# NON-LINEAR DYNAMICS MODEL FOR THE ESS LINAC SIMULATOR 

## Abstract

The ESS Proton Linac will run a beam with 62.5 mA of current. In the first meters of the accelerator, the nonlinear space-charge force dominates the dynamics of the beam. The Drift Tube Linac, the Spoke resonators and the elliptical cavities, which are responsible for the $99.8 \%$ of the total energy gained by the beam along the accelerator, produce a significant longitudinal non-linear force on the proton beam. In this paper, we introduce a new theory to transport the probability density function of the beam under the effect of non-linear forces. A model based on this theory can be implemented in the ESS Linac Simulator for the fast simulations to be performed during the operations of the proton Linac.

## INTRODUCTION

The success of the Courant-Snyder theory with particle accelerators is due to the simple connection between the dynamics of one particle and the dynamics of a beam. A single particle is fully described by the vector of its coordinates and momenta at a given time:

$$
\begin{equation*}
\vec{v}=\left(q_{1} q_{2} \ldots q_{n} p_{1} p_{2} \ldots p_{n}\right)^{T} . \tag{1}
\end{equation*}
$$

If $\mathcal{H}$ is the Hamiltonian, the equations of motion can be expressed as

$$
\begin{equation*}
\frac{d}{d t} \vec{v}=S \cdot \vec{\partial} \mathcal{H} \tag{2}
\end{equation*}
$$

where $\vec{\partial}$ and $S$ are defined as

$$
\begin{gather*}
\vec{\partial}=\left(\partial / \partial q_{1} \partial / \partial q_{2} \ldots \partial / \partial q_{n} \partial / \partial p_{1} \partial / \partial p_{2} \ldots \partial / \partial p_{n}\right)^{T}  \tag{3}\\
S=\left(\begin{array}{cc}
0 & I \\
-I & 0
\end{array}\right) . \tag{4}
\end{gather*}
$$

When the Hamiltonian is quadratic in coordinates and momenta, $\mathcal{H}=f\left(q_{i}{ }^{2}, p_{i}{ }^{2}\right)$, it can be written as $\vec{\partial} H=A \cdot \vec{v}$, where A is a matrix. The equations of motion become

$$
\begin{equation*}
\frac{d}{d t} \vec{v}=S \cdot A \cdot \vec{v} \tag{5}
\end{equation*}
$$

with the solution

$$
\begin{array}{r}
\vec{v}(t)=e^{t S A} \cdot \vec{v}(0) \\
M(t)=e^{t S A} \\
\vec{v}(t)=M(t) \cdot \vec{v}(0) . \tag{8}
\end{array}
$$

In this case, $M(t)$ is the transport matrix that effects the changes of coordinates and momenta for each linear element of the accelerator.

Because of the linear nature of Eq. (8), it is possible to use the same matrix $M(t)$ to transport the r.m.s. of a bunch

[^0]of particles using equation [1]:
\[

\left($$
\begin{array}{cc}
\sigma_{x}^{2} & \sigma_{x} \sigma_{x^{\prime}} \\
\sigma_{x} \sigma_{x^{\prime}} & \sigma_{x^{\prime}}^{2}
\end{array}
$$\right)_{t}=M\left($$
\begin{array}{cc}
\sigma_{x}^{2} & \sigma_{x} \sigma_{x^{\prime}} \\
\sigma_{x} \sigma_{x^{\prime}} & \sigma_{x^{\prime}}^{2}
\end{array}
$$\right)_{0} M^{T}
\]

(9)
here we only consider one dimension, using the standard notation $x=q_{x}$ and $x^{\prime}=\frac{p_{x}}{p_{z}}$, where $q_{x}$ and $p_{x}$ are the respective conjugate coordinate and momentum in the horizontal plane $x$ and $p_{z}$ is the momentum in the direction of motion of the particles.

When the force is non-linear, $\mathcal{H} \neq f\left(q_{i}{ }^{2}, p_{i}{ }^{2}\right)$, Eqs. (8) and (9) are no longer valid. In the following sections, we will show how to construct a general solution for the equations of motion of a bunch of particles, starting from the solution of the equation for a single particle, generalising the Eq. (9) for the case of non-linear forces.

## BEAM DENSITY

Let us assume that we were able to solve the equation of motion in (2) in the case of a non-linear force, that is, when $\mathcal{H} \neq f\left(q_{i}{ }^{2}, p_{i}{ }^{2}\right)$. We will then have an equation of motion for a single particle in the form

$$
\begin{equation*}
\vec{v}(t)=f(\vec{v}(0)) \tag{10}
\end{equation*}
$$

where $f$ is

$$
\begin{equation*}
f: \mathbb{R}^{2 n} \rightarrow \mathbb{R}^{2 n} \tag{11}
\end{equation*}
$$

with $n$ coordinates and momenta; for all the practical cases $n=3$.

