Chapter 1

Vortex Analogue of Molecules

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Kelvin's theory of vortex atoms, in which Kelvin considered knotted strings as atoms, has been debunked and considered to be a failure. A theory of atoms as vortices is incapable of explaining stability and vibrational properties of atoms. With electrons representing ethereal vortices, the vortex atom theory tries to explain the relation between magnetic field and electrical current. In recent years, this simple Kelvin model has been shown to bear resemblance to the superstring theory. Although the vortex atom theory is considered to be scientifically incorrect (in the sense of its being unable to explain atomic properties), it may still be valid in a dynamical sense as for an example considered in this paper. With atomic potentials of logarithmic type, a dynamically stable vortex buckyball is 'grown' here. If stability is considered only from point of view of Huckel theory and eigenvalues of adjacency matrix, it may not be a sufficient test. It will be shown that such a vortex molecule is stable when Floquet theory of periodic orbits is used as a test of stability.

1.1 Introduction

Buckminsterfullerene, C_{60}, is a perfectly symmetrical molecule made up of 60 carbon atoms arranged in the shape of a soccer ball and resembling a geododesic dome [2]. Hexagonal and pentagonal patches on a soccer ball are sewn together such that there are exactly 60 vertices with 3 edges intersecting at each vertex. In 1996, the Nobel Prize in chemistry was awarded to Smalley, Curl and Kroto for their discovery of this molecule. Structure of C_{60} is a truncated icosahedron with carbon atoms occupying each vertex. Such a structure is obtained from an

icosahedron by truncation of each of its 12 vertices resulting in a 5-membered ring at the location of each vertex and a 6-membered ring corresponding to each icosahedral face. Icosahedral configuration itself is a fixed equilibrium configuration when each of its vertices is replaced by a vortex of strength Γ. C_{60} exhibits an unusually high stability since all its valencies are satisfied by truncated icosahedral structure. Bonding environment of each carbon atom is identical and each carbon atom is located at the intersection of two hexagons and a pentagon.

In a buckyball, double bonds connect the pentagons and each pentagonal ring is made up of single bonds. The bond lengths r_d and r_s are 1.401 and 1.458 Åwith cage radius

$$R_c = \frac{1}{2}[g^2(r_d + 2r_s)^2 + r_d^2]^{1/2} \tag{1.1}$$

g is the golden ratio [3].
For point vortex calculations, these points are projected onto a unit sphere.

The molecule is the largest possible symmetric molecule, 60 being the largest number of proper rotations in the icosahedral group which is the largest group in which symmetry operations leave a point fixed. C_{60} is a very stable molecule with a high binding energy. Regular truncated icosahedron has $r_s = r_d$ and a circumscribing (normalized) unit sphere and is one of the Archimedian solids [4]. There are four Archimedian solids with 60 vertices :

solid	v	e	f	configuration
truncated icosahedron	60	90	32	5-6-6
truncated dodecahedron	60	90	32	3-10-10
rhombicosidodecahedron	60	120	62	3-4-5-4
sunb dodecahedron	60	150	92	3-3-3-3-5

Configuration a-b-c is vertex connectivity with a, b and c-sided regular polygon in cyclic order a-b-c.

With atomic interactions of the logarithmic type, the governing Hamiltonian is

$$H = -\sum_{i<j} \Gamma_i \Gamma_j log(l_{ij}^2) \tag{1.2}$$

which is the so-called point-vortex Hamiltonian of N-vortex theory [1]. Here, l_{ij} denotes the chord distance between a particle of strength Γ_i and one with strength Γ_j, which in standard cartesian co-ordinates is

$$l_{ij}^2 = \|\vec{x}_i - \vec{x}_j\|^2 \tag{1.3}$$

The numerical integrations used in this paper were carried out using a symplectic time-splitting method based on 3-vortex integrable subclusters which suppress numerical instabilities [5], then corroborated using variable time-step Runge-Kutta methods.

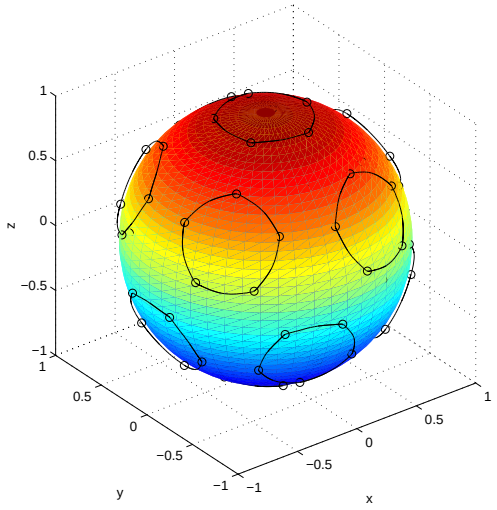

Figure 1.1: The vortex buckyball is made up of 12 clusters of 5 vortices each. A stable icosahedral equilibrium structure is formed by joining the centers of vorticity of each of the 12 clusters.

