihedral spatial symmetries. More precisely, we used the method of gradient equivariant degree \([11, 3, 8, 18]\) to investigate the existence of periodic solution to (7), where \( V \) is the Lennard-Jones and Coulomb potential, around an equilibrium admitting dihedral \( D_n \) symmetries. The dynamics of system (7) can be very complicated with a large number of different periodic solutions exhibiting various spatio-temporal symmetries. The equivariant degree provides equivariant invariants for system (7) allowing a complete symmetric topological classification of the emanating (or bifurcating) branches of periodic solutions from a given equilibrium state. First, the critical periods \( p_{j,l} > 0 \), which are the limit periods for those bifurcation branches can be identified from the so called critical
Figure 3. Relative motions of all particles with $\lambda^2_0 = \frac{l^2}{\mu}$, $l = 1$ and $\mu$ near the eigenvalue $\mu = 6.442637681$ of $\nabla^2 V(u^0)$

Figure 4. Relative motions of all particles with $\lambda^2_0 = \frac{l^2}{\mu}$, $l = 1$ and $\mu$ near the eigenvalue $\mu = 8.469351217$ of $\nabla^2 V(u^0)$

set $\Lambda := \{\lambda_{jl} = \frac{l^2}{\mu_j}, \ l \in \mathbb{N}, \ \mu_j \in \sigma(\nabla^2 V(u^0))\}$, where $\sigma(\nabla^2 V(u^0))$ denotes the set of eigenvalues of the Hessian $\nabla^2 V(u^0)$, and the symmetries of topologically possible solutions to (7) can be identified from the equivariant invariants $\omega_G(\lambda_{jl})$. The explicitly computed Hessian $\nabla^2 V(u^0)$ facilitated the formulation of general results for dihedral molecular configurations.

We developed a method using the isotypical decomposition of the phase space combined with block decompositions and the usual complex operations in order to represent $\nabla^2 V(a)$ as a product of simple $2 \times 2$-matrices. Therefore, the spectrum $\sigma(\nabla^2 V(a))$ is explicitly computed and these computations do not depend on a
particular form of the potential $\mathbf{V}$. In addition, we provided an exact formula for computation of the equivariant invariants $\omega_G(\lambda_{jl})$. We should also mention that for larger groups $D_n$, the actual computations of $\omega_G(\lambda_{jl})$ can be quite complicated but still possible with the use of computer software. Such software was already developed for several types of groups $G = \Gamma \times O(2)$ and it is available at [21].

We remark that elements $\lambda_{jl}$ of the critical set $\Lambda$ correspond to the values of transitional frequencies. The equivariant invariant $\omega_G(\lambda_{jl})$ provides a full topological classification of symmetric modes corresponding to the branches of molecular vibrations emerging from the equilibrium state at the critical frequency $\lambda_{jl}$. This method can be applied to create, for a molecule with dihedral symmetries, an atlas of topologically possible symmetric modes of vibrations, the collection of actual distinct molecular vibrations (related the maximal symmetric types) emerging from the equilibrium state and the corresponding limit frequencies.

This paper provides complementing results to those obtained in [10] (where the orthogonal degree for abelian actions was used).

**Appendix A.** $G$-equivariant gradient degree. In this Appendix we provide a description of the equivariant gradient degree and its properties. For more details we refer to [11, 2, 18, 3]. In what follows $G$ will stand for a compact Lie group.

**Euler and Burnside Rings.** Let $U(G) := \mathbb{Z}[\Phi(G)]$ denote the free $\mathbb{Z}$-module generated by $\Phi(G)$. Define a ring multiplication on generators $(H), (K) \in \Phi(G)$ as follows:

$$(H) \ast (K) = \sum_{(L) \in \Phi(G)} n_L (L), \quad (41)$$

where

$$n_L := \chi_c((G/H \times G/K)_L/N(L)), \quad (42)$$
with \( \chi_c \) being the Euler characteristic taken in Alexander-Spanier cohomology with compact support (cf. [20]). The \( \mathbb{Z} \)-module \( \mathcal{U}(G) \) equipped with the multiplication (41), (42) is a ring called the Euler ring of the group \( G \) (cf. [7]).

The \( \mathbb{Z} \)-module \( A(G) = A_0(G) : = \mathbb{Z}\langle \Phi_0(G) \rangle \), equipped with a similar multiplication as in \( \mathcal{U}(G) \) but restricted only to generators from \( \Phi_0(G) \), is called a Burnside ring. Notice that for \((H), (K), (L) \in \Phi_0(G)\), the formula (42) can be simply written as \( n_L = |(G/H \times G/K)_L/N(L)| \), where \( |X| \) stands for the number of elements in the set \( X \). As opposed to the complicated multiplicative structure of the Euler ring \( \mathcal{U}(G) \), the Burnside ring structure \( A(G) \) can be explicitly computed, as it is illustrated by multiple examples in [1].

