Efficient Calculation of Actions

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Abstract

We present a method to numerically calculate the action variables of a completely integrable Hamiltonian system with N degrees of freedom. It is a constructification of the Liouville-Arnol'd theorem for the existence of tori in phase space. By introducing a metric on phase space the problem of finding N independent irreducible paths on a given torus is turned into the problem of finding the lattice of zeroes of an N-periodic function. This function is constructed using the flows of all constants of motion. For $N = 2$ we use a Poincaré surface of section to scan all tori with a continuation method. As an example the energy surface in the space of action variables of a Hamiltonian showing resonances is calculated.

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1 Introduction

The Liouville-Arnol'd theorem proves that action-angle variables can always be found for completely integrable systems. In practice it can be very hard to do the necessary calculations, e.g. for the Kovalevskaya top this has not been achieved for 100 years. It might not be worth the effort doing a long analytical calculation to obtain the action-angle variables, but the energy surface in the space of action variables can be considered the most concise and comprehensive representation of the global dynamical properties of the system. We therefore want to calculate this surface by numerical methods that also work when analytical manipulations would be unmanageable.

For a system with one degree of freedom the action integral is calculated by integrating along the orbit, which is always closed if it is compact. The case $N = 2$ with compact energy surface is our main interest in this article. Systems with more than two degrees of freedom that are separable except for two freedoms can also be treated like $N = 2$. If the system is completely separable the calculations are as simple as for one freedom. For a generic integrable system with $N \geq 2$ the problem in calculating the actions is to find N independent irreducible paths around each torus. One brute force approach would be to integrate a single trajectory for a long time and then to analyze at the Fourier spectrum. We present a method that is much more efficient.

The main idea in the calculation of actions is to use the flows generated by each constant of motion. At every point these flows give a local coordinate system. The goal is to find a coordinate transformation from the local coordinate systems to one global coordinate system where each coordinate line corresponds to going around one irreducible path of the torus. The flows corresponding to these coordinate lines can be constructed from a linear combination of the original flows of the constants of motion. This combination is given by a matrix of "mixing coefficients" which have to be determined. In fact the matrix entries are the coordinates of the generating vectors of a lattice, each of its cells corresponding to one copy of the torus. The task is to find the generators of this lattice. To solve this problem numerically we introduce a metric on phase space, which allows us to construct a multiply periodic function on that lattice whose zeroes correspond to the corners of the cells. Once the lattice is determined we have: 1) A way to calculate the actions for the torus going around its irreducible paths. 2) The frequencies of the Hamiltonian flow and the winding numbers. 3) An explicit parametrization of the torus which can be used for visualization.

We proceed as follows: first we recall the definition of a completely integrable Hamiltonian system giving some intuitive interpretations. In order to introduce our method and the notation used, it is necessary to give a sketch of Arnold's proof [1] of the existence of tori for completely integrable systems (see also Ozorio de Almeida [2] whose geometric discussion inspired this work) – this is done in section 3. The method itself is then described for the general case of N freedoms and is summarized in a sketch of the algorithm. The discussion of some special features of calculating energy surfaces for $N = 2$ follows, and finally we apply our method to the Walker and Ford Hamiltonian [3] with a 2-2 resonance. For this system the actions are also calculated by standard methods and compared to our results.

Our motivation in developing this method was the study of integrable spinning tops. It is possible to analytically calculate the energy surfaces in action variables for the cases of Euler and Lagrange [4]. This has not yet been achieved for the Kovalevskaya top. We have included some illustrations from that system, but the whole picture will be presented in a forthcoming paper [5]. The complicated structure of phase space in that case deserves some special attention.

2 Completely Integrable Systems

Since our method follows the lines of the proof of the Liouville-Arnol'd theorem, we review it briefly beginning with the definition of a completely integrable system. Consider a Hamiltonian system with N degrees of freedom and canonical variables $(\boldsymbol{q}, \boldsymbol{p}) =: \boldsymbol{x}$ in phase space $\mathcal{P}$, $\dim \mathcal{P} = 2N$, with a time independent smooth Hamiltonian $H : \mathcal{P} \to \mathbf{R}$. The time development of this system is governed by the system of differential equations

$$\dot{\boldsymbol{x}} = \boldsymbol{J}\nabla H =: \boldsymbol{v}_H \qquad \text{with} \qquad \boldsymbol{J} = \begin{pmatrix} 0 & 1_N \\ -1_N & 0 \end{pmatrix}$$

where ∇ is the gradient with respect to $\boldsymbol{x}$ and 1_N the $N \times N$ identity matrix. By $\boldsymbol{v}_H$ we denote the Hamiltonian vector field and by g_H^t the corresponding flow. For any two smooth functions $F_i : \mathcal{P} \to \mathbf{R}$, $i = 1, 2$, their Poisson bracket is defined as

$$\{F_1, F_2\} := \nabla F_1 \boldsymbol{J} \nabla F_2$$

so that the time evolution of any function can be written as

$$\dot{F} = \nabla F \dot{\boldsymbol{x}} = \nabla F \boldsymbol{J} \nabla H = \{F, H\}.$$

