

Nonlinear Single-Particle Dynamics in High Energy Accelerators

Part 5: Lie Transformations

Nonlinear Single-Particle Dynamics in High Energy Accelerators

There are six lectures in this course on nonlinear dynamics:

1. First example: nonlinear dynamics in a bunch compressor
2. Second example: nonlinear dynamics in storage rings
3. Hamiltonian mechanics
4. Canonical perturbation theory
5. Lie transformations
6. Symplectic integrators

We have seen how nonlinear dynamics can play an important role in some diverse and common accelerator systems.

Nonlinear effects have to be taken into account when designing such systems.

A number of powerful tools for analysis of nonlinear systems are developed from Hamiltonian mechanics.

We have reviewed the principles of Hamiltonian mechanics in the context of accelerator beam dynamics, and have looked in particular at symplecticity, canonical transformations, and generating functions.

In this lecture...

In the final two lectures, we shall discuss methods for constructing transfer maps for accelerator elements. We have already seen how to do this for a drift space: but this is a special case, because the equations of motion can be solved exactly.

In this lecture, we shall discuss two powerful techniques for constructing (and representing) maps for accelerator elements:

- Lie transformations;
- mixed-variable generating functions.

We shall use a sextupole as an example, but the techniques we develop are quite general.

Recall the general Hamiltonian for an accelerator element:

$$H = -(1 + hx) \sqrt{\left(\frac{1}{\beta_0} + \delta - \frac{q\phi}{P_0 c}\right)^2 - (p_x - a_x)^2 - (p_y - a_y)^2} - \frac{1}{\beta_0^2 \gamma_0^2} - (1 + hx) a_s + \frac{\delta}{\beta_0}. \quad (1)$$

For a drift space, this becomes:

$$H = -\sqrt{\left(\frac{1}{\beta_0} + \delta\right)^2 - p_x^2 - p_y^2} - \frac{1}{\beta_0^2 \gamma_0^2} + \frac{\delta}{\beta_0}. \quad (2)$$

The equations of motion are given by Hamilton's equations:

$$\frac{dx}{ds} = \frac{\partial H}{\partial p_x}, \quad \frac{dp_x}{ds} = -\frac{\partial H}{\partial x}, \quad (3)$$

and similarly for (y, p_y) and (z, δ) .

Transfer map for a drift space

The equations of motion for a drift space are easy to solve, because the momenta p_x , p_y and δ are constants of the motion. The solution can be expressed as a map in closed form: the Hamiltonian is integrable.

For the transverse variables:

$$x_1 = x_0 + \frac{p_{x0}}{p_s} \Delta s, \quad p_{x1} = p_{x0}, \quad (4)$$

$$y_1 = y_0 + \frac{p_{y0}}{p_s} \Delta s, \quad p_{y1} = p_{y0}. \quad (5)$$

And for the longitudinal variables, we have:

$$z_1 = z_0 + \left(\frac{1}{\beta_0} - \frac{\frac{1}{\beta_0} + \delta}{p_s}\right) \Delta s, \quad \delta_1 = \delta_0. \quad (6)$$

The value of p_s (a constant of the motion) is given by:

$$p_s = \sqrt{\left(\frac{1}{\beta_0} + \delta_0\right)^2 - p_{x0}^2 - p_{y0}^2} - \frac{1}{\beta_0^2 \gamma_0^2}.$$

A sextupole field can be derived from the vector potential:

$$A_x = 0, \quad A_y = 0, \quad A_s = -\frac{1}{6} \frac{P_0}{q} k_2 (x^3 - 3xy^2). \quad (7)$$

This potential gives the fields:

$$B_x = \frac{P_0}{q} k_2 xy, \quad B_y = \frac{1}{2} \frac{P_0}{q} k_2 (x^2 - y^2), \quad B_s = 0. \quad (8)$$

Note that the sextupole strength k_2 is given by:

$$k_2 = \frac{q}{P_0} \frac{\partial^2 B_y}{\partial x^2}. \quad (9)$$

The normalised potential \vec{a} is given by:

$$\vec{a} = \frac{q}{P_0} \vec{A}. \quad (10)$$

Hence, the Hamiltonian for a sextupole can be written:

$$H = -\sqrt{\left(\frac{1}{\beta_0} + \delta\right)^2 - p_x^2 - p_y^2 - \frac{1}{\beta_0^2 \gamma_0^2}} + \frac{1}{6} k_2 (x^3 - 3xy^2) + \frac{\delta}{\beta_0}. \quad (11)$$

Since the coordinates x and y appear explicitly in the Hamiltonian, the momenta p_x and p_y are not constants. The equations of motion are nonlinear, and rather complicated. We will not even bother to write them down, since we cannot find an exact solution in closed form: the Hamiltonian is not integrable.

To track a particle through a sextupole, we have to take one of two approaches:

1. integrate the equations of motion numerically (e.g. using a Runge–Kutta algorithm) with given initial conditions, or,
2. make some approximations that will enable us to write down an *approximate* map in closed form.

Numerical techniques, such as Runge–Kutta algorithms, for integrating equations of motion are standard. The drawback in their use for accelerator beam dynamics is that they tend to be rather slow. Often, we are interested in tracking tens of thousands of particles, thousands of times around storage rings consisting of thousands of elements. Numerical integration is no good for this.

We shall therefore focus on the second approach. We shall make some approximations that will enable us to write down a map in closed form. There are various ways to do this: we begin by developing the idea of *Lie transformations*.

Lie transformations provide a means to construct a transfer map in closed form, even from a Hamiltonian that is not integrable. It is necessary to make some approximations, and these need to be understood in some detail.

Lie operators

Suppose we have a function f of the phase space variables, coordinates \vec{q} and conjugate momenta \vec{p} :

$$f = f(\vec{q}, \vec{p}). \quad (12)$$

Suppose we evaluate f at the location in phase space for a particle whose dynamics are governed by a Hamiltonian H .