Notice that \( A(G) \) is a \( \mathbb{Z} \)-submodule of \( \mathcal{U}(G) \) but not a subring. Define \( \pi_0 : \mathcal{U}(G) \to A(G) \) on generators \((H) \in \Phi(G)\) by

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

(43)

Then we have,

**Lemma A.1.** (cf. [2]) The map \( \pi_0 \) defined by (43) is a ring homomorphism, i.e.

\[
\pi_0((H) \ast (K)) = \pi_0((H)) \cdot \pi_0((K)),
\]

where \((H), (K) \in \Phi(G)\).

Lemma A.1 allows us to use the Burnside ring multiplicative structure in \( A(G) \) to partially describe the Euler ring multiplication structure in \( \mathcal{U}(G) \). In the case of the group \( G = \Gamma \times O(2) \) (here \( \Gamma \) stands for a finite group), the full multiplicative structure of \( U(G) \) can be obtain by using the properties of the Euler ring homomorphism \( \Psi : U(\Gamma \times O(2)) \to U(\Gamma \times S^1) \) (see [6]).

**G-Equivariant Degrees.** Assume that \( G \) is a compact Lie group, \( V \) an orthogonal (final-dimensional) \( G \)-representation and \( f : V \to V \) a continuous \( G \)-equivariant map. Suppose that \( \Omega \subset V \) is an open bounded \( G \)-invariant set such that \( f(x) \neq 0 \) for all \( x \in \partial \Omega \), then \( f \) is called \( \Omega \)-admissible \( G \)-map, and \((f, \Omega)\) – an admissible \( G \)-pair. We denote by \( \mathcal{M}^G \) the set of all admissible \( G \)-pairs. In the case \( f = \nabla \varphi \) for some \( G \)-invariant \( \varphi : V \to \mathbb{R} \), the pair \((f, \Omega)\) is called an admissible gradient \( G \)-pair. We denote by \( \mathcal{M}_{ad}^G \) the set of all admissible gradient \( G \)-pairs \( (\nabla \varphi, \Omega) \).

Then we have the following theorem:

**Theorem A.2.** (cf. [11]) There exists a unique map \( \nabla_G \text{-deg} : \mathcal{M}_{ad}^G \to U(G) \), which assigns to every \((f, \Omega) \in \mathcal{M}_{ad}^G \) an element \( \nabla_G \text{-deg} (f, \Omega) \in U(G) \), called the \( G \)-gradient degree of \( f \) on \( \Omega \),

\[
\nabla_G \text{-deg} (f, \Omega) = \sum_{(H_i) \in \Phi(G)} n_{H_i} (H_i) = n_{H_1} (H_1) + \cdots + n_{H_m} (H_m),
\]

(44)

satisfying the following properties:

**P1** *(Existence)* If \( \nabla_G \text{-deg} (f, \Omega) \neq 0 \), i.e. \( n_{H_i} \neq 0 \) for some \( (H_i) \) in (44), then there exists \( x \in \Omega \) such that \( f(x) = 0 \) and \( (G_x) \geq (H_i) \).

**P2** *(Additivity)* Let \( \Omega_1 \) and \( \Omega_2 \) be two disjoint open \( G \)-invariant subsets of \( \Omega \) such that \( (f)^{-1}(0) \cap \Omega \subset \Omega_1 \cup \Omega_2 \). Then,

\[
\nabla_G \text{-deg} (f, \Omega) = \nabla_G \text{-deg} (f, \Omega_1) + \nabla_G \text{-deg} (f, \Omega_2).
\]
(P3) (Homotopy) If \( f_t : [0, 1] \times V \to V, t \in [0, 1], \) is a \( G \)-gradient \( \Omega \)-admissible homotopy, then
\[
\nabla_G \deg(f_t, \Omega) = \text{a constant}.
\]

(P4) (Normalization) Let \( \varphi \in C^2_G(V, \mathbb{R}) \) be a special \( \Omega \)-Morse function (see [11]) such that \( (\nabla \varphi)^{-1}(0) \cap \Omega = G(v_0) \) and \( Gv_0 = H. \) Then,
\[
\nabla_G \deg(\nabla \varphi, \Omega) = (-1)^{m_-} (\nabla^2 \varphi(v_0)) : (H),
\]
where "\( m_- (\cdot) \)" stands for the total dimension of eigenspaces for negative eigenvalues of a symmetric matrix.