A Hamiltonian system is completely integrable if the following conditions hold:

1. There are N smooth constants of motion F_i, i.e. $\{F_i, H\} = 0$, $i = 1, ..., N$.
2. The F_i are in involution, i.e. $\{F_i, F_j\} = 0$.
3. The F_i are independent, i.e. $\operatorname{rank}(\nabla F_1 ... \nabla F_N) = N$ almost everywhere.

A point $\boldsymbol{x}$ in $\mathcal{P}$ is called a critical point if $\operatorname{rank} \partial \boldsymbol{F}/\partial \boldsymbol{x}|_{\boldsymbol{x}} < N$ where $\boldsymbol{F} = (F_1, ..., F_N)$. The corresponding $\boldsymbol{c} = (c_1, ..., c_N) = \boldsymbol{F}(\boldsymbol{x})$ is called a critical value. The set

$$M_c := \{\boldsymbol{x} \in \mathcal{P} \mid \boldsymbol{F}(\boldsymbol{x}) = \boldsymbol{c}\}. \tag{1}$$

is a manifold if $\boldsymbol{c}$ is not critical since the tangent space of M_c then has dimension N at every point. If the ∇F_i are linearly independent, so are the $\boldsymbol{J}\nabla F_i$. As the gradient is perpendicular to M_c, and $\nabla F_i \cdot \boldsymbol{J}\nabla F_i = \{F_i, F_i\} = 0$, the N linearly independent vectors $\boldsymbol{J}\nabla F_i$ give a local coordinate system (they locally span the tangent space).

The first condition merely states that a constant of motion is to be invariant under the flow g_H^t, generated by the Hamiltonian. M_c is invariant under the flow of

H because the Hamiltonian vector field is always perpendicular to all the gradients: $\nabla F_i \cdot \boldsymbol{v}_H = \nabla F_i \boldsymbol{J} \nabla H = \{F_i, H\} = 0$ by assumption. This is a geometrical interpretation of the Poisson bracket.

The second condition requires that every constant of motion is invariant under the flow of every other one. The flow generated by F_i is denoted by g_i^t and corresponds to the vector field $\boldsymbol{v}_i := \boldsymbol{J}\nabla F_i = dg_i^t/dt|_{t=0}$. So in the above argument we can replace H by *any* other constant of motion. It turns out that this is the main ingredient of the proof and of our application to calculate actions (see figure 1 for an illustration), although it might seem strange to look at these flows because they have no physical meaning. Condition two has yet another geometrical interpretation that is just as important: the Lie bracket of any two of the above vector fields is zero, $[\boldsymbol{v}_i, \boldsymbol{v}_j] = 0$ which can be deduced from $\{F_i, F_j\} = 0$ using the Jacobi identity. Thus the flows commute, i.e. $g_i^t g_j^s = g_j^s g_i^t$ – see [1] for the details.

Finally, the third condition requires that the critical points of $\boldsymbol{F} : \mathcal{P} \to \mathbf{R}^N$ have measure zero. We already used this in order to establish that for the generic non critical case M_c is a manifold of dimension N. The condition makes sure that there are regions where M_c changes smoothly under a change of $\boldsymbol{c}$, and that action-angle variables can be defined in these regions. In general there can be an arbitrary number of disjoint component manifolds for one fixed $\boldsymbol{c}$. Even for a critical value there can exist non critical components. We shall denote a non critical connected component of M_c by M_c^0. For $N = 2$ critical components are equilibrium points, isolated periodic orbits, and separatrices. Note that a point $\boldsymbol{x}$ on a separatrix is in general not a critical point (the dimension of the tangent space is N), but there is a critical point on this component: the unstable periodic orbit. Therefore a separatrix is not a manifold.

3 Liouville-Arnol'd Theorem

The Liouville-Arnol'd theorem states:

If an integrable Hamiltonian system has a compact[1] invariant manifold M_c^0 then M_c^0 is an N-Torus T^N. There exist angle variables which trivialize the flow, and which can be found by quadratures. In a neighborhood of M_c^0 which does not contain critical points a new symplectic coordinate system – the action-angle variables – can be introduced [1, 6].

