THE CONVERGENCE AND ACCURACY OF THE MATRIX FORMALISM APPROXIMATION*

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Abstract

To the present time there has been developed a large number of different codes for the particles beam dynamics modeling. However, their precision, accuracy and reliability of the numerical results are not sufficiently guaranteed in the case of long-term evolution of particle beams in circular accelerators. Here we discuss convergence estimates of the matrix presentation for Lie series. We also consider some problems of the matrix formalism accuracy for constructing the evolution operator of the particle beam. In this article there is paid a special attention to problems of symplecticity and energy conservation for long time evolution of particles beams.

INTRODUCTION

The well known Lie methods for nonlinear dynamics allow us to constructive evaluate the corresponding maps and use them for accelerator physics [1]. But it should be note that evaluation procedures of corresponding Lie maps is enough time-consuming process. Besides, it is very difficult to evaluate corresponding procedures and estimate the required accuracy of the corresponding evaluations. This procedure is necessary for correct calculation for different problems of accelerator physics, particularly for long time beam evolution. Unfortunately the most popular methods have not enough practical instruments for accuracy estimates. The trend of accelerator physics leads us to necessity to have a tool to assess not only the accuracy of computational procedures, but also to preserve certain qualitative properties of the computational procedures (such as symplecticity, energy conservation and so on). Usually these problems are solved only in numerical mode up to some order of integration steps $\mathcal{O}(h^n)$. In the present paper we demonstrate some analytical estimates for the corresponding solutions using the matrix formalism for Lie approach [2, 3]. We also consider some problems of the matrix formalism accuracy for constructing the evolution operator of the particle beam.

THE ACCURATE EVALUATION OF TRUNCATED LIE MAPS

Matrix Series Presentations for Lie Maps

In some previous papers we presented the matrix formalism for Lie maps generated by ordinary differential equations, which can be written in the the following form

$$\frac{d\mathbf{X}}{dt} = \mathbf{F}(\mathbf{X},t) = \sum_{k=1}^{\infty} \mathbb{P}_k(t)\mathbf{X}^{[k]}, \quad \mathbf{X}_0 = \mathbf{X}(t_0), \qquad (1)$$

where $\mathbf{F} = \{F_1,\dots,F_{2n}\}^{\mathrm{T}}$ and $\mathbf{X}^{[k]}$ is a vector of all phase moments for the phase vector $\mathbf{X}$ $(\dim \mathbf{X} = 2n)$, for example, $\mathbf{X} = \{x,p_x,y,p_y\}^{\mathrm{T}}$ and $\mathbb{P}^{1k}$ $\left(\text{with matrix size } \dim \mathbb{P}^{1k} = \binom{2n+k-1}{k}\right)$ are matrices containing partial derivatives

$$\left\{\mathbb{P}^{1k}(t)\right\}_{ij} = \frac{1}{k_1!\dots k_{2n}!}\left.\frac{\partial^k F_i(x_j,t)}{\partial x_1^{k_1}\dots\partial x_n^{k_{2n}}}\right|_{x_1=\dots=x_{2n}=0}.$$

The eq. (1) generates the Lie operator [1] in according the following equality

$$\mathcal{L}_{\mathbf{F}} = \mathbf{F}^*(\mathbf{X},t)\frac{\partial}{\partial\mathbf{X}} = \sum_{k=1}^{\infty}\left(\mathbf{X}^{[k]}\right)^{\mathrm{T}}\mathbb{P}_{1k}^{\mathrm{T}}\frac{\partial}{\partial\mathbf{X}} = \sum_{k=1}^{\infty}\mathcal{L}_{\mathbf{F}_k}.$$