The time evolution of f is:

$$\frac{df}{dt} = \frac{d\vec{q}}{dt} \frac{\partial f}{\partial \vec{q}} + \frac{d\vec{p}}{dt} \frac{\partial f}{\partial \vec{p}}. \quad (13)$$

Using Hamilton's equations, this becomes:

$$\frac{df}{dt} = \frac{\partial H}{\partial \vec{p}} \frac{\partial f}{\partial \vec{q}} - \frac{\partial H}{\partial \vec{q}} \frac{\partial f}{\partial \vec{p}}. \quad (14)$$

We define the *Lie operator* $:g:$ for any function $g(\vec{q}, \vec{p})$:

$$:g: = \frac{\partial g}{\partial \vec{q}} \frac{\partial}{\partial \vec{p}} - \frac{\partial g}{\partial \vec{p}} \frac{\partial}{\partial \vec{q}} \quad (15)$$

Constructing a Lie operator from the Hamiltonian, we can write:

$$\frac{df}{dt} = -:H: f. \quad (16)$$

Equation (16) suggests that given f at time $t = t_0$, we can evaluate f at any later time $t_0 + \Delta t$:

$$f(t_0 + \Delta t) = e^{-\Delta t :H:} f \Big|_{t=t_0}. \quad (17)$$

Here, the exponential of the Lie operator is defined in terms of a series expansion:

$$e^{-\Delta t :H:} = 1 - \Delta t :H: + \frac{\Delta t^2}{2} :H:^2 - \frac{\Delta t^3}{3!} :H:^3 + \dots \quad (18)$$

Equation (16) does indeed give us the value of f at any time $t_0 + \Delta t$, given the value of f at $t = t_0$.

We can see this by simply making a Taylor series expansion:

$$f(t_0 + \Delta t) = f(t_0) + \Delta t \frac{df}{dt} \Big|_{t=t_0} + \frac{\Delta t^2}{2} \frac{d^2 f}{dt^2} \Big|_{t=t_0} + \frac{\Delta t^3}{3!} \frac{d^3 f}{dt^3} \Big|_{t=t_0} + \dots \quad (19)$$

Then, since from (16) we can write:

$$\frac{d}{dt} = -:H: \quad (20)$$

equation (18) follows.

The operator $e^{:g:}$ is called a *Lie transformation*.

To see how to use Lie transformations to solve the equations of motion for a given system, consider a familiar example: a simple harmonic oscillator in one degree of freedom.

The Hamiltonian is:

$$H = \frac{1}{2}p^2 + \frac{1}{2}\omega^2q^2. \quad (21)$$

Suppose we want to find the coordinate q as a function of time t . Of course, in this case, we could simply write down the equations of motion (from Hamilton's equations) and solve them (because the Hamiltonian is integrable). However, we can also write:

$$q(t_0 + \Delta t) = e^{-\Delta t :H:} q \Big|_{t=t_0}. \quad (22)$$

Lie transformation example: harmonic oscillator

To evaluate the Lie transformation, we need $:H:q$. This is given by (15):

$$:H:q = \frac{\partial H}{\partial q} \frac{\partial q}{\partial p} - \frac{\partial H}{\partial p} \frac{\partial q}{\partial q} = -\frac{\partial H}{\partial p} = -p. \quad (23)$$

Similarly, we find:

$$:H:p = \omega^2q. \quad (24)$$

This means that:

$$:H:^2q = :H:(-p) = -\omega^2q, \quad (25)$$

$$:H:^3q = :H:(-q) = \omega^2p, \quad (26)$$

and so on.

Using the above results, we find:

$$q(t_0 + \Delta t) = q|_{t=t_0} - \Delta t:H:q|_{t=t_0} + \frac{\Delta t^2}{2}:H:^2q|_{t=t_0} - \dots \quad (27)$$

$$= q(t_0) + \Delta t p(t_0) - \omega^2 \frac{\Delta t^2}{2} q(t_0) - \dots \quad (28)$$

Collecting together even and odd powers of t , we find that equation (28) can be written:

$$q(t_0 + \Delta t) = q(t_0) \cos(\omega \Delta t) + \frac{p(t_0)}{\omega} \sin(\omega \Delta t). \quad (29)$$

Similarly (an exercise for the student!) we find that:

$$p(t_0 + \Delta t) = e^{-\Delta t:H:} p(t_0)|_{t=t_0} = -\omega q(t_0) \sin(\omega \Delta t) + p(t_0) \cos(\omega \Delta t). \quad (30)$$

Equations (29) and (30) are the solutions we would have found using the conventional approach of integrating the equations of motion: but note that we have not performed any integrations, only differentiations (though we have had to sum an infinite series...)

Lie operators and Lie transformations have many interesting properties that makes them useful for analysing the behaviour of dynamical systems. We shall explore these properties further in the next lecture; but for now, we shall simply see how to apply the technique demonstrated for the harmonic oscillator, to a particle moving through a sextupole.

Recall the Hamiltonian for a sextupole (11):

$$H = -\sqrt{\left(\frac{1}{\beta_0} + \delta\right)^2 - p_x^2 - p_y^2 - \frac{1}{\beta_0^2 \gamma_0^2}} + \frac{1}{6} k_2 (x^3 - 3xy^2) + \frac{\delta}{\beta_0}.$$

Using Lie operator notation, we can write the map for a particle moving through the sextupole as:

$$\vec{x}(s_0 + \Delta s) = e^{-\Delta s : H :} \vec{x} \Big|_{s=s_0}. \quad (31)$$

Since the Lie transformation evolves the dynamical variables according to Hamilton's equations (for the Hamiltonian H) the map expressed in the form (31) is necessarily symplectic. Since application of a Lie transformation just involves differentiation and summation (of an infinite series) we can, in principle, apply the map in this form, for any Hamiltonian.

However, a map expressed as a Lie transformation is not explicit: it requires algebraic manipulation before we can simply put in the values of the dynamical variables at the entrance of the magnet, and obtain the values at the exit of the magnet.

For tracking simulations, it is much more useful to have an *explicit* map, which we can apply by simply substituting numbers into a given formula. For example, equations (29) and (30) give an explicit map for the harmonic oscillator.