Since the constants of motion F_i are in involution all the flows g_i^t form a commutative N parameter group $G^{\mathbf{t}} := g_1^{t_1} ... g_N^{t_N}$. For every flow g_i there is a time t_i, so that $\mathbf{t} = (t_1, ..., t_N) \in \mathbf{R}^N$. The space $\mathbf{R}^N$ is now considered as a commutative group and is used to define an action on M_c^0 by

$$\begin{aligned} \mathcal{G} : \mathbf{R}^N \times M_c^0 &\to M_c^0 \\ (\mathbf{t}, x_0) &\mapsto G^{\mathbf{t}} x_0. \end{aligned}$$

As G is commutative, we can reach any point on M_c^0: since M_c^0 is a non critical component we can locally reach any point $\boldsymbol{x}_1$ in the neighborhood of $\boldsymbol{x}_0$ with say

[1] If instead of compactness completeness of the flows on M_c is assumed, one can show that instead of tori one obtains cylinders $T^k \times \mathbf{R}^{N-k}$

$G^{\mathbf{t}_1}$, using the local coordinate system generated by the flows g_i. We can do this again, starting from $\boldsymbol{x}_1$, reaching any nearby $\boldsymbol{x}_2$ with $G^{\mathbf{t}_2}$, and so on. Since G is commutative the final point then is $\boldsymbol{x} = G^{\mathbf{T}}\boldsymbol{x}_0$ where $\boldsymbol{T} = \sum \mathbf{t}_i$. The flows are complete, i.e. defined for all times, because M_c^0 is compact and non critical; therefore we can reach any point on M_c^0, and the map $\mathcal{G}(\cdot, \boldsymbol{x}_0)$ is surjective. Since M_c^0 is by assumption compact and $\mathbf{R}^N$ is not, the map can not be injective: there must be times for which the corresponding group action maps $\boldsymbol{x}_0$ onto itself. They form the so called stationary subgroup of $\mathbf{R}^N$ for any fixed $\boldsymbol{x}_0$:

$$L = \left\{ \mathbf{t} \in \mathbf{R}^N \;\middle|\; G^{\mathbf{t}}\boldsymbol{x}_0 = \boldsymbol{x}_0 \right\} \tag{2}$$

L is independent of $\boldsymbol{x}_0$ because the flows commute. Since $\dim(M_c^0) = \dim(\mathbf{R}^N) = N$ we must have $\dim(L) = 0$, thus L is a discrete subgroup of $\mathbf{R}^N$ (it is commutative since G is), and therefore it is generated by N linearly independent vectors $\mathbf{l}_i$,

$$L = \left\{ \mathbf{t} \in \mathbf{R}^N | \; \mathbf{t} = \sum m_i \mathbf{l}_i; \;\; m_i \in \mathbf{Z} \right\},$$

and forms a lattice in $\mathbf{R}^N$ since lattices are the only discrete subgroups of $\mathbf{R}^N$. To complete the proof we transform the generators $\mathbf{l}_i$ of L into the generators (unit basis vectors) $\boldsymbol{z}_i$ of $\mathbf{Z}^N$ by a linear change of coordinates:

$$\mathbf{l}_i = \boldsymbol{A}\boldsymbol{z}_i, \quad \boldsymbol{A} = (\mathbf{l}_1 ... \mathbf{l}_N) \in \mathbf{R}^{N \times N}.$$

We have thus constructed a diffeomorphism that maps the N-Torus $T^N = \mathbf{R}^N / \mathbf{Z}^N$ to M_c^0.

Less formally, the above procedure can be viewed like this: the $\mathbf{t}$ give a local coordinate system. The coordinate lines are given by the integral curves of the flows (see figure 1). Since the flows commute, almost every linear combination of them also gives a local coordinate system. These coordinate systems can be turned into a global one by making each new coordinate line close on itself. This is achieved by the above transformation matrix $\boldsymbol{A}$. Instead of $\mathbf{t}$ we use $\boldsymbol{A}^{-1}\mathbf{t}$ as coordinates. Since each new coordinate line is a circle S^1 it is natural to measure length in radians, thus introducing

$$\boldsymbol{\varphi} = 2\pi \boldsymbol{A}^{-1}\mathbf{t}$$

as new coordinates. In figure 2 the coordinate lines φ_i ($\varphi_j = \text{const}, \forall j \neq i$) are shown. Compare these to the coordinate lines t_i which are of course the solutions of our Hamiltonian equations shown in figure 1. The coordinate lines of φ_i can be viewed as a flow ϕ_i expressed in the $\mathbf{t}$ coordinates as (introducing the curve parameter τ)

$$\phi_i^\tau := G^{\boldsymbol{A}\mathbf{e}_i\tau} = G^{\mathbf{l}_i\tau} = g_1^{\tau l_{i1}} ... g_N^{\tau l_{iN}}$$

with the unit vector $\mathbf{e}_i$ in $\mathbf{R}^N$.

