Efficient calculation of actions

H R Dullin† and A Wittek‡

Institut für Theoretische Physik, Universität Bremen, Postfach 330440, 28344 Bremen, Germany

Abstract. We present a method to calculate numerically the action variables of a completely integrable Hamiltonian system with N degrees of freedom. It is a construction 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 zeros of an N-periodic function. This function is constructed using the flows of all constants of motion. Using the fact that neighbouring tori and their irreducible paths are related by some continuous deformation, a continuation method is constructed which allows a systematic scan of the actions. For $N = 2$ we use a Poincaré surface of section to define paths which cross neighbouring tori. Close to isolated periodic orbits the generators are either constructed explicitly or their asymptotic behaviour is given. As an example, the energy surface in the space of action variables of a Hamiltonian showing resonances is calculated.

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 which 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 a compact energy surface is our main interest in this paper. 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 $N \geqslant 2$ the problem in calculating the actions is to find N independent irreducible paths around each torus. In the past some numerical algorithms have been devised which try to determine these paths for $N = 2, 3$ using phase-space projections or Poincaré surfaces of section which work for Liouville tori as well as for KAM tori (see, for example, Noid and Marcus [10] or Knudson and Noid [11]). We present a method which is much more efficient for integrable systems and also works for any number of degrees of freedom.

† E-mail address: hdullin@theo.physik.uni-bremen.de
‡ E-mail address: awittek@theo.physik.uni-bremen.de

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 zeros correspond to the corners of the cells. Once the lattice is determined, we have (i) a way to calculate the actions for the torus going around its irreducible paths, (ii) the frequencies of the Hamiltonian flow and the winding numbers, and (iii) 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. 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 the energy surfaces of integrable spinning tops. For the cases of Euler and Lagrange this has been done analytically [4]. For the Kovalevskaya top this task is considerably more difficult. We have included some illustrations from that system, to which the method has been successfully applied, but the whole picture is presented in [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 $(q, p) =: x$ in phase space $\mathcal{P}$, $\dim \mathcal{P} = 2N$, with a time-independent smooth Hamiltonian $H : \mathcal{P} \to \mathbb{R}$. The time development of this system is governed by the system of differential equations

$$\dot{x} = J\nabla H =: v_{\mathrm{H}} \qquad \text{with} \quad J = \begin{pmatrix} 0 & 1_N \\ -1_N & 0 \end{pmatrix} \tag{1}$$

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

$$\{F_1, F_2\} := \nabla F_1 J \nabla F_2 \tag{2}$$

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

$$\dot{F} = \nabla F \dot{x} = \nabla F J \nabla H = \{F, H\}. \tag{3}$$

A Hamiltonian system is completely integrable if the following conditions hold.
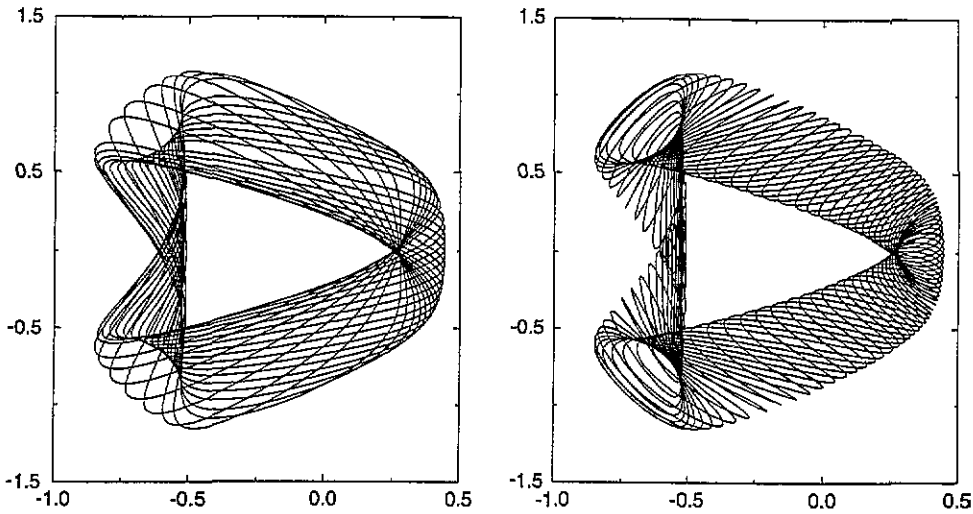
Figure 1. This figure (as well as figures 2 and 3) has been obtained from the Kovalevskaya top. It shows projections of the flows of the Hamiltonian (left) and the Kovalevskaya constant of motion (right) covering the same torus. The orbits can also be viewed as the coordinate lines of the (t_K, t_H) 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 corresponds to a transformation to action-angle variables. See figure 3 for the preimages of these lines in $\mathbb{R}^2$.

