CLASSIFICATION OF NONLINEAR VIBRATIONS IN SYMMETRIC MOLECULES: EQUIVARIANT DEGREE METHOD

by

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This thesis is dedicated to my family who encouraged me to finish my degree and to my teacher Dr. Wieslaw Krawcewicz who helped me every step of the way.

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DISSERTATION

Presented to the Faculty of

The University of Texas at Dallas

in Partial Fulfillment

of the Requirements

for the Degree of

DOCTOR OF PHILOSOPHY IN

MATHEMATICS

THE UNIVERSITY OF TEXAS AT DALLAS

May 2019

ACKNOWLEDGMENTS

I would like to thank my dissertation committee – Wieslaw Krawcewicz, Zalman Balanov, Mieczyslaw Dabkowski, Yifei Lou, and Dmitry Rachinskiy – for their advice and support through the entire process of creating and formalizing this work. My special thanks go to Carlos García-Azpeitia who inspired my interests in this topic and gave me the strength to undertake the task of working on this project. I owe a great debt to Hao-Pin Wu for instructing me how to use his G.A.P. Equivariant Library for the related computations of the equivariant gradient degree. Finally I would like to thank Qingwen Hu, Pavel Kravetz for their help, advice, encouragement and continuous support.

April 2019

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The University of Texas at Dallas, 2019

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This dissertation is devoted to the study of nonlinear periodic vibrations of a group of particles within symmetric molecular conformations governed by the Lennard-Jones and Coulomb forces. In particular, the author investigates nonlinear vibrational modes of oscillations for molecules with tetrahedral and dihedral configurations of atoms. Using the gradient equivariant degree, the author provides the full topological classification of the periodic solutions with both temporal and spatial symmetries for the above configurations. In the process, the general formulae for processing the equivariant spectral data of the linearized system and obtaining the critical frequencies of the particle motions are devised. The obtained frequencies constitute the set of all critical periods for small amplitude periodic solutions emerging from a given stationary symmetric orbit of solutions. The evaluated equivariant invariants provide a complete list of the spatio-temporal symmetries of the periodic solutions emerging from the ground state symmetric equilibria. The proposed method can be applied to study nonlinear vibrations in other symmetric molecules with general force fields.

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CHAPTER 1

INTRODUCTION

1.1 Subject

Mathematical models of molecules describing their dynamical properties play an important role in molecular chemistry. 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. Theoretical and experimental understanding of the molecular dynamics is crucial for scientific applications. Many molecules exhibit natural spacial symmetries — their impact on the actual molecular dynamics is a problem of a formidable complexity. Typically, these symmetries are reflected by the so-called modes (spatio-temporal patterns) of molecular vibrations (periodic solutions). The classification of these patterns constitutes one of the main problems of molecular spectroscopy. Providing such a classification for the systems describing symmetric (tetrahedral and polygonal) molecules, governed by the Lennard-Jones and Coulomb forces, is the main *subject* of this dissertation.

1.2 Mathematical Challenges and Objectives

The complexity of the mathematical models (molecular symmetries, complicated atomic interactions, etc) may result in a **high** number of involved equations and **multiple resonances**, which may create obstacles for applications of commonly used *analytic* methods. The *linear* vibrational modes can be measured using IR and Raman spectroscopy, increasing attention has been given to the mathematical study of other vibrational modes that cannot be measured experimentally (see [20, 8, 24, 40, 41, 44, 37] and the large bibliography therein). A typical practice in studying molecular vibrations is just to analyze the *linear modes* but, as it is well known in the case of resonance, this approach may not reflect the

real nonlinear character of the molecular dynamics. In fact, until recently, there was no universal method that provides a classification of *nonlinear vibrational modes*. Developing such effective topological methods for studying of non-linear vibrational modes in symmetric molecular systems is the main *objective* of this dissertation.

1.3 Classification of Non-linear Modes as a Symmetric Bifurcation Problem

Classical mechanics offers various mathematical molecular models expressed in a form of Newtonian system $\ddot{u} = -\nabla \boldsymbol{\mathcal{V}}(u)$ (with an appropriate choice of the potential $\boldsymbol{\mathcal{V}}$) for examining molecular motions. In particular, such models describe molecular interactions characterized by bond stretching, bond bending, torsion and van der Waals forces. To identify different modes of vibrations (i.e. periodic solutions) corresponding to specific symmetric molecular conformation, one can normalize the period by introducing an additional parameter λ (unknown frequency), i.e., the problem can be reduced to finding 2π-periodic solutions to the system $\ddot{u} = -\lambda^2 \nabla \boldsymbol{\mathcal{V}}(u)$. Consequently, the problem of identification of different modes of vibrations corresponding to specific symmetric molecular conformation can be reduced to a symmetric bifurcation problem, where nonlinear vibrational modes appear as continuous branches of periodic solutions.

1.4 Method

Let us make a distinction between *local* and *global* bifurcation in the context relevant to our discussion. For systems with *discrete spacial symmetries*, local bifurcation is about studying periodic solutions in a proximity (possibly, at a very small neighborhood) of the bifurcation point. Local symmetric bifurcation problems traditionally are studied by using the equivariant normal form classification combined with Center Manifold Theorem/averaging method/Lyapunov-Schmidt reduction (see, for example, [18] and references therein). The global bifurcation, contrary to the local one, is related to solutions living far away from

the point they originated. Studying the global bifurcations involves, in particular, the following problems: (a) existence of *global connected* branches of solutions with prescribed spatio-temporal symmetry, and (b) boundedness/unboundedness of the branches.

In this dissertation a new rigorous method (motivated by classical work of P. Rabinowitz [34]) is proposed for a systematic studying of nonlinear vibrational modes (in both, local and global context) in symmetric molecules. This method allows establishing a comprehensive 'atlas' classifying these modes according to their symmetric properties and providing tools to recognize unbounded (non-compact) branches of such vibrations. Our method is supported by programs in GAP, which provide effective and exact computations of all the equivariant bifurcation invariants.

It should be stressed that the global behavior of bifurcating branches of molecular vibrations was never studied. Therefore, such analysis can be counted as one of the **novelties** of this work.

1.5 Results

In this dissertation, the problem of classification of global nonlinear vibrations in certain symmetric molecules is addressed. In particular, the author examines molecular mechanics of tetrahedral and dihedral molecules – some of the simplest existing molecular configurations. There is an abundance of such molecules in nature which makes it important for molecular vibration analysis. The most popular examples are tetraphosphorus and methane molecules. 2-dimensional dihedral symmetries are common in nature as well: various so called ring compounds such as cyclohexahexaene as well as benzene represent a polygonal class of molecules.

For the tetrahedral molecular configuration, which is the simplest among 3-dimensional symmetric molecules, we established the global existence of branches of periodic solutions emerging from the symmetric equilibrium and classify their symmetries. This dissertation

also provides a full analysis of 2-dimensional n-gonal molecular configurations, for which a classification of molecular vibrations is obtained.

Let us point out that previous research in molecular vibrations never employed topological methods such as the equivariant degree – in fact, as it was already mentioned, most of analysis in molecular chemistry was done by describing only the linear modes of vibrations. Current work opens new possibilities in studying nonlinear molecular vibrations and their symmetric classification – the proposed method can be applied in a standard way to all kinds of the molecular models, even for the most sophisticated potentials. Current dissertation may serve as a basis for extending vibrational analysis to more complex symmetric molecules.

1.6 Outline

This introduction is followed by Chapter 2 containing the preliminaries, which includes a short presentation of the gradient equivariant degree, some of its computational formulae, and examples. General models for atomic interactions are discussed in Chapter 3 together with an outline of the gradient equivariant degree treatment. In Chapter 4, there follows an analysis of the tetrahedral molecule, for which we provide a complete symmetric classification of the nonlinear vibrational modes. Chapter 5 is devoted to the analysis of a polygonal configuration of n identical atoms admitting dihedral symmetries. Classification of nonlinear vibrational modes is accompanied by some computational examples and numerical simulations for several symmetric periodic vibrations.

CHAPTER 2

PRELIMINARIES

2.1 Basic Definitions

For an Euclidean space V, $B(V)$ stands for the open unit ball in V. For $x, y \in V := \mathbb{R}^n$, we denote by $x \bullet y$ the standard inner product in V. In addition, G will stand for a compact Lie group. In what follows, all considered subgroups of G are closed. For a subgroup $H \leq G$, $N(H)$ denotes the *normalizer* of H in G, and $W(H) = N(H)/H$ denotes the *Weyl group* of H in G. We say K is *conjugate* to H if $\exists_{g\in G}\ K = g^{-1}Hg$, and we will write that $K \sim H$, i.e., $(H) := \{K : K \sim H\}$. By (H) we denote the *conjugacy class* of H in G. $\Phi(G) := \{(H) : H \text{ is a subgroup of } G\}$ and $\Phi_n(G) := \{(H) \in \Phi(G) : \dim W(H) = n\}$. The set $\Phi(G)$ has a natural partial order given by: $(H) \leq (K) \iff \exists_{g\in G}\ gHg^{-1} \leq K$.

For a G-space X and $x \in X$, we use $G_x := \{g \in G :\ gx = x\}$ to denote the *isotropy group* of x, $G(x) := \{gx :\ g \in G\}$ to denote the orbit of x, and the conjugacy class (G_x) is called the *orbit type* of x. $\Phi(G;X) := \{(G_x) : x \in X\}$ denotes the set of all the orbit types in X, and $\Phi_n(G;X) := \Phi(G;X) \cap \Phi_n(G)$. Moreover, for a subgroup $H \subset G$, we use the following notations:

$$X_H := \{x \in X :\ G_x = H\},$$

$$X^H := \{x \in X :\ G_x \supset H\},$$

$$X_{(H)} := \{x \in X :\ (G_x) = (H)\},$$

$$X^{(H)} := \{x \in X :\ (G_x) \geq (H)\}.$$

For two G-spaces X and Y, we say that a continuous map $f : X \to Y$ is G-equivariant if and only if $\forall_{g\in G}\forall_{x\in X}\ f(gx) = gf(x)$. We also say that $f : X \to \mathbb{R}$ is G-invariant if $\forall_{g\in G}\forall_{x\in X}$

$f(gx) = f(x)$. One can easily notice that for a G-equivariant map $f := X \to Y$, we have $\forall_{H \leq G}\ f(X^H) \subset Y^H$.

A G-space V is called a *G-representation* if V is an Euclidean space and $\forall_{g \in G}$ the translation map $T_g : V \to V$ is a linear isomorphism where $T_g x := gx$, $x \in X$. Whenever T_g is an orthogonal operator, V is called an *orthogonal* G-representation. An invariant linear subspace $\tilde{V} \subset V$ is called a *subrepresentation* of V, and V is an *irreducible* representation if it has no subrepresentation different from $\{0\}$ and V. Any compact Lie group G admits countably many non-equivalent (real) irreducible G-representations. Given a compact Lie group G, we denote by $\mathcal{V}_i$, $i = 0, 1, 2, \ldots$ a complete list of its all (real) irreducible G-representations, starting with the trivial representation $\mathcal{V}_0$.

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

$$V = V_0 \oplus V_1 \oplus \cdots \oplus V_r, \tag{2.1}$$

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 $\mathcal{V}_j$. The component V_j is commonly called an *isotypical* (or *isotypic*) component of V *modeled* on $\mathcal{V}_j$. One can easily show (see [3]) that the decomposition (2.1) is unique.

For a linear operator $A : V \to V$, we denote by $\sigma(A)$ the real spectrum of A. For $\mu \in \sigma(A)$, we denote by $E(\mu) \subset V$ the generalized eigenspace associated with μ. Since any G-equivariant linear operator $A : V \to V$ preserves the G-isotypical decomposition (2.1), i.e., $A(V_j) \subset V_j$, and the eigenspace $E(\mu)$ is G-invariant, we can introduce the integers

$$m^j(\mu) := \dim \Big(E(\mu) \cap V_j \Big) / \dim V_j, \quad j = 0, 1, 2, \ldots, r, \tag{2.2}$$

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

2.2 Amalgamated Notation

Given two groups G_1 and G_2, we consider the product group $G_1 \times G_2$. The well-known result (see [10, 19]) provides a description of the product group $G_1 \times G_2$. Namely, for any subgroup $\mathscr{H}$ 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

$$\mathscr{H} = \{(h, k) \in H \times K : \varphi(h) = \psi(k)\}. \tag{2.3}$$

In this case, we will use the notation

$$\mathscr{H} =: H \,{}^{\varphi}\!\times_{L}^{\psi} K$$

and the group $H \,{}^{\varphi}\!\times_{L}^{\psi} K$ will be called an *amalgamated* subgroup of $G_1 \times G_2$.

2.3 Conjugacy Classes of Subgroups in $S_4 \times O(2)$

Any closed subgroup $\mathscr{H}$ 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 $\mathbb{Z}_n$, $n \geq 1$. Since we are interested in describing conjugacy classes of $\mathscr{H}$, we can identify the epimorphism $\varphi : H \to L$ by indicating

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

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

$$\mathscr{H} =: H^{Z} \times_{L}^{R} K \ , \tag{2.4}$$

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

$$V_4 = \{(1), (12)(34), (13)(24), (14)(23)\} ,$$

$$D_4 = \{(1), (1324), (12)(34), (1423), (34), (14)(23), (12), (13)(24)\} ,$$

$$Z_4 = \{(1), (1324), (12)(34), (1423)\} ,$$

$$D_3 = \{(1), (123), (132), (12), (23), (13)\} ,$$

$$D_2 = \{(1), (12)(34), (12), (34)\} ,$$

$$D_1 = \{(1), (12)\} .$$

If all the epimorphisms φ with the kernel Z are conjugate, there is no need to use the symbol R in (2.4). Therefore, we will simply write $\mathscr{H} = H^Z \times_L K$. In addition, if all epimorphisms φ from H to L are conjugate, we can also omit the symbol Z, i.e., we will write $\mathscr{H} = H \times_L K$.

2.4 Conjugacy Classes of Subgroups in $D_n \times O(2)$

The conjugacy classes of subgroups in $D_6 \times O(2)$, which will be used in this dissertation, are listed in the Table 2.1.

2.5 Euler and Burnside Rings

The concept of the *Euler ring* was introduced by T. tom Dieck in [39]. For a general compact group G, computations of the Euler ring $U(G)$ may be quite complicated. However, when $G := \Gamma \times O(2)$ (here Γ is a finite group), the Euler ring structure can be described with the help of the reduction techniques and the properties of the Euler ring homomorphisms (see [9] for more details).

Table 2.1. Conjugacy Classes of Subgroups in $D_6 \times O(2)$

ID	(S)	$\lvert W(S)\rvert$	ID	(S)	$\lvert W(S)\rvert$	ID	(S)	$\lvert W(S)\rvert$
1	$(\mathbb{Z}_1 \times \mathbb{Z}_n)$	∞	35	$(D_6{}^{D_3}\times_{D_1} D_n)$	4	69	$(D_6{}^{\tilde{D}_3}\times_{\mathbb{Z}_2} D_{2n})$	2
2	$(D_1 \times \mathbb{Z}_n)$	∞	36	$(D_6{}^{\mathbb{Z}_6}\times_{D_1} D_n)$	4	70	$(\mathbb{Z}_1 \times SO(2))$	24
3	$(\mathbb{Z}_2 \times \mathbb{Z}_n)$	∞	37	$(D_6{}^{\tilde{D}_3}\times_{D_1} D_n)$	4	71	$(D_1 \times SO(2))$	4
4	$(\tilde{D}_1 \times \mathbb{Z}_n)$	∞	38	$(D_2{}^{\mathbb{Z}_1}\times^{D_1}_{D_2} D_{2n})$	4	72	$(\mathbb{Z}_2 \times SO(2))$	12
5	$(\mathbb{Z}_3 \times \mathbb{Z}_n)$	∞	39	$(D_2{}^{\mathbb{Z}_1}\times^{\mathbb{Z}_2}_{D_2} D_{2n})$	4	73	$(\tilde{D}_1 \times SO(2))$	4
6	$(D_2 \times \mathbb{Z}_n)$	∞	40	$(D_2{}^{\mathbb{Z}_1}\times^{\tilde{D}_1}_{D_2} D_{2n})$	4	74	$(\mathbb{Z}_3 \times SO(2))$	8
7	$(D_3 \times \mathbb{Z}_n)$	∞	41	$(D_6{}^{\mathbb{Z}_3}\times^{D_3}_{D_2} D_{2n})$	4	75	$(D_2 \times SO(2))$	2
8	$(\mathbb{Z}_6 \times \mathbb{Z}_n)$	∞	42	$(D_6{}^{\mathbb{Z}_3}\times^{\mathbb{Z}_6}_{D_2} D_{2n})$	4	76	$(D_3 \times SO(2))$	4
9	$(\tilde{D}_3 \times \mathbb{Z}_n)$	∞	43	$(D_6{}^{\mathbb{Z}_3}\times^{\tilde{D}_3}_{D_2} D_{2n})$	4	77	$(\mathbb{Z}_6 \times SO(2))$	4
10	$(D_6 \times \mathbb{Z}_n)$	∞	44	$(D_3{}^{\mathbb{Z}_1}\times_{D_3} D_{3n})$	4	78	$(\tilde{D}_3 \times SO(2))$	4
11	$(D_1{}^{\mathbb{Z}_1}\times_{\mathbb{Z}_2} \mathbb{Z}_{2n})$	∞	45	$(\tilde{D}_3{}^{\mathbb{Z}_1}\times_{D_3} D_{3n})$	4	79	$(D_6 \times SO(2))$	2
12	$(\mathbb{Z}_2{}^{\mathbb{Z}_1}\times_{\mathbb{Z}_2} \mathbb{Z}_{2n})$	∞	46	$(D_6{}^{\mathbb{Z}_2}\times_{D_3} D_{3n})$	2	80	$(D_1{}^{\mathbb{Z}_1}\times_{D_1} O(2))$	4
13	$(\tilde{D}_1{}^{\mathbb{Z}_1}\times_{\mathbb{Z}_2} \mathbb{Z}_{2n})$	∞	47	$(D_6{}^{\mathbb{Z}_1}\times_{D_6} D_{6n})$	2	81	$(\mathbb{Z}_2{}^{\mathbb{Z}_1}\times_{D_1} O(2))$	12
14	$(D_2{}^{D_1}\times_{\mathbb{Z}_2} \mathbb{Z}_{2n})$	∞	48	$(\mathbb{Z}_1 \times D_n)$	24	82	$(\tilde{D}_1{}^{\mathbb{Z}_1}\times_{D_1} O(2))$	4
15	$(D_2{}^{\mathbb{Z}_2}\times_{\mathbb{Z}_2} \mathbb{Z}_{2n})$	∞	49	$(D_1 \times D_n)$	4	83	$(D_2{}^{D_1}\times_{D_1} O(2))$	2
16	$(D_2{}^{\tilde{D}_1}\times_{\mathbb{Z}_2} \mathbb{Z}_{2n})$	∞	50	$(\mathbb{Z}_2 \times D_n)$	12	84	$(D_2{}^{\mathbb{Z}_2}\times_{D_1} O(2))$	2
17	$(D_3{}^{\mathbb{Z}_3}\times_{\mathbb{Z}_2} \mathbb{Z}_{2n})$	∞	51	$(\tilde{D}_1 \times D_n)$	4	85	$(D_2{}^{\tilde{D}_1}\times_{D_1} O(2))$	2
18	$(\mathbb{Z}_6{}^{\mathbb{Z}_3}\times_{\mathbb{Z}_2} \mathbb{Z}_{2n})$	∞	52	$(\mathbb{Z}_3 \times D_n)$	8	86	$(D_3{}^{\mathbb{Z}_3}\times_{D_1} O(2))$	4
19	$(\tilde{D}_3{}^{\mathbb{Z}_3}\times_{\mathbb{Z}_2} \mathbb{Z}_{2n})$	∞	53	$(D_2 \times D_n)$	2	87	$(\mathbb{Z}_6{}^{\mathbb{Z}_3}\times_{D_1} O(2))$	4
20	$(D_6{}^{D_3}\times_{\mathbb{Z}_2} \mathbb{Z}_{2n})$	∞	54	$(D_3 \times D_n)$	4	88	$(\tilde{D}_3{}^{\mathbb{Z}_3}\times_{D_1} O(2))$	4
21	$(D_6{}^{\mathbb{Z}_6}\times_{\mathbb{Z}_2} \mathbb{Z}_{2n})$	∞	55	$(\mathbb{Z}_6 \times D_n)$	4	89	$(D_6{}^{D_3}\times_{D_1} O(2))$	2
22	$(D_6{}^{\tilde{D}_3}\times_{\mathbb{Z}_2} \mathbb{Z}_{2n})$	∞	56	$(\tilde{D}_3 \times D_n)$	4	90	$(D_6{}^{\mathbb{Z}_6}\times_{D_1} O(2))$	2
23	$(\mathbb{Z}_3{}^{\mathbb{Z}_1}\times_{\mathbb{Z}_3} \mathbb{Z}_{3n})$	∞	57	$(D_6 \times D_n)$	2	91	$(D_6{}^{\tilde{D}_3}\times_{D_1} O(2))$	2
24	$(\mathbb{Z}_6{}^{\mathbb{Z}_2}\times_{\mathbb{Z}_3} \mathbb{Z}_{3n})$	∞	58	$(D_1{}^{\mathbb{Z}_1}\times_{\mathbb{Z}_2} D_{2n})$	4	92	$(\mathbb{Z}_1 \times O(2))$	12
25	$(\mathbb{Z}_6{}^{\mathbb{Z}_1}\times_{\mathbb{Z}_6} \mathbb{Z}_{6n})$	∞	59	$(\mathbb{Z}_2{}^{\mathbb{Z}_1}\times_{\mathbb{Z}_2} D_{2n})$	12	93	$(D_1 \times O(2))$	2
26	$(D_1{}^{\mathbb{Z}_1}\times_{D_1} D_n)$	8	60	$(\tilde{D}_1{}^{\mathbb{Z}_1}\times_{\mathbb{Z}_2} D_{2n})$	4	94	$(\mathbb{Z}_2 \times O(2))$	6
27	$(\mathbb{Z}_2{}^{\mathbb{Z}_1}\times_{D_1} D_n)$	24	61	$(D_2{}^{D_1}\times_{\mathbb{Z}_2} D_{2n})$	2	95	$(\tilde{D}_1 \times O(2))$	2
28	$(\tilde{D}_1{}^{\mathbb{Z}_1}\times_{D_1} D_n)$	8	62	$(D_2{}^{\mathbb{Z}_2}\times_{\mathbb{Z}_2} D_{2n})$	2	96	$(\mathbb{Z}_3 \times O(2))$	4
29	$(D_2{}^{D_1}\times_{D_1} D_n)$	4	63	$(D_2{}^{\tilde{D}_1}\times_{\mathbb{Z}_2} D_{2n})$	2	97	$(D_2 \times O(2))$	1
30	$(D_2{}^{\mathbb{Z}_2}\times_{D_1} D_n)$	4	64	$(D_3{}^{\mathbb{Z}_3}\times_{\mathbb{Z}_2} D_{2n})$	4	98	$(D_3 \times O(2))$	2
the 31	$(D_2{}^{\tilde{D}_1}\times_{D_1} D_n)$	4	65	$(\mathbb{Z}_6{}^{\mathbb{Z}_3}\times_{\mathbb{Z}_2} D_{2n})$	4	99	$(\mathbb{Z}_6 \times O(2))$	2
32	$(D_3{}^{\mathbb{Z}_3}\times_{D_1} D_n)$	8	66	$(\tilde{D}_3{}^{\mathbb{Z}_3}\times_{\mathbb{Z}_2} D_{2n})$	4	100	$(\tilde{D}_3 \times O(2))$	2
33	$(\mathbb{Z}_6{}^{\mathbb{Z}_3}\times_{D_1} D_n)$	8	67	$(D_6{}^{D_3}\times_{\mathbb{Z}_2} D_{2n})$	2	101	$(D_6 \times O(2))$	1
34	$(\tilde{D}_3{}^{\mathbb{Z}_3}\times_{D_1} D_n)$	8	68	$(D_6{}^{\mathbb{Z}_6}\times_{\mathbb{Z}_2} D_{2n})$	2			