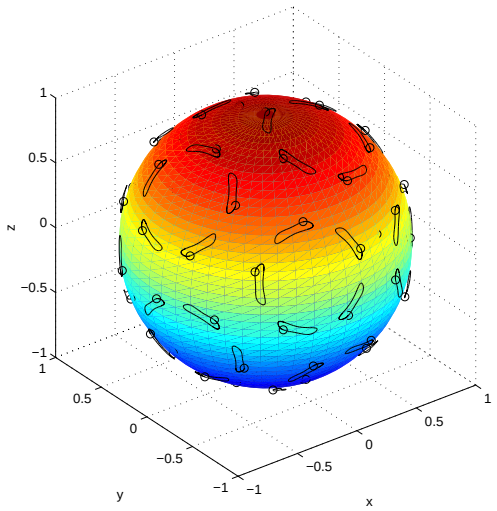

Figure 1.2: Snub Dodecahedron made up of 60 clusters each containing a single vortex.

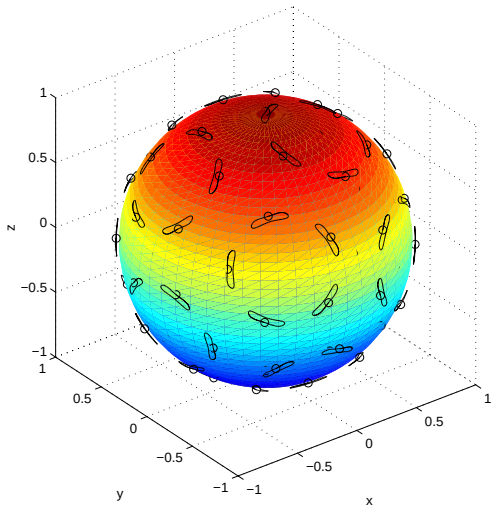

Figure 1.3: Rhombicosidodecahedron made up of 60 clusters each containing a single vortex.

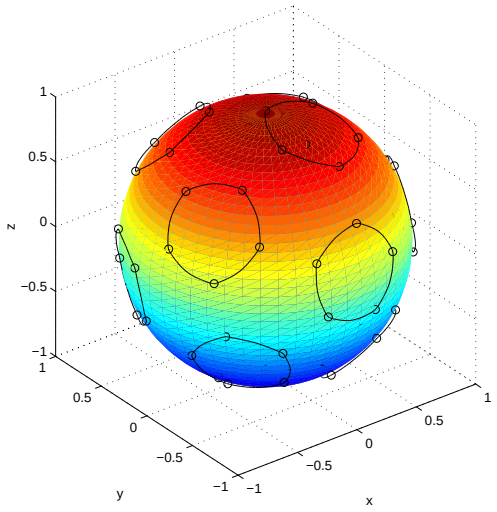

Figure 1.4: Truncated Icosahedron made up of 12 clusters of 5 vortices each.

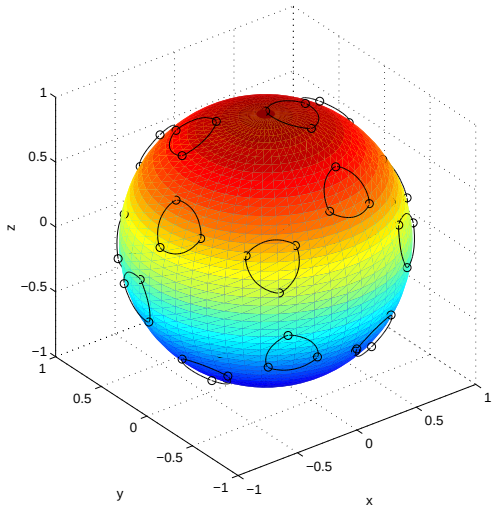

Figure 1.5: Truncated Dodecahedron made up of 20 clusters of 3 vortices each.