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

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

$$M_c := \{x \in \mathcal{P} \mid F(x) = c\} \tag{4}$$

is a manifold if 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 $J\nabla F_i$. As the gradient is perpendicular to M_c, and $\nabla F_i \cdot J\nabla F_i = \{F_i, F_i\} = 0$, the N linearly independent vectors $J\nabla F_i$ 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: $\nabla F_i \cdot v_H = \nabla F_i J\nabla H = \{F_i, H\} = 0$ 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 $v_i := J\nabla F_i = \mathrm{d}g_i^t/\mathrm{d}t|_{t=0}$. 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 (ii) has yet another geometrical interpretation that is just as important: the Lie bracket of any two of the above vector fields is zero, $[v_i, v_j] = 0$, 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 details.

Finally, the third condition requires that the critical points of $F : \mathcal{P} \to \mathbb{R}^N$ have measure zero. We have 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 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 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 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† 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 neighbourhood 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 $G^t := g_1^{t_1} \dots g_N^{t_N}$. For every flow g_i there is a time t_i, so that $t = (t_1, \dots, t_N) \in \mathbb{R}^N$. The space $\mathbb{R}^N$ is now considered as a commutative group and is used to define an action on M_c^0 by

$$
\begin{aligned}
&\mathcal{G} : \mathbb{R}^N \times M_c^0 \to M_c^0 \\
&(t, x_0) \mapsto G^t x_0 .
\end{aligned}
\tag{5}
$$

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 x_1 in the neighbourhood of x_0 with say G^{t_1}, using the local coordinate system generated by the flows g_i. We can do this again, starting from x_1, reaching any nearby x_2 with G^{t_2}, and so on. Since G is commutative the final point then is $x = G^T x_0$, where $T = \sum t_i$. 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 $\mathcal{G}(\cdot, x_0)$ is surjective. Since M_c^0 is by assumption compact and $\mathbb{R}^N$ is not, the map cannot be injective: there must be times for which the corresponding group action maps x_0 onto itself. They form the so-called stationary subgroup of $\mathbb{R}^N$ for any fixed x_0,

$$
L = \left\{ t \in \mathbb{R}^N \mid G^t x_0 = x_0 \right\}
\tag{6}
$$

where L is independent of x_0 because the flows commute. Since $\dim(M_c^0) = \dim(\mathbb{R}^N) = N$ we must have $\dim(L) = 0$, thus L is a discrete subgroup of $\mathbb{R}^N$ (it is commutative since G is), and therefore it is generated by N linearly independent vectors l_i,

$$
L = \left\{ t \in \mathbb{R}^N \mid t = \sum m_i l_i; \ m_i \in \mathbb{Z} \right\}
\tag{7}
$$

† If, instead of compactness, completeness of the flows on M_c is assumed, one can show that, instead of tori, one obtains cylinders $T^k \times \mathbb{R}^{N-k}$.
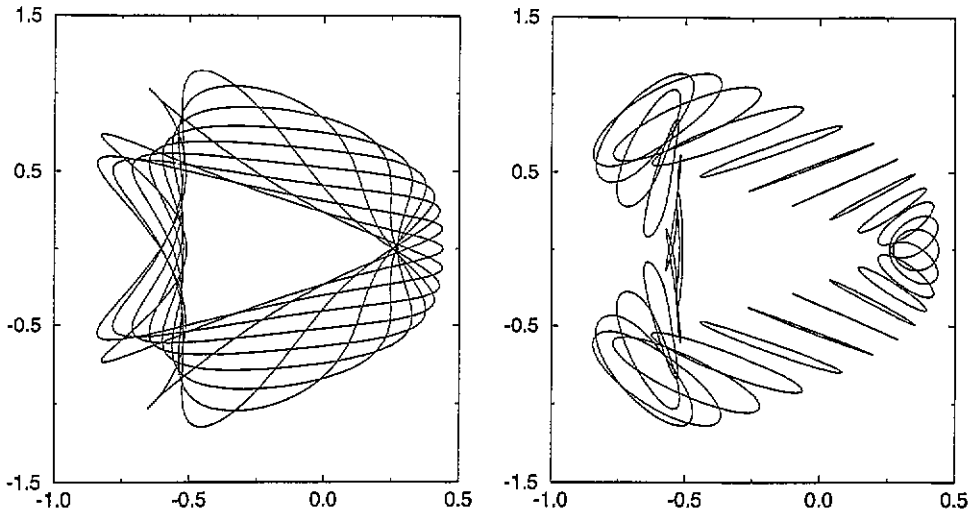
Figure 2. The same torus as shown in figure 1—using the same projection—covered by a grid of coordinate lines of the angle variables: 10 coordinate lines of φ_1 (left) and 30 coordinate lines for φ_2 (right) are shown. These coordinate lines can also be viewed as the orbits of a flow given by a linear 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 $\mathbb{R}^2$.