The formal definition of the Euler ring involve advanced concepts from algebraic topology which are not relevant for the topic of this dissertation. Therefore, only a few notions related to this concept are discussed below. In short, the Euler ring $U(G)$ can be defined as a free $\mathbb{Z}$-module $U(G) := \mathbb{Z}[\Phi(G)]$ generated by $\Phi(G)$. In addition, the ring multiplication in

$U(G)$ is defined on generators (H), $(K) \in \Phi(G)$ by

$$(H) * (K) = \sum_{(L) \in \Phi(G)} n_L (L), \tag{2.5}$$

where

$$n_L := \chi_c \left((G/H \times G/K)_L / N(L) \right) \tag{2.6}$$

with χ_c standing for the Euler characteristic taken in Alexander-Spanier cohomology with compact support (cf. [38]). For more details, refer to [1, 9, 39].

Another algebraic structure related to $U(G)$ is called the Burnside ring of G. It is a $\mathbb{Z}$-module $A(G) := \mathbb{Z}[\Phi_0(G)]$ equipped with the same multiplication as in $U(G)$ but limited to the generators of $\Phi_0(G)$. Thus, in the case of $A(G)$, the formulae for the multiplication can be significantly simplified. Namely, on the generators we have

$$(H) \cdot (K) = \sum_{(L)} n_L (L), \qquad (H), (K), (L) \in \Phi_0(G),$$

where n_L denotes the number of (L) orbits in $G/H \times G/K$, i.e.,

$$n_L := |(G/H \times G/K)_L / G|$$

(here $|X|$ denotes the number of elements in the set X). For n_L, there is the following recurrence formula

$$n_L = \frac{n(L,K)\,|W(K)|\,n(L,\ H)\,|W(H)| - \sum\limits_{(\widetilde{L})>(L)} n\left(L,\widetilde{L}\right) n_{\widetilde{L}} \left|W\left(\widetilde{L}\right)\right|}{|W(L)|}, \tag{2.7}$$

where

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

and (H), (K), (L), $(\widetilde{L})$ come from $\Phi_0(G)$.

The number $n(L,K)$ has very simple interpretation – the number of different subgroups $K' \in (K)'$ such that $L \leq K'$.

Unlike the composition of the Euler ring, the structure of the Burnside ring $A(G)$ can be computed more easily. Computer programs containing G.A.P. routines are very effective for evaluating Burnside rings products. The G.A.P. Equivariant Libraries were created by H.-P. Wu (cf.[9]), allowing effective computation of $A(G)$, theoretically, for any finite group G. Even in the case of some continuous groups G, the G.A.P routines can provide effective tools for the computation of the multiplicative structure of $A(G)$.

One needs to stress that $A(G)$ is a $\mathbb{Z}$-submodule of $U(G)$ but not a subring. However (see [1]), the projection $\pi_0 : U(G) \to A(G)$ defined on generators $(H) \in \Phi(G)$ by

$$\pi_0((H)) = \begin{cases} (H) & \text{if } \ (H) \in \Phi_0(G), \\ 0 & \text{otherwise,} \end{cases} \tag{2.8}$$

is a ring homomorphism, i.e.,

$$\pi_0((H) * (K)) = \pi_0((H)) \cdot \pi_0((K)), \qquad (H), (K) \in \Phi(G),$$

where '$\cdot$' stands for the multiplication in the Burnside ring $A(G)$.

In the recent paper, M. Dabkowski et al. ([9]) proposed new techniques for effective computations of Euler rings $U(G)$ for $G = \Gamma \times O(2)$, where Γ is a finite group. These techniques are based on the known structure of the Euler ring $U(\Gamma \times SO(2))$ (cf. [35]), the Euler ring homomorphism

$$\Psi : U(\Gamma \times O(2)) \to U(\Gamma \times SO(2))$$

induced by inclusion

$$\Gamma \times SO(2) \hookrightarrow \Gamma \times O(2),$$

and the information given by the Burnside ring $A(\Gamma \times O(2))$. The developed in [9] algorithms allow to create G.A.P routines and programs that can be effectively used to handle the sturcture of the Euler ring $U(\Gamma \times O(2))$. The homomorphism π_0 leads to identification of

the Burnside ring $A(G)$ as a part of the Euler ring $U(G)$. With the help of G.A.P. and computer programming, the Euler ring structure for $G = \Gamma \times O(2)$ can be easily and fully calculated (cf. [9]).

2.6 Equivariant Gradient Degree

The gradient equivariant degree – a generalization of the Brouwer/Leray-Schauder degree, was developed in [16] for the gradient maps (see also [9] and [36]). The gradient equivariant degree is just one of many equivariant degrees that were introduced in the last three decades for various types of differential equations (see [2], [4], [22], [26] and references therein).

For a compact Lie group G and a G-representation V, we consider a continuously differentiable G-invariant function $\phi : V \to \mathbb{R}$. Then, clearly $\nabla\phi : V \to V$ is a G-equivariant map. Let $\Omega \in V$ be an open bounded G-invariant set. A pair (∇, Ω) is called an *admissible gradient G-pair* if and only if for all $x \in \partial\Omega$ we have $\nabla\phi(x) \neq 0$. In such a case, we will also say that $\nabla\phi$ is Ω-*admissible* G-map. We denote by $\mathcal{M}^G_\nabla(V)$ the set of all admissible gradient G-pairs in V and put

$$\mathcal{M}^G_\nabla := \bigcup_V \mathcal{M}^G_\nabla(V)$$

where V runs over all possible G-representations. In other words, $\mathcal{M}^G_\nabla$ is the set of all admissible gradient G-pairs.

The existence and basic properties of G-equivariant gradient degree are presented in the following result from [16]:

Theorem 2.6.1. *There exists a unique map $\nabla_G\text{-deg} : \mathcal{M}^G_\nabla \to U(G)$, which assigns to every $(\nabla\varphi, \Omega) \in \mathcal{M}^G_\nabla$ an element $\nabla_G\text{-deg}\,(\nabla\varphi, \Omega) \in U(G)$, called the G-gradient degree of $\nabla\varphi$ on Ω,*

$$\nabla_G\text{-deg}\,(\nabla\varphi, \Omega) = \sum_{(H)\in\Phi(G)} n_H(H_i) = n_{H_1}(H_1) + \cdots + n_{H_m}(H_m), \tag{2.9}$$

satisfying the following properties:

(Existence) *If* $\nabla_G\text{-deg}\,(\nabla\varphi,\Omega)\neq 0$, *i.e., there is in* (2.9) *a non-zero coefficient* n_{H_i}, *then there exists* $u_0\in\Omega$ *such that* $\nabla\varphi(u_0)=0$ *and* $(G_{u_0})\geq(H_i)$.

(Additivity) *Let* Ω_1 *and* Ω_2 *be two disjoint open* G*-invariant subsets of* Ω *such that* $(\nabla\varphi)^{-1}(0)\cap\Omega\subset\Omega_1\cup\Omega_2$. *Then,* $\nabla_G\text{-deg}\,(\nabla\varphi,\Omega)=\nabla_G\text{-deg}\,(\nabla\varphi,\Omega_1)+\nabla_G\text{-deg}\,(\nabla\varphi,\Omega_2)$.

(Homotopy) *If* $\nabla_x\psi:[0,1]\times V\to V$ *is a* G*-gradient* Ω*-admissible homotopy, then*

$$\nabla_G\text{-deg}\,(\nabla_x\psi,\Omega)=\textit{constant}.$$

(Normalization) *Let* $\varphi:V\to\mathbb{R}$ *be a* G *be a special* Ω*-Morse function* [1] *such that* $(\nabla\varphi)^{-1}(0)\cap\Omega=G(u_0)$ *and* $G_{u_0}=H$. *Then,*

$$\nabla_G\text{-deg}\,(\nabla\varphi,\Omega)=(-1)^{\mathrm{m}^-(\nabla^2\varphi(u_0))}\cdot(H),$$

where "$\mathrm{m}^-(\cdot)$*" stands for the Morse index of* $\nabla^2\phi(u_0)$, *i.e., the total dimension of all the eigenspaces corresponding to negative eigenvalues of a (symmetric) matrix.*

(Multiplicativity) *For all* $(\nabla\varphi_1,\Omega_1)$, $(\nabla\varphi_2,\Omega_2)\in\mathcal{M}^G_\nabla$,

$$\nabla_G\text{-deg}\,(\nabla\varphi_1\times\nabla\varphi_2,\Omega_1\times\Omega_2)=\nabla_G\text{-deg}\,(\nabla\varphi_1,\Omega_1)*\nabla_G\textit{-deg}\,(\nabla\varphi_2,\Omega_2)$$

where the multiplication '$*$*' is taken in the Euler ring* $U(G)$.

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

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

where $\Psi:U(G)\to U(G_0)$ *is the Euler ring homomorphism induced by the inclusion* $\psi:G_0\hookrightarrow G$ *(see [1]).*

[1]For the definition and properties of the so-called Morse function, refer to [16].

2.7 Equivariant Gradient Degree in Hilbert Spaces

Using a standard finite-dimensional approximation scheme, the G-equivariant gradient degree can be expanded to the Leray-Schauder type of a degree for admissible gradient G-pairs in Hilbert G-representation. To be more precise, assume that $\mathscr{H}$ is a Hilbert G-representation and $f : \mathscr{H} \to \mathbb{R}$ is a G-invariant continuously differentiable function. $\Omega \in \mathscr{H}$ is an open bounded G-invariant set. We say that $(\nabla f, \Omega)$ is an admissible gradient G-pair in $\mathscr{H}$ if and only if $\forall_{x\in\partial\Omega}\ \nabla f(x) \neq 0$ and $\nabla f(x) = x - F(x)$ where $F : \mathscr{H} \to \mathscr{H}$ is a completely continuous map[2]. In such a case, we will also say that ∇f is an Ω admissible completely continuous field on $\mathscr{H}$.

In order to achieve this expantion, consider a Hilbert G-representation $\mathscr{H}$, a G-equivariant completely continuous gradient field $\nabla f : \mathscr{H} \to \mathscr{H}$, and an open bounded G-invariant set $\Omega \subset \mathscr{H}$ such that ∇f is Ω-admissible. Then, the pair $(\nabla f, \Omega)$ is called a *G-admissible pair* in $\mathscr{H}$. This degree also possesses properties of the Theorem 2.6.1 (cf. [2, 9]).

One of the most important properties of the G-equivariant gradient degree $\nabla_G\text{-deg}(\nabla f, \Omega)$ is its ability to provide a full equivariant topological classification of the solution set for $\nabla f(x) = 0$ and $x \in \Omega$.

Let $\mathscr{H}$ be a Hilbert G-representation and $\Omega \subset \mathscr{H}$ an open bounded G-invariant set. A C^1-differentiable G-invariant functional $f : \mathscr{H} \to \mathbb{R}$ given by $f(x) = \frac{1}{2}\|x\|^2 - \varphi(x)$, $x \in \mathscr{H}$, is called Ω-*admissible* if $\nabla\varphi : \mathscr{H} \to \mathscr{H}$ 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 $\mathscr{H}$, we mean a sequence of G-equivariant orthogonal projections $P_n : \mathscr{H} \to \mathscr{H}$, $n = 1, 2, \ldots$, such that:

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

[2] F is completely continuous means that F is continuous and $\overline{F(A)}$ is compact for any bounded set $A \subset \mathscr{H}$

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

(c) $\lim\limits_{n\to\infty} P_n x = x$ for all $x \in \mathscr{H}$.

Then for an Ω-admissible G-map $f : \mathscr{H} \to \mathbb{R}$, one can define a sequence $f_n : \mathscr{H}_n \to \mathbb{R}$ by $f_n(x) := \frac{1}{2}\|x\|^2 - \varphi(x)$, $x \in \mathscr{H}_n$. By a standard argument, for sufficiently large $n \in \mathbb{N}$, the maps $\nabla f_n(x) := x - P_n \nabla\varphi(x)$, $x \in \mathscr{H}_n$, are Ω_n-admissible, where $\Omega_n := \Omega \cap \mathscr{H}_n$. 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

$$\nabla_G\text{-deg}\,(\nabla f, \Omega) := \nabla_G\text{-deg}\,(\nabla f_n, \Omega_n), \tag{2.10}$$

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 $\mathscr{H}$, for instance see [10]. We should mention that the ideas behind the usage of the approximation methods to define topological degree can be rooted to [7].

2.8 Degree on the Slice

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

Then we have (cf. [6])

Theorem 2.8.1. *(Slice Principle) Let $\mathscr{H}$ be a Hilbert G-representation, Ω – an open G-invariant subset in $\mathscr{H}$, and $\varphi : \Omega \to \mathbb{R}$ – a continuously differentiable G-invariant functional such that $\nabla\varphi$ is a completely continuous field. Suppose that $u_o \in \Omega$ and $G(u_o)$ is an finite-dimensional isolated critical orbit of φ with S_o being the slice to the orbit $G(u_o)$ at u_o, and $\mathcal{U}$ 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*

$$\nabla_G\text{-deg}\,(\nabla\varphi, \mathcal{U}) = \Theta(\nabla_{G_{u_o}}\text{-deg}\,(\nabla\varphi_o, \mathcal{U} \cap S_o)), \tag{2.11}$$

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

Proof. Since the gradient equivariant degree in Hilbert **G**-representations is defined using finite-dimensional approximation scheme, one can assume that $\mathscr{H}$ is a finite-dimensional orthogonal G-representation. Then, $\nabla\varphi_o(u) = P\nabla\varphi(u)$, where $P : \mathscr{H} \to S_o$ is an orthogonal projection. Since $G(u_o)$ is orthogonal to S_o, one can assume that $\mathcal{U}$ is taken sufficiently small so $G(u)$ is transversal to S_o for all $u \in \mathcal{U}$. Then, clearly, if $\nabla\varphi_o(v) = 0$ for some v such that $u := u_o + v \in \mathcal{U} \cap S_o$ then $\nabla\varphi(u) = 0$. Next, we approximate φ_o on $\mathcal{U} \cap S_o$ by a generic map (see [16]), which can be extended equivariantly on $\mathcal{U}$. In such a case, this extension is also generic, and the formula (2.11) follows directly from the definition of the gradient degree for generic maps. □

2.9 Equivariant Basic Degrees

For each irreducible G-representation $\mathcal{V}_i$, the *basic gradient degree* is defined by

$$\nabla_G\text{-deg}_{\,\mathcal{V}_i} := \nabla_G\text{-deg}\,(-\mathrm{Id}\,, B(\mathcal{V}_i))$$

A direct usage of topological definition (see [16]) of the gradient G-equivariant degree to compute the basic degrees $\nabla_G\text{-deg}_{\mathcal{V}_i}$ may be very complicated for infinite compact Lie

groups G. However, in the case of the group $G := \Gamma \times O(2)$ (Γ being a finite group), we have effective reduction techniques (see [9, 35]), using the homomorphism π_0 and the Euler ring homomorphism $\Psi : U(\Gamma \times O(2)) \to U(\Gamma \times S^1)$, which allow to establish the exact values of the gradient $\Gamma \times O(2)$-equivariant basic degrees.

