Nonlinear Single-Particle Dynamics in High Energy Accelerators

Part 4: Integrators I

This course consists of eight lectures:

1. Introduction – some examples of nonlinear dynamics
2. Basic mathematical tools and concepts
3. Representations of dynamical maps
4. Integrators I
5. Integrators II
6. Phase space portraits and "phenomenology"
7. Normal form analysis
8. Some numerical techniques

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 seen how, using these tools, the solutions to the equations of motion for a particle moving through a component in an accelerator beamline may be represented in various ways, including: (truncated) power series; Lie transformation; (implicit) generating function.

Neglecting radiation and interactions between particles, the map for a particle moving through an accelerator component should be *symplectic*.

The representations of maps we have seen so far all have some drawbacks.

- A Lie transformation provides a symplectic representation of a map, but is not explicit (it is not in a form that can be applied directly).

- We can "evaluate" a Lie transformation as a power series; but in general the power series contains an infinite number of terms, and if we truncate the series, the map is no longer symplectic.

- We can construct a generating function from a truncated power series, but this provides an implicit representation of the map, that requires numerical iteration for its application.

In this lecture, we shall develop one of several possible methods for constructing representations that are both explicit (can be applied directly, without iteration) and symplectic. Such a representation is sometimes known as a "symplectic integrator."

The method we shall develop here, known as "symmetric" or "Yoshida" factorisation, is one of the most common and most useful. It takes the Lie transformation as its starting point.

A Lie transformation is written as:

$$\mathcal{M} = e^{-s:h:} \tag{1}$$

where the Lie operator $:h:$ is defined by:

$$:h: = \frac{\partial h}{\partial \vec{q}}\frac{\partial}{\partial \vec{p}} - \frac{\partial h}{\partial \vec{p}}\frac{\partial}{\partial \vec{q}}. \tag{2}$$

$\vec{q}$ are the coordinates and $\vec{p}$ the conjugate momenta; h is a function of $\vec{q}$ and $\vec{p}$. The exponential operator is defined in terms of its series expansion:

$$e^{-s:h:} = 1 - s{:}h{:} + \frac{s^2}{2}{:}h{:}^2 - \frac{s^3}{3!}{:}h{:}^3 + \cdots \tag{3}$$

If h is the Hamiltonian of the system, then the evolution of any function of the phase space variables is given by:

$$\frac{df}{ds} = -{:}h{:}f, \qquad f(s) = e^{-s:h:}f(0). \tag{4}$$

Given a Hamiltonian, we can construct a map in the form of a power series, using a Lie transformation. We showed how to do this in the previous lecture. Unfortunately, in general, the power series contains an infinite number of terms. To apply the map in practice, we either have to sacrifice symplecticity, or resort to an implicit representation that requires a (slow!) numerical iteration process for its solution. In either case, we end up with an approximate representation of the map.

An alternative approach, which we shall now develop, makes an approximation to the Hamiltonian, instead of to the power series constructed from the Lie transform. The goal is to make an approximation in such a way that the resulting Lie transformation can be expressed as a power series with a finite number of terms.

We begin by stating five rules for algebraic manipulation of Lie transformations. It is convenient at this point to introduce the notation $[\cdot,\cdot]$, which is called the *Poisson bracket*:

$$[f,g] = \frac{\partial f}{\partial \vec{q}}\frac{\partial g}{\partial \vec{p}} - \frac{\partial f}{\partial \vec{p}}\frac{\partial g}{\partial \vec{q}}. \tag{5}$$

Clearly, with our previous definition (2) for the Lie operator, we have:

$$:f\!:g = [f,g]\,. \tag{6}$$

It is possible to show (by writing out the derivatives explicitly) that for any functions f, g and h, we have the Jacobi identity:

$$[f,[g,h]] + [g,[h,f]] + [h,[f,g]] \equiv 0 \tag{7}$$

The first rule is simply the series expression for a Lie transformation with *generator* f:

$$e^{:f:}g = g + [f,g] + \frac{1}{2}[f,[f,g]] + \cdots \tag{8}$$

The second rule tells us how to take the Lie transformation of a product of two functions:

$$e^{:f:}(gh) = \left(e^{:f:}g\right)\left(e^{:f:}h\right). \tag{9}$$

This result may be obtained by writing the Lie transformation as a series, and applying the product rule for differentiation. It may also be obtained without lengthy algebra, by considering the role of a Lie generator in obtaining the value of a function at time t from the value of the function at time $t = 0$ (see Exercise 1).

