SELF-CONSISTENT SPACE CHARGE TRACKING METHOD BASED ON LIE TRANSFORM

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Abstract

In this paper we propose to describe the self-force of a particles beam, known as space charge, as a Hamiltonian term dependent on the distribution of the particles' coordinates: $H_{sc} \equiv H_{sc}(\rho(x, y, z))$. This Hamiltonian is then used, together with the kinetic component H_k in a Lie transform to generate a transport map by $e^{-L:H_k+H_{sc}:}$ where the Lie operator $: H_k + H_{sc} :$ is defined according to the Dragt's notation [1]. Then the Lie transform is used to transport directly the distribution function $\rho(x, y, z)$ in a self-consistent iterative algorithm. The result of this proof-of-concept idea is verified on a drift space and on a FODO channel and compared with a traditional multi-particles simulation code.

INTRODUCTION

The research in particle accelerator is moving towards the high intensity particle accelerators in order to have frontier machine in terms of beam power such the European Spallation Source proton Linac, currently under construction in Lund, Sweden [2, 3]. The increasing in beam intensity rises the issue of a proper treatment of the space-charge force in the beam dynamic simulations. Today these simulations are mainly treated with multi-particle codes with various algorithm, like the so-called Particle-In-Cell (PIC), requiring an intensive computational power. In this paper we apply a different approach to simulate a beam, without transporting multi-particle, under the effect of intense space-charge force using the Lie transform as described in [1, Chapter 5], and [4, Chapter 5]. The idea is to start from the beam distribution; find the associated potential solving the Maxwell equations; using the potential in a Hamiltonian to propagate the beam distribution itself in the next step and iterate it for all the required steps using a symbolic calculator. The article will introduce the Lie transform as formal solution of the Hamilton equations then it will be applied to a general function of the beam and finally to the specific cases of the transport of the space charge. The results are compared with the program TraceWin [5].

THE LIE TRANSFORM

We start considering the dynamics expressed by the Hamilton equations in form of Poisson brackets as

$$\dot{q} = \frac{\partial H}{\partial p} = -\{H, q\}; \qquad \dot{p} = -\frac{\partial H}{\partial q} = -\{H, p\} \qquad (1)$$

for any pair of conjugate variables q, p. We call the Poisson bracket "waiting" operator $\{H, \cdot\} =: H :$ as the Lie operator.

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Then the equations of Hamilton are

$$\dot{q} = - : H : q; \qquad \dot{p} = - : H : p. \qquad (2)$$

Moreover, because the Lie operator is a canonical transformations, it sends canonical variables in new canonical variables such that the time evolution of the new variable is obtained again applying the Lie operator

$$\ddot{q} = - : H : \dot{q} =: H :^2 q; \qquad \ddot{p} = - : H : \dot{p} =: H :^2 p \quad (3)$$

with the powers of the Lie operator are calculated iterating the operation as $: H :^2 q =: H : (: H : q)$. If we consider the Taylor expansion of the canonical variables in time, we have

$$q(t) = \sum_{n=0}^{\infty} \frac{t^n}{n!} \frac{d^n q}{dt^n}\bigg|_{q=q_0} = e^{-t:H:} q\big|_{q=q_0;p=p_0} \qquad (4)$$

$$p(t) = \sum_{n=0}^{\infty} \frac{t^n}{n!} \frac{d^n p}{dt^n}\bigg|_{p=p_0} = e^{-t:H:} p\big|_{q=q_0;p=p_0} \qquad (5)$$

where the exponential is defined with the usual Euler formula. The operator $e^{:f:}g$ is general called the Lie transform of g through f. The Lie transform can be used to calculate the time evolution of every infinite derivable function of the canonical coordinates. To prove this fact, let us consider $f = f(q, p)$, its time derivative is given by