To be more precise, let us recall the *G-equivariant Brouwer degree* $G\text{-deg}(f, \Omega) \in A(G)$, which is defined for admissible G-pairs $(f, \Omega) \in \mathcal{M}^G(V)$ and has similar existence, additivity, homotopy and multiplicativity properties as the gradient degree. It can be computed by applying the following recurrence formula to the usual Brouwer degrees of maps $f^H : V^H \to V^H$, $(H) \in \Phi_0(G; V)$, i.e.,

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

and

$$n_H = \frac{\deg(f^H, \Omega^H) - \sum_{(L)>(H)} n_L \, n(H, L) \, |W(L)|}{|W(H)|}. \tag{2.12}$$

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

$$\pi_0 \left(\nabla_G\text{-deg}(\nabla\varphi, \Omega) \right) = G\text{-deg}(\nabla\varphi, \Omega). \tag{2.13}$$

Moreover, the *Brouwer G-equivariant basic degrees*

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

satisfy

$$\deg_{\mathcal{V}_i} = \pi_0 \left[\nabla_G\text{-deg}_{\mathcal{V}_i} \right], \quad i = 0, 1, 2, 3 \ldots \tag{2.14}$$

Therefore, by (2.14),

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

with the integers x_H that need to be determined by other means.

Since the gradient basic degrees $\nabla_{G'}\text{-deg}_{\mathcal{V}_i}$ for the group $G' := \Gamma \times S^1$ are well-known (cf. [35]), one can apply the Euler ring homomorphism $\Psi : U(\Gamma \times O(2)) \to U(\Gamma \times S^1)$ to determine these coefficients (see [9]) by using the relation

$$\nabla_{G'}\text{-deg}_{\mathcal{V}_i} = \Psi\left[\text{deg}_{\mathcal{V}_i}\right] + \sum_{(H)\in\Phi_1(G;\mathcal{V}_i)} x_H \Psi(H),$$

(here we assume that S^1 acts nontrivially on $\mathcal{V}_i$). The Euler ring homomorphism $\Psi : U(\Gamma \times O(2)) \to U(\Gamma \times S^1)$ is defined on the generators by

$$\Psi(H) = \begin{cases} 2(K) & \text{if} \quad K = H \text{ and } K \sim K' \text{ in } \Gamma \times SO(2), \\ (K) + (K') & \text{if} \quad K = H \text{ and } K \not\sim K' \text{ in } \Gamma \times SO(2), \\ (K) & \text{if} \quad K \neq H, \end{cases} \tag{2.15}$$

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

The formula (2.12) allows the usage of computational programs based on G.A.P. platform to obtain exact symbolic evaluation of the G-equivariant Brouwer degree of linear isomorphisms for a large class of classical groups and their products (see [43]).

2.10 G-Equivariant Gradient Degree of Linear Maps

Consider an orthogonal (finite-dimensional) G-representation V. Computational formula to evaluate the G-equivariant degree $\nabla_G\text{-deg}\,(\mathscr{A}, B(V))$, can be easily established. Indeed, consider $\mathscr{A} : V \to V$ a symmetric G-equivariant linear isomorphism, i.e., $\mathscr{A} = \nabla\varphi$ for $\varphi(v) = \frac{1}{2}(\mathscr{A}v \bullet v)$, $v \in V$. Then, by using the G-isotypical decomposition (2.1) of V, we can define

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

Next, by the multiplicativity property,

$$\nabla_G\text{-deg}(\mathscr{A}, B(V)) = \prod_i^r \nabla_G\text{-deg}(\mathscr{A}_i, B(V_i)). \tag{2.16}$$

We denote by $\sigma_-(\mathscr{A})$ the negative spectrum of the operator $\mathscr{A}$. For $\xi \in \sigma_-(\mathscr{A})$, we denote by $E(\xi) := \ker(\mathscr{A} - \xi \mathrm{Id})$ the corresponding to ξ eigenspace of $\mathscr{A}$, and consider the numbers $m_i(\xi)$ given by (2.2). Then,

$$\nabla_G\text{-deg}(\mathscr{A}, B(V)) = \prod_{\xi \in \sigma_-(\mathscr{A})} \prod_{i=0}^{r} \left(\nabla_G\text{-deg}_{\mathcal{V}_i}\right)^{m_i(\xi)}. \tag{2.17}$$

CHAPTER 3

MODELS FOR ATOMIC INTERACTION, MOLECULAR VIBRATIONS AND EQUIVARIANT DEGREE METHOD

A molecule M is a group of atoms, say u_1, u_2, ..., u_n, held together by chemical bonds. These bonds can be described as a subset $\mathscr{B} \subset \mathscr{N} \times \mathscr{N}$, where $\mathscr{N} := \{1, 2, \ldots, n\}$, i.e., the atoms u_i and u_j are bonded if and only if $(i, j) \in \mathscr{B}$. Clearly, we have

$$(i, i) \notin \mathscr{B} \quad \text{and} \quad (i, j) \in \mathscr{B} \;\Leftrightarrow\; (j, i) \in \mathscr{B}.$$

It is possible that the molecule M is a configuration of different atoms and there may be also different types of bonding (e.g. simple or double). We illustrate such molecules on a picture below. However, for sake of simplicity, in this dissertation we assume that all the atoms are identical with the the same mass m.

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. Let us point out that although 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. [27]). 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. In order to be relatively general, the atomic interactions in the molecule M can be described by the following Newtonian system

$$m\ddot{u} = -\nabla \boldsymbol{\mathcal{V}}(u), \tag{3.1}$$

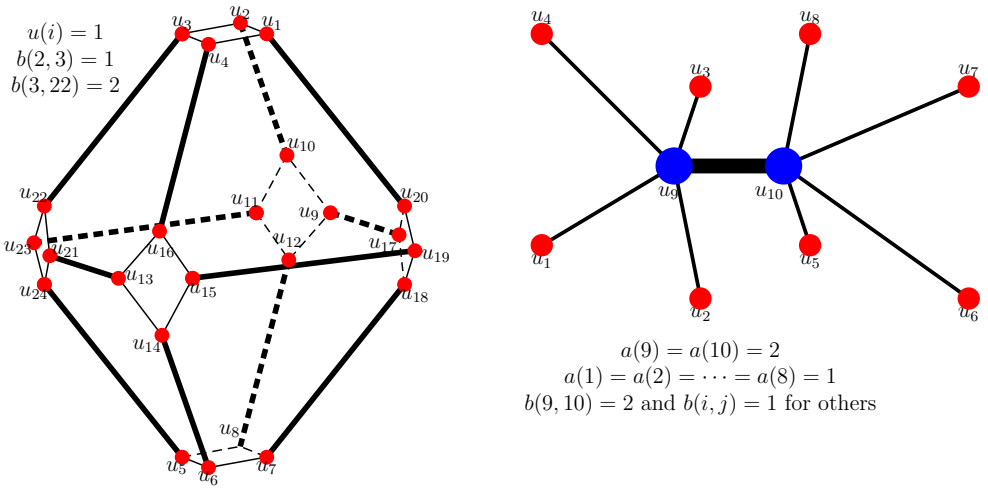


Figure 3.1. Two symmetric molecules with identical atoms and mixed atoms. Bold lines denote double bonding.

where $u(t) = (u_1(t), u_2(t), \ldots, u_n(t)) \in (\mathbb{R}^3)^n$, $u_i(t) \neq u_j(t)$ for $i \neq j$, and

$$\boldsymbol{\mathcal{V}}(u) := \frac{1}{2} \sum_{(i,j)\in\mathscr{B}} U(|u_i - u_j|^2) + \sum_{1\leq i<j\leq n} W(|u_i - u_j|^2). \tag{3.2}$$

Here the function U is the potential expressing bonding between adjacent atoms, while W models the atomic, electric, and other interactions. For the sake of simplicity, in what follows we will assume (by rescaling the equation (3.1)) that all the atoms are identical with the unit mass $m = 1$, i.e. the equation (3.1) can be written as

$$\ddot{u} = -\nabla \boldsymbol{\mathcal{V}}(u). \tag{3.3}$$

Consider the permutation group S_n acting on the set $\mathscr{N}$. Then, by the *symmetry group of the molecule* M we understand the maximal subgroup $\Gamma \subset S_n$ such that

$$\forall_{\sigma\in\Gamma}\ \forall_{(i,j)\in\mathscr{B}}\ \ (\sigma(i), \sigma(j)) \in \mathscr{B}.$$

Notice that the system (3.1) is symmetric with respect to the group action $\Gamma \times O(3)$. Put $\widetilde{V} := (\mathbb{R}^3)^n$

In order to make system (3.3) reference point dependent, we define the subspace

$$V := \{x = (x_1, x_2, \ldots, x_n) \in \mathbb{R}^{3n} : \sum_{i=1}^{n} x_i = 0\}.$$

and the subset

$$\Omega_o := \{(x_1, x_2, \ldots, x_n) \in V :; x_i \neq x_j \ \text{ for } i \neq j\},$$

i.e., we exclude from V the collision orbits.

The Lennard-Jones and Coulomb potentials can be described using the following potential

$$\boldsymbol{\mathcal{V}}(u) := \frac{1}{2} \sum_{(i,j)\in\mathscr{B}} U(|u_i - u_j|^2) + \sum_{1\leq i<j\leq n} W(|u_i - u_j|^2),$$
$$W(t) := \frac{B}{t^6} - \frac{A}{t^3} + \frac{\sigma}{\sqrt{t}}, \quad U(t) = t - 2\sqrt{t}, \quad t > 0.$$

There are many examples of symmetric atomic molecules: octahedral compounds of sulfur hexafluoride SF_6, the molybdenum hexacarbonyl $Mo(CO)_6$, the tetraphosphorus P_4, a spherical fullerene molecule with the formula C_{60} with icosahedral symmetry, or a dihedral molecule with 2-D interactions such as carbon rings, etc. One can find multiple example of symmetric molecule clusters at `http://symmetry.otterbein.edu/gallery/`. In this dissertation, we will consider two types of molecular configurations: tetrahedral and dihedral. However, the proposed method can be effectively applied to any kind of symmetric molecular model.

We are interested in studying molecular vibrations or the so-called modes (i.e., periodic solutions) for the system (3.3). To identify different modes of vibrations (i.e. periodic solutions) corresponding to specific symmetric molecular conformation, one can normalize the period of unknown periodic solutions by introducing an additional parameter λ (unknown frequency), i.e., the problem can be reduced to finding 2π-periodic solutions to the system

$$\ddot{u} = -\lambda^2 \nabla \boldsymbol{\mathcal{V}}(u). \tag{3.4}$$

Clearly, the system (3.4) is a symmetric bifurcation problem, which can be reformulated as a symmetric variational problem.

3.1 Variational Reformulation

Using the system (3.4), the problem of finding periodic solutions to (3.3) can be reformulated as a variational problem on the Sobolev space $H^1_{2\pi}(\mathbb{R}; V)$ (of 2π-periodic V-valued functions) with the functional

$$J_\lambda(u) := \int_0^{2\pi} \left[\frac{1}{2}|\dot{u}(t)|^2 - \lambda^2 \boldsymbol{\mathcal{V}}(u(t))\right] dt, \quad u \in H^1_{2\pi}(\mathbb{R}; \Omega_o),$$

where $\boldsymbol{\mathcal{V}}$ is the potential given by (3.2), λ^{-1} the frequency, and u is the renormalized 2π-periodic solution. The existence of periodic solutions (with fixed frequency λ^{-1}) is equivalent to the existence of critical points of J_λ. We observe that the functional J_λ is invariant under the action of the group

$$G := \Gamma \times O(3) \times O(2),$$

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

3.2 Analysis of Nonlinear Molecular Vibrations

The mathematical analysis of a molecular model includes two objectives: *identification of the normal frequencies* λ^{-1} when the energy state of a molecule is changing from ground vibrational state to excited vibrational states and the *equivariant topological classification of different nonlinear vibrational modes of oscillation* (such as families of periodic solutions with various spatio-temporal symmetries) emerging from the equilibrium configuration (ground vibrational state) of the molecule. The classification of molecular vibrations is a central problem of the molecular spectroscopy. Let us point out that in order to properly describe the vibrational modes occurring in the system (3.3), it is not enough to analyze its linearization at the ground vibrational state. It is a well-known fact that the existence of nonlinear normal modes is not guaranteed under the presence of resonances. Indeed, an example of a

Hamiltonian systems with resonances was presented by Moser [32], in which a linearization of the system had many periodic solutions, while the nonlinear system had none. Therefore, the existence of linear modes does not lead to the existence of nonlinear normal modes under the presence of resonances. Let us point out that due to the occurrence of symmetries, resonances is highly expected in the system (3.3). Therefore, one needs a good methods for classification of nonlinear normal modes.

3.3 Gradient Equivariant Degree Method

To provide an alternative to the equivariant singularity theory (cf. [18]) and other geometric methods that have been used to analyze the existence of relative equilibria in molecules (see [21], [23], [31] and references), the following method based on the equivariant gradient degree was proposed. To describe the main idea of this method, let us point out that the gradient equivariant degree satisfies all the standard properties expected from a degree theory (existence, additivity, homotopy, and multiplicativity properties). The G-equivariant gradient degree $\nabla_G\text{-Deg}(\nabla J_\lambda, \mathscr{U})$ of ∇J_λ on $\mathscr{U}$ can be expressed elegantly as an element of the Euler ring $U(G)$ (which is the free $\mathbb{Z}$-module generated by the conjugacy classes (H) of closed subgroups $H \leq G$) in the form

$$\nabla_G\text{-Deg}(\nabla J_\lambda, \mathscr{U}) = n_1(H_1) + n_2(H_2) + \cdots + n_m(H_m), \quad n_k \in \mathbb{Z},$$

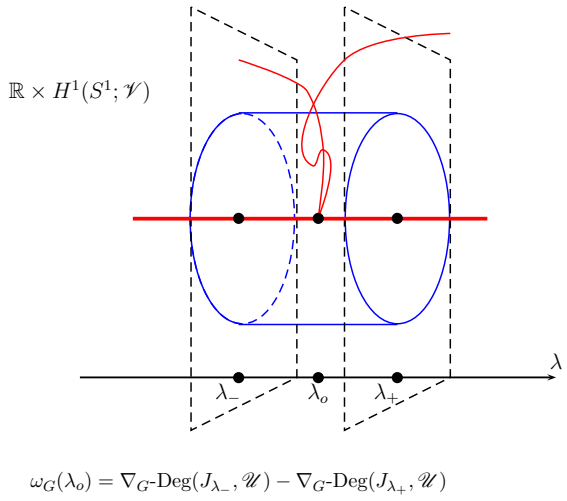
where $\mathscr{U}$ is a neighborhood of the G-orbit of the equilibrium u_o (for some non-critical frequency λ^{-1}) and (H_j) are the orbit types in $\mathscr{U}$. When λ^{-1} crosses a critical frequency λ_o^{-1}, the changes of the $\nabla_G\text{-deg}(\nabla J_\lambda, \mathscr{U})$ allow to establish the existence of various families of orbits of periodic molecular vibrations and their symmetries emerging from the ground state. In fact, the equivariant topological invariant

$$\omega_G(\lambda_o) := \nabla_G\text{-Deg}\left(\nabla J_{\lambda_-}, \mathscr{U}\right) - \nabla_G\text{-Deg}\left(\nabla J_{\lambda_+}, \mathscr{U}\right) \tag{3.5}$$

provides an invariant that contains a full equivariant topological characterization of the families of periodic solutions (together with their symmetries) emerging from the ground state at λ_o (cf. [11]). More precisely, for every non-zero coefficient m_j in

$$\omega_G(\lambda_o) = m_1(K_1) + m_2(K_2) + \dots m_r(K_r),$$

there exists a global family of periodic molecular vibrations with symmetries at least K_j (see the figure below). Moreover, if (K_j) is a maximal orbit type then this family has exact symmetries K_j.



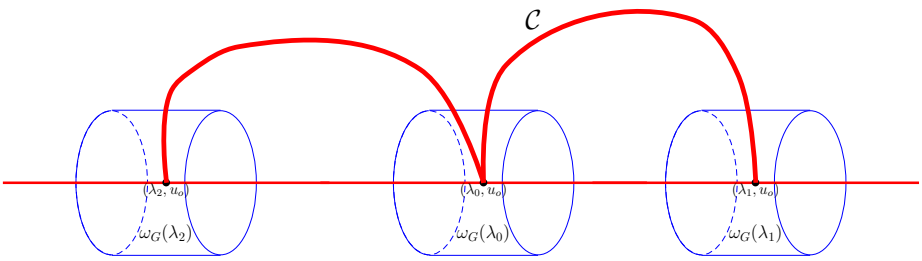
3.4 Global Bifurcation Result

The so-called classical Rabinowitz Theorem [34] establishes occurrence of a global bifurcation from purely local data for compact perturbations of the identity. Its main idea is that if the maximal connected set $\mathcal{C}$ bifurcating from a trivial solution is compact (i.e. bounded), then the sum of the local Leray-Schauder degrees at the set of bifurcation points of $\mathcal{C}$ is zero. Since such maximal connected set $\mathcal{C}$ is either unbounded or comes back to another bifurcation point, this result is also referred to as the *global Rabinowitz alternative* (we refer to Nirenberg's book [33] where a simplified proof of this statement is presented in Theorem 3.4.1).

The classical Rabinowitz's global bifurcation argument can be easily adapted in the equivariant setting for the gradient G-equivariant degree (cf. [17]). That is, for any G-orbit of a compact (bounded) branch $\mathcal{C}$ in $\mathbb{R}_+ \times H^1_{2\pi}(\mathbb{R};\Omega_o)$ containing (λ_0, u_o) we have

$$\sum_{k=0}^{m} \omega_G(\lambda_k) = 0 \tag{3.6}$$

(see the picture below), where λ_k^{-1} are the normal modes belonging to $\mathcal{C}$. In this context the *global property* means that a family of periodic solutions, represented by continuous branch $\mathcal{C}$ in $\mathbb{R}_+ \times H^1_{2\pi}(\mathbb{R};\Omega_o)$, is not compact or come back to another bifurcation point from the equilibrium. The non-compactness of $\mathcal{C}$ implies that the norm or period of solutions from $\mathcal{C}$ goes to the infinity, $\mathcal{C}$ ends in a collision orbit, or goes to a different equilibrium point.



By applying formula (3.6) one can establish an effective criterium allowing to determine the existence of the global (non-compact) branches of molecular vibrations with particular (e.g. maximal) orbit types. To be more precise, it is sufficient to consider all the critical frequencies λ_k^{-1} corresponding to the first Fourier mode and simply show that for some of them, say λ_0^{-1}, the sum in (3.6) can never be zero. Of course, in order to achieve such a task, one would need the exact values of all $\omega_G(\lambda_o)$ for such critical frequencies λ_o^{-1}. Although, this is a very complex task, involving enormous computations, it can be achieve with help of GAP programming. In fact such programs are already developed (see [43]) and were used in this dissertation.

CHAPTER 4

SYMMETRIES OF NONLINEAR VIBRATIONS IN TETRAHEDRAL MOLECULAR CONFIGURATIONS[1]

4.1 Introduction

In this chapter 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 four particles at time t. Such system satisfies the Newtonian equation

$$\ddot{u}(t) = -\nabla \boldsymbol{\mathcal{V}}(u(t)), \tag{4.1}$$

where the potential energy $\boldsymbol{\mathcal{V}}$ represents the force field given by

$$\boldsymbol{\mathcal{V}}(u) := \sum_{1 \le j < k \le 4}^{n} U(|u_j - u_k|^2).$$

When these four particles interact by bond stretching, van der Waals and electrostatic forces [6, 15], 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 $\nabla \boldsymbol{\mathcal{V}}(a) = 0$. To detect possible periodic vibrations around the configuration a, a natural method is to investigate the existence of periodic solutions to (4.1) near a. An important property of this molecular configuration is that it admits tetrahedral spatial symmetries, and thus the bifurcated/emerging

[1] ©2019 AIMS. Portions Adapted, with permission, from I. Berezovik, C. Garca-Azpeitia, and W. Krawcewicz, "Symmetries of Nonlinear Vibrations in Tetrahedral Molecular Configurations," DCDS-B, June 2019.

periodic motions will have both spatial and temporal symmetry. In this case, the equation (4.1) 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.

