Analyzing Charged Particle Beams using Lie Transform Perturbation Theory

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Abstract. This paper briefly reviews the use of Lie transform perturbation theory applied to the dynamics of charged particle beams. Several details not provided here can be found in [1] and [2]. The work analyzes influences due to nonlinear components in external focusing of beams, a regime where the Courant-Snyder invariants are broken [3] for single particle dynamics. The Lie transform analysis is also used to analyze beams with space charge effects, which satisfy the Vlasov-Poisson system of equations. Equilibrium distributions may be obtained even in the nonlinear focusing regime, where simple solution such as the Kapchinskij-Vladimirskij [4] are no longer valid. The work utilizes results that were obtained earlier as part of the research activities of Prof. Allan Kaufman and members of his group.

1. Lie Transform Perturbation Methods for Hamiltonian Systems - A Brief Review

In this section, we outline the Hamiltonian perturbation method described in detail in Ref. [5] and more briefly in Ref. [6]. This method is based on previous work [7, 8, 9, 10, 11] that introduced Lie transform theory as a convenient method to perform Hamilton perturbation analysis. The Lie transformation is defined with respect to a phase space function $w$ such that it satisfies the following Poisson bracket relationship,

$$\frac{dZ}{d\epsilon} = \{Z, w(Z(z, t, \epsilon), t, \epsilon)\},$$

where $Z = (P, Q)$ is a phase space vector representing the generalized positions and momenta of the system, $w$ is the Lie generating function and $\epsilon$ is a continuously varying parameter such that $Z(\epsilon = 0) = z$, the original phase space vector. The above relationship resembles Hamilton’s equation with respect to a “Hamiltonian”, $w$ and “time”, $\epsilon$. This guarantees that the transformation is canonical for all values of $\epsilon$.

The Lie operator $L$ is defined such that it performs a Poisson bracket operation with respect to $w$. Symbolically,

$$L = \{w, \}.$$
A transformation operator $T$ is defined such that its role is to replace the variables of a function by the new canonical variables. For the identity function this is simply,

$$Tz = Z(z, \epsilon, t).$$  \hfill (3)

The operator $T$ is analogous to the “evolution” operator with respect to $\epsilon$. Using Eq. (1) it can be verified that $T$ satisfies

$$\frac{dT}{d\epsilon} = -TL.$$  \hfill (4)

For a similar relationship involving the inverse transformation operator $T^{-1}$, we differentiate the equation $TT^{-1} = 1$ and use the above equation to obtain

$$\frac{dT^{-1}}{d\epsilon} = T^{-1}L.$$  \hfill (5)

The transformed Hamiltonian $K$ can be expressed in terms of the original Hamiltonian $H$ as

$$K(\epsilon) = T^{-1}(\epsilon)(H) + T^{-1}(\epsilon)\int_0^\epsilon d\epsilon'T(\epsilon')\frac{\partial w}{\partial t}(').$$  \hfill (6)

This expression was obtained by Dewar [10].

Using Eq. (4), and the Deprit [9] series expression for the operators $L$ and $T$, gives us the following recursion relationship

$$T_n = -\frac{1}{n} \sum_{m=0}^{n-1} T_m L_{n-m}.$$  \hfill (7)

Similarly, using Eq. (5), and the Deprit series expression for the operators $L$ and $T^{-1}$, the inverse transformation operator may be expressed recursively as

$$T^{-1}_n = \frac{1}{n} \sum_{m=0}^{n-1} L_{n-m} T^{-1}_m.$$  \hfill (8)

It may be noted that when $L$, $T$ and $T^{-1}$ act upon any phase space function, they are expressed in the form of Poisson brackets, which are independent of the canonical variables used. This makes the whole formulation canonically invariant.

To obtain the nth order perturbation equation, we premultiply Eq. (6) by $T$ and differentiate with respect to $\epsilon$ to obtain

$$\frac{\partial T}{\partial \epsilon}K + T \frac{\partial K}{\partial \epsilon} = \frac{\partial H}{\partial \epsilon} + T \frac{\partial w}{\partial t}.$$  \hfill (9)

Using Eq. (4) to eliminate $\partial T/\partial \epsilon$ (with $dT/d\epsilon \to \partial T/\partial \epsilon$, since here $T$ also depends explicitly on $t$) and premultiplying by $T^{-1}$,

$$\frac{\partial w}{\partial t} = \frac{\partial K}{\partial \epsilon} - LK - T^{-1} \frac{\partial H}{\partial \epsilon}.$$  \hfill (10)