The third rule is a little subtle: it tells us how to take the Lie transformation of a function of a function:

$$e^{:f:}g(h) = g\left(e^{:f:}h\right). \tag{10}$$

This result may be shown in a similar way to Rule 2 (see Exercise 2). The subtlety becomes apparent when we want to concatenate maps, i.e. apply one map after another. Consider the map for a drift space of length L:

$$\mathcal{R} = e^{-\frac{1}{2}L:p^2:}, \tag{11}$$

and the map for a thin sextupole, of strength k_2L:

$$\mathcal{S} = e^{-\frac{1}{6}k_2L:q^3:}. \tag{12}$$

The total map for a drift followed by a sextupole is:

$$\mathcal{R}\cdot\mathcal{S} = e^{-\frac{1}{2}L:p^2:}\,e^{-\frac{1}{6}k_2L:q^3:}. \tag{13}$$

Note that we write the Lie transformations in the order that the elements appear in the beamline: we do not reverse the order, as we would for transfer matrices (see Exercise 3).

The fourth rule tells us how to take the Lie transformation of a Poisson bracket:

$$e^{:f:}\,[g,h] = \left[e^{:f:}g, e^{:f:}h\right]. \tag{14}$$

This result may be shown in a similar way to Rules 1 and 2. (Note that if g and h are functions of the phase space variables, then so are their derivatives with respect to those variables.)

The fifth rule is very important and useful:

$$e^{:f:}\, e^{:g:}\, e^{-:f:} = \exp :e^{:f:}g: \tag{15}$$

Unfortunately, it is not easy to show this result; and for a rigorous proof, the student is referred to the literature, e.g. Dragt. However, we can "sketch a proof" as follows. First, consider the operator:

$$\mathcal{M}(\tau) = e^{\tau :f:} :g: e^{-\tau :f:} \tag{16}$$

where τ is a parameter. Note that:

$$\mathcal{M}(0) = :g:. \tag{17}$$

We can take derivatives of $\mathcal{M}$ with respect to τ:

$$\frac{d}{d\tau}\mathcal{M}(0) = :f::g: - :g::f: = :(:f:g): \tag{18}$$

where, in the final step, we have applied the Jacobi identity (7).

Lie transformation algebra: Rule 5

We find that higher derivatives are given by:

$$\frac{d^n}{d\tau^n}\mathcal{M}(0) = :(:f:^n g): \tag{19}$$

Hence, we can write:

$$\begin{aligned}
\mathcal{M}(\tau) &= :g: + \tau\frac{d}{dt}\mathcal{M}(0) + \frac{1}{2}\tau^2\frac{d^2}{dt^2}\mathcal{M}(0) + \frac{1}{3!}\tau^3\frac{d^3}{dt^3}\mathcal{M}(0) + \cdots \\
&= :g: + \tau:(:f:g): + \frac{1}{2}\tau^2:(:f:^2g): + \frac{1}{3!}\tau^3:(:f:^2g): + \cdots \\
&= :(e^{\tau:f:}g): \qquad (20)
\end{aligned}$$

In particular, putting $\tau = 1$, we find:

$$e^{:f:} :g: e^{-:f:} = :(e^{:f:}g): \tag{21}$$

Now, since the Lie operator is a differential operator, we can generalise this result, for any function F:

$$e^{:f:}\, F(:g:)\, e^{-:f:} = F(:(e^{:f:}g):) \tag{22}$$

In particular, with $F(x) = e^x$, we have (15):

$$e^{:f:}\, e^{:g:}\, e^{-:f:} = \exp :e^{:f:} g:$$

This equation is important because it allows us to combine Lie transformations. However, it is special in the sense that it involves "squeezing" one Lie transformation ($e^{:g:}$) between another Lie transformation ($e^{:f:}$) and its inverse ($e^{-:f:}$).

More generally, we can look for the combination of two Lie transformations:

$$e^{:A:}\, e^{:B:} = e^{:C:}. \tag{23}$$

The expression for C in terms of A and B is known as the *Baker-Campbell-Hausdorff formula*, or the BCH formula, for short.