and forms a lattice in $\mathbb{R}^N$ since lattices are the only discrete subgroups of $\mathbb{R}^N$. To complete the proof we transform the generators l_i of L into the generators (unit basis vectors) z_i of $\mathbb{Z}^N$ by a linear change of coordinates,

$$l_i = A z_i \qquad A = (l_1 \ldots l_N) \in \mathbb{R}^{N \times N} . \tag{8}$$

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

Less formally, the above procedure can be viewed like this: the 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 A. Instead of t we use $A^{-1}t$ as coordinates. Since each new coordinate line is a circle S^1, it is natural to measure length in radians, thus introducing

$$\varphi = 2\pi A^{-1} t \tag{9}$$

as new coordinates. In figure 2 the coordinate lines φ_i ($\varphi_j = $ constant, $\forall j \neq i$) 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 t coordinates as (introducing the curve parameter τ)

$$\phi_i^\tau := G^{A e_i \tau} = G^{l_i \tau} = g_1^{\tau l_{i1}} \cdots g_N^{\tau l_{iN}} \tag{10}$$

with the unit vector e_i in $\mathbb{R}^N$.

Every coordinate line φ_i is an irreducible path γ_i around the torus. It can be constructed by using the generators 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

$$I_i := \frac{1}{2\pi} \oint_{\gamma_i} p \, dq . \tag{11}$$

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 t coordinates

$$\frac{dt_j}{d\tau} = \delta_{ij} \qquad \text{with solution} \quad g_i^\tau t_0 = t_0 + e_i \tau . \tag{12}$$

If we transform to angle variables we find

$$g_i^\tau \varphi_0 = \varphi_0 + 2\pi A^{-1} e_i \tau . \tag{13}$$

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

$$\dot{\varphi} = \omega = 2\pi A^{-1} e_1 . \tag{14}$$

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

$$\nu := \frac{\omega_1}{\omega_2} = \frac{(A^{-1})_{11}}{(A^{-1})_{21}} = \frac{l_{22}}{-l_{12}} . \tag{15}$$

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 l_i of the lattice L in 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 x_0 to $G^t x_0$ in phase space

$$\begin{aligned} D_{x_0} &: \mathbb{R}^N \to \mathbb{R} \\ t &\mapsto d(x_0, G^t x_0) \end{aligned} \tag{16}$$

for any fixed 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 $D_{x_0}(t) = 0$ for $t \in L$. Thus we need to find the zeros of $D(t)$ in $\mathbb{R}^N$. Since L does not depend on x_0, the zeros of D do not depend on it and we omit the index x_0. We only need to find N zeros 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 $SL_N(\mathbb{Z})$, the $N \times N$ matrices with det $= 1$ and coefficients in $\mathbb{Z}$.