To produce an explicit map, we can simply evaluate the Lie transformation for each of the dynamical variables, keeping terms in the series expansion up to some order in s .

To see how this works, let us apply the technique to a sextupole.

First of all, dealing with the full Hamiltonian for the sextupole makes things unnecessarily complicated. Let us assume that $\delta = 0$, and that $y = p_y = 0$. Then, we have motion in only one degree of freedom (x). Further, let us take the limit $\beta_0 \rightarrow 1$. Then, the Hamiltonian (11) becomes:

$$H = -\sqrt{1 - p_x^2} + \frac{1}{6}k_2x^3.$$

Now let us evaluate the Lie transformations of x and p_x . To first order in Δs , we find:

$$x(s_0 + \Delta s) = e^{-\Delta s:H}x\Big|_{s=s_0} = x_0 + \frac{p_{x0}\Delta s}{\sqrt{1 - p_{x0}^2}} + O(\Delta s^2), \tag{32}$$

$$p_x(s_0 + \Delta s) = e^{-\Delta s:H}p_x\Big|_{s=s_0} = p_{x0} - \frac{1}{2}k_2x_0^2\Delta s + O(\Delta s^2). \tag{33}$$

where $x_0 = x(s_0)$, etc.

If we truncate the sextupole map (32) and (33) to first order in Δs , we obtain:

$$x(s_0 + \Delta s) = x_0 + \frac{p_{x0}\Delta s}{\sqrt{1 - p_{x0}^2}},$$

$$p_x(s_0 + \Delta s) = p_{x0} - \frac{1}{2}k_2x_0^2\Delta s.$$

This map looks like the map for a drift space of length Δs , but with the addition of a momentum “kick” of size $-\frac{1}{2}k_2x_0^2\Delta s$. Note that the deflection is proportional to the square of the initial co-ordinate: this reflects the nonlinear nature of the field.

It is possible to use the above map for a sextupole in a tracking code. But we can expect to have lost a lot of accuracy by truncating the series expansion for the Lie transformation at first order in Δs . In fact, the truncation has a rather unpleasant consequence...

If we calculate the Jacobian J of the truncated map, and check for symplecticity, we find:

$$J^T S J = \begin{pmatrix} 0 & 1 + \Delta \\ -1 - \Delta & 0 \end{pmatrix} \quad (34)$$

where

$$\Delta = \frac{k_2 x_0 \Delta s^2}{(1 - p_{x0}^2)^{\frac{3}{2}}}. \quad (35)$$

There is a “symplectic error” of order Δs^2 . If we require symplectic maps (for a tracking code, for example), this is bad news. However, we know that the full map, including all terms in the Lie transformation, must be symplectic. This implies that, if we keep more terms, the symplectic error must appear in higher order in Δs .

To reduce the “symplectic error” we can construct the map to second order in s . The result is:

$$x(s_0 + \Delta s) = x_0 + \frac{p_{x0} \Delta s}{\sqrt{1 - p_{x0}^2}} - \frac{k_2 x_0^2 \Delta s^2}{4 (1 - p_{x0}^2)^{\frac{3}{2}}} + O(\Delta s^3), \quad (36)$$

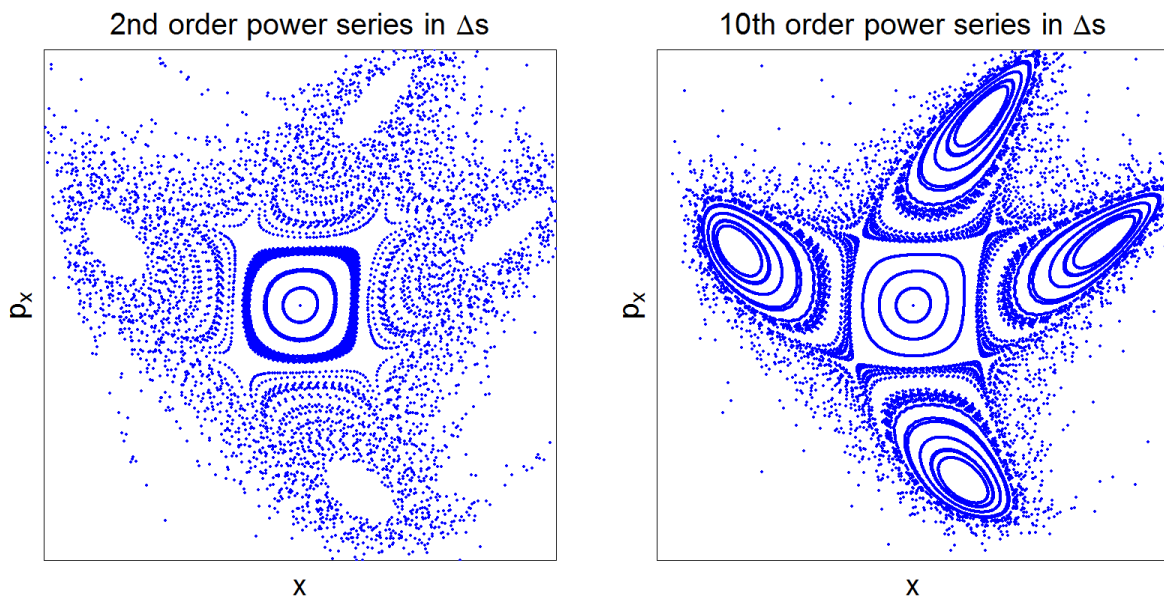
$$p_x(s_0 + \Delta s) = p_{x0} - \frac{1}{2} k_2 x_0^2 \Delta s - \frac{k_2 x_0 p_{x0} \Delta s^2}{2 \sqrt{1 - p_{x0}^2}} + O(\Delta s^3). \quad (37)$$

The higher order terms get increasingly complicated and difficult to interpret. It also very quickly gets cumbersome to work out the symplectic error — but we find, as expected, that if we work out the map to order N , then the symplectic error is of order $N + 1$.