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 $D^2V(u_o)$ are computed to be $4\nu_0^2$ with multiplicity 1, $2\nu_0^2$ with multiplicity 3, and ν_0^2 with multiplicity 2. Then, the normal modes of (4.1) are $2\nu_0$, $\sqrt{2}\nu_0$, and ν_0, which correspond to the irreducible representations A_1, T_1, and E (Mulliken Symbols), respectively.

Observe that the normal mode ν_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 $2\nu_0$ [28]. On the other hand, since the equilibrium corresponds to a local minimizer of the Hamiltonian, the Weinstein-Moser theorem [42] 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_o, starting with the frequencies of the normal modes $2\nu_0$, $\sqrt{2}\nu_0$, and ν_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, it will be proved that the tetrahedral equilibrium u_o 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 ν_0. If there were no resonances at ν_0, the number of solutions arising from ν_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 π-rotation and π-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 $\sqrt{2}\nu_0$, is not a brake orbit, while three particles move in the form of a traveling wave along a triangle, and another one makes a counterbalance movement. The family from ν_0 has symmetries of brake orbits with two symmetries by inversion at any time. The exact description of the symmetries is given later.

The article [12] presents an extensive study of existence and stability of nonlinear modes for tetraphosphorus molecules. However, in this article, the authors assume the absence of resonances in the normal form of the Hamiltonian. Since in this study, we consider the nonlinear normal modes of a force field which expresses mutual interaction between the atoms, we obtain a Hamiltonian with resonances (refer to [5]).

Methane is a common example of a 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 [29, 30] 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 [29, 30] for each frequency coincide with the obtained

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 [29, 30, 12].

4.2 Model for Tetrahedral 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

$$\tilde{\Omega}_o := \{u \in \mathbb{R}^{12} : \forall_{k \neq j} \;\; u_k \neq u_j\}.$$

The Newtonian equation that describes the interaction between these 4-particles is

$$\ddot{u} = -\nabla \boldsymbol{\mathcal{V}}(u), \quad u \in \tilde{\Omega}_o. \tag{4.2}$$

The potential energy $V : \tilde{\Omega}_o \to \mathbb{R}$,

$$\boldsymbol{\mathcal{V}}(u) := \sum_{1 \leq j < k \leq 4}^{n} U(|u_j - u_k|^2), \tag{4.3}$$

is well defined, and when $U \in C^2(\mathbb{R}^+)$, U satisfies

$$\lim_{x^+ \to 0} U(x) = \infty, \qquad \lim_{x \to \infty} U(x) = \infty. \tag{4.4}$$

Classical forces used in molecular mechanics are associated with bending between adjacent particles, electrostatic interactions, and van der Walls forces. The condition (4.4) holds when U is determined by these force fields.

4.2.1 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

$$(\sigma, A)(u_1, u_2, u_3, u_4)^T = (Au_{\sigma(1)}, Au_{\sigma(2)}, Au_{\sigma(3)}, Au_{\sigma(4)})^T, \tag{4.5}$$

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 $\mathbf{T} \subset \mathbb{R}^3$. More precisely, consider the regular tetrahedron given by

$$\mathbf{T} := \{\gamma_1, \gamma_2, \gamma_3, \gamma_4\},$$

where

$$\gamma_1 = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}, \quad \gamma_2 = \begin{pmatrix} \frac{2}{3}\sqrt{2} \\ 0 \\ -\frac{1}{3} \end{pmatrix}, \quad \gamma_3 = \begin{pmatrix} -\frac{1}{3}\sqrt{2} \\ \frac{1}{3}\sqrt{6} \\ -\frac{1}{3} \end{pmatrix}, \quad \gamma_4 = \begin{pmatrix} -\frac{1}{3}\sqrt{2} \\ -\frac{1}{3}\sqrt{6} \\ -\frac{1}{3} \end{pmatrix}.$$

The tetrahedral group $\{A \in O(3) : A(\mathbf{T}) = \mathbf{T}\}$ can be identified with the group S_4. Indeed, any A such that $A(\mathbf{T}) = \mathbf{T}$ permutes the vertices of $\mathbf{T}$, i.e.,

$$A\gamma_j = \gamma_{\sigma(j)}$$

for $j = 1, 2, 3, 4$. Thus, we can identify A_σ 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

$$A_{(1,2)} = \begin{bmatrix} \frac{1}{3} & 0 & \frac{2\sqrt{2}}{3} \\ 0 & 1 & 0 \\ \frac{2\sqrt{2}}{3} & 0 & -\frac{1}{3} \end{bmatrix} \quad \text{and} \quad A_{(2,3,4)} = \begin{bmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{2} & 0 \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} & 0 \\ 0 & 0 & 1 \end{bmatrix}.$$

These generators define an explicit isomorphism $A_\sigma : S_4 \to O(3)$.

Notice that the function $\boldsymbol{\mathcal{V}} : \tilde{\Omega}_o \to \mathbb{R}$ is invariant with respect to the action of $c \in \mathbb{R}^3$ on $(\mathbb{R}^3)^4$ by shifting, $\boldsymbol{\mathcal{V}}(u + c) = \boldsymbol{\mathcal{V}}(u)$. Therefore in order to fix the center of mass at the origin in the system (4.2), we define the subspace

$$\mathscr{V} := \{(u_1, u_2, u_3, u_4)^T \in (\mathbb{R}^3)^4 : u_1 + u_2 + u_3 + u_4 = 0\} \tag{4.6}$$

and $\Omega_o = \tilde{\Omega}_o \cap \mathscr{V}$. Then, one can easily notice that $\mathscr{V}$ and Ω_o are invariant under the nonlinear dynamics of (5.3), and, in addition, Ω_o is G-invariant.

Consider the point $v_0 := (\gamma_1, \gamma_2, \gamma_3, \gamma_4) \in \Omega_o$. The isotropy group $\mathfrak{G}_{v_o}$ 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_σ. Since $\tilde{S}_4$ is a finite group, $\mathscr{V}^{\tilde{S}_4}$ is a one-dimensional subspace of $\mathscr{V}$, and we have that

$$\mathscr{V}^{\tilde{S}_4} = \mathrm{span}_{\mathbb{R}}\{(\gamma_1, \gamma_2, \gamma_3, \gamma_4)^T\}.$$

Then, by Symmetric Criticality Principle, a critical point of $\boldsymbol{\mathcal{V}}^{\tilde{S}_4} : \Omega_o^{\tilde{S}_4} \to \mathbb{R}$ is also a critical point of $\boldsymbol{\mathcal{V}}$. Since $\mathscr{V}^{\tilde{S}_4}$ is one-dimensional, we denote its vectors by $rv_o \in \mathbb{R}^{12}$ for $r \in \mathbb{R}$. Notice that

$$\phi(r) := \sum_{1 \le j < k \le 4} U\left(\frac{8}{3} r^2\right), \quad r > 0.$$

is exactly the restriction of $\boldsymbol{\mathcal{V}}$ to the fixed-point subspace $\mathscr{V}^{\tilde{S}_4} \cap \Omega_o$. Thus in order to find an equilibrium for (5.3), by Symmetric Criticality Principle, it is sufficient to identify a critical point r_o of $\phi(r)$. Clearly by (4.4),

$$\lim_{r \to 0^+} \phi(r) = \lim_{r \to \infty} \phi(r) = \infty.$$

Then, there exists a minimizer $r_o \in (0, \infty)$, which is clearly a critical point of φ. Consequently,

$$u_o := r_o v_o \in \Omega_o \tag{4.7}$$

is the $\tilde{S}_4$-symmetric equilibrium of $\boldsymbol{\mathcal{V}}$. 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 (4.2), see Figure 5.1.

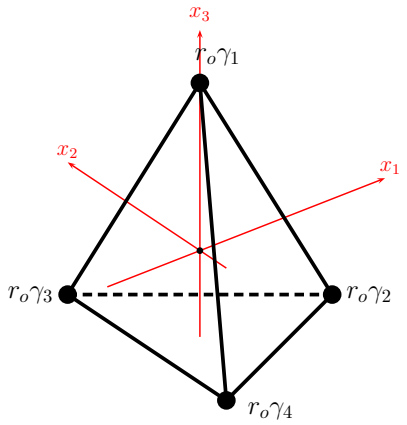


Figure 4.1. Stationary solution to equation (5.3) with tetrahedral symmetries.

4.2.2 Isotypic Decomposition

Since the system (5.3) is symmetric with respect to the group action $\mathfrak{G} := S_4 \times O(3)$, we have that the orbit of equilibria $\mathfrak{G}(u_o)$ is a 3-dimensional submanifold in $\mathscr{V}$. The slice S_o to the orbit $\mathfrak{G}(u_o)$ at u_o is

$$S_o := \{x \in \mathscr{V} : x \bullet T_{u_o}\mathfrak{G}(u_o) = 0\}.$$

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

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

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 $\mathfrak{G}$-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 (5.5). We have the following table of characters χ_j, $j = 0, 1, 2, 3, 4$, for all irreducible $\tilde{S}_4$-representations $\mathcal{V}_j$ (all of them of real type) and the character χ_V of the representation V:

Rep.	Character	(1)	$(1,2)$	$(1,2)(3,4)$	$(1,2,3)$	$(1,2,3,4)$
$\mathcal{V}_0$	χ_0	1	1	1	1	1
$\mathcal{V}_1$	χ_1	3	1	-1	0	-1
$\mathcal{V}_2$	χ_2	2	0	2	-1	0
$\mathcal{V}_3$	χ_3	3	-1	-1	0	1
$\mathcal{V}_4$	χ_4	1	-1	1	1	-1
V	χ_V	12	2	0	0	0

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

$$V = \mathcal{V}_0 \oplus (\mathcal{V}_1 \oplus \mathcal{V}_1) \oplus \mathcal{V}_2 \oplus \mathcal{V}_3 \ .$$

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 $\mathcal{V}_1$, we have the the $\tilde{S}_4$-isotypic decomposition

$$\mathscr{V} = V_0 \oplus V_1 \oplus V_2 \oplus V_3, \qquad V_j = \mathcal{V}_j \ . \tag{4.8}$$

In order to determine the $\tilde{S}_4$-isotypic type of the tangent space $T_{u_0}\mathfrak{G}(u_o)$ (which has to be an irreducible $\tilde{S}_4$-representation of dimension 3), we apply the isotypic projections $P_j : V \to V_j$, $j = 1$ and 3, given by

$$P_j v := \frac{\dim(V_j)}{72} \sum_{g \in S_4} \chi_j(g)\, gv, \quad v \in V,$$

to conclude that $T_{u_0}\mathfrak{G}(u_o) \simeq \mathcal{V}_3$. Therefore, the $\tilde{S}_4$-isotypic decomposition of the slice S_o is

$$S_o = V_0 \oplus V_1 \oplus V_2 \ . \tag{4.9}$$

4.2.3 Computation of the Spectrum $\sigma(\nabla^2 V(u_o))$

Since the potential $\boldsymbol{\mathcal{V}}$ is given by (5.2), we have

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

Notice that we have $\nabla\boldsymbol{\mathcal{V}}(u_o) = 0$ when $U'(r_0^2) = 0$.

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

$$\mathfrak{m}_v := \begin{bmatrix} x \\ y \\ z \end{bmatrix}[x, y, z] = \begin{bmatrix} x^2 & xy & xz \\ xy & y^2 & yz \\ xz & yz & z^2 \end{bmatrix}.$$

Then one can easily see that the matrix $\mathfrak{m}_v$ 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

$$\mathfrak{m}_{j,k} := \mathfrak{m}_{(\gamma_j-\gamma_k)}.$$

Clearly, $\mathfrak{m}_{j,k} = \mathfrak{m}_{k,j}$. Notice that

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

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

$$M := \nabla^2 V(u_o) = 4r_o^2 U''(r_o)\begin{bmatrix} \sum_{j\neq 1}\mathfrak{m}_{1j} & -\mathfrak{m}_{12} & -\mathfrak{m}_{13} & -\mathfrak{m}_{1,4} \\ -\mathfrak{m}_{2,1} & \sum_{j\neq 2}\mathfrak{m}_{2,j} & -\mathfrak{m}_{23} & -\mathfrak{m}_{2,4} \\ -\mathfrak{m}_{3,1} & -\mathfrak{m}_{3,2} & \sum_{j\neq 3}\mathfrak{m}_{3,j} & -\mathfrak{m}_{3,4} \\ -\mathfrak{m}_{4,1} & -\mathfrak{m}_{3,2} & -\mathfrak{m}_{4,3} & \sum_{j\neq 4}\mathfrak{m}_{4,j} \end{bmatrix}.$$

Since $M : \mathscr{V} \to \mathscr{V}$ 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 $V_j = \mathcal{V}_j$ are absolutely irreducible, we have that

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

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

To find explicit formulae for the eigenvalues μ_j, we notice that

$$\mathfrak{v}_0 := \begin{bmatrix} \gamma_1 \\ \gamma_2 \\ \gamma_3 \\ \gamma_4 \end{bmatrix} \in V_0, \quad \mathfrak{v}_1 := \begin{bmatrix} -2\gamma_1 \\ \gamma_1 + \gamma_2 \\ \gamma_1 + \gamma_3 \\ \gamma_1 + \gamma_4 \end{bmatrix} \in V_1, \quad \mathfrak{v}_2 := \begin{bmatrix} \gamma_2 - \gamma_3 \\ \gamma_1 - \gamma_4 \\ \gamma_4 - \gamma_1 \\ \gamma_3 - \gamma_2 \end{bmatrix} \in V_2.$$

By direct application of the matrix $\mathscr{L}$ on the vectors $\mathfrak{v}_j$, $j = 0, 1, 2$, we obtain that

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

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

4.3 Equivariant Bifurcation

In what follows, we are interested in finding non-trivial T-periodic solutions to (4.2), bifurcating from the orbit of equilibrium points $\mathfrak{G}(u_o)$. By normalizing the period, i.e., by making the substitution $v(t) := u\left(\frac{T}{2\pi}t\right)$ in (4.2), we obtain the following system

$$\begin{cases} \ddot{v} = -\lambda^2 \nabla \boldsymbol{\mathcal{V}}(v), \\ v(0) = v(2\pi), \quad \dot{v}(0) = \dot{v}(2\pi), \end{cases} \tag{4.10}$$

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

4.3.1 Equivariant Gradient Map

Since $\mathscr{V}$ is an orthogonal $\mathfrak{G}$- representation, we can consider the first Sobolev space of 2π-periodic functions from $\mathbb{R}$ to $\mathscr{V}$, i.e.,

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

equipped with the inner product

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

Let $O(2)=SO(2)\cup\kappa SO(2)$ denote the group of 2×2-orthogonal matrices, where

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

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., κ, as a linear transformation of $\mathbb{C}$ into itself, acts as complex conjugation.

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

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

Indeed, for $u\in H^1_{2\pi}(\mathbb{R},\mathscr{V})$ and $(\sigma,A)\in\mathfrak{G}$ (see (5.5)), we have

$$\begin{aligned}(\sigma,A)\,u(t) &= (\sigma,A)u(t),\\ e^{i\tau}u(t) &= u(t+\tau),\\ \kappa u(t) &= u(-t).\end{aligned}\tag{4.11}$$

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

Put

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

Then, the system (4.10) can be written as the following variational equation

$$\nabla_u J(\lambda, u) = 0, \quad (\lambda, u) \in \mathbb{R} \times \Omega, \tag{4.12}$$

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

$$J(\lambda, u) := \int_0^{2\pi} \left[\frac{1}{2} |\dot{u}(t)|^2 - \lambda^2 \boldsymbol{\mathcal{V}}(u(t)) \right] dt. \tag{4.13}$$

Assume that $u_o \in \mathbb{R}^{12}$ is the equilibrium point of (4.2) described in subsection 4.2.1. Then, clearly, u_o is a critical point of J. We are interested in finding non-stationary 2π-periodic solutions bifurcating from u_o, i.e., non-constant solutions to system (4.3.1).

We consider the G-orbit of u_o in the space $H^1(S^1, \mathscr{V})$. By $\mathcal{S}_o$, we denote the slice to $G(u_o)$ in $H^1(S^1, \mathscr{V})$. By

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

we will also denote the restriction of J to the set $\mathcal{S}_o \cap \Omega$. Clearly, $\mathscr{J}$ is G_{u_o}-invariant. Then, since the orbit $G(u_o)$ is orthogonal to the slice $\mathcal{S}_o$, critical points of $\mathscr{J}$ are critical points of J in a small tubular neighborhood of the orbit $G(u_o)$. Consequently, these critical points are solutions to system (4.3.1). This property allows to establish the Slice Criticality Principle (see Theorem 2.8.1) 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 $L : H^2(S^1; \mathscr{V}) \to L^2(S^1; \mathscr{V})$, given by $Lu = -\ddot{u} + u$, $u \in H^2(S^1, \mathscr{V})$. Then, the inverse operator L^{-1} exists and is bounded. Let $j : H^2(S^1; \mathscr{V}) \to H^1(S^1, \mathscr{V})$ be the natural embedding operator. Clearly, j is a compact operator. Then, one can easily verify that

$$\nabla_u J(\lambda, u) = u - j \circ L^{-1}(\lambda^2 \nabla \boldsymbol{\mathcal{V}}(u) + u), \tag{4.14}$$

where $u \in H^1(S^1, \mathscr{V})$. Consequently, the bifurcation problem (4.3.1) can be written as $u - j \circ L^{-1}(\lambda^2 \nabla \boldsymbol{\mathcal{V}}(u) + u) = 0$. Moreover, we have

$$\nabla_u^2 J(\lambda, u_o)v = v - j \circ L^{-1}(\lambda^2 \nabla^2 \boldsymbol{\mathcal{V}}(u_o)v + v) \ , \tag{4.15}$$

where $v \in H^1(S^1, \mathscr{V})$.

Consider the operator

$$\mathscr{A}(\lambda) := \nabla_u^2 J(\lambda, u_o)|_{\mathcal{S}_o} : \mathcal{S}_o \to \mathcal{S}_o. \tag{4.16}$$

Notice that

$$\nabla_u^2 \mathscr{J}(\lambda, u_o) = \mathscr{A}(\lambda).$$

Thus, by implicit function theorem, $G(u_o)$ is an isolated orbit of critical points of J whenever $\mathscr{A}(\lambda)$ is an isomorphism. Therefore, if a point (λ_o, u_o) is a bifurcation point for (4.3.1), then $\mathscr{A}(\lambda_o)$ cannot be an isomorphism. In such a case we put

$$\Lambda := \{\lambda > 0 : \mathscr{A}(\lambda_o) \text{ is not an isomorphism}\} \ ,$$

and we call the set Λ the *critical set* for the trivial solution u_o.

