Four Lectures in Particle Dynamics

Lecture 3: The Non-Linear Solution

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From Linear to Non-Linear solution

So far, our approach to beam dynamics was to use the electromagnetic Hamiltonian with the correct magnetic and electric field for the element that we want to simulate. Then expand the Hamiltonian to the second order to benefit of the linear solution. In equations we summarize it as:

$$\begin{aligned}
H &= \frac{\delta}{\beta_0} - \sqrt{\left(\delta + \frac{1}{\beta_0} - \frac{q_c \phi}{c p_0}\right)^2 - (p_x - a_x)^2 - (p_y - a_y)^2 - \frac{1}{\beta_0^2 \gamma_0^2}} - a_z \\
H_2 &= \mathrm{Taylor(H, 2)} + \cancel{\mathcal{O}(3)} \\
\frac{d\vec{v}}{ds} &= S \vec{\nabla}^T H \approx S \vec{\nabla}^T H_2 = S W \vec{v} \\
\vec{v}_L &= e^{LSW} \vec{v}_0
\end{aligned}$$

we now want to explore the possibility to solve the Hamilton equations without using the Taylor expansion truncated at the order 2.

The Lie operator also known as Poisson Bracket

Given the two functions $f(\vec{q},\vec{p})$, $g(\vec{q},\vec{p})$ we define the Poisson Bracket [2] of f and g as

$$\{f,g\} = \sum_{i=1}^{n} \left(\frac{\partial f}{\partial q_i} \frac{\partial g}{\partial p_i} - \frac{\partial f}{\partial p_i} \frac{\partial g}{\partial q_i} \right) \tag{1}$$

Then we will define the Lie operator such as the "waiting" Poisson Bracket as

$$:f := \sum_{i=1}^{n} \left(\frac{\partial f}{\partial q_i} \frac{\partial}{\partial p_i} - \frac{\partial f}{\partial p_i} \frac{\partial}{\partial q_i} \right) \tag{2}$$

such as

$$:f:g = \{f,g\}. \tag{3}$$

This notation and everything about the Lie operator as well as the following Lie transform is addressed in [1]. The theory used here is also discussed in Chapter 9 of [3].

Exercise: Hamilton's equations from Lie operator

Verify that the equations of Hamilton are

$$\dot{q}_i = - : H : q_i \tag{4}$$

$$\dot{p}_i = - : H : p_i \tag{5}$$

Time derivative

The Hamilton equations are only a special case of the application of the Lie operator used with the Hamiltonian. If we have a function $f(\vec{q}, \vec{p})$ then, recalling that $\vec{q}$ and $\vec{p}$ are functions of t we can calculate its time derivative applying the chain rule

$$\begin{aligned} \frac{df}{dt} &= \sum_{i=1}^{n}\left(\frac{\partial f}{\partial q_i}\dot{q}_i + \frac{\partial f}{\partial p_i}\dot{p}_i\right) \\ &= \sum_{i=1}^{n}\left(\frac{\partial f}{\partial q_i}\frac{\partial H}{\partial p_i} - \frac{\partial f}{\partial p_i}\frac{\partial H}{\partial q_i}\right) \\ &= -:H:f. \end{aligned} \tag{6}$$

Time derivative

The consequence of Eq. (6) is the possibility to calculate the higher order time derivatives of q and p as

$$\frac{d^n}{dt^n} q_i = -:H: \frac{d^{n-1}}{dt^{n-1}} q_i = (-1)^n :H:^n q_i \tag{7}$$

$$\frac{d^n}{dt^n} p_i = -:H: \frac{d^{n-1}}{dt^{n-1}} p_i = (-1)^n :H:^n p_i \tag{8}$$

where we defined the power of the Lie operator as the iterations $:H:^2 f =:H:(:H:f)$. Now we have all the ingredients for our non-linear theory.

The non-linear solution

Let say that we found the solution $\vec{v}(t)$ of the Hamilton equations

$$\frac{d\vec{v}}{dt} = S\vec{\nabla}^T H \tag{9}$$

we can always express this solution as the Taylor expansion in time

$$\vec{v}(t) = \vec{v}(0) + t\, \frac{d\vec{v}}{dt}\bigg|_{t=0} + \frac{t^2}{2}\, \frac{d^2\vec{v}}{dt^2}\bigg|_{t=0} \dots \tag{10}$$

and applying the Eqs. (7,8) to every coordinates of $\vec{v}$ we have

$$\begin{aligned} \vec{v}(t) &= \vec{v}(0) - t\,(:H:\vec{v})_{t=0} + \frac{t^2}{2}\left(:H:^2\vec{v}\right)_{t=0} \dots \\ \vec{v}(t) &= e^{-t:H:}\vec{v}(0). \end{aligned} \tag{11}$$

The differential operator $e^{:f:}$ is called the Lie transform through f, so in our case we are doing the Hamiltonian Lie transform of the initial vector in order to obtain the dynamics. The solution (11) is only formal because it does not exist an easy way to calculate the exponential of the Lie operator and the Taylor series of the exponential has to be evaluated truncating the series.

