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A Code to Compute the Action-Angle Transformation for a Particle in an Arbitrary Potential Well*

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Abstract

For a Vlasov treatment of longitudinal stability under an arbitrary wake field, with the solution of the Haïssinski equation as the unperturbed distribution, it is important to have the action-angle transformation for the distorted potential well in a convenient form. We have written a code that gives the transformation $q, p \to J, \phi$, with $q(J, \phi)$ as a Fourier series in ϕ, the Fourier coefficients and the Hamiltonian $H(J)$ being spline functions of J in C^2 (having continuous second derivatives).

I. The Canonical Transformation

We suppose that the Hamiltonian has the form

$$H = \frac{p^2}{2} + V(q), \tag{1}$$

where $V(q)$ is a potential well with continuous derivative. We discuss only values of the constant H such that the motion consists entirely of oscillations between two turning points at which $p = 0$. We denote the turning points by q_0 and q_1, with $q_0 < q_1$, and exclude values of H for which either $V'(q_0)$ or $V'(q_1)$ is zero. We define

$$p(q, H) = \pm\sqrt{2[H - V(q)]}, \tag{2}$$

where $p > 0$ as q moves from q_0 to q_1, and $p < 0$ as it returns from q_1 to q_0. The action integral, which extends over a full period of the motion, is

$$J(H) = \frac{1}{2\pi}\oint p(q, H)dq = \frac{1}{\pi}\int_{q_0}^{q_1} p(q, H)dq. \tag{3}$$

Thanks to our assumption that $V'(q_i) \neq 0$, there is a well-defined inverse function $H(J)$.

Hamilton's equations imply that $p = dq/dt$. If $t = 0$ at $q = q_1$, the time t for displacement q is

$$t = \int_{q_1}^{q} \frac{dq'}{p(q', H)} \tag{4}$$

where the integration path is understood to follow all oscillations that occur by time t: $q_1 \longrightarrow q_0 \longrightarrow q_1 \longrightarrow \cdots \longrightarrow q(t)$. Since H depends only on J, Hamilton's equations in action-angle variables give $\Phi = \Phi_0 + H'(J)t$. Choosing $\Phi(q_1) = 0$, we have

$$\Phi(q, H) = H'(J(H))\int_{q_1}^{q} \frac{dq'}{p(q', H)} \tag{5}$$

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We wish to find the functions $q(J, \Phi)$, $p(J, \Phi)$, and $H(J)$ in a form that will be convenient for repeated and fast numerical evaluations, with 2π-periodicity in Φ guaranteed. We also want these functions to have continuous second derivatives in both variables. These requirements arise from an intended application in solutions of the Vlasov equation with Fokker-Plank term, as discussed below. A convenient expression of the functions is

$$q(J, \Phi) = \sum_{m=0}^{\infty} q_m(J)\cos m\Phi \tag{6}$$

$$p(J, \Phi) = \frac{\partial q(J, \Phi)}{\partial \Phi} H'(J) \tag{7}$$

with $q_m(J)$ and $H(J)$ expanded in terms of some C^2 basis functions $B_k(J)$ and $C_k(J)$:

$$q_m(J) = \sum_k q_{mk} B_k(J) \tag{8}$$

$$H(J) = \sum_k h_k C_k(J) \tag{9}$$

The formula (7) follows from the derivative of (5) with respect to Φ, if we recall that H is only a function of J when written in action-angle coordinates.

If the series (6), (8), and (9) are truncated at a finite number of terms, the resulting transformation $J, \Phi \longrightarrow q, p$ will not be precisely canonical (i.e., symplectic). A measure of symplecticity is the agreement of p as given in (7) with

$$p(J, \Phi) = \pm\sqrt{2[H(J) - V(q(J, \Phi))]}. \tag{10}$$

If p is given by (10), a calculation of the Poisson bracket yields

$$[q, p] = \frac{1}{p}\frac{\partial q}{\partial \Phi}\frac{dH}{dJ}. \tag{11}$$

Thus, if p from (7) agrees with p from (10), we have a canonical transformation, since $[q, p] = 1$. With a moderate number of terms in the series (6), (8), and (9), the transformation can be made to satisfy the canonical condition with sufficient precision for our purposes.

II. The Primary Integrations

We first evaluate the integrals (3) and (5) on a regular mesh in H: $\{H_i | i = 1, \ldots, K\}$. The turning points $q_0(H_i)$ and $q_1(H_i)$ are easily found by a Newton iteration. The factor $H'(J(H_i))$ is defined at each i by

$$\pi = H'(J(H_i))\int_{q_1}^{q_0} \frac{dq}{p(q, H_i)}. \tag{12}$$

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For numerical integration, it is useful to change the variable to

$$u = \cos^{-1} \frac{q_1 + q_0 - 2q}{q_0 - q_1}. \tag{13}$$

The inverse of this transformation is

$$q = \frac{q_0 + q_1}{2} + \frac{q_1 - q_0}{2} \cos u. \tag{14}$$

Then (5) becomes

$$\Phi(q, H_i) = \frac{q_1 - q_0}{2} H'(J(H_i)) \int_0^{u(q)} \frac{\sin u'\, du'}{\sqrt{2[H_i - V(q(u'))]}}. \tag{15}$$

The integrand is now free of singularities. For a nearly quadratic potential, Φ is close to u. The same change of variable is used to compute $J(H_i)$ by (3).