Every coordinate line φ_i is an irreducible path γ_i around the torus. It can be constructed by using the generators $\mathbf{l}_i$ of L which tell us which flows to integrate for what times if we are to go around M_c^0 once, and they give us N different ways to do this.

New constants of motion can now be chosen in a way that they generate the flows that evolve on the coordinate lines φ_i. These are the actions that are given by

measuring the symplectic area of the torus

$$I_i := \frac{1}{2\pi} \oint_{\gamma_i} p\, dq.$$

One usually proceeds to show that a generating function exists which achieves the transformation to these canonical variables. In our context, however, we are done. Having constructed the paths γ_i we can evaluate the path integral numerically and thus compute the actions.

On a given torus we can now express the original flows, especially the Hamiltonian flow, in the angle variables and obtain the frequencies. By definition we get the differential equation for the flow corresponding to F_i in the $\mathbf{t}$ coordinates

$$\begin{aligned} \frac{dt_j}{d\tau} &= \delta_{ij} \quad \text{with solution} \\ g_i^\tau \mathbf{t}_0 &= \mathbf{t}_0 + \mathbf{e}_i \tau. \end{aligned}$$

If we transform to angle variables we find

$$g_i^\tau \boldsymbol{\varphi}_0 = \boldsymbol{\varphi}_0 + 2\pi \boldsymbol{A}^{-1} \mathbf{e}_i \tau. \tag{3}$$

In particular we obtain for the time derivative of the angle variables generated by the Hamiltonian ($H = F_1$)

$$\dot{\boldsymbol{\varphi}} = \boldsymbol{\omega} = 2\pi \boldsymbol{A}^{-1} \mathbf{e}_1.$$

The lattice contains all the information about the frequencies. E.g. for $N = 2$ we obtain explicitly the rotation number ν

$$\nu := \frac{\omega_1}{\omega_2} = \frac{(\boldsymbol{A}^{-1})_{11}}{(\boldsymbol{A}^{-1})_{21}} = \frac{l_{22}}{-l_{12}}.$$

Besides the natural interest of physicists in frequencies they are also useful for the graphical display of the energy surface in the space of action variables, as they are by definition normal to that surface.

Note that the group action $\mathcal{G}$ defines a map from the fundamental cell to the torus and thus gives an explicitly computable parametric representation of that surface.

4 Calculating Actions

The proof shows that the problem of finding the paths is equivalent to finding generating vectors $\mathbf{l}_i$ of the lattice L in $\mathbf{t}$-space. To do so we introduce a metric d on phase space $\mathcal{P}$ and define a map D which measures the distance from $\boldsymbol{x}_0$ to $G^{\mathbf{t}}\boldsymbol{x}_0$ in phase space

$$\begin{aligned} D_{\boldsymbol{x}_0} : \mathbf{R}^N &\to \mathbf{R} \\ \mathbf{t} &\mapsto d(\boldsymbol{x}_0, G^{\mathbf{t}}\boldsymbol{x}_0) \end{aligned}$$

for any fixed $\boldsymbol{x}_0$. A Hamiltonian system does not have a natural metric associated with it in phase space. For our purpose we are free to chose any metric, e.g. the Euclidean one. By definition of L we have $D_{\boldsymbol{x}_0}(\mathbf{t}) = 0$ for $\mathbf{t} \in L$. Thus we need to

find the zeroes of $D(\mathbf{t})$ in $\mathbf{R}^N$. Since L does not depend on $\boldsymbol{x}_0$ the zeroes of D do not depend on it and we omit the index $\boldsymbol{x}_0$. We only need to find N zeroes $\mathbf{l}_i$ that are linearly independent, and form a basis of the lattice L. There are different sets of generators that produce the same lattice. All these generators can be transformed into each other via matrices from $\mathrm{SL}_N(\mathbf{Z})$, the $N \times N$ matrices with $\det = 1$ and coefficients in $\mathbf{Z}$. Any set of generators $\boldsymbol{A}$ defines a valid set of action-angle variables. Rules for the selection of a specific fundamental cell for $N = 2$ are presented in the next section.

Finding minima in N dimensions is a formidable numerical problem. We can, however, use the following simplification which reduces the computation time for the function evaluation considerably.

Consider a zero of D:

$$\begin{aligned} & 0 &=& D(\mathbf{t}) = d(\boldsymbol{x}_0, g_N^{t_N} ... g_1^{t_1} \boldsymbol{x}_0) \\ \Leftrightarrow \quad & \boldsymbol{x}_0 &=& g_N^{t_N} ... g_1^{t_1} \boldsymbol{x}_0 \\ \Leftrightarrow \quad & g_N^{-t_N} \boldsymbol{x}_0 &=& g_{N-1}^{t_{N-1}} ... g_1^{t_1} \boldsymbol{x}_0 \\ \Leftrightarrow \quad & 0 &=& d(g_N^{-t_N} \boldsymbol{x}_0, g_{N-1}^{t_{N-1}} ... g_1^{t_1} \boldsymbol{x}_0). \end{aligned}$$

For $N = 2$ this means that we integrate the flow of $F_1 = H$ forward in time, and the flow of the second constant of motion F_2 backward in time until we find an intersection of the two trajectories.