The Baker-Campbell-Hausdorff formula

The BCH formula applies to any non-commutative algebra, not just the algebra of Lie operators. There is a general expression for the BCH formula, but this is not very enlightening. The first few terms are given as follows:

$$e^{:A:}\, e^{:B:} = e^{:C:}$$

where:

$$\begin{aligned} C &= A + B + \frac{1}{2}[A,B] + \frac{1}{12}[A,[A,B]] + \frac{1}{12}[B,[B,A]] \\ &\quad + \frac{1}{24}[[[A,B],A],B] + \cdots \end{aligned} \tag{24}$$

An expression related to the BCH formula, known as the Zassenhaus formula, tells us how to factorise a Lie transformation whose generator is expressed as a sum:

$$e^{:A+B:} = e^{:A:}\, e^{:B:}\, e^{-\frac{1}{2}:[A,B]:}\, e^{\frac{1}{3}:[B,[A,B]]:+\frac{1}{6}:[A,[A,B]]:} \ldots \tag{25}$$

The BCH formula is immediately useful for us, in our goal of constructing explicit symplectic integrators for accelerator beamline components, as we shall now show. As an example, we will consider motion of a particle through a sextupole magnet.

Consider a simplified Hamiltonian for a sextupole in one degree of freedom:

$$H = \frac{1}{2}p_x^2 + \frac{1}{6}k_2\,x^3. \tag{26}$$

The equations of motion for this Hamiltonian have no closed form solution. The map obtained from the Lie transformation:

$$\mathcal{S} = e^{-L:H:} \tag{27}$$

(for a sextupole of length L) can be expressed as a power series, but this series contains an infinite number of terms.

However, we notice that each of the two terms in the Hamiltonian (26) on its own *does* generate a Lie transformation that can be expressed in closed form:

$$\begin{aligned} e^{-L:H_d:}\,x &= x + Lp_x, & e^{-L:H_d:}\,p_x &= p_x, \\ e^{-L:H_k:}\,x &= x, & e^{-L:H_k:}\,p_x &= p_x - \tfrac{1}{2}k_2Lx^2, \end{aligned} \tag{28}$$

where $H_d = \frac{1}{2}p_x^2$ and $H_k = \frac{1}{6}k_2x^3$. Using the BCH formula:

$$e^{-L:H_d:}\,e^{-L:H_k:} = e^{-L:H - \frac{1}{2}L[H_d,H_k]+O(L^2):}. \tag{29}$$

In other words, we can represent the map for a sextupole as a concatenation of Lie transformations (each of which can be expressed explicitly in closed form) with an "error" of order L^2 in the generator for the complete map.

If the sextupole is short, then the above map (29) may be good enought. However, we can ask the question: is it possible to express the map for a sextupole as the concatenation of Lie transformations, each of which may be expressed explicitly in closed form, but with error of order L^3, or higher?

The answer (of course) is *yes!* Consider the map:

$$e^{-d_1 L:H_d:} e^{-L:H_k:} e^{-d_2 L:H_d:} = e^{-d_1 L:H_d:} e^{-L:d_2 H_d + H_k - \frac{1}{2} d_2 L[H_k, H_d] + O(s^2):}$$

$$= e^{-L:(d_1+d_2)H_d + H_k - \frac{1}{2}(d_1-d_2)L[H_k,H_d] + O(L^2):}. \quad (30)$$

Clearly, if we choose:

$$d_1 = d_2 = \frac{1}{2}, \quad (31)$$

then we find:

$$e^{-\frac{1}{2}L:H_d:} e^{-L:H_k:} e^{-\frac{1}{2}L:H_d:} = e^{-L:H + O(L^2):}. \quad (32)$$

Let us just pause to consider what we have achieved. We have seen that the map (29):

$$e^{-L:H_d:} e^{-L:H_k:} = e^{-L:H + O(L):}$$

allows us to construct an explicit symplectic map in closed form for a sextupole, but with error of order L^2 in the generator. Inspecting the left hand side, we see that the map may be interpreted as a drift (for the length of the sextupole) followed by a transverse momentum kick (by an amount corresponding to the integrated strength of the sextupole).

Similarly, we find that the map (32):

$$e^{-\frac{1}{2}L:H_d:}\, e^{-L:H_k:}\, e^{-\frac{1}{2}L:H_d:} = e^{-L:H+O(L^2):}$$

allows us to construct an explicit symplectic map in closed form for a sextupole, but with error of order L^3 in the generator. Inspecting the left hand side, we see that the map may be interpreted as a drift (for *half* the length of the sextupole), followed by a transverse momentum kick (by an amount corresponding to the integrated strength of the sextupole), followed again by a drift (for *half* the length of the sextupole).