So, for corresponding Lie map [1] we can write

$$\mathcal{M}\left(t|t_0;\mathcal{L}_{\mathbf{F}}\right) = \mathrm{T}\exp\int_{t_0}^{t}\mathcal{L}_{\mathbf{F}}(\mathbf{X},\tau)d\tau =$$

$$= \mathrm{T}\exp\sum_{k=1}^{\infty}\int_{t_0}^{t}\mathcal{L}_{\mathbf{F}_k}d\tau = \mathcal{M}\left(t|t_0;\sum_{t_0}^{t}\mathcal{L}_{\mathbf{F}_k}\right) =$$

$$= \prod_{k=1}^{\infty}\mathcal{M}\left(t|t_0;\sum_{t_0}^{t}\mathcal{L}_{\mathbf{G}_k}\right), \qquad (2)$$

where the symbol "T" denotes the so called chronological ordering exponent Lie operator [3] (or the Dyson operator). Here k indicates the order of corresponding homogeneous polynomials. Evaluation of (2) can be realized in the frame of two following approaches:

1. The Magnuss representation for chronological exponent operators [3, 4].
2. The Zassenhaus formula for homogeneous polynomials $\mathbf{G}_k$, $k \geq 1$ calculation). Using these approaches we can write some symbolic formulas for Lie map $\mathcal{M}$ evaluation. For example, if we introduce the following notations [3] $\mathbb{P}_m^{k\,1} = \prod_{j=1}^{k}\mathbb{G}_m^{\oplus((j-1)(m-1)+1)}$ (here $\oplus$ denotes the Kronecker sum), then we have the following equality

$$\exp\left(\mathcal{L}_{\mathbf{G}_m}\right)\circ\mathbf{X} = \mathbf{X} + \sum_{k=1}^{\infty}\frac{\mathbb{P}_m^{k\,1}}{k!}\mathbf{X}^{[k(m-1)+1]}.$$

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Similar formulae allow us to write the following formulae

$$\mathcal{M}_{\leq 3} \circ \mathbf{X} = \mathbb{R}^{11} \left(\mathbf{X} + \sum_{m=2}^{3} \sum_{k=1}^{\infty} \frac{\mathbb{P}_m^{k1}}{k!} \mathbf{X}^{[k(m-1)+1]} + \right.$$
$$\left. + \sum_{l=1}^{\infty} \sum_{k=1}^{\infty} \frac{1}{k!l!} \mathbb{P}_2^{kl}\, \mathbb{P}_3^{l\,(k+1)}\, \mathbf{X}^{[2l+k+1]} \right), \quad (3)$$

where $\mathbb{R}^{11}$ is a fundamental matrix for linear approximation for motion equations. The formulae similar to (3) allow us to evaluate the necessary maps constructively and use them up to required order. Here we should mention additionally that the corresponding matrices $\mathbb{P}_m^{k1}$ in symbolic or numerical modes up to necessary order on phase vector $\mathbf{X}$.

The formulae similar to (3) allow us to evaluate up to necessary order corresponding matrix expansion for Lie maps. But for many beam physics problems it is very important to conserve some properties, for example the symplecticity property for hamiltonian systems. The symplecticity property imposes special conditions on the corresponding matrices, which have the form of linear algebraic equations [3]. It is necessary to emphasize that these restrictions of the corresponding matrices can not influence on the accuracy estimations.

The Problems of Accuracy Evaluations

The Lie Map. The above pointed methods of Lie maps evaluation will guarantee necessary convergence. As an example, we can give some estimates for convergence of Lie map evaluation in accordance with Magnus presentation of Lie map. According to this approach the chronological presentation (2) can written in the form of ordinary exponential operator [4]:

$$\mathcal{M}(t|t_0) = \exp \mathcal{W}(t|t_0; \mathcal{A}), \quad (4)$$

where $\mathcal{W}(t|t_0;\mathcal{A})$ – is a new vector field, generated by "old" vector field $\mathcal{A} = \mathcal{L}_{\mathbf{F}}$. Differentiation of eq. (4) gives us

$$\frac{d\mathcal{W}(t|t_0)}{dt} = \left[\mathcal{A}(t) \circ \frac{\mathcal{W}(t|t_0)}{1 - \exp\left(-\mathcal{W}(t|t_0)\right)} \right]. \quad (5)$$