In general the function

$$D'(t_1, t_2) := d(g_N^{-t_N} \boldsymbol{x}_0, g_{N-1}^{t_{N-1}} ... g_1^{t_1} \boldsymbol{x}_0)$$

will not be periodic, but the zeroes of D' still are. D' does depend on $\boldsymbol{x}_0$ but its zeroes do not. We can picture $D'(\mathbf{t})$ as a contour plot (figure 3).

Let n be the number of points calculated by the ODE solver on a typical trajectory. By the above trick the dependence of computing time on n reduces from quadratic to linear for $N = 2$, and in general by one order.

In our implementation of the method we calculate actions not just for one, but for all tori on a given energy surface. Using a continuation method we then have a good guess for the zeroes of D'. Therefore we construct "almost angle variable type" flows $\tilde{\phi}_i$: let $\tilde{\mathbf{l}}_i = (\tilde{\mathrm{l}}_{i1}, ..., \tilde{\mathrm{l}}_{iN})^t$ be the guessed zeroes. Analogous to (3) we define

$$\begin{aligned} \tilde{\phi}_i^\tau &:= g_1^{\tau \tilde{\mathrm{l}}_{i1}} ... g_N^{\tau \tilde{\mathrm{l}}_{iN}} \quad \text{and for the vector fields} \\ \tilde{\boldsymbol{v}}_i &:= \sum_{j=1}^{N} \tilde{l}_{ij} \boldsymbol{v}_j \end{aligned}$$

If the guess is correct, i.e. $\tilde{\mathbf{l}}_i = \mathbf{l}_i$, we have $\phi_i = \tilde{\phi}_i$. The search for zeroes of D' is done by integrating the flows $\tilde{\phi}_i$. In these coordinates the zeroes are expected to be close to the corners of the unit cube in $\mathbf{R}^N$. If there is no guess available we set $\tilde{\mathbf{l}}_i = \mathbf{e}_i$ and reobtain the original flows g_i. Since $D'(\mathbf{t}) \geq 0$ always, numerically we look for the minima of $D'(\mathbf{t})$ close to zero, instead of looking for the zeroes themselves.

5 Algorithm

The central part of the numerical procedure for finding the actions, frequencies and parametrization of tori can now be summarized as follows:

1. Choose an initial condition $\boldsymbol{x}_0$ on a non critical torus.
2. Cover "time space" $\mathbf{R}^N$ by a grid $\mathbf{t}_{m_1,...,m_N} = (m_1\tau_1, ..., m_N\tau_N)$, where τ_i (> 0) is a suitable time step and $m_i = 0, 1, ..., M_i$ depending on some estimation for the maximum time necessary to integrate the flows. If there is some estimate available for the $\mathbf{l}_i$, only a grid in the neighborhood of the $\mathbf{l}_i$ is necessary.
3. By integrating the vector fields $\boldsymbol{J}\nabla F_i$, transport $\boldsymbol{x}_0$ to the phase space grid points $g_1^{m_1\tau_1}...g_1^{m_{N-1}\tau_{N-1}}\boldsymbol{x}_0$, e.g. by first generating a 1-D grid $\boldsymbol{x}_{m_1} = g_1^{m_1\tau_1}\boldsymbol{x}_0$, then generating a 2-D grid $\boldsymbol{x}_{m_1,m_2} = g_1^{m_2\tau_2}\boldsymbol{x}_{m_1}$ and so on until an (N-1)-D grid $\boldsymbol{x}_{m_1,...,m_{N-1}}$ is produced; also generate a trajectory $\boldsymbol{x}_{m_N} = g_N^{-m_N\tau_N}\boldsymbol{x}_0$.
4. Find the zeroes (minima which "are zero") of the the scalar function D' on the N dimensional grid $(\boldsymbol{x}_{m_N}, \boldsymbol{x}_{m_1,...,m_{N-1}})$. Additional intermediate points to find the zeroes with better precision are calculated, e.g., by spline interpolation.
5. Identify the generators $\mathbf{l}_i$ as the vectors which generate the lattice of zeroes of D', i.e. check that they are linearly independent and that they do not only generate a sublattice.
6. Construct the irreducible paths γ_i in phase space by integrating the vector fields $\sum_k l_{ik}\boldsymbol{J}\nabla F_k$ for time $t = 1$ with initial condition $\boldsymbol{x}_0$, and calculate the actions by numerically evaluating $\oint_{\gamma_i} p\, dq$.
7. The frequencies $\boldsymbol{\omega}$ of the Hamiltonian flow in action-angle variables can be determined by the first column of the inverse of $\boldsymbol{A} = (\mathbf{l}_1...\mathbf{l}_N)$.
8. The torus in phase space can be parametrized by using the flows $G^{\mathbf{l}_i\tau}$, $0 \leq \tau \leq 1$, using the procedure outlined in 3 (generating an N dimensional grid $\boldsymbol{x}_{m_1,...,m_N}$ instead of the $(N-1)$ dimensional one, however).
9. If desired repeat the procedure with a slightly changed parameter using a continuation method for the zeroes of D'. This might be an intrinsic parameter of the Hamiltonian, the energy or any other constant of motion. Observe that usually this implies that also x_0 has to be changed in order to keep the other constants at the same values. As described in the next section for a two degree of freedom system this could mean: keep the energy constant and change $\boldsymbol{x}_0$ in such a way that another torus with a different second constant of motion is selected.

