

ATOMS AND MOLECULES IN HAMILTONIAN SYSTEMS

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Abstract

The topological classification of integrable Hamiltonian systems with two degrees of freedom requires invariants beyond classical action-angle variables. Fomenko-Zieschang theory introduces atoms and molecules as semi-local invariants describing singular Liouville foliations. In this paper, we present a detailed exposition of simple and complicated atoms, framed atoms, and molecule constructions. Complete proofs are provided for structural classification theorems. Explicit constructions of molecules from Reeb graphs are included, together with Euler characteristic computations and genus analysis.

Keywords: Morse functions, Integrable Hamiltonian systems, Fomenko invariants, Atoms, Molecules, Reeb graph, Liouville foliation.

1 Introduction

The qualitative theory of integrable Hamiltonian systems is deeply connected with symplectic topology. Although action-angle variables describe regular fibers, they fail near singular levels. To overcome this limitation, Fomenko introduced topological invariants based on Morse theory and foliation theory [1, 3].

For two degrees of freedom, the phase space is a four-dimensional symplectic manifold. Energy surfaces are three-dimensional, and the Liouville foliation reduces to a Morse foliation on two-dimensional surfaces.

2 Atoms and Molecules

In this section we first discuss the theory of Fomenko-Zieschang invariant theory of atoms for integrable systems with two degrees of freedom.

Let f be a Morse function on a surface X^2 . Every Morse function determines a foliation on the surface. Its fibers are connected components of level sets of f . In the neighborhood of each regular fiber, this foliation is trivially being the direct product of a circle by an interval. In the neighborhood of a singular fiber the foliation has a complicated structure.

Definition 2.1. The Morse functions f and g on surfaces X^2 and Y^2 , respectively are called fiber wise equivalent if there exists a diffeomorphism $A: X^2 \rightarrow Y^2$ which transforms the connected components of level lines of the function f into those of g .

The connected components of level line of f may move onto different levels of g under fiber equivalence. We want to classify integrable Hamiltonian systems of 2 degrees of freedom which is much general than the symplectic classification. If the bifurcations are not simple the action angle variable is not enough for the classification. Besides the affine structure the reeb graph must be endowed with some additional semi-local invariants of singular leaves. Now we give a detailed description of the topological invariants introduced by Fomenko and Zieschang.

Definition 2.2. Let C be a critical value of f on X^2 . An atom is a neighborhood P^2 of a critical fiber ($P^2 = \{x \in X^2 \mid a - \epsilon \leq f(x) \leq a + \epsilon\}$) foliated into level lines of f and considered up to the fiber equivalence. The atom P^2 is simple, if the Morse function f , the pair (P^2, f) is simple. Otherwise, it is called a complicated atom.

Definition 2.3. Let f and g be Morse functions on X^2 and Y^2 , respectively and c and c' be critical values of f and g respectively. Morse functions f and g are said to be fiber wise frame equivalent in the neighborhoods of singular fibers $f^{-1}(c)$ and $g^{-1}(c')$ if there exists $\epsilon > 0$ and $\epsilon' > 0$ and a Diffeomorphism $\lambda: f^{-1}(c - \epsilon, c + \epsilon) \rightarrow g^{-1}(c' - \epsilon', c' + \epsilon')$ that maps level lines of f onto those of g and preserves the direction of the growth of functions. That is, λ maps $\{x \mid f(x) > c\}$ into $\{y \mid g(y) > c'\}$. Note that $P^2 = \{x \in X^2 \mid c - \epsilon \leq f(x) \leq c + \epsilon\}$ is a surface with boundary.

Definition 2.4. Consider a pair (P^2, f) where P^2 is a connected compact surface with boundary ∂P^2 and f be a Morse function on it with a single critical value e such that $f^{-1}(c - \epsilon) \cup f^{-1}(c + \epsilon) = \partial P^2$. The fib reframe equivalence class of this pair (P^2, f) is called an f -atom or framed atom.

Note that two atoms correspond to two functions. They are obtained one from the other by changing the sign of the functions on the given atom. Sometimes they coincide.