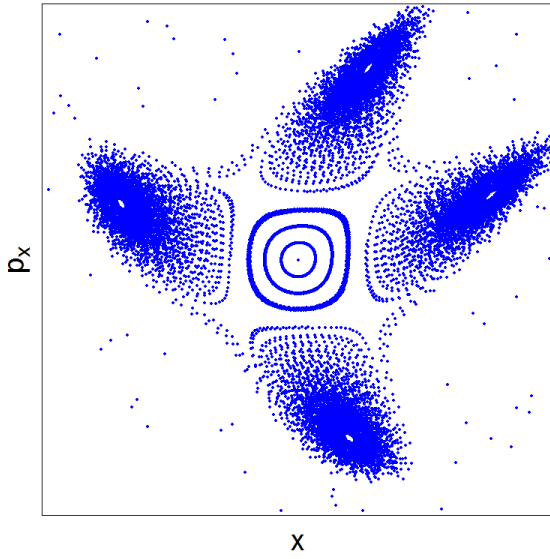
How important is the symplectic error? The only real way to find out for a particular case is to do a convergence test. For example, we can consider one of the examples from an earlier lecture: a sextupole in a periodic beamline. In effect, we construct a lattice from a sequence of sextupoles, with a linear phase advance of some value from one sextupole to the next.

To illustrate the dynamics, we construct a phase-space portrait by “launching” particles with different amplitudes (in x), and tracking them for a few thousand periodic cells, plotting in phase space the values of the dynamical variables for each particle after each cell.

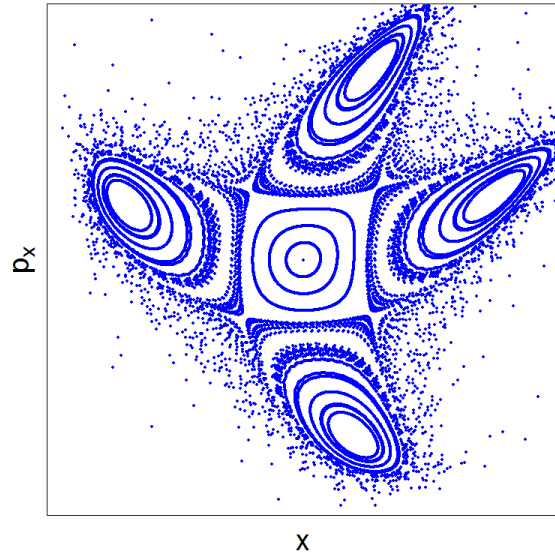
The following plots compare the results using sextupole maps of different orders in Δ_s . Note that we use a linear phase advance of $0.246 \times 2\pi$ between sextupoles, a sextupole length of 0.1 m, and a sextupole strength $k_2 = -6000 \text{ m}^{-3}$.