Equation (5) can be written as a series:

$$\frac{d\mathcal{W}(t|t_0)}{dt} = \sum_{k\geq 0} \alpha_k \left[\mathcal{A} \circ \mathcal{W}^k \right] = \mathcal{A} + \frac{1}{2} \{\mathcal{A}, \mathcal{W}\} +$$
$$+ \frac{1}{12} \left[\mathcal{A} \circ \mathcal{W}^2 \right] + \ldots, \quad (6)$$

where $\alpha_{2k+1} = 0$, $k \geq 1$, $\alpha_0 = 1$, $\alpha_1 = 1/2$, $\alpha_{2k} = (-1)^{k-1} B_{2k}/(2k)!$, B_{2k} – Bernoulli numbers. We can rewrite eq. (6) in the following integral equation:

$$\mathcal{W}(t|t_0) = \sum_{k\geq 0} \alpha_k \int_{t_0}^{t} \left[\mathcal{A}(\tau) \circ \mathcal{W}^k(\tau|t_0) \right] d\tau. \quad (7)$$

Let be $\mathcal{W}_1(t|t_0) = \int_{t_0}^t \mathcal{A}(\tau) d\tau$, then the solution of (7) can be written using the the method of successive approximations:

$$\mathcal{W}_k(t|t_0) = \int_{t_0}^{t} \mathcal{A}(\tau) d\tau + \sum_{l\geq 2} \int_{t_0}^{t} \left[\mathcal{A} \circ \mathcal{W}_{k-1}^l(\tau|t_0) \right] d\tau, \quad (8)$$

where $k \geq 2$, $t \in [t_0, T_1] \subset [t_0, T] \subset R^1$.

We introduce the multiplicative norm, which coordinates with functional dependence elements on $t \in [t_0, T_2]$, $t_0 \leq T_2 \leq T_1$, that is $\|\mathcal{A} \circ \mathcal{B}\|_\Phi \leq \|\mathcal{A}\|_\Phi \|\mathcal{B}\|_\Phi \ \ \forall\ \mathcal{A}, \mathcal{B} \in \mathcal{L}\mathfrak{A}[\mathfrak{X}]$, where the index "$\Phi$" means a norm in the corresponding functional space. Let be, for example, $\mathcal{A}(t)$ – a summable function on the interval $[t_0, T_2]$, then we can define $A(t) = \int_{t_0}^t \|\mathcal{A}(\tau)\| d\tau$, $\forall\ t \in [t_0, T_2]$, where $\|\cdot\|$ – an arbitrary multiplicative norm in $\mathcal{L}\mathfrak{A}[\mathfrak{X}]$ and $A(t)$ – a scalar nonnegative continuous function $\forall\, t \in [t_0, T_2]$. According to the step-by-step method we should prove the sequence convergence. For these aim we use recurrent relation (8) and receive for $\mathcal{W}$:

$$\mathcal{W}(t|t_0) = \int_{t_0}^{t} \mathcal{A}(\tau) d\tau + \alpha_1 \int_{t_0}^{t} \left\{ \mathcal{A}(\tau), \int_{t_0}^{\tau} \mathcal{A}(\tau') \right\} d\tau +$$
$$+ \alpha_1^2 \int_{t_0}^{t} \left\{ \mathcal{A}(\tau), \int_{t_0}^{\tau} \left\{ \mathcal{A}(\tau'), \int_{t_0}^{\tau'} \mathcal{A}(\tau'') d\tau'' \right\} d\tau' \right\} d\tau + \ldots$$