For the integration, minimization and interpolation we use standard methods as e.g. presented in [7].

6 Calculating Energy Surfaces for $N = 2$

Once a set of linearly independent zeroes has been found, the question whether these are the "right" ones has to be addressed. This question can only be answered in a meaningful way in the context of the energy surface as a whole. We have chosen the following properties for the fundamental cell:

1. On stable isolated periodic orbits we require one action to be zero.
2. The fundamental cell varies smoothly under smooth changes of $\boldsymbol{c}$ ($\boldsymbol{c}$ non critical).
3. If there is a smooth path of non critical values of $\boldsymbol{c}$ connecting one stable periodic orbit to another we require different actions to be zero at the endpoints.

We think that these rules can be fulfilled for all energy surfaces.

What happens to the lattice, respectively the fundamental cell, at the critical values of $\boldsymbol{c}$? Near stable periodic orbits we know that the distance measured along the short path around the torus becomes zero. Thus the function D (or D') has flat valleys along the corresponding direction, and all contour lines are approximately parallel to this direction. The action corresponding to this direction should be zero.

Close to the unstable fixed points (respectively separatrices) the time of integration goes to infinity and therefore also the points on the lattice L. This corresponds to the singularity of the frequencies on the separatrix. In our numerical experiments it turned out that the lattice generators tend to infinity on a linear asymptote. The direction of this asymptote seems to be the same on both sides of the separatrix.

To calculate the energy surface of any system we have to make sure that we choose initial conditions $\boldsymbol{x}_0$ for the action calculation on every torus in $\mathcal{P}$. For systems with two degrees of freedom an efficient way to do this is to start on a Poincaré surface of section.

Assume that it is possible to find a Poincaré surface of section that contains every torus of a given energy surface. The Poincaré surface of section itself can be obtained as a contour plot of the second constant of motion restricted to the intersection of the energy surface and the Poincaré surface of section – without doing any integration. The separatrices divide the surface of section into regions. In each of these regions we can introduce a smooth set of actions (see figure 4). Define a path that transversally crosses every torus of that region. Let the path start and terminate at the periodic orbits inside or at the border of this region. Let us consider these paths as the edges of a graph. At the endpoints of each edge (i.e. at the vertices of the graph) there are stable or unstable periodic orbits. If there is a stable periodic orbit the graph has an endpoint there. If there is an unstable periodic orbit the graph has a node and can branch into any number of edges. Draw the graph in such a way that points corresponding to the same value of the second constant of motion have the same height. The graph constructed in this way is actually a topological invariant of an integrable Hamiltonian system, as is shown by Fomenko [8]. The energy surface in $\mathcal{P}$ can be pictured as the graph with a torus attached to every point of the edges. Fomenko also classifies the possible invariant sets at the

vertices of the graphs, corresponding to the critical values of $\boldsymbol{F}$. For our purposes we just use the edges of the graph to do a continuation algorithm for the actions defined in these regions.

7 An Example

In order to show the applicability of our method we have chosen a Hamiltonian showing a 2-2 resonance as described in Walker and Ford [3], which gives rise to a phase space divided by separatrices. For this system the actions and therefore the energy surfaces can be determined by other means and then compared to the results of our method.