Exercise: the drift space with Lie transform

Even if in general the solution (11) requires to truncate the series, this is not always the case. To see this calculate the one dimensional dynamics of a particle through a classical drift space with Hamiltonian

$$H = \frac{p^2}{2m} \tag{12}$$

and with the relativistic Hamiltonian

$$H = \sqrt{p^2c^2 + m^2c^4}. \tag{13}$$

Finally, calculate the full 6D drift space using the electromagnetic Hamiltonian when $\vec{a} = 0$ and $\phi = 0$

$$H = \frac{\delta}{\beta_0} - \sqrt{\left(\delta + \frac{1}{\beta_0}\right)^2 - p_x^2 - p_y^2 - \frac{1}{\beta_0^2\gamma_0^2}}. \tag{14}$$

Beam transport

In the linear dynamic we were able to transport not only a single particle, but also some statistical function of the beam such as the RMS. Can we do something similar with the formalism of Lie transform? The short answer is yes. We have the following equalities

$$f(e^{-t:H:}\vec{v}(0)) = f(\vec{v}(t)) = e^{-t:H:} f(\vec{v}(0)) \tag{15}$$

where the first is due to the Eq. (11) while the second is the combination of Eq. (11) with the Eq. (6). This also means that the following property

$$e^{-t:H:} f(\vec{v}) = f(e^{-t:H:}\vec{v}). \tag{16}$$

holds for any solution $\vec{v}$ of the Hamilton's equations.

Now let us consider a curve defined on the initial phase space, for example we can evaluate the ellipse around the initial beam

$$\xi(x, p_x) = \gamma x^2 + 2\alpha x p_x + \beta p_x^2 - \pi\epsilon = 0. \tag{17}$$

If we want to know how this curve appears in the transformed space we have to consider that the new canonical coordinates will be transformed according to

$$x_{new} = e^{-t:H:}x; \quad p_{x_{new}} = e^{-t:H:}p_x \tag{18}$$

that means

$$x = e^{t:H:}x_{new}; \quad p_x = e^{t:H:}p_{x_{new}} \tag{19}$$

where we used the property $e^{:f:}e^{-:f:} = \mathbb{1}$.

Then $\xi(x, p_x)$ can be written as

$$\xi(x, p_x) = \xi\left(e^{t:H:} x_{new}, e^{t:H:} p_{x_{new}}\right) \tag{20}$$

but we know, from the Eq. (16) that

$$\xi\left(e^{t:H:} x_{new}, e^{t:H:} p_{x_{new}}\right) = e^{t:H:} \xi(x_{new}, p_{x_{new}}) \tag{21}$$

and this means that to evaluate the ellipse on the new space we have to evaluate the function

$$e^{t:H:} \xi(x_{new}, p_{x_{new}}) = 0. \tag{22}$$

Summary Scheme

Define an Hamiltonian

Is quadratic (or Taylor expanded)

$M(t) = e^{tSW}$

Single-particle dynamics:
$\vec{v}(t) = M(t) v_0$

Multi-particle dynamics:
$\Sigma_t = M \Sigma_0 M^T$

Is not quadratic

Transfer map $e^{-t:H:}$

Single-particle dynamics:
$\vec{v}(t) = e^{-t:H:} v_0$

Multi-particle dynamics:
$f(\vec{v}) = e^{t:H:} f(\vec{v_0})$.

Computational Exercise: quadrupole with Lie transform

Considering the 1D Hamiltonian for a quadrupole

$$H = \frac{p_x^2}{2} + k^2 \frac{x^2}{2} \tag{23}$$

generate 10000 random particles in one dimension (x, p_x) with $0 \leq x \leq 5e-3$ m and $0 \leq p_x \leq 5e-6$ and transport them with a quadrupole of length $L = 1$ m and k=0.05 T/m using the Lie transform tecnique truncating the series at the order 20.

Calculate the Twiss parameters α, β, γ, the emittance, and transport the ellipse

$$\gamma x^2 + 2\alpha x p_x + \beta p_x^2 - 1.5\pi\epsilon = 0 \tag{24}$$

using the Lie transform.