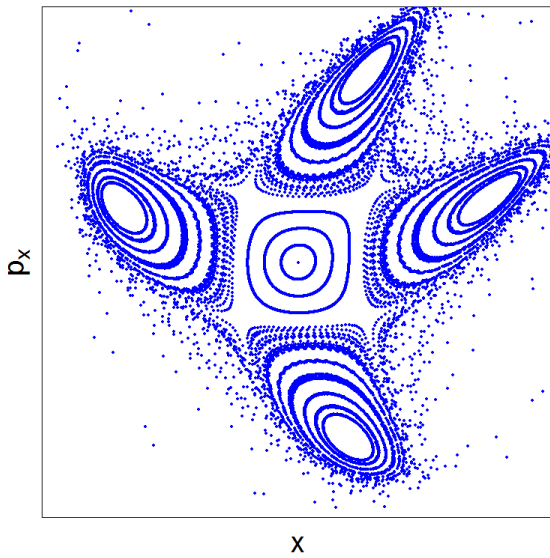
3rd order power series in Δs



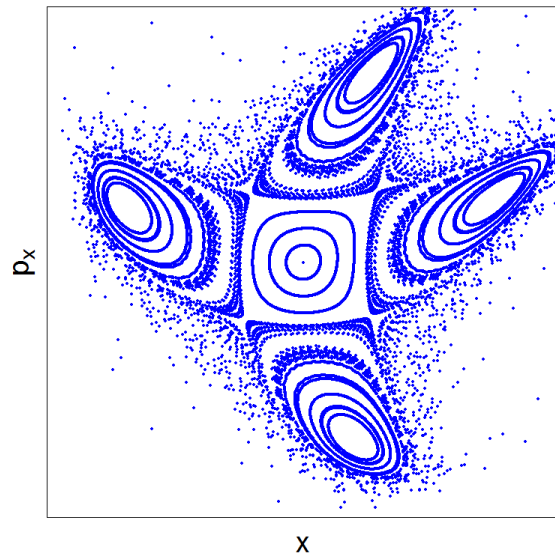
10th order power series in Δs



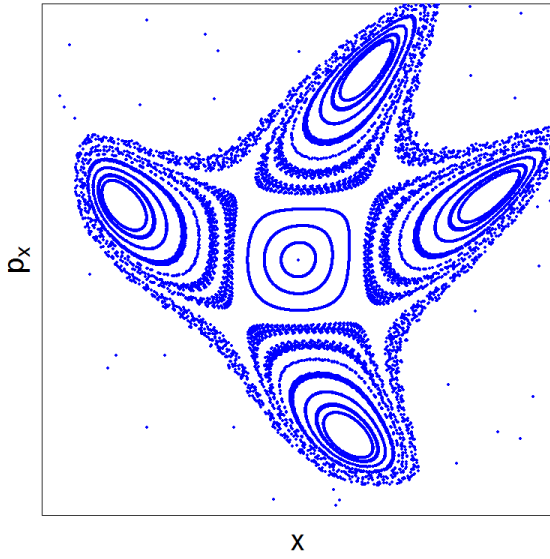
4th order power series in Δs



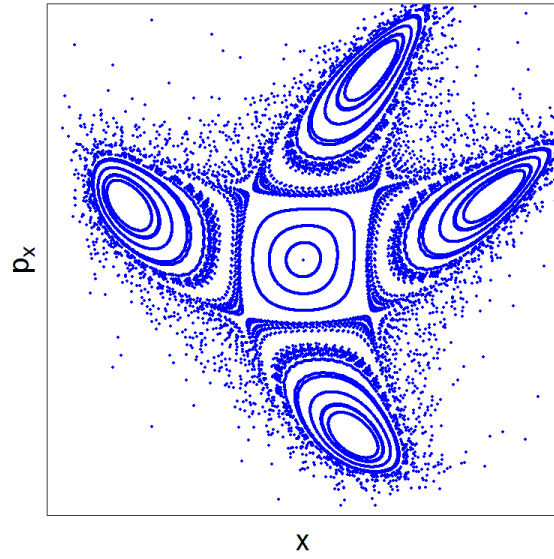
10th order power series in Δs



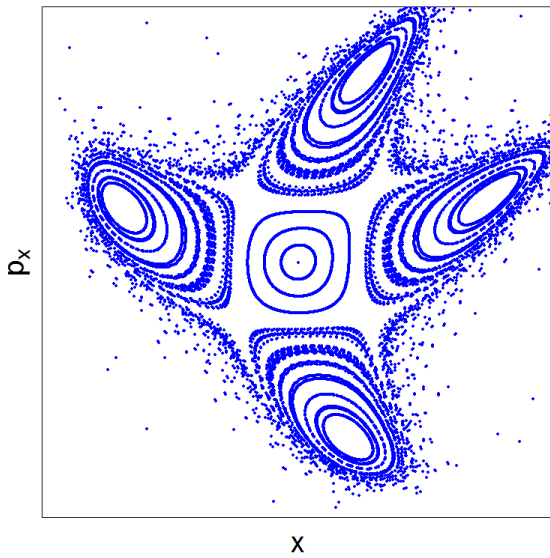
5th order power series in Δs



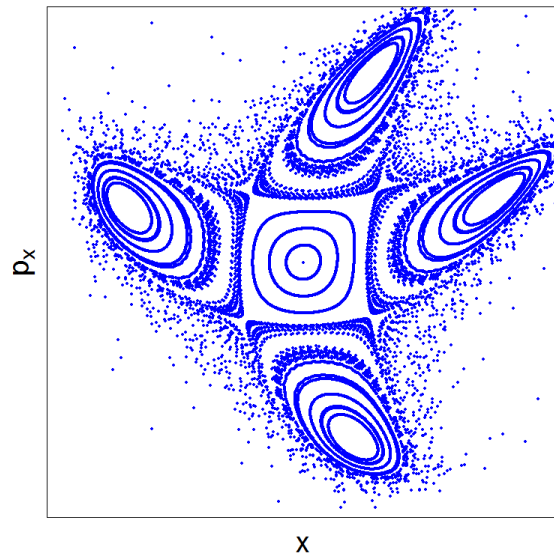
10th order power series in Δs

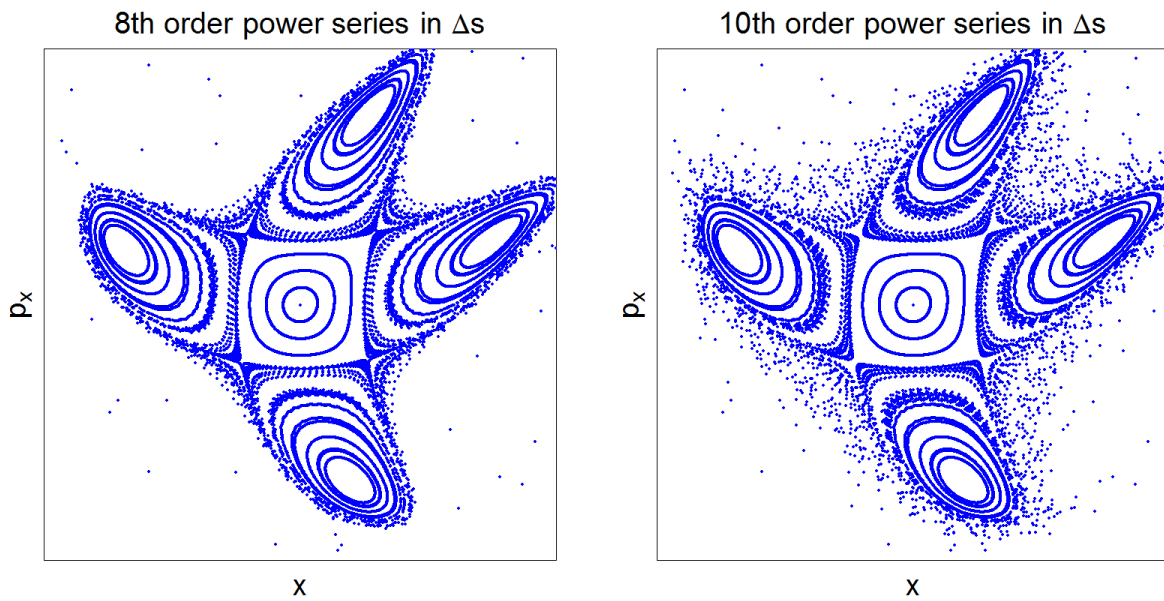


6th order power series in Δs



10th order power series in Δs





It appears that convergence is rather slow. This means that we will need maps of very high order (possibly higher than 12th order) to obtain reliable results.

The problem we encounter is that the high order maps are very cumbersome. They will be difficult to implement in a tracking code, and slow to evaluate.

The problem of finding a “fast symplectic integrator” is one that we shall return to in the final lecture. In the remainder of this lecture, we shall discuss the use of mixed variable generating functions as a means of representing symplectic maps.

As a first step towards representing a transfer map in the form of a mixed variable generating function, we consider again the representation of the map in the form of a power series.

In particular, we note that we can represent the sextupole map (32) and (33) as power series in x_0 and p_{x0} , by making Taylor expansions in x_0 and p_{x0} .