The Hamiltonian is given by

$$H = J_1 + J_2 - J_1^2 - 3J_1J_2 + J_2^2 + \alpha J_1 J_2 \cos(2\varphi_1 - 2\varphi_2)$$

J_i and φ_i are the action-angle variables of the unperturbed system ($\alpha = 0$) and are related to Cartesian variables via

$$\begin{aligned} q_i &= \sqrt{2J_i}\cos\varphi_i \\ p_i &= -\sqrt{2J_i}\sin\varphi_i. \end{aligned}$$

We therefore only allow $J_i \geq 0$. As in the discussion of Walker and Ford the energy will be restricted to the range $0 < E < E_c$ where E_c is the lowest critical energy. Assuming that $0 \leq \alpha \leq \sqrt{5}$ we find that E_c is given by $(3+\alpha)/(13+6\alpha+\alpha^2)$. We also choose the branch of the allowed energies for which the J_i tend to zero as the energy vanishes.

With $\alpha > 0$ the J_i are no longer constants of motion. However, the system is still integrable, and in addition to the Hamiltonian the combination $I = J_1 + J_2$ is easily identified as a new constant of motion. Using a suitable canonical transformation the Hamiltonian is separable, with I already being one of the new actions. The second action can then explicitly be found by quadrature, and the integrals can be solved numerically or – after some manipulations – using elliptic integrals.

In order to employ our method we follow the program outlined above. We find that a Poincaré surface of section with $\varphi_1 = 3\pi/2$ gives a complete overview of phase space and its foliation by tori for all allowed energies (the alternative $\varphi_2 = 3\pi/2$ does not). As illustrated in figure 4, phase space is split into four regions, each of them centered around a simple stable periodic orbit. The central periodic orbit Γ_1 as well as the two (distinct) periodic orbits Γ_3, Γ_4 intersect the surface of section transversally. The fourth periodic orbit Γ_2 does not intersect transversally but lies entirely in the surface of section, it is the boundary of the energy shell in this section. The four regions around the stable periodic orbits are separated by separatrices.

In the Poincaré surface of section the critical points of the constant of motion I are given by $\nabla I = 0$ – corresponding to $\mathrm{rank}(\nabla H, \nabla I) < 2$ in phase space. In order to find the central periodic orbit and the periodic orbit on the boundary by this method we have to resort to the original variables (p_i, q_i) because the transformation from (p_i, q_i) to the action-angle variables (J_i, φ_i) is not invertible at these points. We find

the following distinct critical points

$$
\begin{aligned}
\Gamma_1 \quad &: \quad J_2 = 0 \\
\Gamma_2 \quad &: \quad 0 \le \varphi_2 < 2\pi \quad \text{(degenerated to a line)} \\
&\qquad J_2 = \frac{-1+\sqrt{1+4E}}{2} \\
\Gamma_{3,4} \quad &: \quad \varphi_2 = 0, \pi \\
&\qquad J_2 = \frac{(1+\alpha)(3+\alpha+\sqrt{9+6\alpha+\alpha^2+E(39+31\alpha+9\alpha^2+\alpha^3)})}{(39+31\alpha+9\alpha^2+\alpha^3)} \\
\Gamma_{5,6} \quad &: \quad \varphi_2 = \pi/2, 3\pi/2 \\
&\qquad J_2 = \frac{(1-\alpha)(3-\alpha+\sqrt{9-6\alpha+\alpha^2+E(39-31\alpha+9\alpha^2-\alpha^3)})}{(39-31\alpha+9\alpha^2-\alpha^3)}
\end{aligned}
$$

Γ_1, Γ_2, Γ_3 and Γ_4 are stable periodic orbits while Γ_5 and Γ_6 are unstable periodic solutions. The regions centered around Γ_3 and Γ_4 are equivalent, i.e. they contain the same type of tori and allow the introduction of the same kind of action-angle variables. In the following only one of these regions will be considered.

In order to find initial conditions on all tori we introduce three paths in the regions R_1, R_2 and R_3: $c_1 = \overline{\Gamma_5\Gamma_1}$, $c_2 = \overline{\Gamma_5\Gamma_2}$ and $c_3 = \overline{\Gamma_5\Gamma_3}$. They are not necessarily straight but have to be transversal to all tori crossed. Instead of joining the critical points themselves we may join critical points corresponding to stable periodic orbits and separatrices carrying the same critical values as the unstable periodic orbits (compare to figure 4).

For a set of initial conditions on these paths the two vector fields $v_1 = \boldsymbol{J}\nabla H$ and $v_2 = \boldsymbol{J}\nabla I$ are integrated forward and backward in time. Intersections of these trajectories are found using the Euclidean metric in the p_i, q_i variables. Note that we do not use the knowledge that I already is an action and therefore generates closed trajectories by itself. However, this effect is unavoidable for separable systems, which we need here for comparison. To illustrate the method I is treated like any other constant of motion.