Simply putting the kick in the centre of the sextupole provides a higher-order approximation than putting the kick at the start, or at the end.

If we wish, we can continue the process to higher order. The algebra gets rather formidable, but we only need to do it once for a given accelerator component. A map accurate to fourth order (in the Lie generator) for a sextupole is given by:

$$e^{-d_1L:H_d:}\, e^{-c_1L:H_k:}\, e^{-d_2L:H_d:}\, e^{-c_2L:H_k:}\, e^{-d_2L:H_d:}\, e^{-c_1L:H_k:}\, e^{-d_1L:H_d:} = e^{-L:H+O(L^4):} \tag{33}$$

where:

$$\begin{aligned} d_1 &= \frac{1}{12}\left(4 + 2\sqrt[3]{2} + \sqrt[3]{4}\right), \\ d_2 &= \frac{1}{2} - d_1, \\ c_1 &= 2d_1, \\ c_2 &= 1 - 4d_1. \end{aligned}$$

The "fourth-order explicit symplectic integrator" (33) is an interesting result. It tells us that if we are to approximate a sextupole (or, indeed, any higher-order multipole) by a sequence of drifts and thin kicks, then there is an optimal way to choose the drift lengths and kick strengths.

Taking a more simplistic approach, one would divide the element into a number of *equal* drifts and kicks; a moment's reflection suggests that this should give an accurate answer in the limit of a large number of drifts and kicks. But we have found from an approach based on Lie transformations that by choosing the drift lengths and kick strengths carefully, we can obtain a more accurate result than we would using a similar number of equally divided drifts and kicks.

The above technique is one of the most useful and practical for constructing explicit symplectic integrators. It is sometimes known as "symmetric factorisation", or "Yoshida factorisation".

Before we make some comparisons between the explicit symplectic integrator we have derived here and the maps we have derived in previous lectures, let us pause to consider more carefully the Hamiltonian for a sextupole.

Properly, the Hamiltonian for a sextupole is given by:

$$H = -\sqrt{\left(\frac{1}{\beta_0} + \delta\right)^2 - p_x^2 - p_y^2 - \frac{1}{\beta_0^2\gamma_0^2}} + \frac{1}{6}k_2\left(x^3 - 3xy^2\right) + \frac{\delta}{\beta_0}. \tag{34}$$

We can express this as a sum of two integrable Hamiltonians:

$$H = H_d + H_k, \tag{35}$$

where

$$H_d = -\sqrt{\left(\frac{1}{\beta_0} + \delta\right)^2 - p_x^2 - p_y^2 - \frac{1}{\beta_0^2\gamma_0^2}} + \frac{\delta}{\beta_0}, \tag{36}$$

and

$$H_k = \frac{1}{6}k_2\left(x^3 - 3xy^2\right). \tag{37}$$

The Hamiltonian H_d is just the Hamiltonian for a drift space, and generates the map that we saw in Lecture 2:

$$
\begin{aligned}
x &\mapsto x + L\tfrac{p_x}{p_s}, & p_x &\mapsto p_x, \\
y &\mapsto y + L\tfrac{p_y}{p_s}, & p_y &\mapsto p_y, \\
z &\mapsto z + L\left(\tfrac{1}{\beta_0} - \tfrac{\frac{1}{\beta_0}+\delta}{p_s}\right), & \delta &\mapsto \delta,
\end{aligned}
\tag{38}
$$

where

$$
p_s = \sqrt{\left(\frac{1}{\beta_0}+\delta\right)^2 - p_x^2 - p_y^2 - \frac{1}{\beta_0^2\gamma_0^2}}. \tag{39}
$$

An explicit symplectic integrator for a sextupole

The Hamiltonian H_k generates the map for a thin sextupole kick:

$$
\begin{aligned}
x &\mapsto x, & p_x &\mapsto p_x - \tfrac{1}{2}k_2 L\left(x^2 - y^2\right), \\
y &\mapsto y, & p_y &\mapsto p_y + k_2 Lxy, \\
z &\mapsto z, & \delta &\mapsto \delta.
\end{aligned}
\tag{40}
$$

Using the Hamiltonians H_d and H_k, we can construct a second-order integrator for a sextupole (32), or a fourth-order integrator (33).