$$\dot{f} = \frac{\partial f}{\partial q}\dot{q} + \frac{\partial f}{\partial p}\dot{p} = \frac{\partial f}{\partial q}\frac{\partial H}{\partial p} - \frac{\partial f}{\partial p}\frac{\partial H}{\partial q} = - : H : f \quad (6)$$

with the solution

$$f[q(t), p(t)] = e^{-t:H:} f[q, p]\big|_{q=q_0;p=p_0}. \qquad (7)$$

It is important to notice that the domain of the function f is the initial phase space. When we "transport" the function, we are interested to know how it acts on the final phase space. So the correct way to evaluate the transport of a function of the particles through the dynamics of a Hamiltonian is to apply the inverse of the Lie transform from the co-domain to the domain. The inverse Lie transform is easy to calculate because we have that $e^{-t:H:}e^{t:H:} = \mathbb{1}$.

An Example: Sextupole in 1D

If we want to transport the Courant-Snyder ellipse under the effect of a sextupole the correct steps are:

- calculate the Hamiltonian of a particle with an external sextupolar force as $H = \frac{p_x^2}{2} + k_3\frac{x^3}{6}$ with k_3 the sextupolar gradient;

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- write the equation of the ellipse for the phase space as $\eta = \beta p_x^2 + 2\alpha x p_x + \gamma x^2 - \epsilon = 0$, with $\alpha, \beta, \gamma, \epsilon$ the usual Twiss parameters and the emittance;
- apply the inverse of the Lie transform for the length of the sextupole L to the ellipse and evaluate when the new function is equal to zero $\eta_L = e^{L:H:}\eta = 0$.

The last step cannot be solved exactly but needs a certain approximation. Or the exponential is truncated at a certain order of L, loosing its property of symplecticity, or the Hamiltonian has to be split in fully integrable components following the prescriptions of the Yoshida integrator [6]. The result of the above steps is shown in Fig. 1.

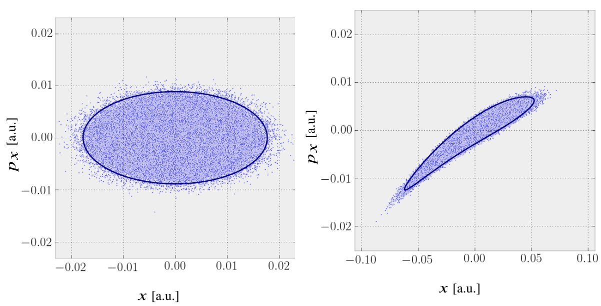

Figure 1: A Gaussian beam [left] is transported through a sextupolar force [right]. The corresponding ellipse is also transported with the inverse Lie transform $e^{L:\frac{p_x^2}{2}+k_3\frac{x^3}{6}:}\left(\beta p_x^2 + 2\alpha x p_x + \gamma x^2 - \epsilon\right)$.

SPACE CHARGE

The formalism presented in the previous section can be used, in principle, to transport the beam under the influence of the space charge. Let's assume that the beam is distributed in the space with a density function given by $\rho(x, y, z)$ traveling with a velocity $\vec{\beta}c$. The density is the projection of the 6D distribution function $n(x, p_x, y, p_y, z, p_z)$ onto the real space

$$\rho(x, y, z) = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} n(x, p_x, y, p_y, z, p_z)\,\mathrm{d}p_x \mathrm{d}p_y \mathrm{d}p_z. \quad (8)$$

The beam will produce an electric scalar potential and a magnetic vector potential that satisfy the Maxwell equations

$$\nabla^2\phi = -\frac{\rho}{\epsilon_0}; \quad \nabla\times\nabla\times\vec{A} = -\mu_0\rho\vec{\beta}c \quad (9)$$

under the assumption that the time derivatives of the electric and magnetic field are zero. We now assume that $\beta_z >> \beta_x, \beta_y$, that means also $\frac{\partial A_z}{\partial z} = 0$, $A_x = A_y = 0$. So the equations for the fields are

$$\frac{\partial\phi}{\partial x} + \frac{\partial\phi}{\partial y} + \frac{\partial\phi}{\partial z} = -\frac{\rho}{\epsilon_0} \quad (10)$$

$$\frac{\partial A_z}{\partial x} + \frac{\partial A_z}{\partial y} = -\frac{\rho}{\epsilon_0}\frac{\beta}{c}. \quad (11)$$

