Nonlinear Beam Dynamics
Part 4: Symplectic Integrators

Chong Shik Park, Ph.D

Korea University, Sejong

In this lecture, we shall develop one of several possible methods for constructing representations that are both explicit (can be applied directly, without requiring numerical solution of equations) 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.

Lie transformations provide a useful starting point for symmetric factorisation.

Reminder: Lie transformations

A Lie transformation is written as:

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

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:

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

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

$$\frac{df}{ds} = -:h: f, \qquad f(s_0 + \Delta s) = e^{-\Delta s :h:} f \Big|_{s=s_0}. \tag{4}$$

Constructing maps from Lie transformations

In a previous lecture, we showed how to construct a map in the form of a power series, using a Lie transformation with a given Hamiltonian.

Unfortunately, the power series usually 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 transformation.

The goal is to make an approximation to the Hamiltonian 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, the Poisson bracket satisfies the Jacobi identity:

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

The first rule that we state 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 $t_0 + \Delta t$ from the value of the function at time $t = t_0$

Lie transformation algebra: Rule 3

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

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

This result may be shown in a similar way to Rule 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_D:

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

and the map for a thin sextupole, of strength $k_2 L_S$:

$$\mathcal{S} = e^{-\frac{1}{6}k_2 L_S :q^3:}. \tag{12}$$

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

$$\mathcal{R}\,\mathcal{S} = e^{-\frac{1}{2}L_D :p^2:}\, e^{-\frac{1}{6}k_2 L_S :q^3:}. \tag{13}$$

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.

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:

$$e^{:f:}\,e^{:g:}\,e^{-:f:} = e^{:h:}, \qquad \text{where} \qquad h = e^{:f:}g. \tag{15}$$

Unfortunately, it is not easy to show this result; and for a rigorous proof, see the literature, e.g. Dragt.

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

$$e^{:f:}\,F(:g:)\,e^{-:f:} = F(:(e^{:f:}g):) \tag{16}$$

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

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

Equation (15) 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:

$$e^{:A:}e^{:B:} = e^{:C:}. \tag{17}$$

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 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 it is not very enlightening. The first few terms are given as follows:

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

where:

$$\begin{aligned} C &= A + B + \frac{1}{2}[A, B] + \frac{1}{12}[A, [A, B]] + \frac{1}{12}[B, [B, A]] \\ &\quad + \frac{1}{24}[[[A, B], A], B] + \cdots \end{aligned} \tag{18}$$

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:

$$e^{:A+B:} = e^{:A:}\, e^{:B:}\, e^{-\frac{1}{2}:[A,B]:}\, e^{\frac{1}{3}:[B,[A,B]]:+\frac{1}{6}:[A,[A,B]]:} \ldots \tag{19}$$

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:

$$H = \frac{1}{2}p_x^2 + \frac{1}{6}k_2 x^3. \tag{20}$$

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

$$\mathcal{S} = e^{-L:H:} \tag{21}$$

(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 (20) on its own *does* generate a Lie transformation that can be expressed in closed form:

$$e^{-L:H_d:}x = x + Lp_x, \qquad e^{-L:H_d:}p_x = p_x,$$

$$e^{-L:H_k:}x = x, \qquad e^{-L:H_k:}p_x = p_x - \tfrac{1}{2}k_2Lx^2, \tag{22}$$

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

$$e^{-L:H_d:}e^{-L:H_k:} = e^{-L:H - \frac{1}{2}L[H_d,H_k] + O(L^3):}. \tag{23}$$

In other words, we can represent the map for a sextupole as a composition 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.

An explicit symplectic integrator for a sextupole

If the sextupole is short, then the above map (23) may be good enough.

However, we can ask the question:

Is it possible to express the map for a sextupole as the composition of Lie transformations, each of which may be expressed explicitly in closed form, and with an error (after composition) of order L^3*, or higher?*

The answer (of course) is *yes!*

Consider the map:

$$e^{-d_1 L:H_d:} e^{-L:H_k:} e^{-d_2 L:H_d:} = e^{-d_1 L:H_d:} e^{-L:d_2 H_d + H_k - \frac{1}{2} d_2 L[H_k, H_d] + O(s^2):}$$
$$= e^{-L:(d_1+d_2)H_d + H_k - \frac{1}{2}(d_1 - d_2) L[H_k, H_d] + O(L^2):}. \tag{24}$$

Clearly, if we choose:

$$d_1 = d_2 = \frac{1}{2}, \tag{25}$$

then we find:

$$e^{-\frac{1}{2}L:H_d:} e^{-L:H_k:} e^{-\frac{1}{2}L:H_d:} = e^{-L:H: + O(L^3)}. \tag{26}$$

Let us just pause to consider what we have achieved.

We have seen that the map (23):

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

allows us to construct an explicit symplectic map in closed form for a sextupole, but with error of order L^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 horizontal kick (with strength corresponding to the integrated strength of the sextupole).