Many tracking codes assume that the transverse momenta are small:

$$\sqrt{p_x^2 + p_y^2} \ll 1. \tag{41}$$

In that case, it is possible to expand the square root in the Hamiltonian for a drift space, H_d (36) to second order in p_x, p_y:

$$H_d = -\sqrt{\left(\frac{1}{\beta_0} + \delta\right)^2 - p_x^2 - p_y^2 - \frac{1}{\beta_0^2\gamma_0^2}} + \frac{\delta}{\beta_0} \approx \frac{p_x^2}{2\Delta} + \frac{p_y^2}{2\Delta} + \frac{\delta}{\beta_0} - \Delta. \tag{42}$$

where

$$\Delta = \sqrt{1 + \frac{2\delta}{\beta_0} + \delta^2} \approx 1 + \frac{\delta}{\beta_0}. \tag{43}$$

The final approximation (for Δ) is valid for $|\delta| \ll 1$. The approximation (42) is known as the paraxial approximation, and is used quite widely. However, as we have seen, it is not always necessary to make the paraxial approximation to obtain higher-order symplectic integrators (at least for common multipole magnets).

We can compare the explicit symplectic integrators for a sextupole derived in this lecture with those derived in previous lectures. Recall that we had three different representations:

- power series truncated at some order in the length of the sextupole;
- power series truncated at some order in the dynamical variables;
- implicit (mixed variable) map.

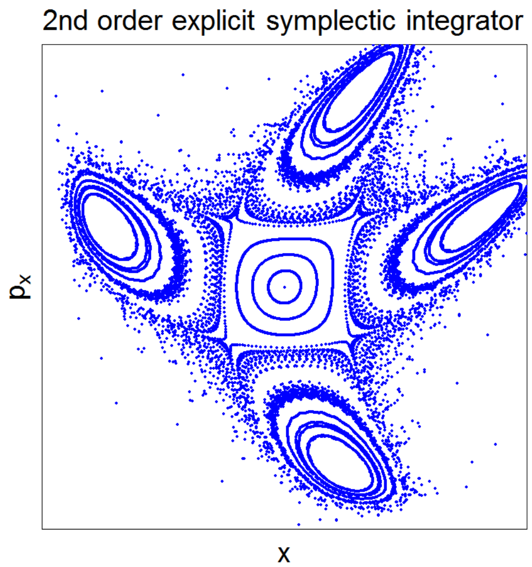
The truncated power series maps are strictly non-symplectic, though we expect the "symplectic error" to get smaller if we truncate at higher order. The implicit map is symplectic, but requires numerical iteration in its application, so tends to be rather slow.

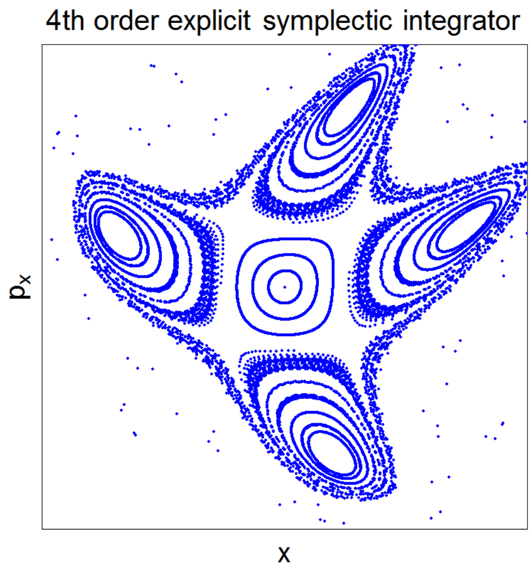
Recall that our "canonical example" is a phase-space rotation through $0.246\times 2\pi$ radians, followed by a sextupole with length $L = 0.1\,\text{m}$, and strength $k_2 = -6000\,\text{m}^{-3}$.

It is a bit difficult to decide exactly which orders to compare. Just for illustration, we shall select the 10^{th} order truncated power series maps, and the 5^{th} order implicit map. We shall compare the 2^{nd} order and 4^{th} order explicit symplectic integrators with these maps.

