INVARIANT SURFACES AND TRACKING BY THE HAMILTON-JACOBI METHOD[†]

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INTRODUCTION

Methods of nonlinear mechanics based on infinite expansions, such as perturbation theory and the Lie-algebraic method, are very cumbersome when carried to high orders. A promising alternative is based on iterative numerical solution of the Hamilton-Jacobi equation.[1,2] In this approach, every iteration is the same calculation, which is not much more complicated than lowest order perturbation theory.

In previous work[1] we applied the Hamilton-Jacobi method to model problems displaying generic difficulties of nonlinear mechanics. Results concerning accuracy and convergence were encouraging, even in difficult regions of phase space close to the onset of chaos. Furthermore, we formulated a criterion for the onset of chaos, and verified its utility in a two-resonance model.

Here we illustrate the method for a model of betatron motion in one degree of freedom, namely, an harmonic oscillator perturbed by a lattice of sextupoles. We obtain invariant surfaces in phase space and also finite time symplectic maps for tracking of single particles. The results indicate that the method will be effective in a full treatment with two degrees of freedom, including arbitrary lattice functions and dispersion.

We anticipate that the method will be useful in lattice design, since it provides a convenient and accurate way of assessing the effect of all resonances up to rather high orders. It could be incorporated in an optimization program, with the goal of determining nonlinear elements so as to eliminate distortions of invariant curves.

HAMILTON-JACOBI EQUATION IN TERMS OF FOURIER AMPLITUDES

In angle-action variables (ϕ, J) of the unperturbed problem, our Hamiltonian has the form

$$H(\phi, J, \theta) = \nu J + f(\theta) U(\phi, J), \tag{1}$$

$$U(\phi, J) = J^{\frac{3}{2}} \cos^3 \phi, \tag{2}$$

where θ, the azimuthal location of a particle, is the independent variable and $f(\theta) = f(\theta + 2\pi)$ consists of a series of rectangular steps, each giving the location, extent, and strength of a sextupole. The unperturbed tune is ν, and normalized Cartesian phase space coordinates are $x = J^{\frac{1}{2}} \cos \phi$, $p = J^{\frac{1}{2}} \sin \phi$.

We seek a canonical transformation $(\phi, J) \mapsto (\psi, K)$ such that the transformed Hamiltonian depends at most on the new action K. The transformation is described by a generating function $F_2(\phi, K, \theta) = \phi K + G(\phi, K, \theta)$ such that

$$\psi = \phi + G_K(\phi, K, \theta), \tag{3}$$

$$J = K + G_\phi(\phi, K, \theta), \tag{4}$$

where subscripts indicate partial derivatives. The Hamilton-Jacobi equation is the requirement that the new Hamiltonian

indeed depend only on K:

$$H(\phi, K + G_\phi, \theta) + G_\theta = H_1(K). \tag{5}$$

For invariant tori we look for solutions G of (5) that are periodic of period 2π in both ϕ and θ. Provided that the Jacobian $1 + G_{\phi K}$ does not vanish, such a solution defines the required transformation via (3) and (4). The new action K will be constant, and the new angle ψ will advance linearly with θ: $\psi = \psi_0 + \nu_1 \theta$, with perturbed tune $\nu_1 = dH_1/dK$. The invariant torus is given in explicit form $J = J(\phi, \theta)$ by (4). One can plot invariant curves, namely surfaces of section at constant θ.

For finite-time maps we look for solutions G of (5) that are periodic in ϕ, but not in θ, and such that $H_1(K) \equiv 0$. Further, we require an initial condition in θ, namely $G(\phi, K, \theta = 0) = 0$. For such solutions both ψ and K are constant, and their constant values are interpreted as initial conditions of (ϕ, J): $\psi = \phi_0$, $K = J_0$. The canonical transformation defined by (3) and (4) is the map $(\phi_0, J_0) \mapsto (\phi(\theta), J(\theta))$, which reduces to the identity at $\theta = 0$. Since (3) is a nonlinear equation for ϕ, the map is not yet given in explicit form. In Sect. 3 we show how to represent it explicitly.