In order to pass from the single-particle solution to one with many particles, we start by considering an invariant of a beam: the number of particles. This number will not change along the accelerator unless the losses are a significant fraction of the total number of particles. If $\rho_{p s}$ is the probability density function of the beam in the phase space, the number of particles can be expressed as:

$$
\begin{equation*}
N=\int_{\mathbb{R}^{2 n}} \rho_{p s} d q_{1} d q_{2} \ldots d q_{n} d p_{1} d p_{2} \ldots d p_{n} \tag{12}
\end{equation*}
$$

We know from the Liouville theorem that if the dynamics is symplectic then the volume of the phase space is preserved. Thus, any dynamics that apply it will keep the quantity $d q_{1} d q_{2} \ldots d q_{n} d p_{1} d p_{2} \ldots d p_{n}$ constant. On the other hand, we also know that the number of particles is preserved in the physical space and in the momentum space separately:

$$
\begin{align*}
N & =\int_{\mathbb{R}^{n}} \rho_{r} d q_{1} d q_{2} \ldots d q_{n}  \tag{13}\\
N & =\int_{\mathbb{R}^{n}} \rho_{m} d p_{1} d p_{2} \ldots d p_{n} \tag{14}
\end{align*}
$$

where $\rho_{r}$ and $\rho_{m}$ are the beam density in the real space and in the momentum space, respectively. These two integrals are invariant all along the machine and we can express this invariance by saying that at any time $t$ the following
equations are valid:

$$
\begin{align*}
\rho_{r}(t) V_{r}(t) & =\rho_{r}(0) V_{r}(0)  \tag{15}\\
\rho_{m}(t) V_{m}(t) & =\rho_{m}(0) V_{m}(0)  \tag{16}\\
V_{r}(t) V_{m}(t) & =V_{r}(0) V_{m}(0) \tag{17}
\end{align*}
$$

where $V_{r}$ and $V_{m}$ are the volume elements given by $V_{r}=$ $d q_{1} d q_{2} \ldots d q_{n}$ and $V_{m}=d p_{1} d p_{2} \ldots d p_{n}$ and Eq. (17) expresses the invariance of the phase-space volume.
We can now see the function $f$ from Eq. (10) as a geometrical transformation of space: $f$ will send the points of $\mathbb{R}^{2 n}$ into new points of $\mathbb{R}^{2 n}$. Consequently, we can calculate how the volume elements $V_{r}$ and $V_{m}$ are transformed under the action of $f . V_{r}$ is an $n$-form and its transformation is such that

$$
\begin{equation*}
V_{r}(t)=\left|J_{r}\right| V_{r}(0) \tag{18}
\end{equation*}
$$

where $\left|J_{r}\right|$ is the determinant of the Jacobian matrix, constructed as

$$
J_{r}=\left(\begin{array}{ccc}
\frac{\partial f_{q_{1}}}{\partial q_{1}} & \ldots & \frac{\partial f_{q_{1}}}{\partial q_{n}}  \tag{19}\\
\vdots & \vdots & \vdots \\
\frac{\partial f_{q_{n}}}{\partial q_{1}} & \ldots & \frac{\partial f_{q_{n}}}{\partial q_{n}}
\end{array}\right) .
$$

The change in the volume $V_{r}$ in Eq. (15) has to be cancelled by the same but opposite change in the density function $\rho_{r}$ in order to keep the number of particles constant (the same applies to $V_{m}$ and $\rho_{m}$ ). We then have

$$
\begin{align*}
\rho_{r}(t) & =\frac{\rho_{r}(0)}{\left|J_{r}\right|}  \tag{20}\\
\rho_{m}(t) & =\frac{\rho_{m}(0)}{\left|J_{m}\right|} . \tag{21}
\end{align*}
$$

Equations (20) and (21) are general equations of motion for a bunch of particles under the influence of linear and non-linear forces.

The technique for expressing the beam dynamics will then require solving the equation of motion for a single particle, calculating the Jacobian matrix and its determinant, and finally dividing the beam density function by this determinant. This technique can mean facing the difficulty that the function $f$ from Eq. (10) will typically depend on $q_{i}$ and $p_{i}$ and the evaluation of the two separate Jacobians will require some assumptions about a possible dependency of the momentum on the position.