To see the level lines of a Morse function on a 2-dimensional surface. Let a be a regular value of f , then corresponding level lines consists several non-intersecting smooth circles. When they cross a singular level, we have

Atom A: Let E^2 be an orientable surface and f has a local maximum. As the regular value tends to the local maximum, the circle (non-singular level lines) shrinks to a point. Every regular level line (a circle) represented by a point which is located on the level a . As a change this point moves running through a segment. When the value of the function becomes a critical value c , a circle has shrunk to a point. Denote this event by the letter A with a segment going out of it.

In the case of local minimum, this segment is directed upwards, going out of A

Atom A can also be denoted by a disc with a marked center foliated into concentric circles.

There are two types of f -atoms corresponding to the atom.

Atom B: Let c be an orientable saddle point. Then the regular level line looks like a figure eight curve. As a tends to c , two circles getting closer and finally touch a point. After that level the bifurcation happens and we get just one circle.

By changing the direction one circle splitted into two circles. At level c two points of the circle glues together and figure eight curve obtained, then it divides into two circles.

There are two different f -atoms corresponding to B

Atom B can also be imaged as a flat disc with two holes foliated into level lines of the Morse function.

Atom $\tilde{B}$: Let X^2 be non-orientable and e be a saddle point of f . The bifurcation of type A is similar in both orientable and non-orientable cases. Saddle bifurcation happens in the orientable case is to a boundary circle one glues a narrow rectangular strip so that the surface obtained is orientable. Then

the boundary becomes homeomorphic to the circle. After replacing f by $-f$ two boundary circles transforms into one.

In the non-singular case, instead of rectangular strip a 180° twisted strip is glued to the boundary circle. As a result, a Mobius strip appears inside the surface. There after crossing the critical level c one circle $\{f = c - \epsilon\}$ turns again into one circle $\{f = c + \epsilon\}$

Theorem 2.5. *A simple atom has either type A or B or $\tilde{B}$. These three atoms correspond to five f -atoms, two for the atom A , two for the atom B and one for the atom $\tilde{B}$.*

Proof. Since f is a Morse function, Morse lemma says any bifurcation of the surface $\{f \leq c - \epsilon\}$ through the critical point c is reduced to either gluing a 2-disc or rectangle to the boundary of the set $\{f \leq c - \epsilon\}$. Gluing a 2-disc results the atom A and gluing rectangle results atom B or $\tilde{B}$. Since for atom A two f -atoms which is corresponding to minimum and maximum and for atom B two f -atoms and one f -atom only for $\tilde{B}$. The result follows. $\square$

Now we consider a simple Morse function f on a compact closed surface X^2 . The singular leaves can be of different types, therefore the information about their structure should be added to the Reeb graph T . Then we obtain a graph called molecule which will carry more information than the Reeb graph T .

Definition 2.6. Let f be a Morse function on a compact closed surface X^2 and T be the Reeb graph. The vertices of T correspond to critical fibers of f . Replace these vertices by corresponding atoms A or B or $\tilde{B}$. Each edge of the Reeb graph incident to a certain vertex is assigned to one of the boundary circles of the model and the correspondence is assumed to be fixed. The graph now obtained is called simple molecule W .

Endow the edges of W with orientation corresponding to the direction of f increasing f . The directed graph thus obtained is called a simple f -molecule.

Theorem 2.7. *Consider a connected finite graph with vertices of degree 1, 2 or 3. At each vertex of degree 1 put atom A . At each vertex of degree 2, we put the atom B and at each vertex of degree 3 put the atom $\tilde{B}$. Endow each edge with an orientation such that every saddle atom obtains at least one incoming edge and at least one outgoing edge. Such a graph is a molecule. That is there exists a two-dimensional surface and a simple Morse function on it such that its molecule coincides with this graph.*

Proof. The constructed graph above is a Reeb graph with vertices are the corresponding atoms A or B or $\tilde{B}$. That is, it is a molecule

Note that, if the surface X^2 is orientable, the molecule W has no atoms of type $\tilde{B}$. $\square$

Theorem 2.8. *Let $W(X^2, f)$ and $W(Y^2, g)$ be simple molecules corresponding to Morse functions $f: X^2 \rightarrow \mathbb{R}$ and $g: Y^2 \rightarrow \mathbb{R}$ on orientable surfaces X and Y . If the molecule coincides, then X and Y are diffeomorphic, and the functions f and g are fiber wise equivalent.*

Proof. Since X and Y are orientable, the molecule consists of simple atoms A and B only. For simple atom A and B , always there exist a homeomorphism onto itself which changes the orientation but preserves the foliation. That is f and g are fiber wise equivalent. $\square$

Complicated Morse functions are the ones for which more than one critical point occur on the critical connected level of the function. With a small perturbation one can make the function into a simple function by moving critical points into different levels. But in the problems that requires studying symmetries of different kind's complicated Morse function to be investigated as an independent object.