We write G as a Fourier series in ϕ, and obtain

$$G_\phi(\phi, K, \theta) = \sum_{m=-\infty}^{\infty} i m g_m(K, \theta) e^{im\phi}. \tag{6}$$

Using (1) and taking the Fourier transform of (5) with $m \neq 0$ we find

$$\left(im\nu + \frac{\partial}{\partial \theta} \right) g_m(\theta) = -f(\theta) V_m(\theta; g), \tag{7}$$

$$V_m(\theta; g) = \frac{1}{2\pi} \int_0^{2\pi} e^{-im\phi} U(\phi, K + G_\phi) \, d\phi. \tag{8}$$

Notice that (6) includes no term with $m = 0$; thus (6) and (8) define V_m as a function of the infinite vector g with components $g_m(\theta)$, $m \neq 0$. We now use a Green function for the operator $im\nu + \partial/\partial\theta$ to convert (7) to an integral equation for $g_m(\theta)$; see Ref. 1.

The periodic Green function gives an equation having solutions automatically periodic in θ; namely,

$$g_m(\theta) = \frac{ie^{-im\nu\theta}}{2\sin m\nu\pi} \int_0^{2\pi} e^{im\nu(\theta' + \pi \operatorname{sgn}(\theta - \theta'))} f(\theta') V_m(\theta'; g) \, d\theta', \tag{9}$$

where $0 \leq \theta \leq 2\pi$, $m \neq 0$, and

$$\operatorname{sgn}(\theta) = \begin{cases} 1 & \theta > 0 \\ -1 & \theta < 0 \end{cases}. \tag{10}$$

On the other hand, the Green function that vanishes at $\theta = 0$ gives an equation having solutions that vanish at $\theta = 0$:

$$g_m(\theta) = -e^{-im\nu\theta} \int_0^\theta e^{im\nu\theta'} f(\theta') V_m(\theta'; g) \, d\theta'. \tag{11}$$

We use (9) to determine invariant tori, and (11) to construct finite-time maps. The unknowns are the $g_m(\theta)$, $m \neq 0$, with θ

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restricted to points inside the magnets, where $f(\theta) \neq 0$. The harmonic oscillator phase advance between magnets, described by the factor $\exp(-im\nu\theta)$, is given automatically once the unknowns have been determined.

Equation (8) or (11) has the form $g = A(g; K)$, where the final action K is a fixed input parameter. We solve the equation by simple iteration $g^{(p+1)} = A(g^{(p)}; K)$, with $g^{(0)} = 0$.[11] The first iterate $g^{(1)}$ coincides with lowest order perturbation theory. To evaluate the nonlinear operator A we perform the sum (6) and the integral (8) as Fast Fourier Transforms. For the θ' integral we represent $V_m(\theta'; g)$ by a linear spline (i.e., as a piecewise-linear function) over each magnet. We then carry out the θ' integral analytically, so as to avoid direct numerical quadrature of the oscillating factor $\exp(im\nu\theta')$, which would be awkward at large $m\nu$. Taking sufficiently many mesh points, we conclude that $V_m(\theta'; g)$ is a very simple function of θ', approximately quadratic over the extent of a sextupole. Better approximations, using cubic splines or a single cubic, are being tested. It appears that very few mesh points will be needed, perhaps 4 or 5 per magnet.

In the case of invariant tori, the number of iterations to achieve a solution of course depends critically on the tune ν, the amplitude K, and the magnet strengths f. Indeed, invariant tori do not exist for all values of these parameters. In the case of finite-time maps, the convergence is much more robust, thanks to the absence of the small divisor $\sin m\nu\pi$; fast convergence appears to be global in regions of interest for accelerators.