Inserting the series expansions and equating like powers of $\epsilon$, we obtain in nth order,

$$\frac{\partial w_n}{\partial t} = nK_n - \sum_{m=0}^{n-1} L_{n-m} K_m - \sum_{m=1}^n mT^{-1}_{n-m} H_m.$$  \hfill (11)

To third order, this equation yields,

$$K_0 = H_0,$$  \hfill (12)
\[
\frac{\partial w_1}{\partial t} + \{w_1, H_0\} = K_1 - H_1, \quad (13)
\]
\[
\frac{\partial w_2}{\partial t} + \{w_2, H_0\} = 2(K_2 - H_2) - L_1(K_1 + H_1), \quad (14)
\]
\[
\frac{\partial w_3}{\partial t} + \{w_3, H_0\} = 3(K_3 - H_3) - L_1(K_2 + 2H_2) - L_2(K_1 + \frac{1}{2}H_1) - \frac{1}{2}L_2^2H_1. \quad (15)
\]

The expression \( \frac{\partial w_n}{\partial t} + \{w_n, H_0\} \) is the variation of \( w_n \) along the unperturbed trajectory described by \( H_0 \). In the following section we use this perturbation scheme to perform time averaging. To do this, we set \( H_0 = 0 \) which reduces the variation of \( w_n \) along a trajectory to a partial derivative with respect to \( t \). Thus, instead of integrating along the unperturbed trajectory, we simply perform an integration over time to determine \( w_n \). At each order, \( K_n \) is chosen such that it cancels the terms that average to a nonzero value over fast oscillations. As a result, the corresponding value of \( w_n \) will have a zero average. This is necessary to prevent \( w_n \) from being secular (unbounded) in time [5]. For a systematic derivation of all these relationships one may refer to Ref. [5] where they are given up to fourth order in \( \epsilon \).

2. Application to a Linear Sinusoidal Focusing System

As an illustration and a test for the validity of the method, we perform the analysis for a linear periodic focusing system. The same example was used in Ref. [12] for the method developed in that paper. The single particle Hamiltonian associated with such a system is given by

\[
H = \frac{p^2}{2} + \frac{kq^2}{2} \sin(\omega t). \quad (16)
\]

This Hamiltonian also describes the motion of a particle in systems such as the Paul trap and the ponderomotive potential. We apply Eqs. (12 - 15) to perform the averaging. As explained in the previous section, we set \( H_0 = 0 \) and \( H_1 = H \). From Eq (12) we get,

\[
K_0 = H_0 = 0, \quad (17)
\]

Applying the first order relationship, Eq (13), we get

\[
\frac{\partial w_1}{\partial t} = K_1 - \frac{p^2}{2} - \frac{kq^2}{2} \sin(\omega t). \quad (18)
\]

The third term on the right averages to zero with respect to time. In order that the net result average to zero, we require

\[
K_1 = \frac{p^2}{2}. \quad (19)
\]

Since \( w_1 \) is relevant only up to an additive constant, it is sufficient to evaluate the indefinite integral to determine \( w_1 \), hence

\[
w_1 = \frac{kq^2}{2\omega} \cos(\omega t). \quad (20)
\]

The second order equation Eq.(14) gives

\[
\frac{\partial w_2}{\partial t} = 2K_2 - \frac{2kpq}{\omega} \cos(\omega t). \quad (21)
\]
Since the second term on the right side averages to zero, we choose

\[ K_2 = 0, \quad (22) \]

and so,

\[ w_2 = -\frac{2kqP}{\omega^2} \sin(\omega t). \quad (23) \]

Applying the third order relationship, Eq. (15) then gives

\[ \frac{\partial w_3}{\partial t} = 3K_3 + \frac{3p^2k}{\omega^2} \sin(\omega t) \]

\[ -\frac{k^2q^2}{\omega^2} \sin^2(\omega t) - \frac{k^2q^2}{2\omega^2} \cos^2(\omega t). \quad (24) \]

Note that the third and fourth terms on the right side do not average to zero. In order that they cancel, we set

\[ K_3 = \frac{1}{4} \frac{k^2q^2}{\omega^2} \quad (25) \]

and as a result,

\[ w_3 = -\frac{3p^2k}{\omega^3} \cos(\omega t). \quad (26) \]