Any set of generators A defines a valid set of action-angle variables. Some possible 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:

$$
\begin{aligned}
0 \qquad &= D(t) = d(x_0, g_N^{t_N} \dots g_1^{t_1} x_0) \\
\Leftrightarrow x_0 \qquad &= g_N^{t_N} \dots g_1^{t_1} x_0 \\
\Leftrightarrow g_N^{-t_N} x_0 &= g_{N-1}^{t_{N-1}} \dots g_1^{t_1} x_0 \\
\Leftrightarrow 0 \qquad &= d(g_N^{-t_N} x_0, g_{N-1}^{t_{N-1}} \dots g_1^{t_1} x_0) .
\end{aligned}
\tag{17}
$$

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

$$
D'(t_1, t_2) := d(g_N^{-t_N} x_0, g_{N-1}^{t_{N-1}} \dots g_1^{t_1} x_0)
\tag{18}
$$

will not be periodic, but the zeros of D' still are. D' does depend on x_0 but its zeros do not. For $N = 2$ we can picture $D'(t)$ 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 practice we are interested in the action integrals not only for one torus but for a family of neighbouring tori which is obtained by varying some of the values of the integrals without crossing any critical values and thereby continuously deforming the torus. A typical example would be to keep the energy fixed and generate an $N - 1$ parameter family of tori by changing the values of the remaining integrals. The energy surface can then be obtained numerically in terms of the action variables.

We use the following continuation method: given a set of fundamental paths $\{l_i\}$ of one torus Γ, where the base $x_0 \in \Gamma$ was used for the determination of the paths, we seek the new paths $\{l'_i\}$ on a neighbouring torus Γ' which are determined using the base $x'_0 = x_0 + \delta x_0$ with δx_0 small. The two tori, as well as the paths, will be related to each other by some continuous deformation.

For a particular time vector $l \in \{l_i\}$ we want to compute $l' = l + \Delta t$ such that $G^{l'} x'_0 = x'_0$. Defining $y = G^l x'_0$ we find as the determining equation for Δt

$$
G^{-\Delta t} x'_0 = y
\tag{19}
$$

with $|\Delta t|$ minimal. Interpreting the difference $\Delta y := y - x'_0$ as a vector in tangent space at x'_0 we can approximate for δx_0 small (and therefore also Δt small) (equation (19)) up to first order in Δt by

$$
M \, \Delta t \approx -\Delta y
\tag{20}
$$

where $M = (v_1, \dots, v_N)|_{x'_0}$ is an $2N \times N$ matrix whose columns are the vector fields at x'_0. Of course equation (20) cannot be solved exactly since the system of equations is overdetermined and usually Δy is not a vector in the tangent space at x'_0. We therefore use singular value decomposition as an approximate solution scheme which yields the best approximate solution for Δt, i.e. $|M \, \Delta t + \Delta y| = \min$ (see for instance [7]).
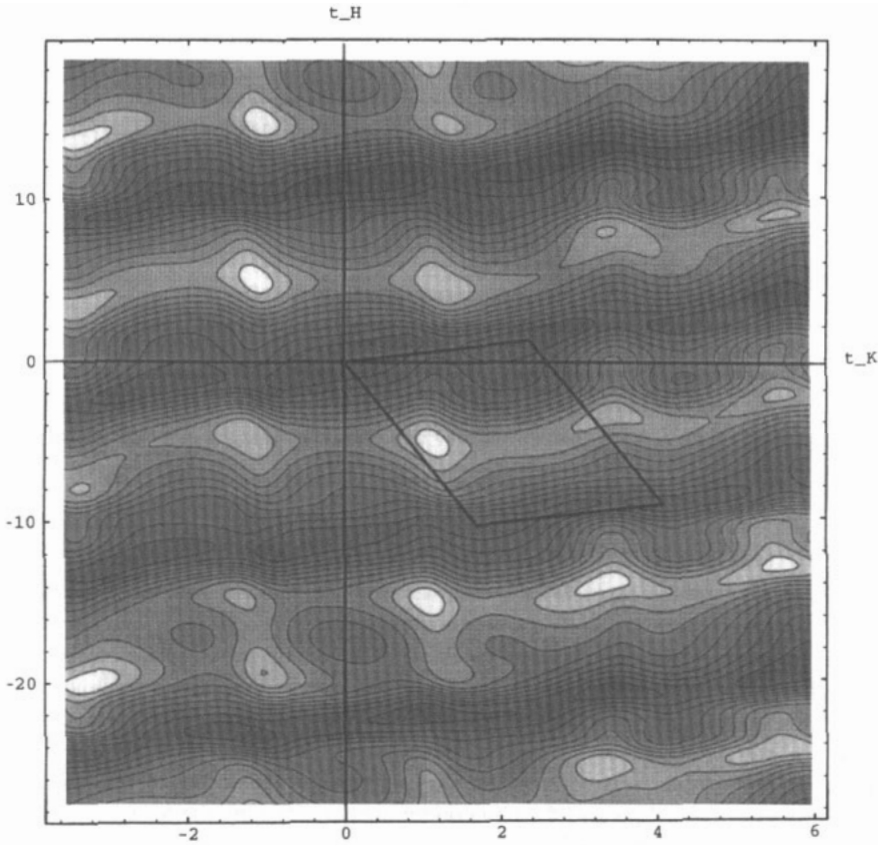
Figure 3. The function D' on (t_K, t_H)-space as a contour plot. Note that the zeros form a periodic lattice L while the function itself is only 'almost periodic'. $\mathcal{G}$ maps the fundamental region indicated onto the torus. The lattice corresponds to the torus shown in figures 1 and 2. Two corners of the fundamental cell give the transformation from t to φ 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.