Solutions

Solutions to proposed exercises.

Solution: Hamilton's equations from Lie operator

Verify that the equations of Hamilton are

$$\dot{q}_i = - : H : q_i \tag{25}$$

$$\dot{p}_i = - : H : p_i \tag{26}$$

Solution: Hamilton's equations from Lie operator

The solution is immediate applying the definition of Lie operator

$$: H : q_i = \sum_{i=1}^{n} \left(\frac{\partial H}{\partial q_i} \frac{\partial}{\partial p_i} - \frac{\partial H}{\partial p_i} \frac{\partial}{\partial q_i} \right) q_i \qquad (27)$$

$$: H : p_i = \sum_{i=1}^{n} \left(\frac{\partial H}{\partial q_i} \frac{\partial}{\partial p_i} - \frac{\partial H}{\partial p_i} \frac{\partial}{\partial q_i} \right) p_i \qquad (28)$$

and recalling that the q_i and p_i variables are all independent, so the cross detivatives are all zero. Then the result is

$$: H : q_i = - \frac{\partial H}{\partial p_i} \qquad (29)$$

$$: H : p_i = \frac{\partial H}{\partial q_i} \qquad (30)$$

that are exactly the Hamilton equations with the flipped sign and this justify the minus sign.

Solution: the drift space with Lie transform

Even if in general the solution (11) requires to truncate the series, this is not always the case. To see this calculate the one dimensional dynamics of a particle through a classical drift space with Hamiltonian

$$H = \frac{p^2}{2m} \tag{31}$$

and with the relativistic Hamiltonian

$$H = \sqrt{p^2 c^2 + m^2 c^4}. \tag{32}$$

Finally, calculate the full 6D drift space using the electromagnetic Hamiltonian when $\vec{a} = 0$ and $\phi = 0$

$$H = \frac{\delta}{\beta_0} - \sqrt{\left(\delta + \frac{1}{\beta_0}\right)^2 - p_x^2 - p_y^2 - \frac{1}{\beta_0^2 \gamma_0^2}}. \tag{33}$$

Solution: the drift space with Lie transform

First the classical case. We start noticing that

$$:H:q=:\frac{p^2}{2m}:q=\frac{\partial\frac{p^2}{2m}}{\partial q}\frac{\partial q}{\partial p}-\frac{\partial\frac{p^2}{2m}}{\partial p}\frac{\partial q}{\partial q}=-\frac{p}{m} \tag{34}$$

and as consequence

$$:H:^2 q=:H:-\frac{p}{m}=0 \tag{35}$$

which means that only the first term of the exponential is different from zero, all the other terms are zero and we do not have to truncate. For the same argument of Eq. (35) we have for the momentum

$$:H:p=0. \tag{36}$$

Solution: the drift space with Lie transform

We can calculate the equations of motion now

$$q(t) = e^{-t:H:}q\big|_{t=0} = q_0 + t\frac{p_0}{m} \quad (37)$$

$$p(t) = e^{-t:H:}p\big|_{t=0} = p_0 \quad (38)$$

where $q_0 = q(0)$ and $p_0 = p(0)$. The result is the same as the exercise in the first lecture as expected for the classical particle.

Solution: the drift space with Lie transform

For the relativistic Hamiltonian we apply the same method

$$
\begin{aligned}
:H:q &= :\sqrt{p^2c^2+m^2c^4}:q \\
&= \frac{\partial\sqrt{p^2c^2+m^2c^4}}{\partial q}\frac{\partial q}{\partial p} - \frac{\partial\sqrt{p^2c^2+m^2c^4}}{\partial p}\frac{\partial q}{\partial q} \\
&= -\frac{pc}{\sqrt{p^2+m^2c^2}} \qquad (39)
\end{aligned}
$$

and again we can see that if we iterate $:H:^2 q$ we obtain zero, as well as for $:H:p=0$. Them the equations of motion are

$$
q(t) = e^{-t:H:}q\big|_{t=0} = q_0 + t\frac{p_0}{\gamma m} \qquad (40)
$$

$$
p(t) = e^{-t:H:}p\big|_{t=0} = p_0 \qquad (41)
$$

using the definition of momentum $p=\gamma\beta mc$ and $\gamma^2-1=\gamma^2\beta^2$.