Let introduce the notation $\mathcal{W} = \sum_{k\geq 0} \mathcal{W}^k$, where $\mathcal{W}^k$ – a group of terms of series comprising k nested Lie brackets, then we obtain the following estimation

$$\|\mathcal{W}^k(t|t_0)\| \leq A(t)\, (2A(t))^k\, C_k, \quad k \geq 0, \quad (9)$$

where C_k satisfies to following recurrent relations: $C_{2l} = \alpha_{2l} + C_{2l-2} C_{2l-4}$, $C_{2l+1} = \alpha_{2l} + C_3 C_{2l-1}$, $l \geq 2$, $C_0 = 1$, $C_1 = 1$, $C_2 = \alpha_1^2 + |\alpha_1|$, $C_3 = \alpha_1^3 + 2|\alpha_1|$. The connection of coefficients α_{2k} with Bernoulli numbers leads us to the estimation

$$|\alpha_{2m}| \leq \frac{2}{(2\pi)^{2m}} \sum_{k\geq 1} \frac{1}{2^{2k}} < \frac{4}{(2\pi)^{2m}}.$$

Introducing the following notation $M = \int_{t_0}^{T_2} A(\tau) d\tau$, one can estimate $\|\mathcal{W}^k\|_{L_1} \leq 2^k M^{k+1} C_k$ under sufficiently great k. The majorant series with general term $2^k M^{k+1} C_k$ will be converge in according to limit test for convergence by D'Alember, if there is satisfied the inequality

$$\lim_{k\to\infty} \frac{2^{k+1} M^{k+2} C_{k+1}}{2^k M^{k+1} C_k} = q < 1.$$

Let be (for definiteness) $k = 2l$, then

$$q = \lim_{l\to\infty} \frac{2MC_{2l+1}}{C_{2l}} = \lim_{l\to\infty} \frac{2M(\alpha_{2l} + C_3 C_{2l-1})}{\alpha_{2l} + C_{2l-2} C_{2l-4}} = 2M.$$

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So the majorant series converges under $M < 1/2$, and the series (7) is a absolutely convergent series. So the equation (5) has a continuous-time solution on the interval $[t_0, T_2]$. From here follows the theorem about absolutely convergence of the series (8).

The Ordinary Differential Equations. It is often the beam dynamics problems are described by the Cauchy problem

$$\frac{d\mathbf{X}}{dt} = \mathbf{G}(\mathbf{X}), \quad \mathbf{X}(t_0) = \mathbf{X}_0,$$

where $\mathbf{G} = \{G_1, \dots, G_n\}^{\mathrm{T}}$ is an analytical function for any $\mathbf{X} \in \mathcal{X}_1 \subset R^{2n}$, $0 \in \mathcal{X}_1$ and $\mathbf{G}(0) = 0$. Then in a neighborhood of zero $\mathbf{X} = 0$ we have

$$\mathbf{G}(\mathbf{X}) = \sum_{k=0}^{\infty} \mathbb{A}_k \mathbf{X}^{[k]}, \tag{10}$$

From the convergence of series (10) follows

$$|(\mathbb{A}_k)^i| \leq \frac{M_i}{(r)^k}, \quad (r)^k = r_1^{k_1} \dots r_n^{k_n}, \tag{11}$$

where $|x_i| \leq r_i$, $i = \overline{1,n}$ and r_i guarantees embedding $\mathcal{P}_r \subset \mathcal{X}_1 \subset R^n$. Here $(\mathbb{A}_k)^i$ – i-th row of matrix $\mathbb{A}_k$ and M_i are some positive constants. Using (11) one can write the following estimations:

$$|G_i(\mathbf{X})| = \left| \sum_{k=0}^{\infty} (\mathbb{A}_k)^i \, \mathbf{X}^{[k]} \right| \leq M_i \sum_{k=0}^{\infty} \left(\frac{x}{r} \right)^k,$$

where $(x/r)^k = \prod_{i=1}^{n} (x_i/r_i)^{k_i}$. Then one can obtain the following estimations $\forall\, i = \overline{1,n}$:

$$\|G_i(\mathbf{X})\| \leq \frac{M_G^m}{1 - (x/r)^m}, r^m = \min_{i=\overline{1,n}} r_i, \; M_G^m = \max_{i=\overline{1,n}} M_i.$$