The map takes the form:

$$x_i(s_0 + \Delta s) = \sum_j R_{ij} x_j(s_0) + \sum_{j,k} T_{ijk} x_j(s_0) x_k(s_0) + \dots \quad (38)$$

where the coefficients R_{ij} , T_{ijk} etc. are functions of the length and strength of the sextupole.

A map expressed in this way is in a convenient form for implementing in a tracking code: we just need to work out the values of the various coefficients.

For a sextupole, we find (for example, by applying the Lie transformations in equations (32) and (32)) that to second order in the dynamical variables:

$$\begin{aligned} x(s_0 + \Delta s) = & x_0 + \Delta s p_{x0} - \frac{1}{4} k_2 \Delta s^2 x_0^2 - \frac{1}{6} k_2 \Delta s^3 x_0 p_{x0} \\ & - \frac{1}{24} k_2 \Delta s^4 p_{x0}^2 + O(3) \end{aligned} \quad (39)$$

$$\begin{aligned} p_x(s_0 + \Delta s) = & p_{x0} - \frac{1}{2} k_2 \Delta s x_0^2 - \frac{1}{2} k_2 \Delta s^2 x_0 p_{x0} \\ & - \frac{1}{6} k_2 \Delta s^3 p_{x0}^2 + O(3) \end{aligned} \quad (40)$$

Here, $O(3)$ means terms of order 3 and higher in the dynamical variables.

We expect the full map (to infinite order) to be symplectic. But if we truncate the map at some given order in the dynamical variables, then we will lose symplecticity.

For example, if we find the Jacobian J of the map truncated at second order in the dynamical variables, then we find that:

$$J^T S J = \begin{pmatrix} 0 & 1 + \Delta \\ -1 - \Delta & 0 \end{pmatrix} \quad (41)$$

where the symplectic error is now:

$$\Delta = \frac{1}{72} k_2^2 \Delta s^4 (\Delta s^2 p_{x0}^2 + 6\Delta s x_0 p_{x0} + 6x_0^2). \quad (42)$$

In general, if we truncate the power series map at order N , then there is a symplectic error of order N .

Sextupole map: mixed variable generating function map

A power series provides a very convenient representation of a map.

The drawback is that in general, a map represented in this way will not be symplectic.

However, if the power series map is of order N , and symplectic to that order, then it is possible to construct a generating function that reproduces the map to order N .

Using this generating function, we can carry out symplectic tracking.

As an example, consider the power series map for the sextupole, truncated to first order (the same as a drift space):

$$x_1 = x(s_0 + \Delta s) = x_0 + \Delta s p_{x0}, \quad (43)$$

$$p_{x1} = p_x(s_0 + \Delta s) = p_{x0}. \quad (44)$$

We can think of the map as a transformation from old variables x_0 and p_{x0} , to new variables, x_1 and p_{x1} .

Since the map is symplectic, it represents a canonical transformation.

We can represent the canonical transformation in the form of a mixed variable generating function.

The canonical transformation can be obtained from a generating function of the third kind:

$$F_3(x_1, p_{x0}) = -x_1 p_{x0} + \frac{1}{2} \Delta s p_{x0}^2. \quad (45)$$

Using the equations for a canonical transformation of this kind:

$$x_0 = -\frac{\partial F_3}{\partial p_{x0}}, \quad p_{x1} = -\frac{\partial F_3}{\partial x_1}, \quad (46)$$

we find that:

$$x_0 = x_1 - \Delta s p_{x0}, \quad p_{x1} = p_{x0}. \quad (47)$$

A method for constructing the generating function (to arbitrary order) starting from a given power series is outlined in Appendix A (using a sextupole in one degree of freedom as an example).

The advantage of representing a map in the form of a mixed variable generating function is that the map is symplectic, and takes a reasonably compact form.

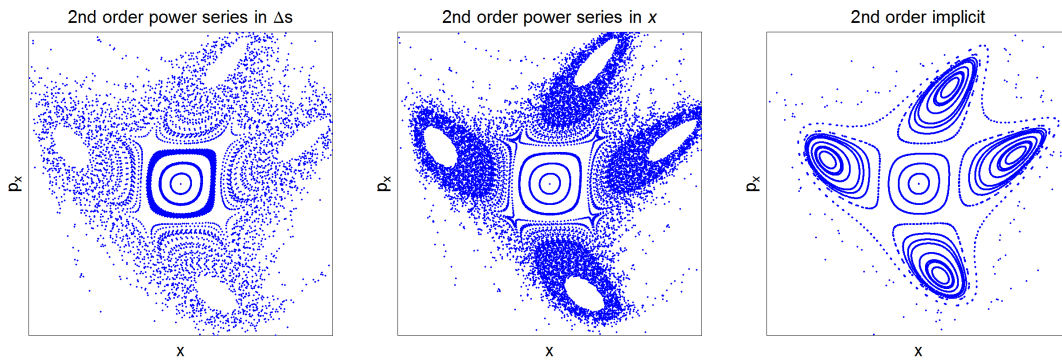
The main disadvantage is that the representation is implicit: rather than a set of expressions into which we just have to substitute the initial values for the variables, we have a set of equations that must be solved (numerically) each time we wish to apply the map.

We now have three representations that are convenient (to a greater or lesser extent) for tracking:

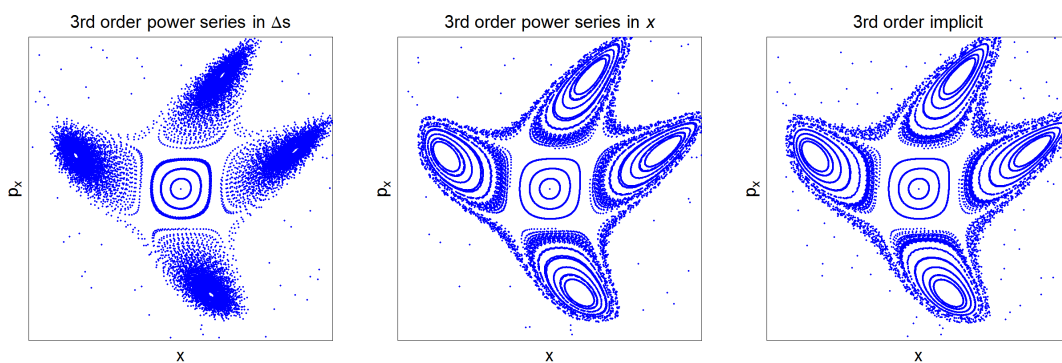
- power series to a specified order in Δs ;
- power series to a specified order in the dynamical variables;
- implicit map to a specified order in the dynamical variables.