Now $u = \pi$ corresponds to $q = q_0$. We divide the interval $[0, \pi]$ into N intervals, and integrate by Simpson's rule [1]. The first and last intervals are treated by an open Newton-Cotes formula [1], to avoid taking the limit of the integrand at the endpoints. We evaluate the integrand (15) for upper limit u at all of the mesh points u_i. The value of N is increased until the integral on $[0, \pi]$ converges to machine precision.

III. Finding the Fourier Coefficients

After the integrations, the angles $\Phi^{(j)} = \Phi(q(u_j), H_i)$ are known, with the u_j on a large regular mesh of $N + 1$ points. To evaluate the Fourier coefficients q_m for $|m| \leq M$, we search through the $\Phi^{(j)}$ to find those that are closest to the points one would normally use in a discrete Fourier transform, namely the points

$$\frac{\pi k}{M}, \qquad k = 0, \ldots, M. \tag{16}$$

Denoting those angles by Φ_k, and the corresponding values of $q(u_j)$ by $q^{(k)}$, we solve the following linear equations for the Fourier coefficients:

$$q^{(k)} = \sum_{m=0}^{M} q_m \cos m\Phi_k, \qquad k = 0, \ldots, M \tag{17}$$

We solve this system as follows: if we assume that the function $q(\phi)$ can be expressed exactly as

$$q(\phi) = \sum_{m=0}^{M} q_m \cos m\phi, \tag{18}$$

then we can write $q(\Phi_k)$ in terms of the values $x_k = q(\pi k/M)$ as

$$\begin{aligned} q(\Phi_k) = \frac{1}{2M} \Bigg\{ & x_0 \cot \frac{\Phi_k}{2} \sin M\Phi_k \\ & + x_M \cot \frac{\Phi_k - \pi}{2} \sin M(\Phi_k - \pi) \\ & + \sum_{n=1}^{M-1} x_n \frac{\sin \Phi_k}{\sin(\Phi_k + \pi k/M)} \frac{\sin M(\Phi_k - \pi k/M)}{\sin[(\Phi_k - \pi k/M)/2]} \Bigg\} \end{aligned} \tag{19}$$

This linear system can then be solved for the x_k, the function values at the mesh points. The discrete Fourier transform of the x_k then gives the coefficients q_m. The advantage of this is that the system (19) is very well conditioned if the Φ_k are close to the mesh points (16); this is why we chose the mesh points Φ_k as described above.

The system (17) can also be solved as a Vandermonde system. There are $O(n^2)$ direct methods for solving such a system which should work very well [2].

IV. Expressing the Transformation as a Function of J

Let $q_m^{(i)}$ and $J^{(i)}$ denote the values of q_m and J at $H = H_i$, as determined by the procedure just described. To get the required functions of J, we invoke the expansions (8) and (9), and determine the coefficients by solving the linear systems

$$\begin{aligned} q_m^{(i)} &= \sum_k q_{mk} B_k(J^{(i)}) && (20) \\ H^{(i)} &= \sum_k h_k C_k(J^{(i)}), && (21) \end{aligned}$$

where $i = 1, \ldots, K$. A possible improvement is to use the values of $H'(J^{(i)})$ as determined in (12) for an additional constraint on the function $H(J)$. One would then use a larger set of basis functions C_k, and augment (21) with the additional equations

$$H'(J^{(i)}) = \sum_k h_k C'_k(J^{(i)}), \qquad i = 1, \ldots, K \tag{22}$$

This step should make the whole scheme more self-consistent, and could be quite worthwhile.

V. Example

We have written a code which finds the transformation described for an arbitrary differentiable potential V. It computes the transformation from $J = 0$ (which is found by finding the minimum of the potential) up through the J corresponding to a given value of H. The basis functions B_j and C_j are both taken to be B-Splines [3] in $\sqrt{J}$, whose knots t_i are chosen to be

$$\begin{aligned} t_0 &= \cdots = t_{k-1} = 0 && (23) \\ t_{i+k} &= \frac{1}{k-1} \sum_{j=i+1}^{i+k-1} \sqrt{J^{(i)}} \quad i = 0, \ldots, n-k-1 && (24) \\ t_n &= \cdots = t_{n+k-1} = \sqrt{J^{(n-1)}} && (25) \end{aligned}$$

as described on pp. 218-9 of [3]. The code computes q_m for $m \leq M$ for a given integer M. We do not use the data for $H'(J^{(i)})$ as described above.