(P5) (Multiplicativity) For all \( (f_1, \Omega_1), (f_2, \Omega_2) \in \mathcal{M}^G_V, \)
\[
\nabla_G \deg(f_1 \times f_2, \Omega_1 \times \Omega_2) = \nabla_G \deg(f_1, \Omega_1) \ast \nabla_G \deg(f_2, \Omega_2)
\]
where the multiplication "\( \ast \)" is taken in the Euler ring \( U(G). \)

(P6) (Suspension) If \( W \) is an orthogonal \( G \)-representation and \( B \) an open bounded invariant neighborhood of \( 0 \in W, \) then
\[
\nabla_G \deg(f \times \text{Id}_W, \Omega \times B) = \nabla_G \deg(f, \Omega).
\]

Remark A.3. The ‘full’ gradient equivariant degree may be difficult to compute. However, it is possible to consider its truncation to \( A(G), \) i.e. we can define
\[
G \text{-deg}(f, \Omega) := \pi_0 (\nabla_G \text{-deg}(f, \Omega)).
\]
In fact, there exists the \( G \)-equivariant degree \( G \text{-deg} : \mathcal{M}^G \to A(G), \) which satisfies in \( A(G) \) the properties (P1)–(P3), (P5)–(P6). This degree can be effectively computed using recurrence formulae presented in [1]. In this paper, for the sake of simplicity, we limit our computations to the \( G \)-equivariant degree only. However, in order to provide the full \( G \)-equivariant classification of the solution set \( (\nabla \varphi)^{-1}(0) \cap \Omega, \) one should use the gradient \( G \)-equivariant degree. We refer to [6] for algorithms allowing the computations of the gradient degree for \( G = \Gamma \times O(2) \) (with \( \Gamma \) being a finite group).

Remark A.4. Assume that \( \mathcal{H} \) is a separable Hilbert \( G \)-representation and \( \Omega \subset \mathcal{H} \) a open bounded \( G \)-invariant set. In a standard way, one can extend the definition of the gradient \( G \)-equivariant degree to admissible gradient \( G \)-pairs \( (\nabla \varphi, \Omega), \) where \( \varphi : \mathcal{H} \to \mathbb{R} \) is a \( G \)-invariant \( C^1 \)-differentiable map such that \( \nabla \varphi : \mathcal{H} \to \mathcal{H} \) is completely continuous field. For more details we refer to [6].

**Computations of the \( G \)-Equivariant Degree.** Consider a symmetric \( G \)-equivariant linear isomorphism \( T : V \to V, \) where \( V \) is an orthogonal \( G \)-representation. Thus, \( T = \nabla \varphi \) for \( \varphi(v) = \frac{1}{2} \langle T_v \cdot v, v \rangle, \) \( v \in V, \) where “\( \cdot \)” stands for the inner product. We will show how to compute \( \nabla_G \text{-deg}(T, B(V)). \) Consider the \( G \)-isotypical decomposition (4) of \( V \) and put
\[
T_i := T|_{V_i} : V_i \to V_i, \quad i = 0, 1, \ldots, r.
\]
Then, by the Multiplicativity property (P5),
\[
\nabla_G \text{-deg}(T, B(V)) = \prod_i \nabla_G \text{-deg}(T_i, B(V_i)). \tag{45}
\]
For each irreducible \( G \)-representation \( V_i, \) the basic gradient degree is defined by
\[
\text{Deg}_{V_i} := \nabla_G \text{-deg}(-\text{Id}, B(V_i)). \tag{46}
\]
The basic degrees $\text{Deg}_V$ can be computed using formulae developed in [6]. Denote by $\sigma(T)$ the real spectrum of $T$ and put $\sigma_-(T) := \{ \xi \in \sigma(T) : \xi < 0 \}$. The set $\sigma_-(T)$ is called the negative spectrum of $T$. Then, using (45) we obtain the following computational formula for the gradient $G$-equivariant degree of the isomorphism $T$

\[
\nabla_{G}\text{-deg}(T, B(V)) = \prod_{\xi \in \sigma_-(T)} \prod_{i} (\text{Deg}_{U_i})^{m_i(\mu)}.
\]

(47)

A.1. Gradient degree on the slice. Let $G$ be a compact Lie group and $\mathcal{H}$ be a separable Hilbert $G$-representation. Let $\varphi : \mathcal{H} \rightarrow \mathbb{R}$ be a continuously differentiable $G$-invariant functional such that $\nabla \varphi : \mathcal{H} \rightarrow \mathcal{H}$ is a completely continuous field.

Since in the infinite-dimensional Hilbert representation $\mathcal{H}$ and orbit $G(u_o)$ may not have a structure of a submanifold, assume that $u_o \in \mathcal{H}$ is such that the orbit $G(u_o)$ is contained in a finite-dimensional $G$-subrepresentation $\mathcal{H}_o$ of $\mathcal{H}$ and put $\hat{G} := G_{u_o}$. In such a case the $G$-action on $\mathcal{H}_o$ is smooth and the orbit $G(u_o)$ is a smooth submanifold of $\mathcal{H}$. Denote by $S_o \subset \mathcal{H}$ the slice to the orbit $G(u_o)$ at $u_o$ and let $V_o := \tau_o G(u_o)$ be the tangent space to $G(u_o)$ at $u_o$. Then clearly, $S_o = V_o^\perp$, and $S_o$ is a smooth Hilbert $G$-representation.