Solution: the drift space with Lie transform

And now for the complicate one. From the previous two cases we learned that when we iterate the Lie operator of an Hamiltonian that depends only by the momentum on the position variable we eventually obtain zero. Moreover, we saw that when we apply the same operator to the momentum we obtain zero. So, we know already

$$p_x(L) = p_{x0}; \quad p_y(L) = p_{y0}; \quad \delta(L) = \delta_0 \tag{42}$$

and for the positions we will have

$$x(L) = x_0 - L : H : x \tag{43}$$

$$y(L) = y_0 - L : H : y \tag{44}$$

$$z(L) = z_0 - L : H : z \tag{45}$$

Solution: the drift space with Lie transform

If we call

$$d = \sqrt{\left(\delta + \frac{1}{\beta_0}\right)^2 - p_x^2 - p_y^2 - \frac{1}{\beta_0^2\gamma_0^2}} \tag{46}$$

then we have

$$\begin{aligned} x(L) &= x_0 + L\frac{p_{x0}}{d} &(47)\\ y(L) &= y_0 + L\frac{p_{y0}}{d} &(48)\\ z(L) &= z_0 + \frac{L}{\beta_0}\left(1 - \frac{1}{d}\right) - L\frac{\delta_0}{d}. &(49) \end{aligned}$$

It is remarkable to see that not even the simplest element of a particle accelerator is linear!

Solution: the drift space with Lie transform

The motion in the three directions depends on d that is a non-linear function of the initial conditions. In particular there is a dependency from the energy offset δ. Such a dependency is called chromaticity of the beam.

In accelerator physics literature, a particle accelerator is frequently seen as an optical system like a set of lenses. This is due to the fact that quadrupolar magnets act in a similar way as a focusing or defocusing lens. But we have to keep in mind that the nature of particles and the one of the light is fundamentally different. The light is massless, and its speed in vacuum is a constant for any color (any energy). A particle beam has an energy spread that produces a velocity spread, and even in the empty space we see a chromatic aberration where particle with different energies travel different lengths in the same time.

Solution: quadrupole with Lie transform

Considering the 1D Hamiltonian for a quadrupole

$$H = \frac{p_x^2}{2} + k^2 \frac{x^2}{2} \tag{50}$$

generate 10000 random particles in one dimension (x, p_x) with $0 \leq x \leq 5e-3$ m and $0 \leq p_x \leq 5e-6$ and transport them with a quadrupole of length $L = 1$ m and k=0.05 T/m using the Lie transform tecnique truncating the series at the order 20.

Calculate the Twiss parameters α, β, γ, the emittance, and transport the ellipse

$$\gamma x^2 + 2\alpha x p_x + \beta p_x^2 - 1.5\pi\epsilon = 0 \tag{51}$$

using the Lie transform.

Solution: quadrupole with Lie transform

We first generate the particles, calculate the standard deviations and the Twiss functions

```
x_array = random.normal(0.0, 5e-3, size=10000)
px_array = random.normal(0, 5e-6, size=10000)

sigma_x = x_array.std()**2
sigma_px = px_array.std()**2
sigma_xpx = sum((x_array-x_array.mean())*(px_array-
    px_array.mean()))/len(x_array)
sigma_x, sigma_xpx, sigma_px

emit = numpy.sqrt(sigma_x*sigma_px-sigma_xpx**2)
alpha = -sigma_xpx/emit
beta = sigma_x/emit
gamma = sigma_px/emit
```

Solution: quadrupole with Lie transform

then we define the ellipse

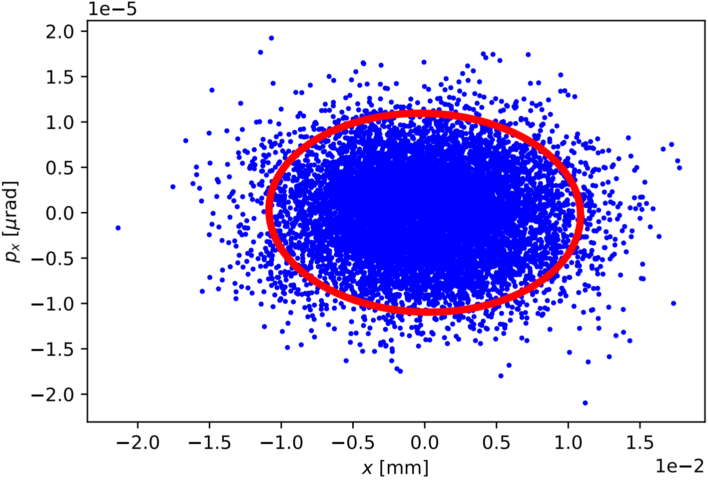
```
x_ellipse = numpy.linspace(x_array.min(), x_array.max()
    , 1000)
p_ellipse = numpy.linspace(px_array.min(), px_array.max
    (), 1000)
x_ellipse, p_ellipse = numpy.meshgrid(x_ellipse,
    p_ellipse)
ellipse = gamma*x_ellipse**2+2*alpha*x_ellipse*
    p_ellipse+beta*p_ellipse**2-1.5*numpy.pi*emit
```