## LIE TRANSFORMATION

So far, nothing has been said about the function $f$ from Eq. (10), which is responsible for the transport of a single particle. The most elegant way to treat a general non-linear Hamiltonian is to use the Lie transformation [2-4]. If $f$ : $\mathbb{R}^{2 n} \rightarrow \mathbb{R}^{2 n}$ and $g: \mathbb{R}^{2 n} \rightarrow \mathbb{R}^{2 n}$ are two differentiable functions, then we say that the Lie operator : $f$ : is applied to $g$

$$
\begin{equation*}
: f: g=\sum_{i=1}^{n}\left(\frac{\partial f}{\partial q_{i}} \frac{\partial g}{\partial p_{i}}-\frac{\partial f}{\partial p_{i}} \frac{\partial g}{\partial q_{i}}\right) . \tag{22}
\end{equation*}
$$

It is also possible to calculate the powers of a Lie operator such as

$$
\begin{equation*}
(: f:)^{2} g=: f:(: f: g) \tag{23}
\end{equation*}
$$

In particular,

$$
\begin{equation*}
e^{: f:} g=\sum_{i=0}^{\infty} \frac{(: f:)^{i}}{i!} g \tag{24}
\end{equation*}
$$

is called the $f$ Lie transformation of $g$. In an element of finite length $L$ with an Hamiltonian $\mathcal{H}$ we have the special relationship

$$
\begin{align*}
q_{i}(L) & =e^{:-L \mathcal{H}:} q_{i}(0)  \tag{25}\\
p_{i}(L) & =e^{:-L \mathcal{H}} p_{i}(0) \tag{26}
\end{align*}
$$

or, in our notation

$$
\begin{equation*}
\vec{v}(L)=e^{:-L \mathcal{H}: \vec{v}(0)} \tag{27}
\end{equation*}
$$

which is the general equation for the transport of a particle, regardless of the linear or non-linear nature of the force. A proof of this equation can be found in [3].

## LINEAR EXAMPLE

The one-dimensional Hamiltonian for a quadrupolar force is

$$
\begin{equation*}
\mathcal{H}=\frac{1}{2}\left(k^{2} x^{2}+p_{x}^{2}\right) . \tag{28}
\end{equation*}
$$

The equations of motion in terms of Lie transform are then

$$
\begin{align*}
x_{L} & =e^{:-\frac{L}{2}\left(k^{2} x^{2}+p_{x}^{2}\right):} x  \tag{29}\\
p_{x_{L}} & =e^{:-\frac{L}{2}\left(k^{2} x^{2}+p_{x}^{2}\right):} p_{x} \tag{30}
\end{align*}
$$

where the $L$ index refers to the variables after the action of a magnet of length $L$. Recalling Eq. (24) we have

$$
\begin{align*}
x_{L} & =\sum_{i=0}^{\infty}(-1)^{i}\left[\frac{(k L)^{2 i}}{(2 i)!} x+\frac{(k L)^{2 i+1}}{(2 i+1)!} \frac{p_{x}}{k}\right]  \tag{31}\\
P_{x_{L}} & =\sum_{i=0}^{\infty}(-1)^{i}\left[-\frac{(k L)^{2 i+1}}{(2 i+1)!} k x+\frac{(k L)^{2 i}}{(2 i)!} p_{x}\right] \tag{32}
\end{align*}
$$

or

$$
\begin{align*}
x_{L} & =x \cos (k L)+\frac{p_{x}}{k} \sin (k L)  \tag{33}\\
p_{x_{L}} & =-k x \sin (k L)+p_{x} \cos (k L) \tag{34}
\end{align*}
$$

which are the well-known expressions for motion through a quadrupole.

We can calculate how the standard deviation of the beam changes under this transformation:

$$
\begin{equation*}
\sigma_{x_{L}}^{2}=\int_{\mathbb{R}^{2}} x_{L}^{2} \rho_{p s} d x d p_{x} \tag{35}
\end{equation*}
$$

We know from Eqs. (20) and (21) that the quantity $\rho_{p s} d x d p_{x}$ is constant, so we have

$$
\begin{align*}
\sigma_{x_{L}}^{2}= & \int_{\mathbb{R}^{2}}\left(x \cos (k L)+\frac{p_{x}}{k} \sin (k L)\right)^{2} \rho_{p s} d x d p_{x}(36) \\
= & \cos ^{2}(k L) \sigma_{x}^{2}+\frac{\sin ^{2}(k L)}{k^{2}} \sigma_{p_{x}^{2}}+  \tag{37}\\
& +\frac{2 \cos (k L) \sin (k L)}{k} \sigma_{x} \sigma_{p_{x}} . \tag{38}
\end{align*}
$$

This result is the same as what we would have obtained if we used the standard equation for the linear transport Eq. (9).