1.2 Clustering Dynamics

With a logarithmic Hamiltonian, the N=60 point vortex atoms associated with the Archimedean solids undergo spontaneous clustering, with each cluster undergoing periodic motion with characteristic frequencies based on the number of vortices, $m < N$, and the ring radius, r, of each cluster. Shown in figure is the vortex buckyball - 60 equal strength ($\Gamma_i = \Gamma_j$=1) particles are placed initially at the co-ordinates of bucky molecule. The vortices form 12 groups of 5 vortices each which co-orbit in periodic motion. Similar clustering occurs when vortices are placed at the vertices of the four Archimedean solids as shown in figures 2,3,4,5. The snub dodecahedron (SD) and the rhombicosidodecahedron (RI) form 60 individual clusters of one vortex per cluster; the truncated icosahedron (TI) forms 12 clusters of 5 vortices each (like the vortex buckyball); the truncated dodecahedron (TD) forms 20 clusters of 3 vortices per cluster.

Figure 6 shows the genesis of the vortex buckyball as it arises from its associated icosahedral equilibrium structure. Equal strength vortices (say 5Γ) placed at the 12 vertices of an icosahedral Platonic solid are known to form a fixed equilibrium structure [5]. Each vertex is then split into 5 equal strength vortices (Γ) along the edges of an icosahedron giving rise to 12 interacting rings of radius r with 5 vortices per ring. The ring parameter r measures the distance from equilibrium and has value $r \approx 0.34$ for the vortex buckyball.
In order to calculate the frequency associated with these periodic orbits, consider an isolated ring of m equal strength evenly spaced point vortices placed on the surface of a unit sphere at co-latitude θ. Frequency of rotation of such a

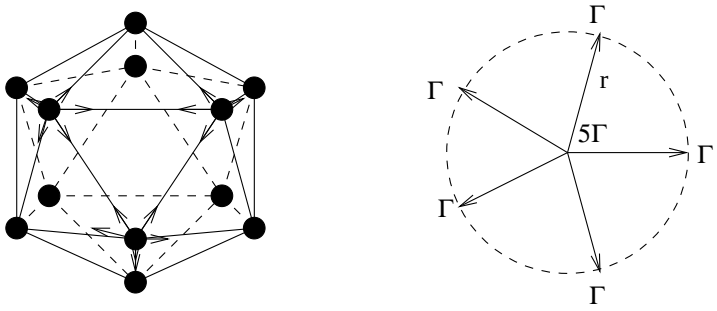

Figure 1.6: The vortex buckyball arises from splitting each of the vortices at the 12 vertices of an icosahedron into 5 equal parts along the adjacent edges. Icosahedral equilibrium structure with arrows denoting the splitting process are shown. Each vortex is split equally among the 5 edges to form a cluster of 5 co-orbiting vortices. The radius r measures the distance from equilibrium and has value r=0.34 for the vortex buckyball.

latitudinal ring can be easily calculated to be equal to

$$\omega = \frac{\cos\theta}{\sin^2\theta} \cdot \frac{(m-1)\Gamma}{2\pi} \tag{1.4}$$

with Γ being the point vortex strength. We know that the co-latitude and ring radius r are related by $\sin\theta$=r, which gives rise to the frequency-radius formula for an isolated ring of m point vortices

$$\omega = k_m \frac{\sqrt{1-r^2}}{r^2} \tag{1.5}$$

Here, k_m is a constant depending only on m. This yields

$$\left(\frac{\omega}{k_m}\right)^2 = \frac{1}{r^4} - \frac{1}{r^2} \tag{1.6}$$

for an isolated ring, shown as the dashed curve in figure 7. Also shown in this figure are the frequencies associated with the interacting clusters, with the rightmost data point representing the vortex buckyball. Assuming these 12 interacting clusters obey a similar scaling law

$$\left(\frac{\omega}{k}\right)^2 = \frac{1}{r^a} - \frac{1}{r^b} \;\; a > b \tag{1.7}$$

the 2 scaling exponents can be computed by making the following observation. If the above equation is multiplied by r^b and a new variable is defined