We can compare the three representations using our “standard” example, that is a periodic lattice constructed from cells with a linear phase advance of $0.246 \times 2\pi$, with a sextupole of length 0.1 m and strength $k_2 = 6000 \text{ m}^{-3}$ in each cell.

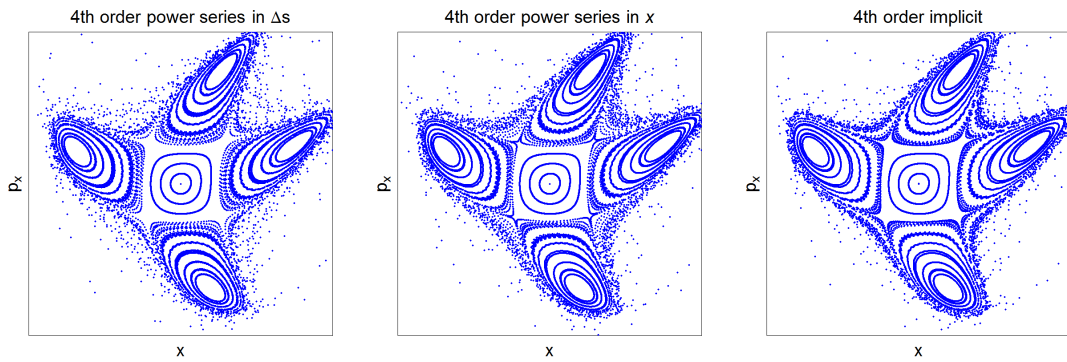
Sextupole map: comparison of different representations



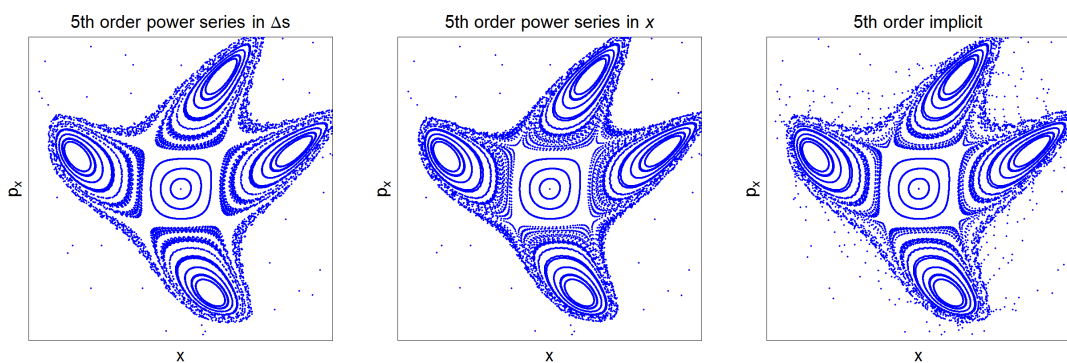
Sextupole map: comparison of different representations



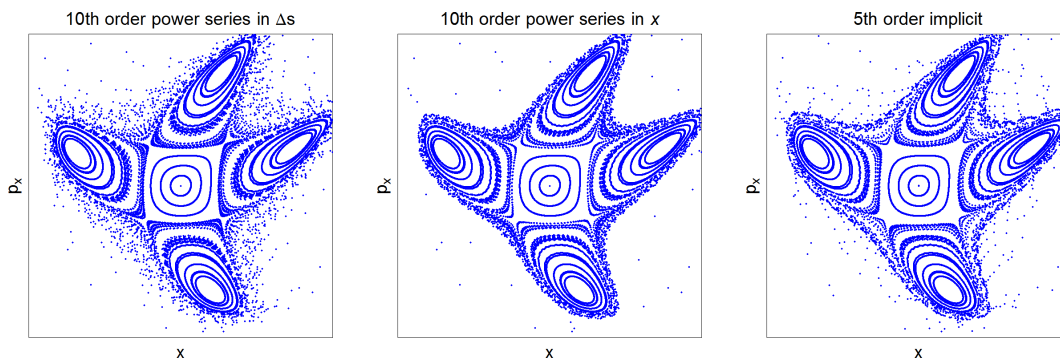
Sextupole map: comparison of different representations



Sextupole map: comparison of different representations



We can compare the 10th order explicit maps with the 5th order implicit map:



There do appear to be some advantages to a symplectic map: the implicit map looks very similar to the explicit (non-symplectic) maps at much higher order. We cannot conclude that a relatively low order implicit map is more accurate than a high order power series map, but symplecticity does seem to be an important feature.

The drawback of the implicit map is that it can be computationally expensive. Tracking is much slower than if an explicit map is used, even if the explicit map is at higher order.

However, we have not yet exhausted all the possibilities. If we go back to the map in the form of a Lie transformation, it turns out that some of the properties of Lie transformations are helpful in constructing explicit symplectic maps. We shall return to this topic in a future lecture, when we discuss “integrators”.

- The transfer map for an accelerator element can be represented in symplectic form as a Lie transformation:

$$\vec{x}(s) = e^{-Hs}\vec{x}(0),$$

where H is the Hamiltonian.

- An explicit map in the form of a power series can be obtained from a Lie transformation, by performing the appropriate differentiations. In general, a map in the form of an infinite series is produced.
- A map in a convenient form for tracking can be obtained by truncating the infinite series obtained by evaluating a Lie transformation. However, it may be necessary to retain high order terms in order to maintain accuracy, and reduce effects arising from the fact that the truncated map is no longer symplectic.
- A finite-order symplectic map in implicit form can be constructed from a truncated (non-symplectic) power series map. Evaluating a map in implicit form requires numerical iteration, which can be slow.