We can now construct a Newton-type iteration scheme to determine the exact Δt numerically. Explicitly

(0) $x'_0 = x_0 + \delta x_0$, $n = 0$, $\Delta t_0 = 0$, $M = (v_1, \ldots, v_N)|_{x'_0}$

(i) $y_{n+1} = G^{l + \Delta t_n} x'_0$

(ii) $\Delta y_{n+1} = y_{n+1} - x'_0$

(iii) 'solve' $M \Delta t_{n+1} = -\Delta y_{n+1}$

(iv) continue with step (i) until $|\Delta y_{n+1}|$ or $|\Delta t_{n+1}|$ is less than some predefined value.

By construction, the points y_n stay on the invariant torus, which is specified by x'_0, and the scheme will converge onto the correct Δt if δx_0 is chosen small enough. We therefore control the method by choosing δx_0 appropriately. Consider

$$\delta \tilde{x} \approx \left(\frac{\partial}{\partial x_0} (G^l x_0) \, \delta x_0 \right) \tag{21}$$

where $\frac{\partial}{\partial x_0}(G^l x_0)$ is the Jacobian matrix of the flow map which is obtained by solving the variational equation,

$$\frac{\mathrm{d}}{\mathrm{d}\tau}\left(\frac{\partial}{\partial x_0}x(\tau)\right) = \left(\frac{\partial}{\partial x}\left(\sum_i l_i v_i\right)\right)\bigg|_{x=x(\tau)}\left(\frac{\partial}{\partial x_0}x(\tau)\right) \qquad \tau \in [0, 1] \tag{22}$$

where

$$x(\tau) = G^{l\tau}x_0. \tag{23}$$

With the approximation $\Delta x_0 \approx \delta\tilde{x}_0 - \delta x_0$ we can solve (20) in order to find some first estimate for Δt_0 used in the iteration scheme. Since only linear equations are involved we can easily control the magnitude of the changes Δy and Δt_0 by adjusting the norm of δx_0.

5. Calculating energy surfaces for $N = 2$

We restrict the discussion to the case of $N = 2$, considering one of the integrals to be the energy which is held constant at a non-critical value. The goal is to determine the energy surface in terms of action variables.

To calculate the energy surface of any system we have to make sure that we choose initial conditions 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
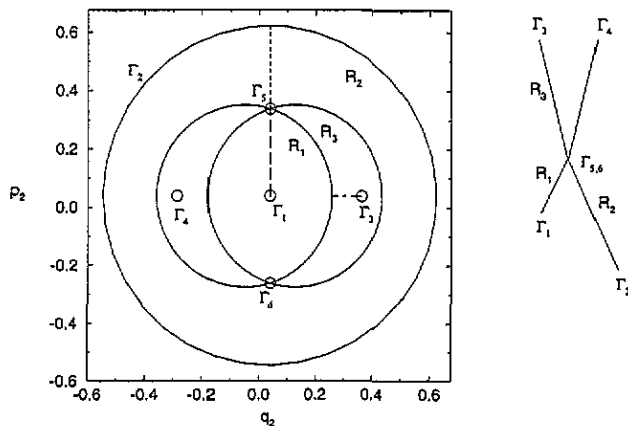
Figure 4. The Poincaré surface of section of the Walker and Ford Hamiltonian, with coordinates (q_2, p_2) corresponding to (φ_2, J_2) for energy $E = 0.2$ and $\alpha = 0.1$. The separatrices and the critical points Γ_i are shown. The pictures of the energy surfaces (figure 6) are obtained by scanning 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.

vertices of the graph) there are stable or unstable periodic orbits. If there is a stable periodic orbit then the graph has an endpoint there. If there is an unstable periodic orbit then 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, 9]. 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 F. In general, they can only be of the following types: stable periodic orbits (minimax circles), minimax tori, unstable periodic orbits (orientable or non-orientable saddles) or minimax Klein bottles. Fomenko shows this assuming the integrals to be so-called Bott integrals, i.e. the critical points of the integrals form non-degenerate critical smooth submanifolds of the energy surface. We will also assume this in the following. For the determination of the actions we use paths in the Poincaré surface of section which are equivalent to the edges of the graphs for the continuation method described in the previous section.