4.3.2 Bifurcation Theorem

Consider the S^1-action on $H^1(S^1, \mathscr{V})$, where S^1 acts on functions by shifting the argument (see (4.11)). Then, $(H^1(S^1, \mathscr{V}))^{S^1}$ is the space of constant functions, which can be identified with the space $\mathscr{V}$, i.e.,

$$H^1(S^1, \mathscr{V}) = \mathscr{V} \oplus \mathscr{W}, \quad \mathscr{W} := \mathscr{V}^{\perp}.$$

Then, the slice $\mathcal{S}_o$ in $H^1(S^1, \mathscr{V})$ to the orbit $G(u_o)$ at u_o is exactly

$$\mathcal{S}_o = S_o \oplus \mathscr{W}.$$

Since the eigenvalues are $\mu_j \neq 0$ for $j = 0, 1, 2$, any $\lambda_o \in \Lambda$ satisfying the condition $\mathscr{A}(\lambda_o)|_{S_o} : S_o \to S_o$ is an isomorphism. This, in its turn, leads to the following theorem:

Theorem 4.3.1. *Consider the bifurcation system* (4.3.1) *and assume that* $\lambda_o \in \Lambda$ *is isolated in the critical set* Λ*, i.e., there exists* $\lambda_- < \lambda_o < \lambda_+$ *such that* $[\lambda_-, \lambda_+] \cap \Lambda = \{\lambda_o\}$*. Define*

$$\omega_G(\lambda_o) := \nabla_{G_{u_o}}\text{-deg}\Big(\mathscr{A}(\lambda_-), B_1(0)\Big) - \nabla_{G_{u_o}}\text{-deg}\Big(\mathscr{A}(\lambda_+), B_1(0)\Big),$$

where $B_1(0)$ *stands for the open unit ball in* $\mathscr{H}$*. 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* (4.3.1) *from the orbit* $\{\lambda_o\} \times G(u_o)$ *with symmetries at least* (H_j)*.*

Consider the S^1-isotypic decomposition of $\mathscr{W}$, i.e.,

$$\mathscr{W} = \overline{\bigoplus_{l=1}^{\infty} \mathscr{W}_l}, \quad \mathscr{W}_l := \{\cos(l\cdot)\mathfrak{a} + \sin(l\cdot)\mathfrak{b} : \mathfrak{a},\, \mathfrak{b} \in \mathscr{V}\}.$$

In a standard way, the space $\mathscr{W}_l$, $l = 1, 2, \ldots$, can be naturally identified with the space $\mathscr{V}^{\mathbb{C}}$ on which S^1 acts by l-folding,

$$\mathscr{W}_l = \{e^{il\cdot} z : z \in \mathscr{V}^{\mathbb{C}}\}.$$

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

$$G_{u_o} = \tilde{S}_4 \times O(2),$$

it is also S^1-equivariant, and thus $\mathscr{A}(\lambda)(\mathscr{W}_l) \subset \mathscr{W}_l$. Using the $\tilde{S}_4$-isotypic decomposition of $\mathscr{V}^{\mathbb{C}}$, we have the G_{u_o}-isotypic decomposition

$$\mathscr{W}_l = W_{0,l} \oplus W_{1,l} \oplus W_{2,l} \oplus W_{3,l}\ , \qquad W_{j,l} = \mathcal{W}_{j,l}\ .$$

Moreover, we have

$$\mathscr{A}(\lambda)|_{W_{j,l}} = \left(1 - \frac{\lambda^2 \mu_j + 1}{l^2 + 1}\right) \mathrm{Id}\ ,$$

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 Λ for the equilibrium u_o of the system (4.2) is

$$\Lambda := \left\{ \frac{l}{\sqrt{\mu_j}} : j = 0, 1, 2, \quad l = 1, 2, 3, \dots \right\},$$

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 Λ

$$\lambda_{0,1} < \lambda_{1,1} < \lambda_{2,1} = \lambda_{0,2} < \lambda_{1,2} < \lambda_{2,2} = \lambda_{0,4} \ .$$

Definition 4.3.2. For simplicity, hereafter, we denote by S_4 the isotropy group $\mathfrak{G}_{u_0} = \tilde{S}_4$, i.e., with this notation we write

$$G_{u_0} = \mathfrak{G}_{u_0} \times O(2) = S_4 \times O(2) \ .$$

From the computation of the gradient degree in (2.17) with G_{u_0}, we obtain

$$\nabla_{G_{u_0}}\text{-deg}\Big(\mathscr{A}(\lambda_o), B_1(0)\Big) = \prod_{\left\{(j,l)\in\mathbb{N}^2 : \lambda_{j,l} < \lambda_o\right\}} \nabla\text{-deg}_{\mathcal{W}_{j,l}} \tag{4.17}$$

for $\lambda \notin \Lambda$.

For each critical number $\lambda_{j,l}$, we choose two numbers $\lambda_- < \lambda_{j,l} < \lambda_+$ such that $[\lambda_-, \lambda_+] \cap \Lambda = \{\lambda_{j,l}\}$. Calculating the difference of the gradient degree at λ_+ and λ_- using (4.17), we obtain that the equivariant invariants are given by

$$\begin{aligned}
\omega_G(\lambda_{0,1}) &= \nabla\text{-deg}_{\mathcal{W}_{0,1}} - (S_4 \times O(2)) \\
\omega_G(\lambda_{1,1}) &= \nabla\text{-deg}_{\mathcal{W}_{0,1}} * \Big(\nabla\text{-deg}_{\mathcal{W}_{1,1}} - (S_4 \times O(2))\Big) \\
\omega_G(\lambda_{2,1}) &= \nabla\text{-deg}_{\mathcal{W}_{0,1}} * \nabla\text{-deg}_{\mathcal{W}_{1,1}} * \Big(\nabla\text{-deg}_{\mathcal{W}_{2,1}} * \nabla\text{-deg}_{\mathcal{W}_{0,2}} - (S_4 \times O(2))\Big)
\end{aligned}$$

4.3.3 Computation of the Gradient Degree

We use the amalgamated notation to describe the conjugacy classes ($\mathscr{H}$) 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 $\omega_G(\lambda_{j_o,1}) \in U(S_4 \times O(2))$ should be considered. In particular, although it is not the case here, the invariant $\omega_G(\lambda_{j_o,1})$ may contain maximal orbit types (H) with infinite Weyl's group $W(H)$. Therefore, we consider the truncation to $A(S_4 \times O(2))$ given by

$$\widetilde{\omega}_G(\lambda_{j_o,1}) := \pi_0\Big(\omega_G(\lambda_{j_o,1})\Big),$$

where $\pi_0 : U(G) \to A(G)$ is a ring homomorphism. Other more complex molecular structures may require the full value of the invariant $\omega_G(\lambda_{j_o})$ 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 [43]) to compute the basic degrees truncated to $A(G)$:

$$\begin{aligned}
\nabla\text{-deg}_{\mathcal{W}_{0,l}} =& -(S_4 \times D_l) + (S_4 \times O(2)),\\
\nabla\text{-deg}_{\mathcal{W}_{1,l}} =& -(D_4{}^{D_2}\times_{\mathbb{Z}_2} D_{2l}) - (D_2{}^{D_1}\times_{\mathbb{Z}_2} D_{2l}) - (D_4{}^{\mathbb{Z}_1}\times_{D_4} D_{4l}) - (D_3 \times D_l)\\
&- (D_3{}^{\mathbb{Z}_1}\times_{D_3} D_{3l}) + 2(D_1 \times D_l) - (\mathbb{Z}_1 \times D_l) + (\mathbb{Z}_2{}^{\mathbb{Z}_1}\times_{\mathbb{Z}_2} D_{2l})\\
&+ (D_2{}^{\mathbb{Z}_1}_{\mathbb{Z}_2}\times_{D_2} D_{2l}) + (V_4{}^{\mathbb{Z}_1}\times_{D_2} D_{2l}) + (D_2{}^{D_1}\times_{D_1} D_l) - (\mathbb{Z}_2{}^{\mathbb{Z}_1}\times_{D_1} D_l)\\
&+ (S_4 \times O(2)),\\
\nabla\text{-deg}_{\mathcal{W}_{2,l}} =& -(S_4{}^{V_4}\times_{D_3} D_{3l}) - (D_4 \times D_l) + (V_4 \times D_l) - (D_4{}^{V_4}\times_{\mathbb{Z}_2} D_{2l})\\
&+ 2(D_4{}^{V_4}\times_{D_1} D_l) + (S_4 \times O(2)),\\
\nabla\text{-deg}_{\mathcal{W}_{3,l}} =& -(D_4{}^{\mathbb{Z}_4}\times_{\mathbb{Z}_2} D_{2l}) - (D_4{}^{\mathbb{Z}_1}\times_{D_4} D_{4l}) - (D_2{}^{D_1}\times_{\mathbb{Z}_2} D_{2l}) + 2(D_1{}^{\mathbb{Z}_1}\times_{\mathbb{Z}_2} D_{2l})\\
&+ (\mathbb{Z}_2{}^{\mathbb{Z}_1}\times_{\mathbb{Z}_2} D_{2l}) - (\mathbb{Z}_1 \times D_l) - (D_3{}^{\mathbb{Z}_3}\times_{\mathbb{Z}_2} D_{2l}) - (D_3{}^{\mathbb{Z}_1}\times_{D_3} D_{3l})\\
&+ (D_2{}^{\mathbb{Z}_1}_{D_1}\times_{D_2} D_{2l}) + (D_2{}^{\mathbb{Z}_1}_{\mathbb{Z}_2}\times_{D_2} D_{2l}) + (V_4{}^{\mathbb{Z}_1}\times_{D_2} D_{2l}) - (\mathbb{Z}_2{}^{\mathbb{Z}_1}\times_{D_1} D_l)\\
&+ (S_4 \times O(2)),\\
\nabla\text{-deg}_{\mathcal{W}_{4,l}} =& -(S_4{}^{A_4}\times_{\mathbb{Z}_2} D_{2l}) + (S_4 \times O(2)),
\end{aligned}$$

Next, we again use GAP programming (see [43]) and the product $*$ of the Euler ring $U(\Gamma)$ to compute the full equivariant invariants $A(S_4 \times O(2))$, where the maximal isotropy classes are colored red:

$$
\begin{aligned}
\widetilde{\omega}_G(\lambda_{0,1}) = & -(S_4 \times D_1),\\
\widetilde{\omega}_G(\lambda_{1,1}) = & -(D_4{}^{D_2}\times_{\mathbb{Z}_2} D_2) - (D_2{}^{D_1}\times_{\mathbb{Z}_2} D_2) - (D_4{}^{\mathbb{Z}_1}\times_{D_4} D_4) + (D_3 \times D_1)\\
& - (D_3{}^{\mathbb{Z}_1}\times_{D_3} D_3) + (D_2 \times D_1) - (D_1 \times D_1) + (\mathbb{Z}_2{}^{\mathbb{Z}_1}\times_{\mathbb{Z}_2} D_2)\\
& + (D_2{}^{\mathbb{Z}_1}_{\mathbb{Z}_2}\times_{D_2} D_2) + (V_4{}^{\mathbb{Z}_1}\times_{D_2} D_2) + (D_4{}^{D_2}\times_{D_1} D_1) + (D_1{}^{\mathbb{Z}_1}\times_{D_1} D_1)\\
& - (\mathbb{Z}_2{}^{\mathbb{Z}_1}\times_{D_1} D_1),\\
\widetilde{\omega}_G(\lambda_{2,1}) = & -(S_4{}^{V_4}\times_{D_3} D_3) - (S_4 \times D_2) + (D_4{}^{V_4}\times_{\mathbb{Z}_2} D_2) - (\mathbb{Z}_4{}^{\mathbb{Z}_2}\times_{\mathbb{Z}_2} D_2)\\
& + 2(D_2{}^{D_1}\times_{\mathbb{Z}_2} D_2) - (D_1{}^{\mathbb{Z}_1}\times_{\mathbb{Z}_2} D_2) - 2(\mathbb{Z}_2{}^{\mathbb{Z}_1}\times_{\mathbb{Z}_2} D_2) + 2(S_4 \times D_1)\\
& - (D_4 \times D_1) - 2(D_3 \times D_1) - (D_2 \times D_1) + (D_1 \times D_1)\\
& + (\mathbb{Z}_1 \times D_1) + 2(D_4{}^{D_2}\times_{\mathbb{Z}_2} D_2) + 2(D_3{}^{\mathbb{Z}_1}\times_{D_3} D_3) - (D_4{}^{\mathbb{Z}_2}_{\mathbb{Z}_4}\times_{D_2} D_2)\\
& - (D_2{}^{\mathbb{Z}_1}_{D_1}\times_{D_2} D_2) - (D_2{}^{\mathbb{Z}_1}_{\mathbb{Z}_2}\times_{D_2} D_2) - (V_4{}^{\mathbb{Z}_1}\times_{D_2} D_2) - (D_4{}^{D_2}\times_{D_1} D_1)\\
& + (D_4{}^{V_4}\times_{D_1} D_1) - (D_2{}^{D_1}\times_{D_1} D_1) + 3(\mathbb{Z}_2{}^{\mathbb{Z}_1}\times_{D_1} D_1).
\end{aligned}
$$

4.4 Description of the Symmetries

The invariants $\omega_G(\lambda_{j,1})$ 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 $\lambda_{2,1} = \lambda_{0,2}$ with maximal group $S_4{}^{S_4}\times_{\mathbb{Z}_1} D_2$ is not independent of minimal period bifurcation from $\lambda_{0,1}$ with maximal group $S_4{}^{S_4}\times_{\mathbb{Z}_1} D_1$, we cannot conclude that these two bifurcations are different from each other.

We can conclude that the other 7 maximal groups in the invariants $\omega_G(\lambda_{j,1})$ 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 $\tilde{S}_4$ with S_4, i.e., in a maximal group, an element $\sigma \in S_4$ acts as

$$\sigma u_j = A_\sigma u_{\sigma(j)} \ .$$

4.4.1 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

$$S_4 \,{}^{S_4}\!\times_{\mathbb{Z}_1} D_1.$$

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.

4.4.2 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

$$D_4 \,{}^{D_2}\!\times_{\mathbb{Z}_2} D_2$$

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 κ implies that the periodic solution is a brake orbit. Thus, $A_{(12)}$ is the inversion over the plane, containing the points γ_3, γ_4, and the middle point of γ_1 and γ_2, which interchanges γ_1 with γ_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 π that interchanges γ_1 with γ_3 and γ_2 with γ_4. Therefore u_1 is the π-rotation and π-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

$$D_2 {}^{D_1}\!\times_{\mathbb{Z}_2} D_2$$

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 κ 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 π-rotation and π-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

$$D_4 {}^{\mathbb{Z}_1}\!\times_{D_4} D_4$$

is generated by $((12), \kappa)$ and $\left((1324), e^{i\pi/2}\right)$ 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 $\left((1324), e^{i\pi/2}\right)$ 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 κ, 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

$$-D_3{}^{\mathbb{Z}_1}\times_{D_3} D_3$$

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: $u_1(t) = A_{(1,2)}u_2(-t) = A_{(1,2)}u_1(-t - 2\pi/3)$.

4.4.3 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 $S_4{}^{V_4}\times_{D_3} D_3$. 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, and u_3 are related by a rotation of $2\pi/3$ and a phase shift of $2\pi/3$.

CHAPTER 5

DIHEDRAL MOLECULAR CONFIGURATIONS INTERACTING BY LENNARD-JONES AND COULOMB FORCES[1]

5.1 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. [27]). 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 SF_6, the molybdenum hexacarbonyl $Mo(CO)_6$, the tetraphosphorus P_4, a spherical fullerene molecule with the formula C_{60} with icosahedral symmetry, or a dihedral molecule with 2-D interactions such as carbon rings, etc. One can find multiple examples of symmetric molecule clusters in [25].

Let us consider n identical atoms u_j, $j \in \{1, 2, \ldots, n-1, n\} =: X$, in the space $\mathbb{R}^3$. Then, a set $\mathscr{B} \subset X \times X$, satisfying the conditions (a) $(i,j) \in \mathscr{B}$ then $(j,i) \in \mathscr{B}$ and (b) $(j,j) \notin \mathscr{B}$, can be considered as a *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 $(i,j) \in \mathscr{B}$. It follows that the symmetries $\Gamma \subset S_n$ of a molecular bonding are the permutation $\sigma \in S_n$ such that

$$\forall_{(i,j)\in\mathscr{B}} \ \ (\sigma(i), \sigma(j)) \in \mathscr{B}.$$

[1]

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

$$\ddot{u} = -\nabla \boldsymbol{\mathcal{V}}(u), \quad u(t) = (u_1(t), u_2(t), \dots, u_n(t)), \quad u_i(t) \neq u_j(t), \ \text{ for } \ i \neq j, \tag{5.1}$$

where

$$\boldsymbol{\mathcal{V}}(u) := \frac{1}{2} \sum_{(i,j)\in\mathscr{B}} U(|u_i - u_j|^2) + \sum_{1\leq i<j\leq n} W(|u_i - u_j|^2),$$
$$W(t) := \frac{B}{t^6} - \frac{A}{t^3} + \frac{\sigma}{\sqrt{t}}, \quad U(t) = t - 2\sqrt{t}, \quad t > 0.$$

In this chapter, we are interested in studying planar molecular interactions for (5.1) in a ring of n identical atoms with the dihedral D_n symmetries. Such model was studied in [15], where a similar (but not complete) classification of nonlinear vibrations was obtained using $\mathbb{Z}_n$-symmetries. Current 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 (5.11)), 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 [1, 10, 13, 14, 15, 28, 35, 36]).

The content of this chapter can be described as follows. First, 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^o and describe the dihedral isotypical decomposition of the slice to the orbit of these equilibria. Next, in the section 5.3, we formulate the problem of finding a periodic vibration to (5.3) as a bifurcation

problem (5.11) and reformulate it as a variational bifurcation problem with $D_n \times O(2)$-symmetries. In the subsection 5.3.1, we introduce the equivariant invariant $\omega_{\mathbf{G}}(\lambda_o)$. In the subsection 5.3.2, we compute the spectrum of $\mathscr{L} := \nabla^2 \boldsymbol{\mathcal{V}}(u^o)$ for a general potential $\boldsymbol{\mathcal{V}}$ and, subsequently in the section 5.4, we formulate the main existence results based on the values of the equivariant invariants $\omega_G(\lambda_o)$ (Theorem 5.4.2). In the section 5.4.2, we consider an example of a particular system (5.11) 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 5.4.3.

5.2 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 $\Omega_o' := \{u \in \mathbb{C}^n : u_k \neq u_j, \text{ if } k \neq j, \text{ with } k, j = 0, 1, 2, \cdots, n-1\}$. The Lennard-Jones and Coulomb potential $\boldsymbol{\mathcal{V}} : \Omega_o' \to \mathbb{R}$ is given by

$$\boldsymbol{\mathcal{V}}(u) := \sum_{j=0}^{n} U(|u_{j+1} - u_j|^2) + \sum_{0 \leq j < k \leq n-1} W(|u_j - u_k|^2), \tag{5.2}$$

where

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

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

$$\ddot{u} = -\nabla \boldsymbol{\mathcal{V}}(u), \quad u \in \Omega_o'. \tag{5.3}$$

Notice that the function $\boldsymbol{\mathcal{V}} : \Omega_o' \to \mathbb{R}$ 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 $\boldsymbol{\mathcal{V}}(z_0+z, z_1+z, \ldots, z_{n-1}+z) =$

$\boldsymbol{\mathcal{V}}(z_0, z_1, \ldots, z_n)$. In order to make system (5.3) independent of reference point (i.e. the choice of the origin in $\mathbb{C}^n$), we put

$$\mathscr{V} := \{(z_0, z_1, z_2, \ldots, z_{n-1}) \in \mathbb{C}^n : z_0 + z_1 + z_2 + \cdots + z_{n-1} = 0\}, \tag{5.4}$$

and $\Omega_o = \Omega'_o \cap \mathscr{V}$, and consider (5.3) 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 $\xi := (0, 1, 2, 3, \ldots, n-1)$ (the "rotation" corresponding to $\gamma = e^{\frac{2\pi i}{n}}$) 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

$$(\sigma, A)(z_0, z_1, \ldots, z_{n-1}) = (Az_{\sigma(0)}, Az_{\sigma(1)}, \ldots, Az_{\sigma(n-1)}), \tag{5.5}$$

where $(\sigma, A) \in D_n \times O(2)$. Notice that $\Omega_o \subset \mathscr{V}$ is $\mathfrak{G}$-invariant and the system (5.3) is $\mathfrak{G}$-equivariant.