Collecting the nonzero terms, the transformed Hamiltonian is now given as a function of the new variables by

\[ K = \frac{P^2}{2} + \frac{\Omega^2Q^2}{2} \quad (27) \]

where \( \Omega = k/\sqrt{2}\omega \). This is the Hamiltonian for a harmonic oscillator with solution

\[ Q(t) = Q(0) \cos(\Omega t) + \frac{P(0)}{\Omega} \sin(\Omega t), \quad (28) \]

\[ P(t) = P(0) \cos(\Omega t) - \Omega Q(0) \sin(\Omega t). \quad (29) \]

To transform back to the original coordinate system, we use the operator \( T^{-1} \) for which we need to know \( L \) up to the desired order. The operators \( L_n \) can be expressed in terms of the values of \( w_n \) as

\[ L_1 = \left\{ \frac{kQ^2}{2\omega} \cos(\omega t), \right\}, \quad (30) \]

\[ L_2 = \left\{ -\frac{2kQP}{\omega^2} \sin(\omega t), \right\}, \quad (31) \]

\[ L_3 = \left\{ -\frac{3kP^2}{\omega^3} \cos(\omega t), \right\}. \quad (32) \]

Using these to perform the inverse transformation as described we get, up to third order,

\[ q = Q + \frac{kQ}{\omega^2} \sin(\omega t) + \frac{2kP}{\omega^3} \cos(\omega t), \quad (33) \]

\[ p = P + \frac{kQ}{\omega} \cos(\omega t) - \frac{kP}{\omega^2} \sin(\omega t) \]

\[ + \frac{1}{3} \frac{k^2}{\omega^3} Q \sin(\omega t) \cos(\omega t). \quad (34) \]
Figure 1. $q$ vs $t$ with $k = 1$, $\omega = (a) 4$, (b) 3, (c) 2.5 and (d) 2. The solid line represents the numerical solution.

The above solution is compared with calculations from a fourth order symplectic integrator [13, 14] and is shown in Fig. (1). The parameters used were the same as those used in Ref. [12]. The accuracy of the approximate solution compares well with that obtained by Channell [12] using a different method. That is, the solution given by Eqs. (33) and (34) overlaps well with the numerical solution for $k/\omega^2 = 1/16$ and the accuracy gradually decreases with decreasing $\omega$.

3. Application to Single Particle Dynamics in Accelerators

For a single particle moving in a particle accelerator under the influence of quadrupoles and sextupoles, the Hamiltonian can be expressed in cylindrical coordinates as

$$H = \frac{1}{2} (p_r^2 + l^2) + \frac{1}{2} \kappa_2(s) r^2 \cos(2\theta) + \frac{1}{3} \kappa_3(s) r^3 \cos(3\theta + \alpha).$$

The variable $s$ is the distance along the axis, which is equivalent to time for constant axial velocity. The momentum in the radial direction is $p_r$, and $l$ is the angular momentum. The values of $\kappa_2(s)$ and $\kappa_3(s)$ depend upon the strength of the quadrupole and sextupole magnets respectively and also the velocity of the particle in the axial direction. The angle $\alpha$ depends upon the relative values of $a_2$ and $b_2$ which is determined by the orientation of the sextupoles with respect to the quadrupoles. We use normalized units in which the charge and mass of the particle are unity. It is assumed that the Hamiltonian is periodic in $s$ with periodicity $S$, i.e., $\kappa_2(s + S) = \kappa_2(s)$ and $\kappa_3(s + S) = \kappa_3(s)$. It is further assumed that the average of $\kappa_2(s)$ and $\kappa_3(s)$ over a period $S$ is zero. That is,

$$\langle \kappa_2 \rangle = \frac{1}{S} \int_{s}^{s+S} \kappa_2(s) ds = 0$$

(36)
and the same for $\kappa_3$. The angle brackets $\langle \cdots \rangle$ denote an average over one period in the rest of this paper.

Employing the same procedure as before, it can be shown [1] that the transformed Hamiltonian gives

$$K = \frac{1}{2}(P_R^2 + \frac{l^2}{R^2}) \frac{1}{2} \langle (\kappa_2 I_2)^2 \rangle R^2 \frac{1}{3} \langle \kappa_2 \kappa_3 \rangle R^3 \cos(\Theta + \alpha) + \frac{1}{2} \langle (\kappa_3 I_3)^2 \rangle R^4. \quad (37)$$

In order for $K$ to be independent of $\Theta$, the transformed azimuthal variable, $\langle \kappa_2 \kappa_3 \rangle$ must vanish. The simplest way to achieve this with real quadrupoles and sextupoles is as shown in Fig 2. One could extend the analysis to more complex systems as well. The separation between the quadrupoles and sextupoles is represented by a term,

$$\psi = \frac{2\pi \Delta s}{S} \quad (38)$$

where $\Delta s$ is the spatial distance between the two of them. The averaged Hamiltonian $K$ is independent of $\Theta$ when $\psi = 90^\circ$, i.e., when the sextupoles are placed halfway between two quadrupoles of opposite sign.