Exercises

1. Show equation (30):

$$p(t_0 + \Delta t) = e^{-\Delta t:H} p \Big|_{t=t_0} = -\omega q(t_0) \sin(\omega \Delta t) + p(t_0) \cos(\omega \Delta t),$$

where H is the harmonic oscillator Hamiltonian:

$$H = \frac{1}{2}p^2 + \frac{1}{2}\omega^2 q^2.$$

2. Find, to second order, the implicit map for a sextupole in two transverse degrees of freedom. What is the generating function for this map?

In this Appendix, we outline a method for constructing a mixed variable generating function that represents a symplectic map, starting from a (truncated) power series approximation for the map.

The method is best explained using an example: we shall use map for a sextupole in one degree of freedom.

It should be clear to see how the technique generalises for more degrees of freedom.

First, we write down the power series map for the sextupole, truncated to first order:

$$x_1 = x(s_0 + \Delta s) = x_0 + \Delta s p_{x0}, \quad (48)$$

$$p_{x1} = p_x(s_0 + \Delta s) = p_{x0}. \quad (49)$$

We can think of the map as a canonical transformation from old variables x_0 and p_{x0} , to new variables, x_1 and p_{x1} .

To simplify the notation, in the remainder of this Appendix we shall write the “old” variables as $x = x_0 = x(s_0)$ and $p_x = p_{x0} = p_x(s_0)$, and the “new” variables as $X = x_1 = x(s_0 + \Delta s)$ and $P_X = p_{x1} = p_x(s_0 + \Delta s)$.

The canonical transformation can be obtained from a mixed variable generating function of the third kind:

$$F_3(X, p_x) = -Xp_x + \frac{1}{2}\Delta s p_x^2. \quad (50)$$

Using the equations for a canonical transformation of this kind:

$$x = -\frac{\partial F_3}{\partial p_x}, \quad P_X = -\frac{\partial F_3}{\partial X}, \quad (51)$$

we find that:

$$x = X - \Delta s p_x, \quad P_X = p_x. \quad (52)$$

In general, suppose we have a generating function:

$$F_3 = -\begin{pmatrix} X & p_x \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \sum_n \frac{\vec{U}^{(n)}}{n+1} \quad (53)$$

where $\vec{U}^{(n)}$ is a vector whose components are power series of order n in the variables X and p_x .

Then, the relationship between the “old” variables (x, p_x) and the “new” variables (X, P_X) is given by:

$$\begin{pmatrix} x \\ P_X \end{pmatrix} = \sum_n \vec{U}^{(n)}. \quad (54)$$

For the sextupole map truncated to first order, we would write:

$$\vec{U}^{(1)} = \begin{pmatrix} X - \Delta s p_x \\ p_x \end{pmatrix}. \quad (55)$$

To generalise to higher orders, we need a means of constructing $\vec{U}^{(2)}$, $\vec{U}^{(3)}$, and so on. We can do this by iteration. The idea is to write x as a function of X and p_x to some order N , and then substitute this expression for x into the terms of order 2 to order $N + 1$ in the original power series map, and truncate at order $N + 1$.

So, from the first order terms for the sextupole map, we have:

$$x = X - \Delta s p_x, \quad (56)$$

$$P_X = p_x. \quad (57)$$

That is,

$$\vec{U}^{(1)} = \begin{pmatrix} X - \Delta s p_x \\ p_x \end{pmatrix}. \quad (58)$$

The second order terms for the sextupole are found from (39) and (40):

$$X = x + \Delta s p_x - \frac{1}{4}k_2\Delta s^2x^2 - \frac{1}{6}k_2\Delta s^3xp_x - \frac{1}{24}k_2\Delta s^4p_x^2 + O(3),$$

$$P_X = p_x - \frac{1}{2}k_2\Delta s x^2 - \frac{1}{2}k_2\Delta s^2xp_x - \frac{1}{6}k_2\Delta s^3p_x^2 + O(3).$$

Rearranging, we have:

$$x = X - \Delta s p_x + \frac{1}{4}k_2\Delta s^2(X - \Delta s p_x)^2 + \frac{1}{6}k_2\Delta s^3(X - \Delta s p_x)p_x + \frac{1}{24}k_2\Delta s^4p_x^2, \quad (59)$$

$$P_X = p_x - \frac{1}{2}k_2\Delta s(X - \Delta s p_x)^2 - \frac{1}{2}k_2\Delta s^2(X - \Delta s p_x)p_x - \frac{1}{6}k_2\Delta s^3p_x^2. \quad (60)$$

Thus, we find:

$$\vec{U}^{(2)} = \begin{pmatrix} \frac{1}{4}k_2\Delta s^2X^2 - \frac{1}{3}k_2\Delta s^3Xp_x + \frac{1}{8}k_2\Delta s^4p_x^2 \\ -\frac{1}{2}k_2\Delta s X^2 + \frac{1}{2}k_2\Delta s^2Xp_x - \frac{1}{6}k_2\Delta s^3p_x^2 \end{pmatrix}. \quad (61)$$

Proceeding in this way, we can construct a map to the same order as the original power series, but in which the *old* coordinate x and *new* momentum P_X are expressed in terms of the *new* coordinate X and *old* momentum p_x (54):

$$\begin{pmatrix} x \\ P_X \end{pmatrix} = \sum_n \vec{U}^{(n)}(X, p_x).$$

A map of this form is called an *implicit* map. If the original power series map is symplectic to order N , then the implicit map (constructed to order N) will be canonical, and can be derived from a generating function, using (53).

Although we do not usually need the generating function, it is often worth while working out what it is, as a check on your calculations.

We now have a way of constructing a symplectic map of order N , given a power series map obtained by truncating a symplectic map of infinite order at order N .

The only problem is that the finite order symplectic map is in implicit form: that is, we cannot simply substitute the initial values of the phase space variables, and obtain the final values by evaluating a power series.

Instead, we need to solve the equations by some numerical technique (such as a Newton–Raphson algorithm).