Theorem A.5. (Slice Principle) Let $\varphi : \mathcal{H} \rightarrow \mathbb{R}$ be a continuously differentiable $G$-invariant functional with $\nabla \varphi$ being a completely continuous field. Assume that $u_o \in \mathcal{H}$ is such that $G(u_o)$ is an isolated critical orbit of $\varphi$ and $G(u_o)$ is contained in a finite-dimensional $G$-subrepresentation. Suppose that $G := G_{u_o}$, $S_o$ is the slice to the orbit $G(u_o)$ at $u_o$, and $U$ is an isolating tubular neighborhood of $G(u_o)$. Define $\varphi_o : S_o \rightarrow \mathbb{R}$ by $\varphi_o (v) = \varphi(u_o + v), v \in S_o$. Then

\[
\nabla_{G}\text{-deg}(\nabla \varphi, U) = \Theta(\nabla_{G}\text{-deg}(\nabla \varphi_o, U \cap S_o)),
\]

(48)

where $\Theta : U(G) \rightarrow U(G)$ is defined on generators $\Theta(K) := (K)^\prime$ with $(K)^\prime$ being the conjugacy of $K$ in $G$ and $(K)^\prime$ being the conjugacy class of $K$ in $G$.

Proof. Since the gradient equivariant degree in Hilbert $G$-representations, is defined using finite-dimensional orthogonal $G$-representation. Then, $\nabla \varphi_o (u) = P \nabla \varphi (u)$, where $P : \mathcal{H} \rightarrow S_o$ is an orthogonal projection. Since $G(u_o)$ is orthogonal to $S_o$, one can assume that $U$ is taken sufficiently small so $G(u)$ is transversal to $S_o$ for all $u \in U$. Then clearly, if $\nabla \varphi_o (v) = 0$ for some $v$ such that $u := u_o + v \in U \cap S_o$, then $\nabla \varphi (u) = 0$. Next, we approximate $\varphi_o$ on $U \cap S_o$ by a generic map (see [11]), which can be extended equivariantly on $U$ and, in such a case, this extension is also generic, formula (48) follows directly from the definition of the gradient degree for generic maps.

A.2. Notation used for the product group $G \times O(2)$. For two groups $G_1$ and $G_2$ all the subgroups $\mathcal{H}$ of the product group $G_1 \times G_2$ can be easily described (see [6, 13]). If $\mathcal{H} \leq G_1 \times G_2$ then there are $H \leq G_1$, $K \leq G_2$, a group $L$ and two epimorphisms $\varphi : H \rightarrow L$ and $\psi : K \rightarrow L$, such that

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

(49)

In this case, we will use the notation

\[
\mathcal{H} =: H \overset{\varphi}{\times}_L K.
\]

(50)

In the case $G_1 = G$ is a finite group and $G_2 = O(2)$, the notation (50) can be simplified. One can denote the conjugacy classes $(\mathcal{H}) \in \Phi(G \times O(2))$ in a more
comprehensive way. Namely, we identify $L$ with $K/\text{Ker}(\psi) \leq O(2)$ and denote by $r$ the rotation generator in $L$. Then the subgroups

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

(here $\langle r \rangle$ stands for the subgroup generated by $r$) allow us to identify the epimorphism $\varphi : H \to L$. This leads to a simpler notation

$$\mathcal{H} := H^Z_R \times_L K.$$  \hfill (51)

In the case when all the epimorphisms $\varphi$ with the kernel $Z$ are conjugate, there is no need to use the symbol $R$ in (51), and we will simply write $\mathcal{H} = H^Z_R \times_L K$. Moreover, whenever all epimorphisms $\varphi$ from $H$ to $L$ are conjugate, we can also omit the symbol $Z$, i.e., we will write $\mathcal{H} = H \times_L K$. For example, $D_2 \times Z_2 \times D_2$ stands for the subgroup $H^Z_R \times_L K$, where $\text{Ker}(\psi) = D_m$ and $\text{Ker}(\varphi) = D_1$. On the other hand, for $D_2 \times Z_2 \times D_2 \times D_2$, we have $\text{Ker}(\psi) = Z_m$, while $\varphi : D_2 \to D_2$ is an isomorphism such that $\varphi(r) = r$ (here $D_2 := \{1, r, \kappa, \kappa r\}$, $\kappa := e^{2\pi i/3} = -1$). Similarly, for the subgroup $D_2 \times Z_2 \times D_2 \times D_2$, we have $\text{Ker}(\psi) = Z_m$, while $\varphi : D_2 \to D_2$ is an isomorphism such that $\varphi(\kappa) = r$.

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