Once ϕ and A_z are known, the contribution of the potential to the Hamiltonian is

$$H_{sc} = q(\phi - \beta c A_z) \quad (12)$$

where q is the charge; the βc factor in front of A_z is due to the dependency of the magnetic field from the speed of the beam and the minus sign is because the magnetic force is the opposite direction with respect to the electric force. The full Hamiltonian is then given by the kinetic component H_k plus the space charge component H_{sc} plus any other external potential H_e. For example the Hamiltonian of the transverse dynamics of a beam passing through a quadrupole is

$$H = \frac{p_x^2}{2} + \frac{p_y^2}{2} + q(\phi - \beta c A_z) - \frac{k_q x^2}{2} + \frac{k_q y^2}{2}. \quad (13)$$

The particles can be transported simply applying Eqs. (4, 5) under the approximation that the time interval (or the length) is small enough such that the force of space-charge can be considered constant. The distribution function n itself is a function of the canonical coordinates, so it can be transported by the Hamiltonian through the inverse Lie transform

$$n_{\text{new}} = e^{L:H:}n_{\text{old}} \quad (14)$$

and can be used to compute the new potential. Once the new potential is calculated it can be replaced in the Hamiltonian restarting the process in an iterative algorithm. This tracking is self-consistent because the potential is transported at each step according to the dynamics described by the Hamiltonian.

TRACKING

KV Distribution

The first application of the tracking method discussed in the previous section is for a beam with a uniform particle distribution within an ellipse; the so-called Kapchinsky-Vladimirsky distribution or KV distribution [7]. This distribution is defined for an infinite long beam with a transverse section represented by an ellipse uniformly filled with particles

$$\rho(x, y, z) = \begin{cases} \frac{I}{\pi\beta c R_x R_y}, & \text{if } \frac{x^2}{R_x^2} + \frac{y^2}{R_y^2} \leq 1 \\ 0, & \text{if } \frac{x^2}{R_x^2} + \frac{y^2}{R_y^2} > 1 \end{cases} \quad (15)$$

where R_x and R_y are the semiaxes of the ellipse. Because the distribution is defined in two dimensions, the Eqs. (10) and (11) differs only for the constant factor $\frac{\beta}{c}$ and we have the solution [8, p. 67]

$$\phi = \frac{A_z\beta}{c} = -\frac{I}{2\pi\epsilon_0\beta c}\left(\frac{x^2}{R_x(R_x+R_y)} + \frac{y^2}{R_y(R_x+R_y)}\right) \quad (16)$$

that leads to the Hamiltonian term

$$H_{\text{sc}} = -\frac{qI}{2\pi\epsilon_0\gamma^2\beta c}\left(\frac{x^2}{R_x(R_x+R_y)} + \frac{y^2}{R_y(R_x+R_y)}\right). \quad (17)$$

An important property of the space charge term due to a KV distribution is that it is quadratic in x and y, which implies that the space charge force is linear.

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An Example: KV in Linear Elements

For this example we are going to assume a round KV distribution ($R_x = R_y$) and will perform the calculations in one dimension.

A self-consistent space charge tracking requires that the length of the element be small enough to ensure that the space charge potential can be considered constant during the time interval. For cases with strong space charge this is in general not the case and the tracking has to be done in small steps. This can be done easily using the Lie transform, as the length L is a parameter. At each step, the space charge potential needs to be re-computed from the density function and updated in the full Hamiltonian.