**Figure 2.** A step function lattice that will lead to a near integrable condition. The shorter steps represent the sextupole function $\kappa_3(s)$ while the higher ones the quadrupole function $\kappa_2(s)$.

The dynamic aperture is defined as the volume in phase space in which all particles remain confined throughout their trajectories in the accelerator. The calculations in this section estimate the projection of the dynamic aperture onto various phase space planes for different values of $\psi$.

In Fig. (3), the left side represents the initial phase space positions of confined particles and the ones on the right represent the unconfined particles from the same initial distribution. It is important to plot the confined and unconfined particles separately in order to ensure that there is no overlap between the two regions, which is true in these simulations. This is expected because all the phase space variables other than those shown in the respective plot were set to zero. Given that the dynamic aperture allows only confined particles and not a mixture of the two, the left side plots represent the projection of the dynamic aperture onto the respective plane.
4. Generalization to Beams with Space Charge Effects

In the study of self consistent systems such as beams with space charge effects, it is often required to solve for the phase space density $f(q,p)$ which satisfies the Vlasov equation,

$$\frac{df}{ds} = \frac{\partial f}{\partial t} + \{H, f\} = 0. \quad (39)$$

Lie transform methods have been used to analyze systems governed by the Vlasov equation in the past (for example see Ref[15]). In self consistent systems, since the Hamiltonian includes the space charge potential, $H$ itself will be a function of $f$. In many cases, it is possible to decompose $H$ as

$$H = H^e + H^{sc}, \quad (40)$$

where $H^e$ is the term arising from external forces and $H^{sc}$ arises from space charge forces. In Vlasov-Poisson systems, $H^{sc}$ is proportional to the electrostatic potential $\phi$ which satisfies Poisson’s equation,

$$\nabla^2 \phi(q,s) = -\epsilon m q \int dp f(q,p,s) \quad (41)$$

where $q$ is the charge of the particle and $\epsilon_0$ is the free-space permittivity. In Eq. (41), we have put in the ordering parameter, $\epsilon^m$ for maximal ordering. Since we are solving for beam equilibria, this factor will be selected so that the lowest-order potential is of the same order as the lowest-order averaged confining forces.

If we define a function

$$F(Q, P, s) = f(q(Q, P, s), p(Q, P, s), s), \quad (42)$$

then it may be easily verified that

$$f(q, p, s) = TF(q, p, s). \quad (43)$$

From the property of canonical invariance of the Vlasov equation (see for example Ref [12]), we then have

$$\frac{dF}{dt} = \frac{\partial F}{\partial s} + \{K, F\} = 0. \quad (44)$$

Using the perturbation expansion terms of the transformation operator $T$ we can in principle expand $f$ in terms of $F$ using Eq. (43) in order to obtain the phase space distribution in the original coordinate system. This gives,

$$f = f_0 + \epsilon f_1 + \epsilon^2 f_2 + \epsilon^3 f_3 + \ldots \quad (45)$$
where

\[ f_n(q, p, s) = T_n F(q, p, s) \quad (46) \]

Combining Eqs. (45) and (41), \( \phi \) may be expressed as a decomposition of its different order terms such that,

\[ \phi = \epsilon^m (\phi_m + \epsilon \phi_{m+1} + \epsilon^2 \phi_{m+2} + \epsilon^3 \phi_{m+3} + \ldots) \quad (47) \]

where

\[ \nabla^2 \phi_n(q, s) = -\frac{q}{\epsilon_0} \int dp f_{n-m}(q, p, s) \quad (48) \]

The different terms in the electrostatic potentials represent contributions arising from the different orders in the perturbation of the charge density. Thus, the lowest nonzero term in \( \phi \) corresponds to the lowest nonzero term in \( f \).

The motivation to carry out the procedure outlined in this section is based on the presumption that it is possible to perform a canonical transformation from \((q, p, s)\) to \((Q, P, s)\) such that the resulting phase space function, \(F(q, p, s)\) is easier to solve for than \(f(q, p, s)\). It is then more convenient to first solve for \(F\) and then transform back to \(f\) rather than solving directly for \(f\). In this study, we solve for an equilibrium, where \(F\) is independent of \(s\). This is achieved through a transformation that depends on \(s\). If the transformation is perturbative, which is true in this context, \(f\) may be obtained only up to a desired order. It has been shown in the appendix that the terms higher than the lowest nonzero term in \(f\) do not change the total number of particles in the distribution. Thus, the total charge is conserved even upon truncation of the series expansion in \(f\).