Using the procedure outlined above we then determine the actions I_1 and I_2 for a given energy. Figure 5 contains the results from direct quadrature and from our method for $E = 0.2$ and $\alpha = 0.1$. For comparison the results were transformed by appropriate matrices from $\mathrm{SL}_N(\mathbf{Z})$. They agree perfectly well. Although the actions are discontinuous at the boundaries of the regions there are sum rules satisfied that can be read off the Poincaré surface of section: $I_2(\Gamma_5 \in R_2) = I_2(\Gamma_5 \in R_1) - 2I_2(\Gamma_5 \in R_3)$. In figure 5 action I_2 of region R_3 is multiplied by -2 to make this relationship more obvious. A comprehensive picture of the energy surfaces in action space for different energies and parameters is given in figure 6.

8 Conclusion

Our method is an efficient recipe to calculate action variables, frequencies and corresponding energy surfaces by purely numerical methods. Furthermore the tori of integrable systems are easily parametrized. Besides giving the correct results for the

trivial example of a separable system, it has also proved to be applicable to the complicated case of Kovalevskaya's top; the results will be published in a forthcoming paper [5].

Currently we have implemented the algorithm for the case of two degrees of freedom, a third degree of freedom is allowed if one variable is cyclic and the corresponding constant of motion is an action. The algorithm is easily extended to the truly three degree of freedom case, although with a significant increase in computing time for the generation of irreducible paths. Also the one dimensional scan of the tori, which corresponds to scanning the values of the second constant of motion in the different regions, becomes a two dimensional scan in the two constants of motion.

In the current state a good knowledge of the bifurcations in phase space (e.g. in the form of Fomenko's graphs) has to be supplied. Future work is directed towards the complete automation of the method in the sense that for two degrees of freedom the Fomenko graph corresponding to the system is generated numerically. Complicated phase space topologies could then be identified and analyzed. The method can then be applied as a black box function to experimentally relevant systems, and e.g. serve as a basis for the calculation of energy levels in a semiclassical approximation.

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Figure 1: This figure (as well as figures 2 and 3) has been obtained from the Kovalevskaya top. It shows projections of the flows of the Hamiltonian (left) and the Kovalevskaya constant of motion (right) covering the same torus. The orbits can also be viewed as the coordinate lines of the (t_K, t_H) coordinates on the torus. Obviously they do not generate a global coordinate system, although the flows are in this case almost "orthogonal" on the torus. Expressing these flows by linear combinations of the ones shown in figure 2 means a transformation to action-angle variables. See figure 3 for the preimages of these lines in $\mathbf{R}^2$.

Figure 2: The same torus as shown in figure 1 – using the same projection – covered by a grid of coordinate lines of the angle variables. 10 coordinate lines of φ_1 (left) and 30 coordinate lines for φ_2 (right) are shown. These coordinate lines can also be viewed as the orbits of a flow given by a linear combination of the flows shown in figure 1. We determine angle variables and thus actions by numerically calculating this transformation. See figure 3 for the preimages of these lines in $\mathbf{R}^2$.

Figure 3: The function D' on (t_K, t_H)-space as a contour plot. Note that the zeroes form a periodic lattice L while the function itself is only "almost periodic". $\mathcal{G}$ maps the fundamental region indicated onto the torus. The lattice corresponds to the torus shown in figures 1 and 2. Two corners of the fundamental cell give the transformation from $\mathbf{t}$ to $\boldsymbol{\varphi}$ coordinates. The orbits (respectively coordinate lines) t_i shown in figure 1 correspond to the t_K- and t_H- axis of this picture. The coordinate lines φ_i (respectively orbits) shown in figure 2 correspond to lines parallel to the edges of the fundamental parallelogram.

Figure 4: The Poincaré surface of section of the Walker and Ford Hamiltonian, with coordinates (q_2, p_2) corresponding to (φ_2, J_2) for energy $E = 0.2$ and $\alpha = 0.1$. The separatrices and the critical points Γ_i are shown. The pictures of the energy surfaces (figure 6) are obtained by scanning the paths c_i in the regions R_i as indicated. We have chosen c_1 and c_2 as described in the text. c_3, however, is chosen differently: it connects Γ_3 and the separatrix, thereby crossing all tori in region R_3 transversally. On the right the corresponding Fomenko graph is shown.

Figure 5: The energy surface of the Walker and Ford Hamiltonian for $E = 0.2$ and $\alpha = 0.1$. The results of a standard (circles) and our computational method (crosses) are both shown. The three pieces of the energy surface correspond to the three regions R_i.

Figure 6: The energy surfaces of the Walker and Ford Hamiltonian for an energy range 0.01 to 0.22 in steps of 0.01. Figure a) shows the unperturbed case, $\alpha = 0$ – the energy surface is smooth. For b) $\alpha = 0.1$ is chosen. As in figure 5 each energy surface is split in three pieces.