We take as an example the potential $V(q) = 1 - \cos q$. We know the transformation for this potential:

$$J = \frac{8}{\pi} \left[\frac{H}{2} K\left(\frac{H}{2}\right) - K\left(\frac{H}{2}\right) + E\left(\frac{H}{2}\right) \right] \tag{26}$$

$$\Phi = \begin{cases} \frac{\pi}{2}\left\{1 - \frac{F(\sin^{-1}[\sqrt{H/2}\sin q/2]|H/2)}{K(H/2)}\right\} & p < 0 \\ \frac{\pi}{2}\left\{\frac{F(\sin^{-1}[\sqrt{H/2}\sin q/2]|H/2)}{K(H/2)} - 1\right\} & p > 0. \end{cases} \quad (27)$$

Here F and K are elliptic integrals [4].

We will check the accuracy of our transformation by computing q and H on a uniform mesh in J of $10K$ points and a uniform mesh in Φ of $10M$ points (excluding $\Phi = 0$ and $\Phi = \pi$). First, we compute $H(J)$ at each J mesh point, then substitute that value in Eq. (26) and compare to the original J. We give the maximum value of $\Delta J = |J(H(J_i)) - J_i|/J_i$ in table I. Next, we take $H(J_i)$

M	K	ΔJ	$\Delta\Phi$	ϵ_S
4	8	2×10^{-5}	8×10^{-4}	4×10^{-3}
4	16	6×10^{-7}	8×10^{-4}	3×10^{-3}
4	32	2×10^{-8}	8×10^{-4}	3×10^{-3}
4	64	8×10^{-10}	8×10^{-4}	3×10^{-3}
4	128	2×10^{-11}	8×10^{-4}	3×10^{-3}
8	8	2×10^{-5}	8×10^{-4}	2×10^{-2}
8	16	6×10^{-7}	4×10^{-5}	9×10^{-4}
8	32	2×10^{-8}	2×10^{-6}	3×10^{-5}
8	64	8×10^{-10}	8×10^{-7}	7×10^{-6}
8	128	2×10^{-11}	8×10^{-7}	7×10^{-6}
16	8	2×10^{-5}	2×10^{-3}	1×10^{-1}
16	16	6×10^{-7}	2×10^{-5}	1×10^{-3}
16	32	2×10^{-8}	5×10^{-7}	2×10^{-5}
16	64	8×10^{-10}	9×10^{-9}	5×10^{-7}
16	128	2×10^{-11}	5×10^{-10}	8×10^{-9}

Table I

Accuracy of the transformation. Quartic B-splines are used throughout. Maximum value of H is 1.

and $q(J_i, \Phi_j)$ on the grid described and compute Φ using Eq. (27) for each of these values. These results are then compared to the original Φ. We record the maximum value of $\Delta\Phi = |\Phi(H(J_i), q(J_i, \Phi_j)) - \Phi_j|$ in the second column of table I. Finally, we check the symplecticity of the resulting transformation by computing

$$\epsilon_S = \left| \frac{\frac{\partial q}{\partial \Phi}\frac{dH}{dJ}}{\sqrt{2[H - V(q)]}} - 1 \right| \quad (28)$$

for values where neither the square root nor $\partial q/\partial\Phi$ is zero. The maximum value of this is recorded in the third column of table I.

VI. Conclusion

We have described a method for determining a transformation of a one-dimensional system described by a Hamiltonian of the form (1) to action-angle variables. A computer program to implement this method has been written, and gives satisfactory results regarding convergence.

We note that this method can be applied even to a $V(q)$ which is only given at a finite number of points q_i. We simply define $V(q)$ to be a function which passes through these values. Any interpolation method may be used to define such a $V(q)$.

This work was motivated by the desire to give a more thorough treatment of the Vlasov equation for longitudinal instabilities, along the lines followed by Oide and Yokoya [5]. These authors linearize the Vlasov equation about the stationary distribution derived from the Haïssinski equation, and then use the action-angle variables J, Φ of the "distorted potential well" implied by that distribution. The perturbed distribution function $\Psi_1(J, \Phi)$ is represented as a Fourier series in Φ with the coefficients being step functions in J. The step function technique has some deficiencies. It gives at best slow convergence as the steps are refined, and makes it difficult to treat the Fokker-Planck term, $-2\delta(\partial/\partial p)(p\Psi_1 + \partial\Psi_1/\partial p)$. We think that it would be better to use a C^2 spline basis for the J dependence of Ψ_1. Then the Fokker-Planck term can be handled easily with the help of our Fourier series (6) for q, since $\partial/\partial p = -(\partial q/\partial J)(\partial/\partial\Phi) + (\partial q/\partial\Phi)(\partial/\partial J)$. Oide's rough treatment of the Fokker-Planck term by a perturbative method suggests that it is very important in determining thresholds of instabilities.

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