Symmetric Equilibrium for (5.3)**:** Consider the point $v^o := (1, \gamma, \gamma^2, \ldots, \gamma^{n-1}) \in \Omega_o$, where $\gamma := e^{i\frac{2\pi}{n}}$. Then

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

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

$$\mathscr{V}^\Gamma = \mathrm{span}_{\mathbb{R}}\{(1, \gamma, \gamma^2, \ldots, \gamma^{n-1})\}.$$

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

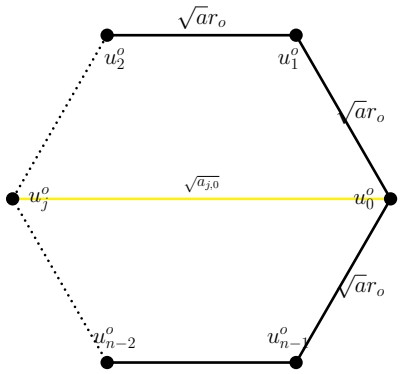


Figure 5.1. Stationary solution to equation (5.3) with dihedral symmetries.

for the orbit of equilibria for (5.3) in this subspace. The restriction of $\boldsymbol{\mathcal{V}}$ to the subspace $\{t(1, \gamma, \gamma^2, \ldots, \gamma^{n-1}) : t > 0\}$ can be written as

$$\phi(t) = nU\left(at^2\right) + \sum_{0 \le j < k \le n-1} W\left(a_{jk}t^2\right), \quad t > 0. \tag{5.6}$$

where

$$a = 4\sin^2\frac{\pi}{n} \quad \text{and} \quad a_{jk} = 4\sin^2\frac{(k-j)\pi}{n}, \tag{5.7}$$

where $0 \le j < k \le n-1$. Since

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

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

$$u^o = r_o(1, \gamma, \gamma^2, \ldots, \gamma^{n-1}) \in \Omega_o \tag{5.8}$$

which is a Γ-symmetric equilibrium of $\boldsymbol{\mathcal{V}}$ (see Figure 5.1). We put

$$u^o = (u_0^o, u_1^o, \ldots, u_{n-1}^o) \in \mathbb{C}^n,$$

i.e., $u_k^o = r_o\gamma^k$, $k = 0, 1, 2, \ldots, n-1$. Consequently we have the orbit of equilibria $M = \mathfrak{G}(u^o)$. The tangent vector to M at $u^o \in M$ is $v^o = i(1, \gamma, \ldots, \gamma^{n-1})$, thus the slice S_o to the orbit

M at u^o is $S_o = \{z \in \mathbb{C}^n : z \bullet v^o = 0\}$, or equivalently

$$S_o = \left\{ (z_0, z_1, \ldots, z_{n-1}) \in \mathbb{C}^n : \mathrm{Re}\left(\sum_{k=0}^{n-1} z_k i\gamma^{-k} \right) = 0 \right\}.$$

Define $\mu : \mathbb{C}^n \to \mathbb{R}$ and $\nu : \mathbb{C}^n \to \mathbb{C}$ by

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

Then $\ker \mu = S_o$ and $\ker \nu \subset \ker \mu$. Notice that μ and ν are Γ-invariant so S_o is a Γ-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 $(z, z\gamma^{-j}, z\gamma^{-2j}, \ldots, z\gamma^{-(n-1)j}) \in \ker \nu$ for $z \in \mathbb{C}$. Next, we define

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

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

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

where '$\cdot$' 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 $\gamma z = \gamma^{j+1} \cdot z$, $\kappa z = \overline{z}$, $z \in \mathbb{C}$. 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_o.

Isotypical Components of S_o for n being an odd number: In this case, the space S_o has the following isotypical components

$$S_o = \mathscr{V}_0 \oplus \mathscr{V}_1 \oplus \mathscr{V}_2 \oplus \cdots \oplus \mathscr{V}_j \oplus \cdots \oplus \mathscr{V}_r, \text{ with } r = \left\lfloor \frac{n}{2} \right\rfloor, \tag{5.9}$$

where $\mathscr{V}_0 = W_{n-1}$, that is,

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

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

$$\mathscr{V}_j = W_{j-1} \oplus W_{n-j-1}.$$

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 $j = 1, 2, \ldots, r$, $\mathscr{V}_j$ is a complex subspace of $\mathbb{C}^n$ such that

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

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

$$S_o = \mathscr{V}_0 \oplus \mathscr{V}_1 \oplus \mathscr{V}_2 \oplus \cdots \oplus \mathscr{V}_j \oplus \cdots \oplus \mathscr{V}_r, \text{ with } r = \frac{n}{2}, \tag{5.10}$$

with the same components $\mathscr{V}_j$ in (5.9) for $j < \frac{n}{2} = r$ and an additional isotypical component $\mathscr{V}_r$ given by

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

5.3 Variational Reformulation

We are interested in finding non-trivial p-periodic solutions to (5.3), bifurcating from the orbit equilibrium points $\mathfrak{G}(u^o)$. By normalizing the period in (5.3) (i.e., by making the substitution $v(t) = u\left(\frac{pt}{2\pi}\right)$) we obtain the following system,

$$\begin{cases} \ddot{v} = -\lambda^2 \nabla \boldsymbol{\mathcal{V}}(v), \\ v(0) = v(2\pi), \;\; \dot{v}(0) = \dot{v}(2\pi), \end{cases} \tag{5.11}$$

where $\lambda = \frac{p}{2\pi}$. The problem (5.11) can be reformulated as a variational problem.

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

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

equipped with the inner product

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

The space $H^1_{2\pi}(\mathbb{R}, \mathscr{V})$ is an orthogonal Hilbert representation of $\mathbf{G} := D_n \times O(2) \times O(2)$ with the $\mathbf{G}$-action given by (see (5.5))

$$\Big((\xi, A, e^{i\tau})x\Big)(t) = (\xi, A)x(t + \tau), \tag{5.12}$$

$$\Big((\xi, A, e^{i\tau}\kappa)x\Big)(t) = (\xi, A)x(-t + \tau). \tag{5.13}$$

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

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

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

Then system (5.11) is equivalent to the following variational equation

$$\nabla_u J(\lambda, u) = 0, \quad (\lambda, u) \in \mathbb{R} \times \Omega, \tag{5.14}$$

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

$$J(\lambda, u) = \int_0^{2\pi} \left[\frac{1}{2}|\dot{u}(t)|^2 - \lambda^2 \boldsymbol{\mathcal{V}}(u(t)) \right] dt. \tag{5.15}$$

Clearly, the equilibrium point $u^o = r_o(1, \gamma, \gamma^2, \gamma^{n-1}) \in \mathbb{C}^n$ of (5.3) (described in subsection 5.2) is a critical point of J. We consider the $\mathbf{G}$-orbit $\mathbf{G}(u^o)$ in the space $H^1(S^1, \mathscr{V})$. We are interested in finding non-stationary 2π-periodic solutions bifurcating from $\mathbf{G}(u^o)$, that is, non-constant solutions to system (5.14).

Consider the operator $L : H^2(S^1; \mathscr{V}) \to L^2(S^1; \mathscr{V})$, given by $Lu = -\ddot{u}+u$, $u \in H^2(S^1, \mathscr{V})$. Then the inverse operator L^{-1} exists and is bounded. Let $j : H^2(S^1; \mathscr{V}) \to H^1(S^1, \mathscr{V})$ be the natural embedding operator. Then j is a compact operator and we have

$$\nabla_u J(\lambda, u) = u - j \circ L^{-1}(\lambda^2 N_{\nabla \boldsymbol{\mathcal{V}}}(u) + u), \quad u \in H^1(S^1, \mathscr{V}), \tag{5.16}$$

where

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

Consequently, the bifurcation problem (5.14) can be written as

$$\mathscr{F}(\lambda, u) := u - j \circ L^{-1}(\lambda^2 N_{\nabla \boldsymbol{\mathcal{V}}}(u) + u) = 0.$$

Notice that $\mathscr{F}$ is a completely continuous gradient field. Moreover, we have

$$D_u \mathscr{F}(\lambda, u^o) = \nabla_u^2 J(\lambda, u^o) = \mathrm{Id} \, - j \circ L^{-1}(\lambda^2 N_{\nabla^2 \boldsymbol{\mathcal{V}}}(u^o) + \mathrm{Id}\,), \tag{5.17}$$

where

$$(N_{\nabla^2 \boldsymbol{\mathcal{V}}}(u^o)v)(t) = \nabla^2 \boldsymbol{\mathcal{V}}(u^o)v(t), \quad v \in H^1(S^1, \mathscr{V});\ t \in \mathbb{R}.$$

In what follows we put

$$\mathscr{L} := \nabla^2 \boldsymbol{\mathcal{V}}(u^o) : \mathscr{V} \to \mathscr{V} \quad \text{and} \quad \mathscr{L}_o : P \circ \mathscr{L}|_{S_o} : S_o \to S_o. \tag{5.18}$$

Put $G := \mathbf{G}_{u^o} = \Gamma \times O(2) \simeq D_n \times O(2)$ and denote by $\mathscr{S}_o$ the slice to $\mathbf{G}(u^o) = \mathfrak{G}(u^o)$ in $H^1(S^1, \mathscr{V})$. We will also denote by $\mathscr{J} : \mathbb{R} \times \widetilde{\Omega} \to \mathbb{R}$ the restriction of J to the set $\mathbb{R} \times \widetilde{\Omega}$, where $\widetilde{\Omega} = \mathscr{S}_o \cap \Omega$ and $\mathscr{J}(\lambda, u) = J(\lambda, u^o + u)$, $u \in \widetilde{\Omega}$. Notice that $\mathscr{J}$ is G-invariant. Consider the operator $\mathscr{A}(\lambda) : \mathscr{S}_o \to \mathscr{S}_o$, given by

$$\mathscr{A}(\lambda) := P(\nabla_u^2 J(\lambda, u^o)). \tag{5.19}$$

Notice that

$$\nabla_u^2 \mathscr{J}(\lambda, u^o) = \mathscr{A}(\lambda),$$

thus, by implicit function theorem, $\mathbf{G}(u^o)$ is an isolated orbit of critical points of J, whenever $\mathscr{A}(\lambda)$ is an isomorphism. Therefore, if a point (λ_o, u^o) is a bifurcation point for (5.14), then $\mathscr{A}(\lambda_o)$ is not an isomorphism. Based on this observation we define $\Lambda = \{\lambda > 0 : \mathscr{A}(\lambda_o)$ is not an isomorphism$\}$. We will call the set Λ the *critical set* for the trivial solution u^o.

Consider the restricted S^1-action on $H^1(S^1, \mathscr{V})$ (see (5.12)). The fixed-point space $(H^1(S^1, \mathscr{V}))^{S^1}$, by identifying it with the subspace of constant functions, is the space $\mathscr{V}$. Thus we have

$$H^1(S^1, \mathscr{V}) = \mathscr{V} \oplus \mathscr{W}, \quad \mathscr{W} := \mathscr{V}^{\perp},$$

so the slice $\mathscr{S}_o$ in $H^1(S^1, \mathscr{V})$ to the orbit $\mathfrak{G}(u^o)$ at u^o is exactly

$$\mathscr{S}_o = S_o \oplus \mathscr{W}.$$

5.3.1 Application of the Equivariant Gradient Degree

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

Define the following equivariant invariants (cf. [17]:

$$\omega_G(\lambda_o) := \nabla_G\text{-deg}\Big(\mathscr{A}(\lambda_-), B_1(0)\Big) - \nabla_G\text{-deg}\Big(\mathscr{A}(\lambda_+), B_1(0)\Big), \tag{5.20}$$

$$\omega_{\mathbf{G}}(\lambda_o) := \Theta\Big(\omega_G(\lambda_o)\Big), \tag{5.21}$$

where $B_1(0)$ stands for the open unit ball in $\mathscr{S}_o$ and $\Theta : U(G) \to U(\mathbf{G})$ 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 2.8.1) that 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 $\omega_{\mathbf{G}}(\lambda_o) = n_1(H_1) + n_2(H_2) + \cdots + n_m(H_m)$ also has non-zero coefficient n_j, and there exists a bifurcating branch of nontrivial solutions to (5.14) from the orbit $\{\lambda_o\} \times \mathbf{G}(u^o)$ with symmetries at least (H_j) (with respect to the $\mathbf{G}$-action).

Consider the S^1-isotypical decomposition of $\mathscr{W}$, that is,

$$\mathscr{W} = \overline{\bigoplus_{l=1}^{\infty} \mathscr{W}_l}, \quad \mathscr{W}_l := \{\cos(l\cdot)\mathfrak{a} + \sin(l\cdot)\mathfrak{b} : \mathfrak{a},\, \mathfrak{b} \in \mathscr{V}\}.$$

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

$$\sigma(\mathscr{A}(\lambda)|_{\mathscr{W}_l}) = \left\{1 - \frac{\lambda^2\mu + 1}{l^2 + 1} : \mu \in \sigma(\mathscr{L}_o)\right\}, \tag{5.22}$$

which under the assumption that $0 \notin \sigma(\mathscr{L}_o)$, implies that $\lambda_o \in \Lambda$ if and only if $\lambda_o^2 = \frac{l^2}{\mu}$ for some $l = 1, 2, 3, \ldots$ and $\mu \in \sigma(\mathscr{L}_o)$. Therefore, in order to apply the formula (2.17), it is essential to know the spectrum $\sigma(\mathscr{L}_o)$.

5.3.2 Computation of the Spectrum $\sigma(\mathscr{L})$

Since the potential $\boldsymbol{\mathcal{V}}$ is given by (5.2), we can write that $\boldsymbol{\mathcal{V}}(u) = \Phi(u) + \Psi(u)$, $u \in \Omega$, 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 $\mathscr{L}$: For a given complex number $z = x + iy$, which we write in a vector form $z = (x, y)^T$, we define the matrix $\mathfrak{m}_z := zz^T$, i.e.

$$\mathfrak{m}_z := \begin{bmatrix} x \\ y \end{bmatrix}[x, y] = \begin{bmatrix} x^2 & xy \\ xy & y^2 \end{bmatrix}.$$

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

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

The 2×2 matrix $\mathfrak{m}_{jk}$ can be described using the complex operators as

$$\mathfrak{m}_{jk} = \frac{|z_{jk}|^2}{2}\Big[1 - \gamma^{j+k}\kappa\Big] = 2\sin^2\frac{\pi(j-k)}{n}\Big[1 - \gamma^{j+k}\kappa\Big].$$

Put

$$
\begin{aligned}
v_{jk} &:= U'(a_{jk}r_o^2), & v_{jj} &:= 0\\
u_{jk} &:= 2U''(a_{jk}r_o^2)\sin^2\frac{\pi(j-k)}{n}, & u_{jj} &:= 0\\
\mathfrak{v}_{jk} &:= W'(a_{jk}r_o^2), & \mathfrak{v}_{jj} &:= 0\\
\mathfrak{u}_{jk} &:= 2W''(a_{jk}r_o^2)\sin^2\frac{\pi(j-k)}{n}, & \mathfrak{u}_{jj} &:= 0
\end{aligned}
$$

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

$$\nabla^2\Phi(u^o) = 2U'(ar_o^2)\mathcal{A} + 4r_o^2U''(ar_o^2)\mathcal{B},$$

where

$$\mathcal{A} := \begin{bmatrix} 2 & -1 & 0 & \dots & -1\\ -1 & 2 & -1 & \dots & 0\\ \vdots & \vdots & \vdots & \ddots & \vdots\\ -1 & 0 & 0 & \dots & 2 \end{bmatrix},$$

and

$$
\begin{aligned}
\mathcal{B} &:= \begin{bmatrix} \mathfrak{m}_{0,n-1}+\mathfrak{m}_{0,1} & -\mathfrak{m}_{01} & 0 & \dots & -\mathfrak{m}_{0,n-1}\\ -\mathfrak{m}_{1,0} & \mathfrak{m}_{1,0}+\mathfrak{m}_{1,2} & -\mathfrak{m}_{1,2} & \dots & 0\\ \vdots & \vdots & \vdots & \ddots & \vdots\\ -\mathfrak{m}_{n-1,0} & 0 & 0 & \dots & \mathfrak{m}_{n-1,n-2}+\mathfrak{m}_{n-1,0} \end{bmatrix}\\
&= 2\sin^2\frac{\pi}{n}\begin{bmatrix} 2-(\gamma^{-1}+\gamma)\kappa & -1+\gamma\kappa & 0 & \dots & -1+\gamma^{-1}\kappa\\ -1+\gamma\kappa & 2-(\gamma^1+\gamma^3)\kappa & -1+\gamma^3\kappa & \dots & 0\\ \vdots & \vdots & \vdots & \ddots & \vdots\\ -1+\gamma^{-1}\kappa & 0 & 0 & \dots & 2-(\gamma^{-3}+\gamma^{-1}) \end{bmatrix}\\
&= 2\sin^2\frac{\pi}{n}\Big(\mathcal{A} - \mathcal{E}_\gamma K\Big),
\end{aligned}
$$

with

$$K = \begin{bmatrix} \kappa & 0 & 0 & \dots & 0 \\ 0 & \kappa & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \dots & \kappa \end{bmatrix}, \ \mathcal{E}_\gamma = \begin{bmatrix} \gamma^{-1}+\gamma & -\gamma & 0 & \dots & -\gamma^{-1} \\ -\gamma & \gamma+\gamma^3 & -\gamma^3 & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ -\gamma^{-1} & 0 & 0 & \dots & \gamma^{-3}+\gamma^{-1} \end{bmatrix}$$