FINITE-TIME MAP IN EXPLICIT FORM

To put the finite-time map in explicit form, we solve (3) and (4) for (ϕ, J) as functions of (ψ, K). This is done using Fourier series in ψ rather than ϕ:

$$\begin{pmatrix} \phi \\ J \end{pmatrix} = \sum_{m=-\infty}^{\infty} \begin{pmatrix} \phi_m(K, \theta) \\ J_m(K, \theta) \end{pmatrix} e^{im\psi} + \begin{pmatrix} \psi \\ K \end{pmatrix}. \quad (12)$$

The coefficients, being integrals over ψ, may be rewritten as integrals over ϕ, in which the integrands are known explicit functions of ϕ; see Ref. 1. We find

$$\begin{pmatrix} \phi_m \\ J_m \end{pmatrix} = \frac{1}{2\pi} \int_0^{2\pi} d\phi (1 + G_{\phi K}) e^{-im(\phi + G_K)} \begin{pmatrix} -G_K \\ G_\phi \end{pmatrix}. \quad (13)$$

A full-turn map $\phi(0), J(0) \mapsto \phi(2\pi), J(2\pi)$ is thus represented as

$$\begin{pmatrix} \phi(2\pi) \\ J(2\pi) \end{pmatrix} = \sum_{m=-\infty}^{\infty} \begin{pmatrix} \phi_m(J(0), 2\pi) \\ J_m(J(0), 2\pi) \end{pmatrix} e^{im\phi(0)} + \begin{pmatrix} \phi(0) \\ J(0) \end{pmatrix}. \quad (14)$$

The coefficients $\phi_m(K, \theta), J_m(K, \theta)$ have a very smooth dependence on K, which we represent by cubic spline functions. Their values at the spline knots $K^{(i)}$ are obtained by solving (11), together with the corresponding equation for $\partial g_m/\partial K$, for $K = K^{(i)}$, $i = 1, 2, \cdots, n$. That yields G_ϕ and G_K, from which we calculate the coefficients via (13).

Evaluation of the map (14) amounts to evaluation of polynomials: first cubic polynomials in $J(0)$ to find the coefficients, and then polynomials of degree m_{max} in $\exp(i\phi(0))$. The maximum required mode number m_{max} is not necessarily greater for a large ring than for a small one. Consequently, for a large

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[11] For better convergence one can employ Newton's method, see Ref. 1.

ring the burden of computation lies in calculating the coefficients ϕ_m, J_m with sufficient accuracy; iteration of the map itself should be relatively inexpensive. At a given level of accuracy, the time to compute the coefficients increases linearly with the number of magnets. Another point worth noting is that the coefficients are also smooth functions of tune and magnet strength. One could therefore evaluate them at discrete values in a continuous range of such parameters, and use spline interpolation for intermediate points. Thus one could compute and store maps for a continuous range of lattices once for all.

NUMERICAL EXAMPLES

To find realistic parameters for the model Hamiltonian (1) we begin with the Hamiltonian for a real lattice with focusing function $K(s)$ and sextupole distribution $S(s)$:

$$H(x, p, s) = \frac{1}{2}p^2 + \frac{1}{2}K(s)x^2 + \frac{1}{6}S(s)x^3, \quad (15)$$

where s is path length and the dimensionless transverse momentum is measured in units of longitudinal momentum: $p = p_x/p_0$. After two canonical transformations and a change of independent variable from s to $\theta = s/R$, where $2\pi R$ is the machine circumference, the Hamiltonian takes the form

$$H(\phi_1, J, \theta) = \nu J + \frac{\sqrt{2}}{3} RS(s)(J\beta(s))^{\frac{3}{2}} \cos^3(\phi_1 - \chi(s)) \quad (16)$$

where

$$x = \sqrt{2J\beta} \cos \phi,$$

$$p = -\sqrt{2J/\beta}(\sin \phi - \frac{1}{2}\beta' \cos \phi),$$

$$\nu = \frac{1}{2\pi} \int_0^{2\pi R} \frac{ds}{\beta(s)},$$

$$\phi_1 = \phi + \chi(s) = \phi + \left[\frac{\nu s}{R} - \int_0^s \frac{ds'}{\beta(s')} \right]. \quad (17)$$