$$\tilde{\omega} = 1 + r^b(\omega/k)^2 \tag{1.8}$$

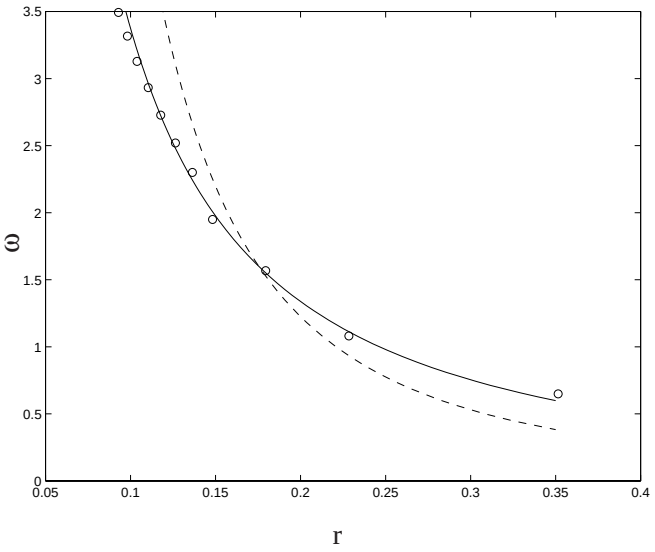

Figure 1.7: Both the dashed and the solid curves obey the formula $(\omega/k)^2 = r^{-a} - r^{-b}$. The dashed curve corresponds to an isolated ring with scaling exponents a=4, b=2 and k=0.05. The solid curve with exponents a=2.65, b=2 and k=0.16 more closely fits the data for cluster-cluster interactions.

then $\tilde{\omega}$ obeys the power law

$$\tilde{\omega} = r^{b-a} \tag{1.9}$$

Thus, if the scaling relation holds, a correct choice for exponent b will force the data (on a log-log plot) to lie with slope s, which is related to the exponents by s=b-a. From this, the remaining exponent a can be computed. The curve with exponents a=2.65 and b=2 is shown (solid) in figure 7 and the fit with the data is excellent.

1.3 Stability Theory

The Huckel molecular orbital formalism allows for quick, albeit crude electronic structure calculations, including information about molecular stability [3]. The theory is based on diagonalizing the Huckel matrix Hm

$$Hm = \beta A + \alpha I \tag{1.10}$$

with co-efficients α being a Coulomb integral and β a resonance integral. The matrix A is the adjacency matrix associated with the configuration, whose eigenvalues for the buckyball are shown in table 2. Eigenvalues of adjacency matrix are one way of chracterizing stability of a molecule. An N-vortex graph will have a size N adjacency matrix with a 1 at position (i,j) if vertices of the corresponding solid are joined by an edge, and 0 otherwise. This simple topological Huckel approach focuses on the topology of bonds which incorporates the interaction laws through co-efficients α and β.

Eigenvalues of adjacency matrix			
λ_{TI}	λ_{TD}	λ_{RI}	λ_{SD}
3 ×1	3 ×1	4 ×1	5 ×1
2.757 ×3	2.842 ×3	3.618 ×3	4.488 ×3
2.303 ×5	2.562 ×5	2.925 ×5	3.577 ×5
1.82 ×3	2.303 ×4	2.236 ×4	2.717 ×4
1.562 ×4	1.618 ×4	1.382 ×3	1.322 ×3
1 ×9	1.507 ×3	1 ×4	1.071 ×4
0.618 ×5	0 ×10	0.552 ×5	0.195 ×5
-0.139 ×3	-0.507 ×3	0 ×6	-0.285 ×5
-0.382 ×3	-0.618 ×4	-0.382 ×8	-1 ×6
-1.303 ×5	-1.303 ×4	-1 ×4	-1.252 ×3
-1.438 ×3	-1.562 ×5	-2.236 ×4	-1.507 ×4
-1.618 ×5	-1.842 ×3	-2.477 ×5	-2.136 ×5
-2 ×4	-2 ×11	-2.618 ×8	-2.28 ×4
-2.562 ×4			-2.351 ×5
-2.618 ×3			-2.558 ×3

In Huckel theory for molecular stability [2], the eigenvalues of adjacency matrix are arranged in decreasing order and conclusion of stability follows if

$$\frac{2\sum_{i=1}^{N/2}\lambda_i}{N} > 1 \tag{1.11}$$

Calculation of adjacency matrix for each of the above solids enables us to form a table as above which lists the eigenvalues for these solids in decreasing order. Adjacency matrix and eigenvalues for buckyball and truncated icosahedron are the same. Since N is same for each solid, the factor h=$\sum_{i=1}^{N/2}\lambda_i$ is an indication of how resilient the structure is.