In order to start the continuation algorithm we need two time vectors l_1 and l_2 which generate the fundamental lattice for one torus on each edge. On a given Liouville torus these generators are only defined up to some linear transformation from $SL_N(\mathbb{Z})$. This is reflected by the fact that action-angle variables are not defined uniquely. We are therefore free to use any two generating vectors found by the method described in the previous section. The obtained actions can then later be transformed via some matrix from $SL_N(\mathbb{Z})$ to some more suitable form.

Often we can do better than this, however. The energy surface around stable periodic orbits looks like a full torus ($D^2 \times S^1$) which is foliated by the Liouville tori. One fundamental path around such a torus can therefore be chosen in such a way that it lies in a plane locally normal to the periodic orbit and collapses onto a point when the torus is 'deformed' into the periodic orbit. This allows a unique definition of that path.

A stable periodic orbit γ is a critical manifold. Therefore there exist some λ_H, λ_K such that

$$v := \lambda_H v_H + \lambda_K v_K = 0 \tag{24}$$

on γ, where v_H and v_K are the vector fields corresponding to the Hamiltonian and the second constant of motion, respectively. In a small neighbourhood of $x^* \in \gamma$, v is approximately given by its linearization at x^*, i.e. by $((\partial/\partial x)v)|_{x^*}$. Two of the eigenvalues of $((\partial/\partial x)v)|_{x^*}$ are 0 (corresponding to eigenvectors parallel to v_H and parallel to ∇H) and two are purely imaginary ($\pm i\omega$—corresponding to the flow on the torus). For a torus close to γ which has a base point $x_0 = x^* + \delta x$, where δx is a real valued combination of the complex eigenvectors, we therefore find that to first order in $|\delta x|$ one of the generators is given by

$$l_1 = (2\pi \lambda_H/\omega, 2\pi \lambda_K/\omega) \qquad \text{with} \quad G^{l_1} x_0 = x_0. \tag{25}$$

The other generator cannot uniquely be defined like this, therefore we use the following method. Determine the simple period of the periodic orbit, i.e. determine the minimal $T > 0$ in $g_H^T x^* = x^*$. Then compute the eigenvalues of the Jacobian of the linearized flow $(\partial/\partial x^*)(g_H^T x^*)$. Two of them are equal to 1, the other two are complex conjugated lying on the unit circle ($\alpha_1 = \exp(i\tilde{\omega})$, $\alpha_2 = \exp(-i\tilde{\omega})$). Now using the results for the first path, choose t such that $(\tilde{\omega} + t\omega) \bmod 2\pi = 0$. The second generator for the base x_0 is then given by

$$l_2 = (T + t\lambda_H, t\lambda_K) \qquad \text{with} \quad G^{l_2} x_0 = x_0. \tag{26}$$

For unstable periodic orbits the situation is different. A path which locally lies in a plane normal to the periodic orbit γ is difficult to construct explicitly, because it will approximately follow the separatrix and the length of its generator will depend on global information. As before, there exist numbers λ_H, λ_K such that $v := \lambda_H v_H + \lambda_K v_K = 0$ on γ. The relevant eigenvalues of the linearized vector field at $x^* \in \gamma$ are real, i.e. $\pm\beta$. As the torus gets closer to the separatrix we therefore expect a logarithmic divergence of the generator for a path normal to the periodic orbit:

$$l_1 = (t_H, t_K) \rightarrow (\lambda_H t, \lambda_K t) \qquad t \rightarrow \infty. \tag{27}$$

The asymptotic behaviour in the plane (t_H, t_K) is therefore given by the slope $t_K/t_H = \lambda_K/\lambda_H$. Choosing the generator with this asymptotic behaviour also ensures that the symplectic area enclosed by the path stays finite. A path which has a component parallel to the periodic orbit would yield, as a limiting behaviour, a path which follows the periodic orbit a number of times n, where n goes to infinity as the periodic orbit is approached.