Solution: quadrupole with Lie transform

and we plot

```
plt.ticklabel_format(style='sci', axis='x', scilimits
    =(0,0))
plt.ticklabel_format(style='sci', axis='y', scilimits
    =(0,0))
plt.xlabel('$x$ [mm]')
plt.ylabel('$p_x$ [$\mu$rad]')
plt.scatter(x_array, px_array,s=3, facecolor='b')
plt.xlim(1.1*x_array.min(),1.1*x_array.max())
plt.ylim(1.1*px_array.min(),1.1*px_array.max())
plt.contour(x_ellipse, p_ellipse, ellipse,[0],
    linewidths=4 ,colors='r')
plt.show()
```

Solution: quadrupole with Lie transform



Solution: quadrupole with Lie transform

We create the symbolic calculator for the Lie transform

```python
import sympy
x, p = sympy.symbols('x,p_x', real=True)
def lie_operator(f, g):
    return f.diff(x)*g.diff(p)-f.diff(p)*g.diff(x)
def lie_transform(f, g, order):
    step = lie_operator(f, g)
    result = g + step
    for i in range(2,order+1,1):
        step = sympy.simplify(lie_operator(f, step))
        result = sympy.simplify(result + step/sympy.factorial(i))
    return result
```

Solution: quadrupole with Lie transform

Now we are ready to transform our beam. We generate the Hamiltonian, transport with the Lie transform and transform it in a numeric function with lambdify.

```
L = 1.0
k = 0.05
H = (p**2/2+k**2*x**2/2)
order=20
xf = sympy.lambdify((x,p),lie_transform(-L*H,x,order))
pf = sympy.lambdify((x,p),lie_transform(-L*H,p,order))

new_x_array = xf(x_array,px_array)
new_px_array = pf(x_array,px_array)
```

Solution: quadrupole with Lie transform

In the same way we transport the ellipse.

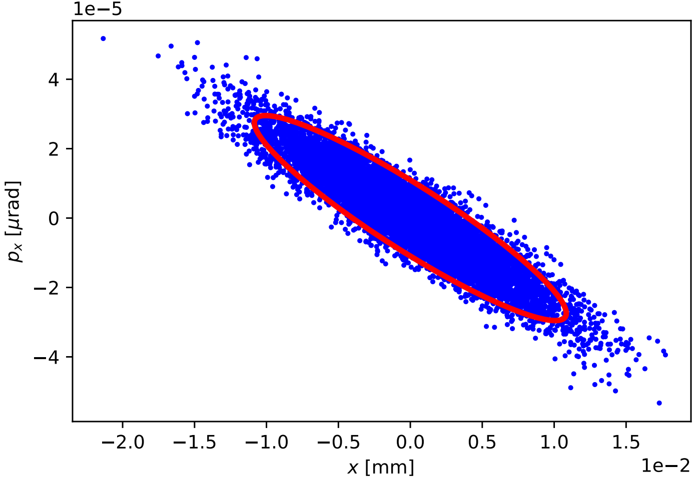
```
x_ellipse = numpy.linspace(new_x_array.min(),
    new_x_array.max(), 1000)
p_ellipse = numpy.linspace(new_px_array.min(),
    new_px_array.max(), 1000)
x_ellipse, p_ellipse = numpy.meshgrid(x_ellipse,
    p_ellipse)
ellipse_sym = sympy.lambdify((x,p), lie_transform(L*H,
    gamma*x**2+2*alpha*x*p+beta*p**2-1.5*numpy.pi*emit,
    order), numpy)
ellipse=ellipse_sym(x_ellipse, p_ellipse)
```

Solution: quadrupole with Lie transform

And finally we plot the result.

```
plt.ticklabel_format(style='sci', axis='x', scilimits=(0,0))
plt.ticklabel_format(style='sci', axis='y', scilimits=(0,0))
plt.xlabel('$x$ [mm]')
plt.ylabel('$p_x$ [$\mu$rad]')
plt.scatter(new_x_array, new_px_array,s=3, facecolor='b')
plt.xlim(1.1*new_x_array.min(),1.1*new_x_array.max())
plt.ylim(1.1*new_px_array.min(),1.1*new_px_array.max())
plt.contour(x_ellipse, p_ellipse, ellipse,[0], linewidths=3 ,colors='r')
plt.show()
```

Solution: quadrupole with Lie transform



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