It is worth noting here that our $\sigma_{x_{L}}$ is a linear combination of the initial $\sigma$ 's because the transport map was linear. When
the map is non-linear, the standard deviation can still be calculated by expanding the non-linear function and evaluating the high-order statistical estimator, such as:
$\left\langle q_{i}(t)\right\rangle=\alpha_{\left\langle q_{i}\right\rangle}\left\langle q_{i}(0)\right\rangle+\alpha_{\left\langle q_{i}{ }^{2}\right\rangle}\left\langle q_{i}(0)^{2}\right\rangle+\alpha_{\left\langle q_{i}{ }^{3}\right\rangle}\left\langle q_{i}(0)^{3}\right\rangle+\ldots$
where the $\alpha$ coefficients are from the Taylor expansion. This evaluation of the standard deviation can be concatenated for different non-linear elements only if after a certain $\alpha$ the terms are negligible. Otherwise, the truncated series will introduce an error that will diverge.

## NON-LINEAR EXAMPLE

The one dimensional Hamiltonian for an octupolar force with a gradient $k_{3}$ is:

$$
\begin{equation*}
\mathcal{H}=\frac{1}{4}\left(k_{3} x^{4}+p_{x}^{2}\right) \tag{40}
\end{equation*}
$$

The equations of motion in terms of the Lie transform are then:

$$
\begin{align*}
x_{L} & =e^{:-\frac{L}{4}\left(k_{3} x^{4}+p_{x}^{2}\right):} x  \tag{41}\\
p_{x_{L}} & =e^{:-\frac{L}{4}\left(k_{3} x^{4}+p_{x}^{2}\right):} p_{x} \tag{42}
\end{align*}
$$

This calculation cannot be performed in the same elegant manner as the linear example because the sum from the Lie transform does not converge to a known function as before. Nevertheless, it is possible to expand the exponential according to Eq. (24), truncate at certain order, and evaluate it. The choice of the order to truncate to and the relative error can be evaluated using the determinant of the full Jacobian for the phase space. In one dimension it is:

$$
\begin{equation*}
|J|=\frac{\partial x_{L}}{\partial x} \frac{\partial p_{x_{L}}}{\partial p_{x_{L}}}-\frac{\partial x_{L}}{\partial p_{x_{L}}} \frac{\partial p_{x_{L}}}{\partial x} \tag{43}
\end{equation*}
$$

This determinant has to be one, $|J|=1$, so the distance of this determinant from 1 is the error due to the approximation of the truncated series in Eqs. (41) and (42). The result is like

$$
\begin{align*}
\tilde{x}_{L} & =\sum_{i=0}^{n} \frac{(:-L \mathcal{H}:)^{i}}{i!} x  \tag{44}\\
\tilde{p}_{x_{L}} & =\sum_{i=0}^{n} \frac{(:-L \mathcal{H}:)^{i}}{i!} p_{x} \tag{45}
\end{align*}
$$

where the $\sim$ express the approximation of the series at the order $n$. Finally the evaluation of the new beam density is performed applying Eq. (20); in the one-dimensional case the determinant of the Jacobian is simply the derivative

$$
\begin{equation*}
\left|J_{r}\right|=\frac{d \tilde{x}_{L}}{d x} \tag{46}
\end{equation*}
$$

$\tilde{x}_{L}$ is a function of $x$ and $p_{x}$ but for the purpose of this paper we evaluate the determinant assuming large-aptitude particles where the approximation $p_{x}=-\frac{\alpha}{\beta} x$ holds.

In Fig. 1 the qualitative behaviour of a Gaussian beam is illustrated, passing through an octupole with the Hamiltonian of Eq. (40) or a sextupole of Hamiltonian $\mathcal{H}=\frac{1}{6} k_{2} x^{3}+\frac{p_{x}^{2}}{2}$.

The characteristics shape for the transit of the beam through a sextupole or an octupole is obtained using the


Figure 1: [Color] Gaussian beam passing through a sextupole or an octupole. The characteristic shift on the beam center is visible for the sextupole, while the folding of the tails is visible for the octupole.
theory illustrated in herein. This shape is in agreement with previous results, as seen in [5] and [6].

## CONCLUSIONS

We presented a new technique for addressing the nonlinear problem of beam dynamics based on the study of beam density. This method is analogous to the standard envelope calculation when the force is linear. In the non-linear case, the modification of the beam density is useful for understanding the behavior of the beam without requiring full multi-particle tracking. The sextupole and octupole calculations are qualitatively in agreement. The future development of this technique will involve the prediction of experimental results, such as the effect of strong non-linear space charges of high-current accelerators like ESS.

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