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

$$\nabla^2\Psi(u^o) = 2\mathcal{C} + 4r_o^2\mathcal{D},$$

where

$$\mathcal{C} := \begin{bmatrix} \sum_{j\neq 0} W'(a_{0j}r_o^2) & -W'(a_{01}r_o^2) & \dots & -W'(a_{0,n-1}r_o^2) \\ -W'(a_{1,0}r_o^2) & \sum_{j\neq 1} W'(a_{1j}r_o^2) & \dots & -W'(a_{2,n-1}r_o^2) \\ \vdots & \vdots & \ddots & \vdots \\ -W'(a_{n-1,0}r_o^2) & -W'(a_{n-1,1}r_o^2) & \dots & \sum_{j\neq n-1} W'(a_{n-1,j}r_o^2) \end{bmatrix}$$

$$= \begin{bmatrix} \sum_j \mathfrak{v}_{0j} & -\mathfrak{v}_{01} & -v_{02} & \dots & -\mathfrak{v}_{0,n-1} \\ -\mathfrak{v}_{10} & \sum_j \mathfrak{v}_{1j} & -\mathfrak{v}_{12} & \dots & -\mathfrak{v}_{1,n-1} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ -\mathfrak{v}_{n-1,0} & -\mathfrak{v}_{n-1,1} & -\mathfrak{v}_{n-1,2} & \dots & \sum_j \mathfrak{v}_{n-1,j} \end{bmatrix}$$

and

$$\mathcal{D} := \begin{bmatrix} \sum_{j\neq 0} W''(a_{0j}r_o^2)\mathfrak{m}_{0j} & -W''(a_{01}r_o^2)\mathfrak{m}_{01} & \dots & -W''(a_{0,n-1}r_o^2)\mathfrak{m}_{0,n-1} \\ -W''(a_{1,0}r_o^2)\mathfrak{m}_{1,0} & \sum_{j\neq 1} W''(a_{1j}r_o^2)\mathfrak{m}_{1,j} & \dots & -W''(a_{1,n-1}r_o^2)\mathfrak{m}_{1,n-1} \\ \vdots & \vdots & \ddots & \vdots \\ -W''(a_{n-1,0}r_o^2)\mathfrak{m}_{n-1,0} & -W''(a_{n-1,1}r_o^2)\mathfrak{m}_{n-1,1} & \dots & \sum_{j\neq n-1} W''(a_{n-1,j}r_o^2)\mathfrak{m}_{n-1,j} \end{bmatrix}$$

$$= \begin{bmatrix} \sum_j \mathfrak{u}_{0j}(1-\gamma^j\kappa) & -\mathfrak{u}_{01}(1-\gamma\kappa) & \dots & -\mathfrak{u}_{0,n-1}(1-\gamma^{n-1}\kappa) \\ -\mathfrak{u}_{10}(1-\gamma\kappa) & \sum_j \mathfrak{u}_{1j}(1-\gamma^{j+1}\kappa) & \dots & -\mathfrak{u}_{1,n-1}(1-\kappa) \\ \vdots & \vdots & \ddots & \vdots \\ -\mathfrak{u}_{n-1,0}(1-\gamma^{-1}\kappa) & -\mathfrak{u}_{n-1,1}(1-\kappa) & \dots & \sum_j \mathfrak{u}_{n-1,j}(1-\gamma^{j-1}\kappa) \end{bmatrix}$$

$$= \widetilde{\mathcal{C}} - \mathcal{F}_\gamma K,$$

with

$$\widetilde{\mathcal{C}} = \begin{bmatrix} \sum_j \mathfrak{u}_{0j} & -\mathfrak{u}_{01} & -\mathfrak{u}_{02} & \dots & -\mathfrak{u}_{0,n-1} \\ -\mathfrak{u}_{10} & \sum_j \mathfrak{u}_{1j} & -\mathfrak{u}_{12} & \dots & -\mathfrak{u}_{1,n-1} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ -\mathfrak{u}_{n-1,0} & -\mathfrak{u}_{n-1,1} & -\mathfrak{u}_{n-1,2} & \dots & \sum_j \mathfrak{u}_{n-1,j} \end{bmatrix}$$

and

$$\mathcal{F}_\gamma := \begin{bmatrix} \sum_j \mathfrak{u}_{0j}\gamma^j & -\mathfrak{u}_{01}\gamma & \dots & -\mathfrak{u}_{0,n-1}\gamma^{-1} \\ -\mathfrak{u}_{10}\gamma & \sum_j \mathfrak{u}_{1j}\gamma^{j+1} & \dots & -\mathfrak{u}_{1,n-1} \\ \vdots & \vdots & \ddots & \vdots \\ -\mathfrak{u}_{n-1,0}\gamma^{-1} & -\mathfrak{u}_{n-1,1} & \dots & \sum_j \mathfrak{u}_{n-1,j}\gamma^{j-1} \end{bmatrix}.$$

Using the above decompositions, we have the following matrix representations: $\mathcal{A}_k := \mathcal{A}|_{\mathscr{V}_k}$, $\mathcal{B}_k := \mathcal{B}|_{\mathscr{V}_k}$, $\mathcal{C}_k := \mathcal{C}|_{\mathscr{V}_k}$, $\widetilde{\mathcal{C}}_k := \widetilde{\mathcal{C}}|_{\mathscr{V}_k}$, and $\mathcal{A}_k := \mathscr{L}|_{\mathscr{V}_k}$.

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

$$\mathcal{A}_0 = [2 - 2\mathfrak{Re}(\gamma)] = \Big[4\sin^2\frac{\pi}{n}\Big], \quad \mathcal{A}_1 = [2 - 2\mathfrak{Re}(\gamma^2)] = \Big[4\sin^2\frac{2\pi}{n}\Big]$$
$$\mathcal{A}_k = \begin{bmatrix} 2 - 2\mathfrak{Re}(\gamma^{k-1}) & 0 \\ 0 & 2 - 2\mathfrak{Re}(\gamma^{k+1}) \end{bmatrix} = \begin{bmatrix} 4\sin^2\frac{\pi(k-1)}{n} & 0 \\ 0 & 4\sin^2\frac{\pi(k+1)}{n} \end{bmatrix},$$

for $1 < k < \lfloor \frac{n}{2} \rfloor$. Since

$$\mathcal{E}_\gamma K\mathbf{u}^k = 2\mathfrak{Re}(\gamma - \gamma^k)\mathbf{v}^k = -4\sin\frac{\pi(1+k)}{n}\sin\frac{\pi(1-k)}{n}\mathbf{v}^k,$$
$$\mathcal{E}_\gamma K\mathbf{v}^k = 2\mathfrak{Re}(\gamma - \gamma^k)\mathbf{u}^k = -4\sin\frac{\pi(1+k)}{n}\sin\frac{\pi(1-k)}{n}\mathbf{u}^k,$$

we get

$$\mathcal{B}_0 = \Big[8\sin^4\frac{\pi}{n}\Big], \quad \mathcal{B}_1 = \Big[8\sin^2\frac{\pi}{n}\sin^2\frac{2\pi}{n}\Big]$$
$$\mathcal{B}_k = \begin{bmatrix} 8\sin^2\frac{\pi}{n}\sin^2\frac{\pi(k-1)}{n} & 8\sin^2\frac{\pi}{n}\sin\frac{\pi(1+k)}{n}\sin\frac{\pi(1-k)}{n} \\ 8\sin^2\frac{\pi}{n}\sin\frac{\pi(1+k)}{n}\sin\frac{\pi(1-k)}{n} & 8\sin^2\frac{\pi}{n}\sin^2\frac{\pi(k+1)}{n} \end{bmatrix},$$

for $1 < k < \lfloor \frac{n}{2} \rfloor$. Put

$$\mathfrak{a}_k := \sum_j \mathfrak{v}_{0j} - \sum_j \mathfrak{v}_{0j}\gamma^{(1-k)j} = \sum_{j=1}^{\lfloor\frac{n-1}{2}\rfloor} 4\mathfrak{v}_{0j}\sin^2\frac{\pi(1-k)j}{n}$$
$$\mathfrak{b}_k := \sum_j \mathfrak{v}_{0j} - \sum_j \mathfrak{v}_{0j}\gamma^{(1+k)j} = \sum_{j=1}^{\lfloor\frac{n-1}{2}\rfloor} 4\mathfrak{v}_{0j}\sin^2\frac{\pi(1+k)j}{n}$$
$$\mathfrak{a}_k := \sum_j \mathfrak{u}_{0j} - \sum_j \mathfrak{u}_{0j}\gamma^{(1-k)j} = \sum_{j=1}^{\lfloor\frac{n-1}{2}\rfloor} 4\mathfrak{u}_{0j}\sin^2\frac{\pi(1-k)j}{n}$$
$$\mathfrak{b}_k := \sum_j \mathfrak{u}_{0j} - \sum_j \mathfrak{u}_{0j}\gamma^{(1+k)j} = \sum_{j=1}^{\lfloor\frac{n-1}{2}\rfloor} 4\mathfrak{u}_{0j}\sin^2\frac{\pi(1+k)j}{n}$$

Since

$$\mathcal{C}\mathbf{u}^k = \left(\sum_j \mathfrak{v}_{0j} - \sum_j \mathfrak{v}_{0j}\gamma^{(1-k)j}\right)\mathbf{u}^k, \quad \mathcal{C}\mathbf{v}^k = \left(\sum_j \mathfrak{v}_{0j} - \sum_j \mathfrak{v}_{0j}\gamma^{(1+k)j}\right)\mathbf{v}^k,$$

thus we obtain

$$\mathcal{C}_0 = [\mathbf{a}_0]\,,\ \mathcal{C}_1 = 0,\ \ \widetilde{\mathcal{C}}_0 = [\mathfrak{a}_0]\,,\ \ \widetilde{\mathcal{C}}_1 = 0$$

$$\mathcal{C}_k = \begin{bmatrix} \mathbf{a}_k & 0 \\ 0 & \mathbf{b}_k \end{bmatrix}, \quad \widetilde{\mathcal{C}}_k = \begin{bmatrix} \mathfrak{a}_k & 0 \\ 0 & \mathfrak{b}_k \end{bmatrix}$$

for $1 < k < \left\lfloor \frac{n}{2} \right\rfloor$. Next, put

$$\mathfrak{c}_k = \sum_j \mathfrak{u}_{0j}\gamma^j - \sum_j \mathfrak{u}_{0j}\gamma^j\gamma^{j(k-1)} = 4\sum_{j=1}^{\lfloor\frac{n-1}{2}\rfloor} \mathfrak{u}_{0j} \sin\frac{\pi j(k+1)}{n} \sin\frac{\pi j(k-1)}{n}.$$

Since

$$\mathcal{F}_\gamma K\mathbf{u}^k = \left(\sum_j \mathfrak{u}_{0j}\gamma^j - \sum_j \mathfrak{u}_{0j}\gamma^j\gamma^{j(k-1)}\right)\mathbf{v}^k$$

$$\mathcal{F}_\gamma K\mathbf{v}^k = \left(\sum_j \mathfrak{u}_{0j}\gamma^j - \sum_j \mathfrak{u}_{0j}\gamma^j\gamma^{j(k-1)}\right)\mathbf{u}^k.$$

we obtain

$$\mathcal{D}_0 = [\mathfrak{a}_0], \ \ \mathcal{D}_1 = [\mathfrak{c}_1] = [0],$$

$$\mathcal{D}_k = \begin{bmatrix} \mathfrak{a}_k & -\mathfrak{c}_k \\ -\mathfrak{c}_k & \mathfrak{b}_k \end{bmatrix}, \quad \text{for } \ 1 < k < \lfloor\frac{n}{2}\rfloor$$

Finally, we get th following matrix representations of $\mathscr{L}_k$

$$\mathscr{L}_0 = [\boldsymbol{\alpha}_0], \quad \mathscr{L}_1 = [\boldsymbol{\alpha}_1], \tag{5.23}$$

where

$$\boldsymbol{\alpha}_0 = 8\left(U'(ar_o^2) + 4r_o^2U''(ar_o^2)\sin^2\frac{\pi}{n}\right)\sin^2\frac{\pi}{n} + \sum_{j=1}^{\lfloor\frac{n-1}{2}\rfloor}(8v_{0j} + 16r_o^2u_{0j})\sin^2\frac{\pi j}{n} \tag{5.24}$$

$$\boldsymbol{\alpha}_1 = 8\left(U'(ar_o^2) + 4r_o^2U''(ar_o^2)\sin^2\frac{2\pi}{n}\right)\sin^2\frac{2\pi}{n} \tag{5.25}$$

and

$$\mathscr{L}_k = \begin{bmatrix} 2\boldsymbol{\alpha}_k & \boldsymbol{\delta}_k \\ \boldsymbol{\delta}_k & 2\boldsymbol{\beta}_k \end{bmatrix}, \quad 1 < k \leq \left\lfloor \frac{n-1}{2} \right\rfloor \tag{5.26}$$

where

$$\begin{aligned} \boldsymbol{\alpha}_k &:= 4U'(ar_o^2)\sin^2\frac{\pi(k-1)}{n} + 16r_o^2U''(ar_o)\sin^2\frac{\pi}{n}\sin^2\frac{\pi(1-k)}{n} \\ &\quad + \sum_{j=1}^{\lfloor\frac{n-1}{2}\rfloor}\left(4\mathfrak{v}_{0j} + 8r_o^2\mathfrak{u}_{oj}\right)\sin^2\frac{\pi(1-k)j}{n} \end{aligned} \tag{5.27}$$

$$\begin{aligned} \boldsymbol{\beta}_k &:= 4U'(ar_o^2)\sin^2\frac{\pi(k+1)}{n} + 16r_o^2U''(ar_o)\sin^2\frac{\pi}{n}\sin^2\frac{\pi(1+k)}{n} \\ &\quad + \sum_{j=1}^{\lfloor\frac{n-1}{2}\rfloor}\left(4\mathfrak{v}_{0j} + 8r_o^2\mathfrak{u}_{oj}\right)\sin^2\frac{\pi(1+k)}{n} \end{aligned} \tag{5.28}$$

$$\begin{aligned} \boldsymbol{\delta}_k &:= 32r_o^2U''(ar_o^2)\sin^2\frac{\pi}{n}\sin\frac{\pi(1+k)}{n}\sin\frac{\pi(1-k)}{n} \\ &\quad - 32r_o^2\sum_{j=1}^{\lfloor\frac{n-1}{2}\rfloor}\mathfrak{u}_{0j}\sin\frac{\pi j(k-1)}{n}\sin\frac{\pi j(k+1)}{n}. \end{aligned} \tag{5.29}$$

Case 2 (n being an even number). In this case we have an additional isotypical component $\mathscr{V}_r$, $r = \frac{n}{2}$. The entries of the matrix $\mathscr{L}_k$, for $0 \leq k < \frac{n}{2}$, given by formulae (5.23) and (5.26), are slightly different, i.e.

$$\begin{aligned} \boldsymbol{\alpha}_0 &= 8\left(U'(ar_o^2) + 4r_o^2U''(ar_o^2)\sin^2\frac{\pi}{n}\right)\sin^2\frac{\pi}{n} + \sum_{j=1}^{\lfloor\frac{n-1}{2}\rfloor}(8v_{0j} + 16r_o^2u_{0j})\sin^2\frac{\pi j}{n}n \\ &\quad + 4v_{0r} + 8u_{0r}r_o^2, \end{aligned} \tag{5.30}$$

$$\boldsymbol{\alpha}_1 = 8\left(U'(ar_o^2) + 4r_o^2U''(ar_o^2)\sin^2\frac{2\pi}{n}\right)\sin^2\frac{2\pi}{n}, \tag{5.31}$$

$$\boldsymbol{\alpha}_k := 4U'(ar_o^2)\sin^2\frac{\pi(k-1)}{n} + 16r_o^2U''(ar_o)\sin^2\frac{\pi}{n}\sin^2\frac{\pi(1-k)}{n}$$
$$+\sum_{j=1}^{\lfloor\frac{n-1}{2}\rfloor}\left(4\mathfrak{v}_{0j}+8r_o^2\mathfrak{u}_{oj}\right)\sin^2\frac{\pi(1-k)j}{n}+\delta(k)(2\mathfrak{v}_{0r}+4r_o^2\mathfrak{u}_{0r}), \tag{5.32}$$

$$\boldsymbol{\beta}_k := 4U'(ar_o^2)\sin^2\frac{\pi(k+1)}{n} + 16r_o^2U''(ar_o)\sin^2\frac{\pi}{n}\sin^2\frac{\pi(1+k)}{n}$$
$$+\sum_{j=1}^{\lfloor\frac{n-1}{2}\rfloor}\left(4\mathfrak{v}_{0j}+8r_o^2\mathfrak{u}_{oj}\right)\sin^2\frac{\pi(1+k)}{n}+\delta(k)(2\mathfrak{v}_{0r}+4r_o^2\mathfrak{u}_{0r}), \tag{5.33}$$

$$\boldsymbol{\delta}_k := 32r_o^2U''(ar_o^2)\sin^2\frac{\pi}{n}\sin\frac{\pi(1+k)}{n}\sin\frac{\pi(1-k)}{n}$$
$$-32r_o^2\sum_{j=1}^{\lfloor\frac{n-1}{2}\rfloor}\mathfrak{u}_{0j}\sin\frac{\pi j(k-1)}{n}\sin\frac{\pi j(k+1)}{n}+16\delta(k)r_o^2\mathfrak{u}_{0r}, \tag{5.34}$$

for $1 < k \leq r-1$. In addition we have $\mathscr{L}_k = [\boldsymbol{\alpha}_r]$, where

$$\boldsymbol{\alpha}_r := 8U'(ar_o^2)\cos^2\frac{\pi}{n} + 32r_o^2U''(ar_o^2)\sin^2\frac{\pi}{n}\cos^2\frac{\pi}{n}$$
$$+\sum_{j=1}^{\lfloor\frac{n-1}{2}\rfloor}(8\mathfrak{v}_{0j}+16r_o^2\mathfrak{u}_{0j})\sin^2\frac{\pi(1-r)j}{n}+(4\mathfrak{v}_{0r}+8r_o^2\mathfrak{u}_{0r}). \tag{5.35}$$

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

Proposition 5.3.1. *For n being an odd number we have the following explicit formulae for the spectrum of the operator $\mathscr{L}$*

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

where

$$\mu_0 := \boldsymbol{\alpha}_0, \quad \mu_1 := \boldsymbol{\alpha}_1,$$
$$\mu_k^{\pm} := \boldsymbol{\alpha}_k + \boldsymbol{\beta}_k \pm \sqrt{(\boldsymbol{\alpha}_k - \boldsymbol{\beta}_k)^2 + \boldsymbol{\delta}_k^2}, \quad 1 < k \leq \left\lfloor\frac{n-1}{2}\right\rfloor.$$

and the coefficients $\boldsymbol{\alpha}_j$, $\boldsymbol{\beta}_j$, $\boldsymbol{\delta}_j$ are given by (5.24), (5.25),(5.27), (5.28) *and* (5.29). *Moreover, all the eigenvalues μ_j, $j = 0, 1$, or $\mu_j^{\pm}$, $1 < j \leq \lfloor\frac{n-1}{2}\rfloor$, are $\mathcal{V}_j$-simple.C*

Proposition 5.3.2. *For n being an even number we have the following explicit formulae for the spectrum of the operator $\mathscr{L}$*

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

where

$$\begin{aligned} &\mu_0 := \boldsymbol{\alpha}_0, \quad \mu_1 := \boldsymbol{\alpha}_1, \quad \mu_r := \boldsymbol{\alpha}_r, \\ &\mu_k^{\pm} := \boldsymbol{\alpha}_k + \boldsymbol{\beta}_k \pm \sqrt{(\boldsymbol{\alpha}_k - \boldsymbol{\beta}_k)^2 + \boldsymbol{\delta}_k^2}, \quad 1 < k \leq \left\lfloor \frac{n-1}{2} \right\rfloor. \end{aligned}$$

and the coefficients $\boldsymbol{\alpha}_j$, $\boldsymbol{\beta}_j$, $\boldsymbol{\delta}_j$ are given by (5.30), (5.31),(5.32), (5.28), (5.34) *and* (5.35). *Moreover, all the eigenvalues μ_j, $j = 0, 1, r$, or $\mu_j^{\pm}$, $1 < j \leq \left\lfloor \frac{n-1}{2} \right\rfloor$, are $\mathcal{V}_j$-simple.*

5.4 Existence Result and Examples

5.4.1 Computation of the Equivariant Bifurcation Invariants

In order to describe the G-isotypical decomposition of the slice $\mathcal{S}_o$ (recall $G := D_n \times O(2)$), first, we identify the irreducible G-representations related to the isotypical decomposition of $\mathscr{W}$. 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 [3]), $j = 0, 1, \ldots, \lfloor \frac{n}{2} \rfloor$, $l = 1, 2, 3, \ldots$. The corresponding to $\mathcal{W}_{jl}$ isotypical components of $\mathscr{W}$ are

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

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

$$\gamma(z_1, z_2) := (\gamma^j \cdot z_1, \gamma^{-j} \cdot z_2),$$
$$\kappa(z_1, z_2) := (z_2, z_1),$$
$$\xi(z_1, z_1) := (\xi^l \cdot z_1, \xi^l \cdot z_2),$$
$$\boldsymbol{\kappa}(z_1, z_2) := (\overline{z}_1, \overline{z}_2),$$