The Hamiltonian for a beam with space charge effects is given by

\[ H = \frac{1}{2} \left( p_r^2 + \frac{l^2}{r^2} \right) + \frac{1}{2} \left( \kappa_2(s) r^2 \cos(2\theta) \right) + \frac{1}{3} \kappa_3(s) r^3 \cos(3\theta + \alpha) + \frac{q}{m_0 v_s^2 \gamma^3} \phi(r, \theta, s). \quad (49) \]

Over here, \(m_0\) is the rest mass, \(q\) the charge and \(v_s\) the axial velocity of the particle, and \(\gamma\) is the Lorentz relativistic factor. Using the same averaging procedure described in this paper, and requiring that the system be azimuthally symmetric, one could obtain the transformed Hamiltonian, which is given by

\[ K = \frac{1}{2} \left( P_R^2 + \frac{L^2}{R^2} \right) + \frac{1}{2} \left( (\kappa_2^I) R^2 + \frac{1}{2} (\kappa_3^I)^2 R^4 \right) - \frac{1}{3} \left( \kappa_2^I \kappa_3^I \right) R^3 \cos(\Theta + \alpha) + \frac{q}{m_0 v_s^2 \gamma^3} \phi_3 \quad (50) \]

As before, the superscript \(I\) represents an integration with respect to “time”, \(s\) with the same conditions as described in the previous section.

The averaged Hamiltonian now has an external potential independent of \(s\) allowing one to compute an equilibrium distribution, which is a steady state solution of Eq. (44) given by

\[ F = F(K(Q, P)). \quad (51) \]

Transforming \(F\) to \(f\) up to the desired order based on the procedure described in the previous section would then yield a near equilibrium distribution function in the original coordinate system.
Figure 4. Purely linear focusing (a) plot number density of $n_0$, (b)$n_0 + n_2$ located in the middle of an x-focusing quadrupole

Figure 5. Nonlinear focusing, (a) plot of number density $n_0$, and (b) $(n_0 + n_2)$ located in the middle of a sextupole

A thermal equilibrium distribution is then given by

$$F(P, Q) = \hat{n} \exp[-K/T_0] = \frac{\hat{n}}{2\pi T_0} \exp\left\{ -\frac{1}{2} (P^2_R + \frac{L^2}{R^2}) + V(R) + \frac{q}{mv^2_s} \right\} / T_0$$

where $\hat{n}$ is the density at $R = 0$, $T_0$ represents the temperature of the beam, in units of the Hamiltonian and the external potential term $V(R)$ is given by

$$V(R) = \frac{1}{2} \langle (\kappa_2^2)^2 \rangle R^2 + \frac{1}{2} \langle (\kappa_3^2)^2 \rangle R^4$$

Transferring this distribution to the original phase space variables, one could get the “s” dependence of the distribution upto the desired order.

Figure 4 shows how the “s” dependence for a purely linear external focusing case changes when one takes into account perturbations over the averaged equilibrium distribution. The
averaged distribution in position space, which is Fig 4(a) is symmetric about $\theta$, while Fig 4(b) shows the dependence of the distribution with respect to $\theta$ inside a quadrupole magnetic field.

Figure 5 shows how the “s” dependence for a nonlinear linear external focusing case changes when one takes into account perturbations over the averaged equilibrium distribution. The averaged distribution in position space (5)(a) is symmetric about $\theta$, while (5)(b) shows the dependence of the distribution with respect to $\theta$ inside a sextupole magnetic field.

It is clear that the symmetry of the distribution reflects the symmetry of the external focusing element. A detailed formulation showing the derivation of the distribution will be presented in a paper under preparation [2].

5. Summary
Lie Transform theory has proved to be a powerful tool for analyzing certain aspects of beams physics. Work in this area is being continued by us and we hope that the effort will lead to a more optimized designs and better understanding of particle accelerators in the future. Nonlinear components such as sextupoles and octupoles are regularly used in storage rings and optimizing the dynamic aperture can greatly help improve the performance of such facilities. Beams with space charge effects are important in heavy ion fusion experiments and spallation neutron sources. The analysis presented in this paper may even find applications in systems other than particle accelerators.

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