Both $\beta(s)$ and $\chi(s)$ will have little variation over the extent of a short sextupole; for present purposes we may assume that they are constant. Furthermore, χ will be the same constant on every sextupole, since we assume that the sextupoles are spaced uniformly, and that the beta function varies periodically with period equal to the spacing. After a rotation of coordinates the Hamiltonian (16) then has exactly the form (1) that we have assumed. Note incidentally that our Hamilton-Jacobi equations (9) and (11) apply just as well to the exact form (16), and would not be harder to solve if it were used. One could also include an arbitrary profile $f(\theta)$ for each magnet, rather than a square step.

To illustrate with a simple but realistic example we take a set of four sextupoles of equal strength and sign, separated by 90 degrees in phase advance: $\nu\Delta\theta = \pi/2$. We choose parameters motivated by the SSC Conceptual Design: $\beta(SF) = 325\,m$, $x_{max} \simeq 1\,cm$, $S = 6.58 \times 10^{-3}/m^3$ for magnets of length $1.5\,m$, sextupoles spaced by $192\,m$ (cell length). The relation $\nu\Delta\theta = \pi/2$ determines the radius R in our model in terms of ν and the cell length.

For $x_{max} = 1\,cm$ we have $J \simeq 1.5 \times 10^{-7}\,m$. We show results for invariant surfaces with $K = 1.5 \times 10^{-7}\,m$, computed from (9) with maximum mode number $m = 31$ and 10 mesh points per magnet for the θ integration. We iterate (9) for various ν, and find convergence except in narrow bands around rational values $\nu = n/m$, $m \leq 31$. Of course, the excluded bands increase in width with increasing K, and tend to zero with increasing m.

As expected, the pairing of sextupoles with 180° phase difference suppresses the third order resonance to high accuracy, for θ outside the group of sextupoles. In most of tune space the dominant residual resonance is 4th order. Near 4th and 5th order resonances we find convergence provided that the fractional part of the tune differs from 1/4 or 1/5, respectively, by greater then 1 %. Figs. 1 and 2 show invariant curves $J(\phi, \theta = 0)$ for $\nu = 3.2475$ and 3.198; $\theta = 0$ is outside the group of magnets at the leading edge of the first magnet. For $\nu^* = 3.198$ there are $m = 4$ and $m = 5$ components in nearly equal amounts. Fig. 3 shows the same data as Fig. 1, but in a polar plot in (x, p) space. In these difficult cases close to strong resonances the convergence is relatively slow; the normalized residual[1] $r = ||g - A(g)||/||g||$ is 10^{-3} after about 12 iterations, and 10^{-7} after about 30.

In Fig. 4 we show results from tracking, obtained in 2000 iterations of the full-turn map of Eq. (14) for $\nu = 3.2475$. The initial condition was a point on the curve of Fig. 1. The agreement between Fig. 1 and Fig. 4 is good, and was obtained without much refinement in numerical technique. Evaluation of the map (14) was quite fast; it required 40 ms of CPU time on a VAX 785, in a single precision computation with Fourier modes $|m| \leq 15$.

We conclude that the Hamilton-Jacobi method for invariant surfaces will probably be useful in real lattice design. The method for finite-time maps seems promising, but it remains to be seen whether sufficient accuracy can be maintained through many thousands of iterations of the map.

REFERENCES

1. R. L. Warnock and R. D. Ruth, "Invariant Tori through Direct Solution of the Hamilton-Jacobi Equation", SLAC-PUB -3865, LBL-21709, to be published in Physica D.

2. S. Chapman, B. C. Garrett, and W. H. Miller, J. Chem. Phys. 64 (1976) 502.

Fig. 1 Invariant Curve, $\nu = 3.2475$

Fig. 4 Tracking with Full-Turn Map, $\nu = 3.2475$

Fig. 2 Invariant Curve, $\nu = 3.198$

Fig. 3 Invariant Curve, $\nu = 3.2475$