Solid	h	Point Vortex Energy (H)	h/H
SD	55.0	65.2	0.84
RI	49.3	65.2	0.76
Bucky	46.6	65.0	0.72
TI	46.6	65.0	0.72
TD	44.5	63.3	0.70

From the table, it is immediately evident that Hamiltonian of the point vortex motion is directly proportional to the sum of eigenvalues of adjacency matrix for a given N. Moreover, if the solids are arranged in the decreasing order of distance between two adjacent vertices, l_{ij},

Solid	l_{ij}
SD	0.46
RI	0.45
Bucky	0.41
TI	0.40
TD	0.34

then too the same arrangement follows.
Stability of such a periodic orbit governed essentially by nonlinear differential equations [6]

$$\dot{\mathbf{x}} = \mathbf{f}(\mathbf{x}) \tag{1.12}$$

can be determined by linearizing it about the periodic orbit, resulting in

$$\dot{\mathbf{y}} = J(t)\,\mathbf{y} \tag{1.13}$$

with

$$J(t) = D\,\mathbf{f} \tag{1.14}$$

the 2N×2N jacobian matrix and $\mathbf{x}$(t+T)=$\mathbf{x}$(t). If Φ(t) is the fundamental matrix associated with this T-periodic system, then the 2N eigenvalues of Φ(T)

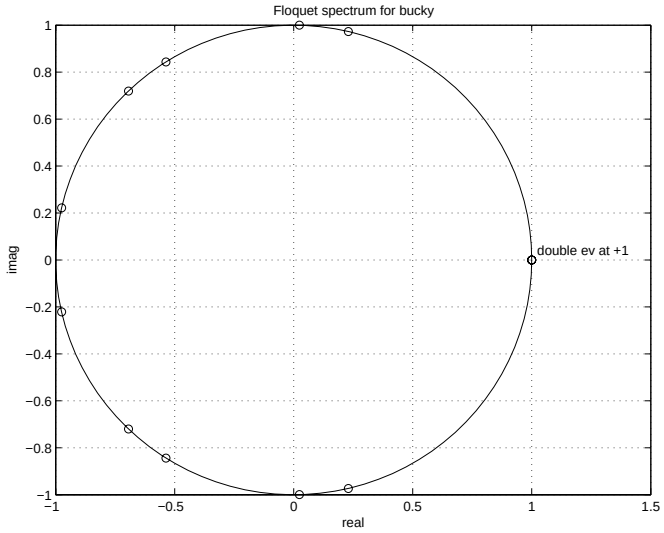

Figure 1.8: Floquet spectrum associated with the vortex buckyball lying on the unit circle. There are 10 multipliers per cluster with 12 clusters making a total of 120 multipliers.

are known as Floquet multipliers and the spectrum of eigenvalues determines linear stability of the periodic orbit. Since the system is Hamiltonian, the characterstic multipliers occur in complex conjugate pairs. All the eigenvalues lie on unit circle and the orbit is linearly stable. 10 (5 vortices with 2 multipliers per vortex) characteristic multipliers shown in figure 1.8 are for one cluster only - they are repeated for each of the 12 clusters yielding a total of 120 multipliers for the vortex buckyball. Thus, adjacency spectrum predicts stability of the truncated icosahedral state and Floquet theory shows stability of periodic orbits in the case of logarithmic interactions.

1.4 Conclusions

With logarithmic interactions, the buckyball configuration leads to periodic orbits of 12 interacting clusters with 5 vortices per cluster. The stability of these orbits is evidenced by their Floquet spectrum. The nonlinear scaling theory accurately predicts the interacting cluster frequencies through the full range of values of ring radii from the icosahedral equilibrium, r=0, to the buckyball value r=0.34. Periodic or quasi-periodic states that arise via symmetric splitting processes of the type described in this paper are generic objects that can be obtained from other regular structures such as Platonic solid equilibria or relative equilibria [5]. Asymmetric splitting processes give rise to much more complex

dynamical states whose properties are not nearly as well understood yet seem rich and well worth pursuing.

Bibliography

[1] V. Bogomolov (1977). Dynamics of vorticity at a sphere, *Fluid Dynamics* **6**, 863-870.

[2] F. Chung, S. Sternberg (1993). Mathematics and the Buckyball, *American Scientist*, Vol 81, 56-71.

[3] J. Cioslowski (1995). *Electronic structure calculations on Fullerenes and their derivatives*, Oxford University Press, Oxford.

[4] H. Coxeter (1963). *Regular polytopes*. MacMillan Co., New York.

[5] B. Khushalani (2004). Symplectic subcluster methods and periodic vortex motion on a sphere, *PhD Dissertation*, University of Southern California.

[6] K. Meyer (1999). *Periodic solutions of the N-body problem*, Springer-Verlag, New York.