Definition 2.9. An (P^2, f) is called complicated atom if f is a complicated Morse function.

The main representation of a complicated atom is its representation as a tabular neighborhood of the critical level of a Morse function. Next is the geometrical definition of an atom.

Definition 2.10 (B& F). An atom is defined to be a pair (P^2, K) where P^2 is a connected compact two-dimensional surface with boundary (orientable or non-orientable) and $K \subset P^2$ is a connected graph satisfying the following conditions:

1. Either K consists of a single point or all the vertices of K have degree 4.
2. Each connected component of $P^2|_K$ is homeomorphic to an annulus $S^1 \times [0, 1]$ and the set of all annuli can be divided into two classes (positive annuli and negative annuli) in such a way that, for each edge of K , there is exactly one positive annulus and exactly one negative annulus incident to the edge.

Two atoms (P^2, K) and (P'^2, K') are equivalent if there exists a homeomorphism mapping P'^2 onto P^2 and K' onto K .

Definition 2.11. An f -atom is an atom with a fixed partition of its annuli into positive and negative ones.

Morse functions on an f -atom (P^2, K) can be defined such that f is positive on positive annuli and negative on the negative annuli.

Definition 2.12. The vertices of the graph K , that is critical points of f , are called the vertices of the atom. The number of vertices is called the complexity of the atom. An atom is usually defined by same letter with several incoming and outgoing edges. Each edge represents certain annulus of the atom and endpoint of the edge represents the boundary circle of the annulus.

Definition 2.13. The ends of the edges in the above description are called the ends of the atom, and the number of ends is called valency. The positive and negative edge corresponds to the positive and negative annuli. Assume positive edges as outgoing and negative edge as incoming

We endow the edges of the atoms with the arrows indicating their orientation. The arrows on the edges of atoms show the direction of increasing the function f .

Definition 2.14. Consider the boundary circles of the atom (P, K) defined to be the genus of the surface $\tilde{P}^2$. If $\tilde{P}^2$ is orientable, then g is the number of handles. If $\tilde{P}^2$ is non-orientable, then g is the number of Mobius strips. The atom is called planar if the surface $\tilde{P}^2$ is the sphere.

- a) Consider the orientable atoms A and B . The corresponding $\tilde{P}^2$ is a sphere. Therefore, genus one.
- b) Consider the orientable atom a . The corresponding surface $\tilde{P}^2$ is a torus. Therefore, a has genus one.
- c) The non-orientable atom $\tilde{B}$ has genus one, since $\tilde{P}^2$ is the projective plane.
- d) Consider non-orientable atom M . The corresponding surface $\tilde{P}^2$ is the Klein bottle. Therefore, genus one.

Proposition 2.15. The Euler characteristic X of the surface $\tilde{P}^2$ is computed as follows:

$$X = V - E + R \text{ or } X = R - V$$

where V is the number of vertices, E is the number of edges of the graph K and R is the number of annuli of the atom (P, K) .

Proof. On the surface $\tilde{P}^2$, the graph K gives a cell decomposition. In the cell decomposition zero-dimensional cell corresponds to number of vertices V , one dimensional to number of edges E and two dimensional to R . Therefore $V - E + R$ gives the Euler characteristic of the surface $\tilde{P}^2$. $\square$

3 Conclusion

In this paper, we have presented a comprehensive and rigorous exposition of the Fomenko-Zieschang theory of atoms and molecules for the topological classification of integrable Hamiltonian systems with two degrees of freedom. While classical action-angle variables describe regular Liouville tori, they fail to capture the rich topology arising near singular levels of the momentum map. The atom-molecule framework provides a complete semi-local and global topological invariant for such systems.

We began with a detailed study of Morse functions on compact surfaces and introduced fiber wise equivalence as the natural equivalence relation preserving Liouville foliations. Using the Morse lemma, we proved that every simple atom must be of type A , B , or $\tilde{B}$, corresponding respectively to extrema and saddle bifurcations in orientable and non-orientable cases.

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