The Hamiltonian of a drift space in 1D $\left(H = \frac{p_x^2}{2}\right)$ is quadratic in p_x. If the space charge term due to a KV distribution is added to this Hamiltonian, we obtain a quadratic function of x and p_x. In this case, since all forces are linear, the result of transporting a KV distribution is another KV distribution. For this reason, instead of transporting the distribution function we can simply transport the Courant-Snyder ellipse as shown above. To compute the new space charge potential after each step, Eq. (16) can be used with the beam radius extracted from the new ellipse.

Figure 2 shows the result of transporting beam with a KV distribution over a 1 m drift space and a beam current of 50 mA. The results are in good agreement with TraceWin.

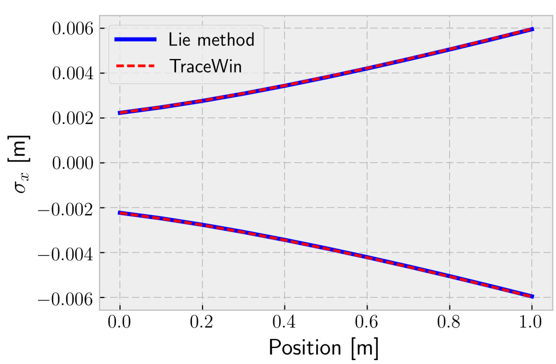

Figure 2: Beam size along 1 m drift space, calculated using Lie method (solid blue) and TraceWin (dashed red). Simulations for a 3 MeV proton beam of 50 mA with a KV distribution, a normalized emittance of 0.1 π mm mrad and Twiss parameters $\alpha = -1\ \pi$ and $\beta = 1\ \pi$ mm / mrad.

For a sequence of linear elements, the method described above can be applied element by element. For illustration, we show here the case of KV distribution transported through a FODO channel. The calculation is done in 2D, as the beam cannot be round all the way through the FODO channel.

The comparison of the simulation of the FODO channel using the method described in this paper and TraceWin is shown in Fig. 3.

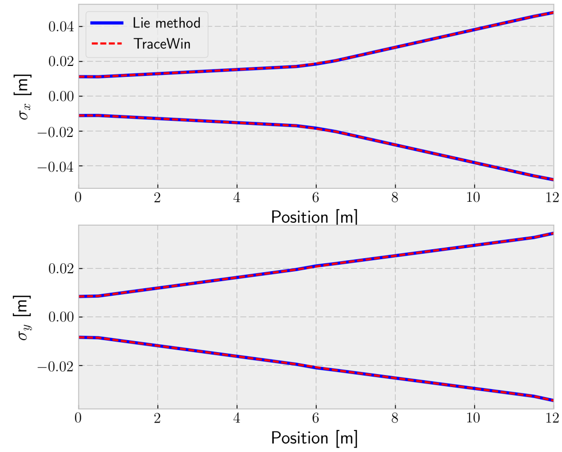

Figure 3: Beam size along a FODO channel for the horizontal (top) and vertical (bottom) planes, calculated using Lie method (solid blue) and TraceWin (dashed red). The FODO channel is composed of two 1 m long quadrupoles with a normalized strength k=0.1 separated by 5 m drift spaces. Simulations for a 3 MeV proton beam of 50 mA with a KV distribution, a normalized emittance of 0.1 π mm mrad (both planes) and Twiss parameters $\alpha_x = \alpha_y = 0\ \pi$, $\beta_x = 25\ \pi$ mm / mrad and $\beta_y = 14.2\ \pi$ mm / mrad.

SUMMARY

This paper presents a self-consistent method to track a high intensity beam relying on the Lie transform and using a symbolic calculator, avoiding the use of multi-particle codes. Examples for the KV distribution with linear elements are in good agreement with other simulation tools.

The application of this method for non-KV distributions and non-linear elements requires the computation of the space charge potential solving the Poisson equation, which is a non-trivial problem. The use of an approximate method that allows to calculate an analytic space charge potential is currently under study.

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