The second generator can be constructed such that its corresponding path smoothly approaches the periodic orbit as the torus approaches the separatrix. In the case of a non-orientable saddle the path actually provides a double covering of the periodic orbit because the periodic orbit is inverse hyperbolic. As in the case of a stable periodic orbit we determine the simple period T of the periodic orbit (in case of a non-orientable saddle we have to take twice the period). Compute the eigenvalues of the linearized flow map; the relevant ones will be $\alpha_1 = \exp(\tilde{\beta})$ and $\alpha_2 = \exp(-\tilde{\beta})$. The second generator is then given by

$$l_2 = (T - \lambda_H \tilde{\beta}/\beta, -\lambda_K \tilde{\beta}/\beta). \tag{28}$$

This construction ensures that the fundamental paths can be 'continuously' deformed across separatrices (the first one only in its asymptotic behaviour, though). It also naturally produces a singularity in the frequencies, one of them approaching zero as the torus approaches the separatrix.

Because the constructions of the generators are only valid in some possibly small neighbourhood of the periodic orbits, the iteration scheme of the previous section should be applied to correct the results to their proper values. Often the Fomenko graph will have a stable periodic orbit on one end of an edge and an unstable periodic orbit on the other end. One usually has to decide which set of generators or which particular combination to use because, in general, the two sets do not have to agree on both vertices. For example, in our numerical studies it often happened that the path transverse to the stable periodic orbit transformed into the path approaching the separatrix and the path parallel to the unstable periodic orbit became a path parallel to the stable periodic orbit. This resembles the behaviour one would expect interpreting the structures one sees in a Poincaré surface of section naively.

The above method of choosing the fundamental cells also agrees with an intuitive picture one has in mind when defining action variables. We would like to define action variables in such a way that one of the actions vanishes on a stable periodic orbit. In case the energy surface contains only two stable periodic orbits as critical manifolds, which, for example, happens when the low-energy limit corresponds to a system of two harmonic oscillators, one of the action variables should vanish on one periodic orbit and the other one should do so on the other periodic orbits. The generators are uniquely defined by this choice and also serve as a natural starting point when the energy is changed.

6. 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

$$H = J_1 + J_2 - J_1^2 - 3J_1 J_2 + J_2^2 + \alpha J_1 J_2 \cos(2\varphi_1 - 2\varphi_2) \tag{29}$$

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

$$q_i = \sqrt{2J_i} \cos \varphi_i \qquad p_i = -\sqrt{2J_i} \sin \varphi_i . \tag{30}$$

Therefore we only allow $J_i \geqslant 0$. 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 $0 \leqslant \alpha \leqslant \sqrt{5}$, 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 be found explicitly 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 centred 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:

$\Gamma_1 : \ J_2 = 0$

$\Gamma_2 : \ 0 \leqslant \varphi_2 < 2\pi \quad$ (degenerated to a line)

$$J_2 = \frac{-1 + \sqrt{1 + 4E}}{2}$$

$\Gamma_{3,4} : \varphi_2 = 0, \pi$

$$J_2 = \frac{(1 + \alpha)(3 + \alpha + \sqrt{9 + 6\alpha + \alpha^2 + E(39 + 31\alpha + 9\alpha^2 + \alpha^3)})}{(39 + 31\alpha + 9\alpha^2 + \alpha^3)} \tag{31}$$

$\Gamma_{5,6} : \varphi_2 = \pi/2, 3\pi/2$

$$J_2 = \frac{(1 - \alpha)(3 - \alpha + \sqrt{9 - 6\alpha + \alpha^2 + E(39 - 31\alpha + 9\alpha^2 - \alpha^3)})}{(39 - 31\alpha + 9\alpha^2 - \alpha^3)}$$