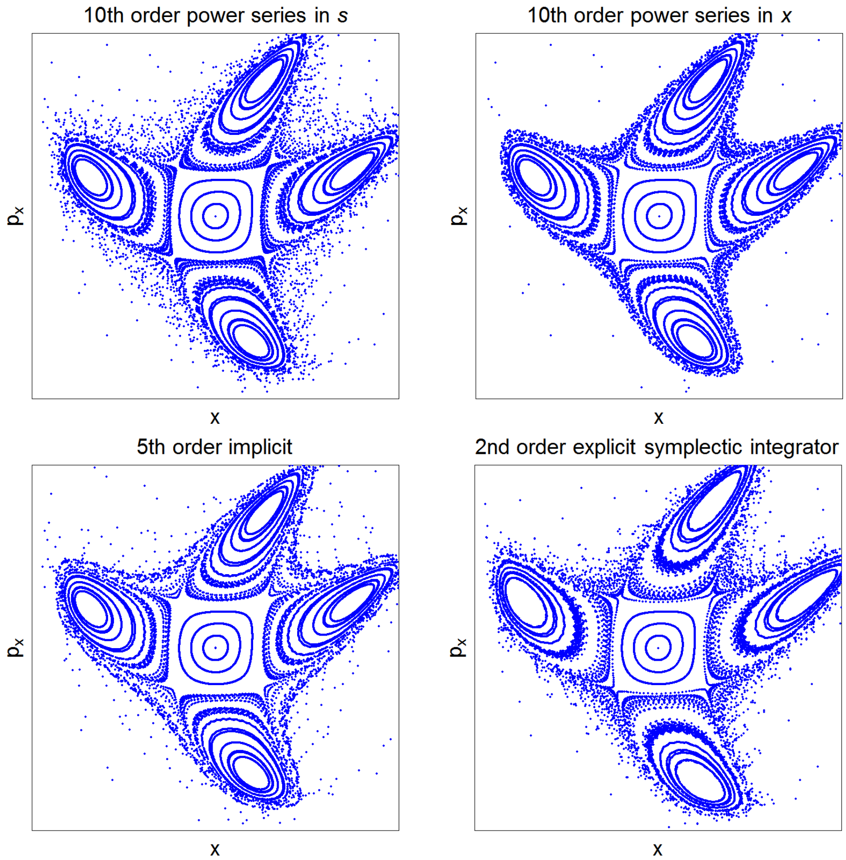
(Note that the order of the symplectic integrator refers to the accuracy of the *generator* of the map, not the accuracy of the power series representation.)

First, we compare the phase space portraits obtained using the 2^{nd} order and 4^{th} order explicit symplectic integrators:

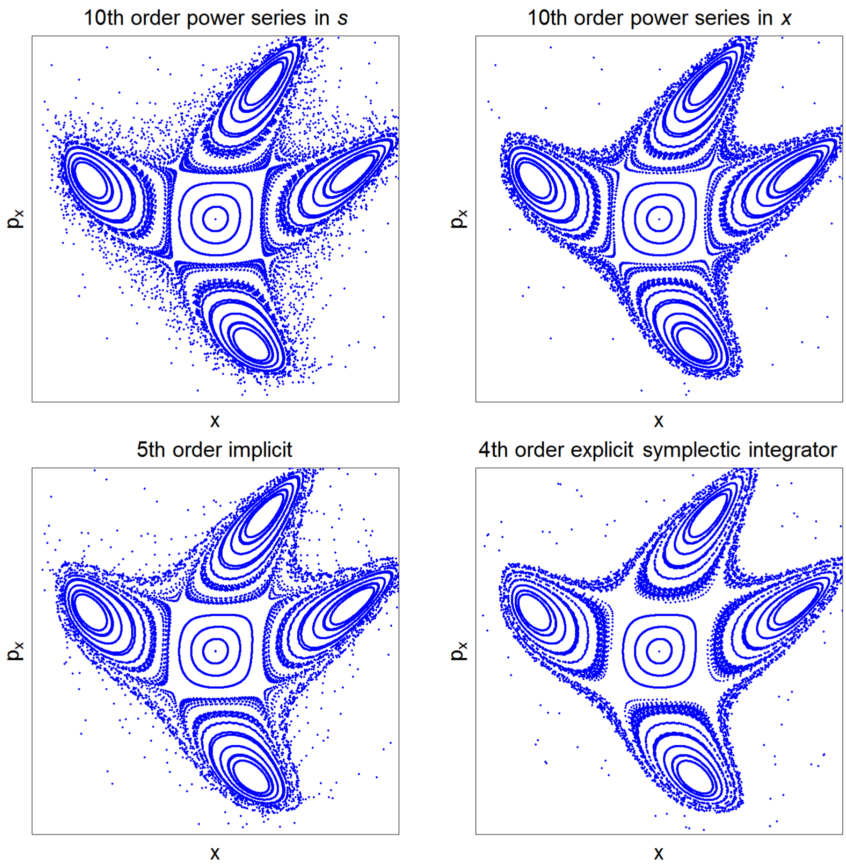




Comparison of maps



Comparison of maps



Clearly, there are some differences between all these maps. What is not so clear, is how significant these differences are.

We should remember that none of the maps shown in these comparisons is an "exact" map for the sextupole: in fact, we are still not capable of constructing an exact map in a form that is appropriate for fast tracking.

You should, by now, have some appreciation of why any two tracking codes will generally disagree about the details of the dynamical behaviour of particles in an accelerator beamline. It is always necessary to make some compromise between speed and accuracy; exactly how that compromise is made will affect the results.

We should mention that many techniques have been developed for converting between power series maps and Lie transformations: there are various applications for these techniques, that we will not go into here.

However, it is worth noting that often, one wishes to factorise a map into linear and nonlinear components. This leads to a Deprit factorisation:

$$\mathcal{M} = \mathcal{R} \cdot e^{:g:}, \tag{44}$$

where $\mathcal{R}$ is a linear map (that may be represented, for example, by a matrix, or by a Lie transformation with a generator that is a second-order polynomial in the phase space variables), and g is a polynomial containing terms that are third-order and higher in the dynamical variables.

Also worth noting is the Dragt-Finn factorisation, that expresses a map as:

$$\mathcal{M} = \prod_{n=2} e^{:g_n:}, \tag{45}$$

where g_n is a homogeneous polynomial of order n in the dynamical variables.

The benefit of a Dragt-Finn factorisation, is that it is possible to "truncate" the map while retaining symplecticity, simply by dropping factors higher than a desired order.

Clearly, the generators appearing in the Dragt-Finn and the Deprit factorisations of a given map are related by the BCH formula. Usually, though, one starts from a given power series map, and constructs the generators for one or other factorisation by following a systematic procedure.

Finally, we note the Irwin factorisation. This is of the form:

$$\mathcal{M} = \prod e^{:r_n:} \cdot e^{:k_n:}, \tag{46}$$

where r_n is a homogeneous second-order polynomial (generating a linear map) and each k_n generates an integrable map. The benefit of the Irwin factorisation is that it is possible to construct an explicit power series map, just by applying the Lie transformations to the dynamical variables.

Again, techniques exist for constructing a map represented as an Irwin factorisation from a given power series map. We then have a technique for "symplectification" of a power series.

Coming next...

We now have a technique for constructing an explicit symplectic map for a multipole magnet. However, accelerator beamlines often use more complex components, such as undulators and wigglers. In the next lecture, we shall study techniques for constructing maps for more complex configurations of magnetic fields than exist in simple multipoles.

Then, in the final lectures of this course, we shall explore what happens when we combine maps for various elements along a beamline.

Exercises

1. Using the Hamiltonian H as a generator for a Lie transformation, write down the the value of a function g at time t in terms of the value of the function at time $t = 0$. Hence, by considering g as the product of two functions, show Rule 2 (9) for the algebra of Lie transformations:
$$e^{:f:}(gh) = \left(e^{:f:}g\right)\left(e^{:f:}h\right).$$
(Hint: write $f = -tH$).

2. Using the same ideas as in Exercise 1, show Rule 3 (9):
$$e^{:f:}g(h) = g\left(e^{:f:}h\right).$$

3. Consider horizontal motion of a particle in a section of accelerator beamline consisting of a drift of length L followed by a thin sextupole of strength k_2L. Show that the map for this section of beamline may be written:
$$\begin{aligned} x &\mapsto x + Lp_x \\ p_x &\mapsto p_x + \frac{1}{6}(x + Lp_x)^2. \end{aligned}$$
Show that this map may be obtained from the Lie transformation (13):
$$\mathcal{R} \cdot \mathcal{S} = e^{-\frac{1}{2}L:p^2:}\, e^{-\frac{1}{6}k_2L:q^3:}.$$