Similarly, we find that the map (26):

$$e^{-\frac{1}{2}L:H_d:}\,e^{-L:H_k:}\,e^{-\frac{1}{2}L:H_d:} = e^{-L:H:+O(L^3)}$$

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 horizontal kick (with strength corresponding to the integrated strength of the sextupole), followed finally by another drift (for *half* the length of the sextupole).

Simply putting the kick in the center 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:

$$e^{-d_1 L:H_d:}\, e^{-c_1 L:H_k:}\, e^{-d_2 L:H_d:}\, e^{-c_2 L:H_k:}\, e^{-d_2 L:H_d:}\, e^{-c_1 L:H_k:}\, e^{-d_1 L:H_d:} = e^{-L:H:+O(L^5)} \tag{27}$$

where:

$$d_1 = \frac{1}{12}\left(4 + 2\sqrt[3]{2} + \sqrt[3]{4}\right), \tag{28}$$

and:

$$d_2 = \frac{1}{2} - d_1, \qquad c_1 = 2d_1, \qquad c_2 = 1 - 4d_1. \tag{29}$$

An explicit symplectic integrator for a sextupole

The “fourth-order explicit symplectic integrator” (27) 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:

$$H = -\sqrt{\left(\frac{1}{\beta_0} + \delta\right)^2 - p_x^2 - p_y^2 - \frac{1}{\beta_0^2\gamma_0^2}} + \frac{1}{6}k_2\left(x^3 - 3xy^2\right) + \frac{\delta}{\beta_0}. \tag{30}$$

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

$$H = H_d + H_k, \tag{31}$$

where

$$H_d = -\sqrt{\left(\frac{1}{\beta_0} + \delta\right)^2 - p_x^2 - p_y^2 - \frac{1}{\beta_0^2\gamma_0^2}} + \frac{\delta}{\beta_0}, \tag{32}$$

and

$$H_k = \frac{1}{6}k_2\left(x^3 - 3xy^2\right). \tag{33}$$

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

$$x_1 = x_0 + L\frac{p_{x0}}{p_{s0}}, \qquad p_{x1} = p_{x0},$$

$$y_1 = y_0 + L\frac{p_{y0}}{p_{s0}}, \qquad p_{y1} = p_{y0},$$

$$z_1 = z_0 + L\left(\frac{1}{\beta_0} - \frac{\frac{1}{\beta_0}+\delta_0}{p_{s0}}\right), \qquad \delta_1 = \delta_0, \tag{34}$$

where

$$p_{s0} = \sqrt{\left(\frac{1}{\beta_0} + \delta_0\right)^2 - p_{x0}^2 - p_{y0}^2 - \frac{1}{\beta_0^2\gamma_0^2}}. \tag{35}$$

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

$$x_1 = x_0, \qquad p_{x1} = p_{x0} - \frac{1}{2} k_2 L \left(x_0^2 - y_0^2 \right),$$

$$y_1 = y_0, \qquad p_{y1} = p_{y0} + k_2 L x_0 y_0,$$

$$z_1 = z_0, \qquad \delta_1 = \delta_0. \tag{36}$$

Using the Hamiltonians H_d and H_k, we can construct a second-order integrator for a sextupole (26), or a fourth-order integrator (27).

When applying these results, it is important to remember that the final values from the application of one Lie transformation become the initial values for the application of the next Lie transformation.

Note: the paraxial approximation

Many tracking codes assume that the transverse momenta are small:

$$\sqrt{p_x^2 + p_y^2} \ll 1. \tag{37}$$

In that case, it is possible to expand the square root in the Hamiltonian for a drift space, H_d (32) to second order in p_x, p_y:

$$H_d = -\sqrt{\left(\frac{1}{\beta_0} + \delta\right)^2 - p_x^2 - p_y^2 - \frac{1}{\beta_0^2\gamma_0^2}} + \frac{\delta}{\beta_0} \approx \frac{p_x^2}{2D} + \frac{p_y^2}{2D} + \frac{\delta}{\beta_0} - D, \tag{38}$$

where

$$D = \sqrt{1 + \frac{2\delta}{\beta_0} + \delta^2} \approx 1 + \frac{\delta}{\beta_0}. \tag{39}$$

The final approximation (for D) is valid for $|\delta| \ll 1$. The approximation (38) 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 two different representations:

- power series truncated at some order in the length of the sextupole;
- power series truncated at some order in the dynamical variables;

The truncated power series maps are strictly non-symplectic, though we expect the "symplectic error" to get smaller if we truncate at higher order.

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.

It is possible to extend some of the techniques developed in this lecture to construct maps for more complex configurations of magnetic fields than exist in simple multipoles.

An example of such a technique is the "explicit symplectic integrator for s-dependent static magnetic field" developed by Wu, Forest and Robin (*Phys. Rev. E* **68**, 046502 (2003)).