where 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 centred around Γ_3 and Γ_4 are equivalent, i.e. they contain the same
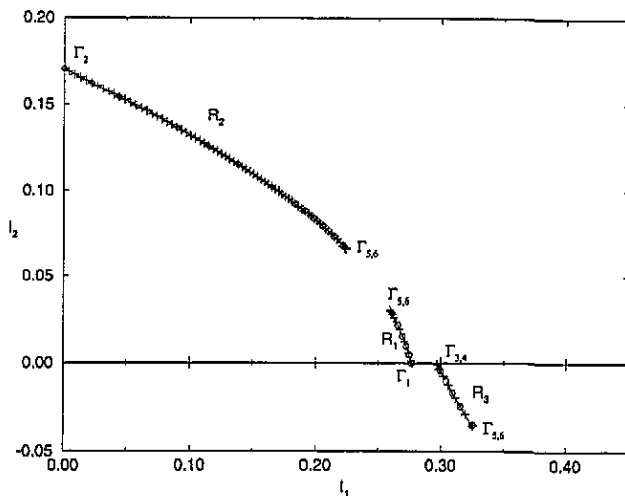
Figure 5. The energy surface of the Walker and Ford Hamiltonian for $E = 0.2$ and $\alpha = 0.1$. The results of a standard (circles) and our computational method (crosses) are both shown. The three pieces of the energy surface correspond to the three regions R_i.
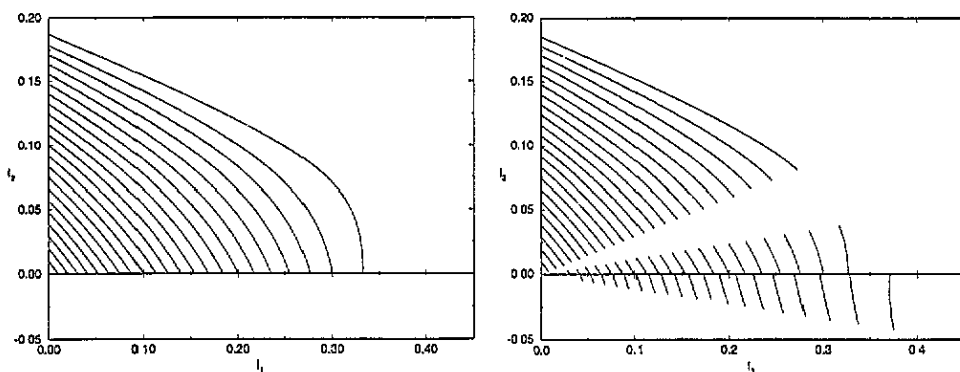

Figure 6. The energy surfaces of the Walker and Ford Hamiltonian for an energy range 0.01 to 0.22 in steps of 0.01. Figure (a) shows the unperturbed case, $\alpha = 0$—the energy surface is smooth. For (b), $\alpha = 0.1$ is chosen. As in figure 5, each energy surface is split in three pieces.

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).

Using the procedures outlined above we then determine the actions I_1 and I_2 for a given energy. For convergence criteria in phase space we use the Euclidean metric in the p_i, q_i variables. Note that we do not use the knowledge that I is already 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.

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

$SL_N(\mathbb{Z})$. 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.

7. Conclusion and outlook

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 [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 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 analysed. The method can then be applied as a black-box function to experimentally relevant systems, and, for example, serve as a basis for the calculation of energy levels in a semiclassical approximation.

Acknowledgment

References

[1] Arnol'd V I 1978 *Mathematical Methods of Classical Mechanics* (New York: Springer)
[2] de Almeida A M O 1988 *Hamiltonian Systems: Chaos and Quantization* (Cambridge: Cambridge University Press)
[3] Walker G H and Ford J 1969 *Phys. Rev.* **188** 416
[4] Richter P H 1990 Die Theorie des Kreisels in Bildern *Institut für Dynamische Systeme report* 226 (Universität Bremen)
[5] Dullin H R, Juhnke M and Richter P H 1994 The Energy Surfaces of the Kovalevskaya Top *Int. J. Bifurcation Chaos* to appear
[6] Abraham R and Marsden J E 1978 *Foundations of Mechanics* (Reading, MA: Benjamin)
[7] Press W H, Flannery B P, Teukolsky S A and Vetterling W T 1988 *Numerical Recipes in C* (Cambridge: Cambridge University Press)
[8] Fomenko A T 1991 *Topological Classification of Integrable Systems* ed A T Fomenko (Providence, RI: American Mathematical Society)
[9] Fomenko A T 1991 *The Geometry of Hamiltonian Systems* ed T Ratiu (New York: Springer)
[10] Noid D W and Marcus R A 1977 *J. Chem. Phys.* **67** 559
[11] Knudson S K and Noid D W 1988 *Chem. Phys. Lett.* **145** 16