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

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

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

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

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

Consequently, for $\lambda_o = \lambda_{j,l}^{\pm}$ or $\lambda_o = \lambda_{j,l}$, by applying formula (2.17), we obtain that

$$\begin{aligned}
\omega_G(\lambda_o) &= \nabla_G\text{-deg}\Big(\mathscr{A}(\lambda_-), B_1(0)\Big) - \nabla_G\text{-deg}\Big(\mathscr{A}(\lambda_+), B_1(0)\Big) \\
&= \prod_{\xi \in \sigma_-(\mathscr{A}(\lambda_-)) \cup \{\lambda_o\}} \prod_{i,k} (\text{Deg}_{\mathcal{W}_{ik}})^{m_{ik}(\xi)} - \prod_{\xi \in \sigma_-(\mathscr{A}(\lambda_-))} \prod_{i,k} (\text{Deg}_{\mathcal{W}_{ik}})^{m_{ik}(\xi)} \\
&= \prod_{\xi \in \sigma_-(\mathscr{A}(\lambda_-))} \prod_{i,k} (\text{Deg}_{\mathcal{W}_{ik}})^{m_{ik}(\xi)} * \Big(\text{Deg}_{\mathcal{W}_{jl}} - (G)\Big). \qquad (5.36)
\end{aligned}$$

Example 5.4.1. In the case of the group $G = D_6 \times O(2)$, we have the following basic degrees[2] $\text{Deg}_{\mathcal{W}_{jk}}$ (which were obtained in [43] using GAP programming)

$$\text{Deg}_{\mathcal{W}_{0,l}} = (D_6 \times O(2)) - (D_6 \times D_l),$$

[2]Let us point out that for practical applications of the gradient $D_n \times O(2)$-degree, it is fully justified (see [10]) to use is values truncated to the Burnside ring $A(D_n \times O(2))$

$$\begin{aligned}
\mathrm{Deg}_{\mathcal{W}_{1,l}} &= (D_6 \times O(2)) - ({D_6}^{\mathbb{Z}_1}\times_{D_6} D_{6l}) - ({D_2}^{D_1}\times_{\mathbb{Z}_2} D_{2l}) - ({D_2}^{\tilde{D}_1}\times_{\mathbb{Z}_2} D_{2l}) + \\
&\quad 2({D_2}^{\mathbb{Z}_1}\times_{D_2}^{\mathbb{Z}_2} D_{2l}) + ({\mathbb{Z}_2}^{\mathbb{Z}_1}\times_{\mathbb{Z}_2} D_{2l}), \\
\mathrm{Deg}_{\mathcal{W}_{2,l}} &= (D_6 \times O(2)) - ({D_6}^{\mathbb{Z}_2}\times_{D_3} D_{3l}) - ({D_2}^{\mathbb{Z}_2}\times_{\mathbb{Z}_2} D_{2l}) - (D_2 \times D_l) + \\
&\quad 2({D_2}^{\mathbb{Z}_2}\times_{D_1} D_l) + (\mathbb{Z}_2 \times D_l), \\
\mathrm{Deg}_{\mathcal{W}_{3,l}} &= (D_6 \times O(2)) - ({D_6}^{\tilde{D}_3}\times_{\mathbb{Z}_2} D_{2l}).
\end{aligned}$$

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

Theorem 5.4.2. *Under the assumptions formulated in section 3, i.e.* $\boldsymbol{\mathcal{V}} : \Omega_o' \to \mathbb{R}$ *is given by* (5.2) *and the* Γ*-symmetric equilibrium* u^o *of* $\boldsymbol{\mathcal{V}}$ *is given* (5.8)*, for every* $\lambda_o = \lambda_{jl}$*,* $0 < j \leq \lfloor \frac{n-1}{2} \rfloor$*, and* $\lambda_o = \lambda_{0,l}$*,* $\lambda_{1,l}$ *or* $\lambda_{r,l}$*there exists an orbit of bifurcating branches of nontrivial periodic solutions to* (5.14) *from the orbit* $\{\lambda_{jl}\} \times \mathfrak{G}(u^o)$*. More precisely, for every orbit type* $(H_{j,l})$ *in* D_{jl} *there exists an orbit of periodic solutions with symmetries at least* $H_{j,l}$*.*

Proof. This result is a direct consequence of the Existence Property (P1) of the gradient equivariant degree formulated in Theorem 2.6.1. □

5.4.2 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 (5.2), we put $A = 0.002205918750$, $B = 0.000004055064608$ and $\sigma = 0.35$. Therefore, we obtain that ϕ defined at (5.6) assumes its minimum at $r_0 = 1.214894009$. The distinct eigenvalues of the Hessian matrix $\nabla^2\boldsymbol{\mathcal{V}}(u^o)$ are $\mu_0 = 10.10496819$, $\mu_1 = 8.469351217$, $\mu_3 = 3.854423919$, $\mu_2^- = 6.442637681$ and $\mu_2^+ = -0.007288929$, Several values of the critical set Λ, particularly for $l = 1, 2, 3, 4$ are listed in table below.

Table 5.1. The values $\lambda_{j,l}$ in the critical set Λ

j	μ_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	1.03085168	1.37446891
3	3.854423919	0.50935463	1.01870927	1.52806390	2.03741854
2^+	6.442637681	0.62767390	1.25534781	1.88302171	2.51069561
2^-	0.007288929	11.7130006	23.4260011	35.1390017	46.8520023

One can notice that we have the following inequalities:

$$\lambda_{0,1} < \lambda_{1,1} < \lambda_{3,1} < \lambda^+_{2,1} < \lambda_{0,2} < \lambda_{1,2} < \lambda_{0,3} < \lambda_{3,2} < \lambda_{1,3} < \lambda^+_{2,2} < \lambda_{0,4} < \lambda_{1,4} < \lambda_{3,3} < \dots$$

Topological Invariants $\omega(\lambda_o)$: In the below table we list the maximal orbit types in $\mathscr{W}_{j,l} \setminus \{0\}$, $l \geq 1$:

Table 5.2. Maximal orbit types in $\mathscr{W}_{j,l}$

$\mathscr{W}_{j,l}$, $l \geq 1$	maximal orbit types
$\mathscr{W}_{0,l}$	$(D_6 \times D_l)$
$\mathscr{W}_{1l}$	$(D_6 \,{}^{\mathbb{Z}_1}\!\times_{D_6} D_{6l})$, $(D_2 \,{}^{D_1}\!\times_{\mathbb{Z}_2} D_{2l})$, $(D_2 \,{}^{\tilde{D}_1}\!\times_{\mathbb{Z}_2} D_{2l})$
$\mathscr{W}_{2,l}$	$(D_6 \,{}^{\mathbb{Z}_2}\!\times_{D_3} D_{3l})$, $(D_2 \,{}^{\mathbb{Z}_2}\!\times_{\mathbb{Z}_2} D_{2l})$, $(D_2 \times D_l)$
$\mathscr{W}_{3,l}$	$(D_6 \,{}^{\tilde{D}_3}\!\times_{\mathbb{Z}_2} D_{2l})$

Next, we list the values of the equivariant invariants $\omega(\lambda_{jl})$ (given by (5.36)):

$$\omega_G(\lambda_{0,1}) = \mathrm{Deg}_{\mathcal{W}_{0,1}} - (G)$$

$$\omega_G(\lambda_{1,1}) = \mathrm{Deg}_{\mathcal{W}_{0,1}} * (\mathrm{Deg}_{\mathcal{W}_{1,1}} - (G))$$

$$\omega_G(\lambda_{3,1}) = \mathrm{Deg}_{\mathcal{W}_{0,1}} * \mathrm{Deg}_{\mathcal{W}_{1,1}} * (\mathrm{Deg}_{\mathcal{W}_{3,1}} - (G))$$

$$\omega_G(\lambda^+_{2,1}) = \mathrm{Deg}_{\mathcal{W}_{0,1}} * \mathrm{Deg}_{\mathcal{W}_{1,1}} * \mathrm{Deg}_{\mathcal{W}_{3,1}} * (\mathrm{Deg}_{\mathcal{W}_{2,1}} - (G))$$

These sequences of equivariant invariants $\omega(\lambda_{j,l})$ can be continued indefinitely due to the the fact 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 Λ. 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 [43]). 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 ware 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^o 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 $A(D_n \times O(2))$)

$$\begin{aligned}
\omega_G(\lambda^+_{2,1}) &= \mathrm{Deg}_{\mathcal{V}_{0,1}} * \mathrm{Deg}_{\mathcal{V}_{1,1}} * \mathrm{Deg}_{\mathcal{V}_{3,1}} * (\mathrm{Deg}_{\mathcal{V}_{2,1}} - (D_6 \times O(2))) \\
&= -(D_2\, {}^{\mathbb{Z}_2}\!\times_{\mathbb{Z}_2} D_2) + (\tilde{D}_1\, {}^{\mathbb{Z}_1}\!\times_{\mathbb{Z}_2} D_2) + (D_2 \times D_1) \\
&\quad - (D_1 \times D_1) - (D_6\, {}^{\mathbb{Z}_2}\!\times_{D_3} D_3) + (\tilde{D}_3\, {}^{\mathbb{Z}_1}\!\times_{D_3} D_3) \\
&\quad + (D_3\, {}^{\mathbb{Z}_1}\!\times_{D_3} D_3) + (D_2\, {}^{\mathbb{Z}_1}\!\times^{\tilde{D}_1}_{D_2} D_2) + (D_2\, {}^{\mathbb{Z}_2}\!\times_{D_1} D_1) \\
&\quad - (D_2\, {}^{D_1}\!\times_{D_1} D_1) - (\tilde{D}_1\, {}^{\mathbb{Z}_1}\!\times_{D_1} D_1) - (D_1\, {}^{\mathbb{Z}_1}\!\times_{D_1} D_1).
\end{aligned}$$

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. In such a way, we can list some types of the branches of periodic vibrations emerging from the equilibrium u^o:

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

$\lambda_{1,1}$: 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 $(D_6\,{}^{D_6}\!\times^{\mathbb{Z}_1} D_6)$, $(D_2\,{}^{D_1}\!\times_{\mathbb{Z}_2} D_2)$, $(D_2\,{}^{\tilde{D}_1}\!\times_{\mathbb{Z}_2} D_2)$.

$\lambda_{3,1}$: For the limit period $3.20036952\,m$ there exists at least the following orbit of p-periodic vibrations with spatio-temporal symmetries at least $(D_6\,{}^{\tilde{D}_3}\!\times_{\mathbb{Z}_2} D_2)$.

$\lambda^{+}_{2,1}$: 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 $(D_6\,{}^{\mathbb{Z}_2}\!\times_{D_3} D_3)$, $(D_2\,{}^{\mathbb{Z}_2}\!\times_{\mathbb{Z}_2} D_2)$, $(D_2 \times D_1)$.

$\lambda_{1,2}$: For the limit period 1.91622311 there exist at least the following three orbits of p-periodic vibrations with spatio-temporal symmetries at least $(D_6\,{}^{\mathbb{Z}_1}\!\times_{D_6} D_{12})$, $(D_2\,{}^{D_1}\!\times_{\mathbb{Z}_2} D_4)$, $(D_2\,{}^{\tilde{D}_1}\!\times_{\mathbb{Z}_2} D_4)$.

$\lambda^{-}_{2,1}$: For the limit period 73.59495327 there exist at least the following three orbits of p-periodic vibrations with spatio-temporal symmetries at least $(D_6\,{}^{\mathbb{Z}_2}\!\times_{D_3} D_3)$, $(D_2\,{}^{\mathbb{Z}_2}\!\times_{\mathbb{Z}_2} D_2)$, $(D_2 \times D_1)$

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.

5.4.3 Numerical Simulations

In this subsection, we present some simulations of the periodic solutions predicted by our theory. On Figures 5.2–5.5. we show the periodic solutions which were found for $\lambda_0^2 = \frac{1}{\mu}$ with μ taking values near the last four eigenvalues. Figures 5.2, 5.3, 5.4, and 5.5 are the relative motions of all particles around the origin where we relocated the centers of the motions to the origin by subtracting their averages of the orbits in the horizontal and vertical directions.

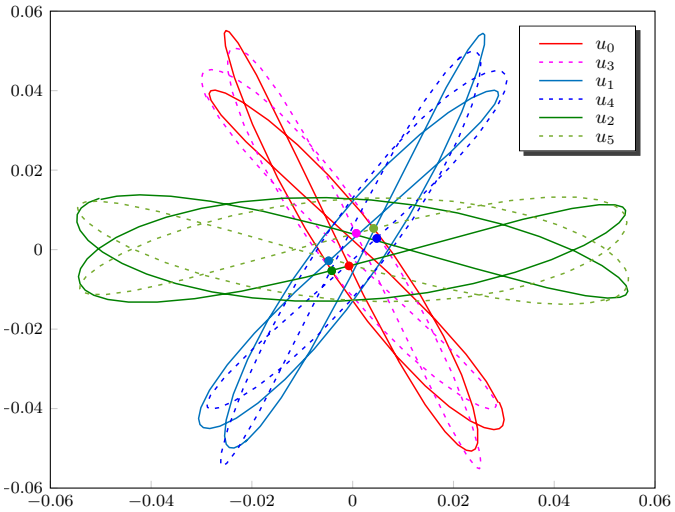


Figure 5.2. Relative motions of all 6 particles with $\lambda_0^2 = \frac{l^2}{\mu}$, $l = 1$ and μ near the eigenvalue $\mu_0 = 10.10496819$ of $\nabla^2 \boldsymbol{\mathcal{V}}(u^o)$

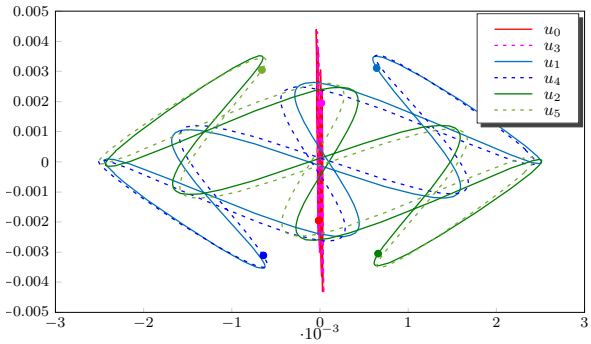


Figure 5.3. Relative motions of all particles with $\lambda_0^2 = \frac{l^2}{\mu}$, $l = 1$ and μ near the eigenvalue $\mu = 6.442637681$ of $\nabla^2 \boldsymbol{\mathcal{V}}(u^o)$

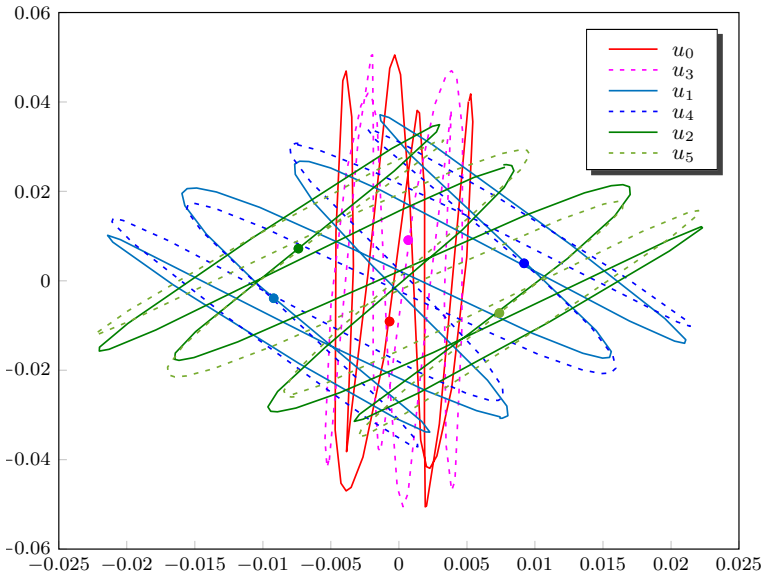


Figure 5.4. Relative motions of all particles with $\lambda_0^2 = \frac{l^2}{\mu}$, $l = 1$ and μ near the eigenvalue $\mu = 8.469351217$ of $\nabla^2 V(u^o)$

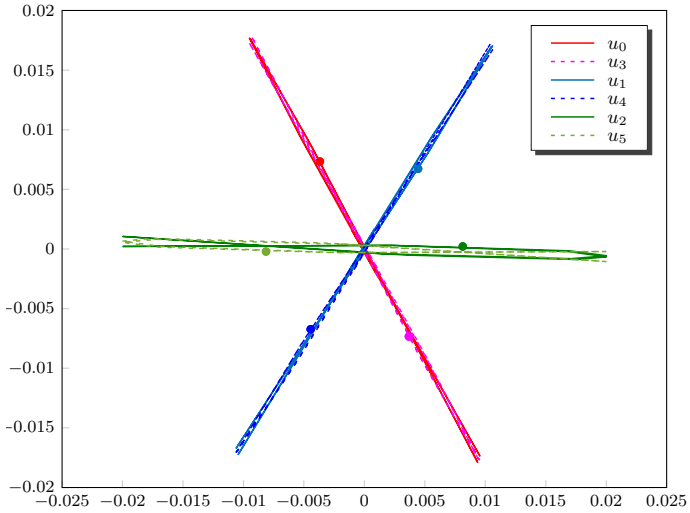


Figure 5.5. Relative motions of all particles with $\lambda_0^2 = \frac{l^2}{\mu}$, $l = 1$ and μ near the eigenvalue $\mu = 3.854423919$ of $\nabla^2 \boldsymbol{\mathcal{V}}(u^o)$

5.4.4 Concluding Remarks

In this dissertation, we analyzed a system (5.3) with n particles in the plane $\mathbb{R}^2$ admitting dihedral spatial symmetries. More precisely, we used the method of gradient equivariant degree [16, 2, 13, 35] to investigate the existence of periodic solution to (5.3), where $\boldsymbol{\mathcal{V}}$ is the Lennard-Jones and Coulomb potential, around an equilibrium admitting dihedral D_n symmetries. The dynamics of system (5.3) 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 (5.3) allowing a complete symmetric topological classification of the emanating (or bifurcating) branches of periodic solutions from a given equilibrium state. First, the critical periods $p_{jl} > 0$, which are the limit periods for those bifurcation branches can be identified from the so called *critical set* $\Lambda := \{\lambda_{jl} = \frac{l^2}{\mu_j},\ l \in \mathbb{N},\ \mu_j \in \sigma(\nabla^2\boldsymbol{\mathcal{V}}(u^o))\}$, where $\sigma(\nabla^2\boldsymbol{\mathcal{V}}(u^o))$ denotes the set of eigenvalues of the Hessian $\nabla^2\boldsymbol{\mathcal{V}}(u^o)$, and the symmetries of topologically possible solutions to (5.3) can be identified from the equivariant invariants $\omega_{\mathbf{G}}(\lambda_{jl})$. The explicitly computed Hessian $\nabla^2\boldsymbol{\mathcal{V}}(u^o)$ 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 $\nabla^2\boldsymbol{\mathcal{V}}(a)$ as a product of simple 2×2-matrices. Therefore, the spectrum $\sigma(\nabla^2\boldsymbol{\mathcal{V}}(a))$ is explicitly computed and these computations do not depend on a particular form of the potential $\boldsymbol{\mathcal{V}}$. In addition, we provided an exact formula for computation of the equivariant invariants $\omega_{\mathbf{G}}(\lambda_{jl})$. We should also mention that for larger groups D_n, the actual computations of $\omega_{\mathbf{G}}(\lambda_{jl})$ 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 [43].

We remark that elements λ_{jl} of the critical set Λ correspond to the values of transitional frequencies. The equivariant invariant $\omega_{\mathbf{G}}(\lambda_{jl})$ provides a full topological classification of symmetric modes corresponding to the branches of molecular vibrations emerging from the

equilibrium state at the critical frequency λ_{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 dissertation provides complementing results to those obtained in [15] (where the orthogonal degree for abelian actions was used).

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