Let x^m satisfies inequalities $|x_i| \leq x^m < r^m$, then $\|\mathbf{G}(\mathbf{X})\| \leq M_G^m / (1 - x^m/r^m)^n = G^m(x^m)$, where $G^m(x^m)$ is a function of single variable x^m, defining the n-dimensional cube $\mathcal{Q}_n \subset \mathcal{P}_n^r \subset R^1$: $|x_i| \leq x^m$. Above mentioned computations allow us to estimate $G_i(\mathbf{X})\partial/\partial x_i$. Let define a Lie operator

$$\mathcal{L}_{\mathbf{G}} = \sum_{i=1}^{n} G_i(\mathbf{X}) \frac{\partial}{\partial x_i} = \left(\mathbf{G}(\mathbf{X}), \frac{\partial}{\partial \mathbf{X}} \right) = \mathbf{G}^*(\mathbf{X}) \frac{\partial}{\partial \mathbf{X}},$$

and $\exp\left(t\mathcal{L}_{\mathbf{G}(\mathbf{X})}\right) \circ \mathbf{F}(\mathbf{X}) = \sum\limits_{k=0}^{\infty} (t^k/k!) \mathcal{L}_{\mathbf{G}(\mathbf{X})}^k \circ \mathbf{F}(\mathbf{X})$, then after some evaluations one can derive

$$\sum_{k=0}^{\infty} \frac{|t|^k}{k!} \left\| \mathcal{L}_{\mathbf{G}}^k \circ \mathbf{F}(\mathbf{X}) \right\| \leq \sum_{k=0}^{\infty} \frac{|t|^k}{k!} \left(\mathcal{L}^m\right)^k \circ F^m(x^m),$$

where $\|\mathbf{X}\| \leq x^m < r^m$. Finally we can obtain

$$\sum_{k=0}^{\infty} \frac{|t|^k}{k!} \left\| \mathcal{L}_{\mathbf{G}}^k \circ \mathbf{F}(\mathbf{X}) \right\| \leq \frac{M_{\mathbf{G}}^m}{(1 - x^m/r^m)^n} \times$$

$$\times \sum_{k=0}^{\infty} \alpha_k \left(|t| \frac{M_{\mathbf{F}}^m (n+1)}{r^m \left(1 - x^m/r^m\right)^{(n+1)}} \right)^k, \tag{12}$$

where $\alpha_k \leq \left(\left(1 - \frac{1}{n+1} \right)^{n+1} \right)^k$, and we obtain a convergent series, if there

$$|t| < \frac{r^m \left(1 - x^m/r^m\right)^{n+1}}{n M_{\mathbf{F}}^m \left(n/n+1\right)^n} < \frac{r^m \left(1 - x^m/r^m\right)^{n+1} e}{n M_{\mathbf{F}}^m}.$$

So, the series (12) converges absolutely, if there are the next inequalities

$$|t| < \frac{r^m \left(1 - x^m/r^m\right)^{n+1}}{n M_{\mathbf{F}}^m} \left(1 + \frac{1}{n+1} \right)^n,$$
$$\|\mathbf{X}\| \leq x^m < r^m.$$

The above mentioned formulae demonstrate the basic restrictions on the parameters of the problem. But on the practice it will be more practically to use the following formula for convergence estimation:

$$\|\overline{\mathbf{X}} - \mathbf{X}_N\| \leq \sum_{k=N+1}^{\infty} \frac{k\, r^k L^{k+1} M}{(k-1)!} J_k(L, M), \tag{13}$$

where N is the truncation error for the given approximation order, r is the region in the phase space under study ($\|\mathbf{X}_0\| \leq r$) and h – an integration step. In the estimation (13) we introduce the following definitions:

$$L = \sup_{t,\tau \in \mathcal{T}} \|\mathbb{R}^{11}(t,\tau)\|, \quad \sup_{t,\tau \in \mathcal{T}} \|\mathbb{R}^{jj}(t,\tau)\| \leq j L^j,$$

$M = \int\limits_{\mathcal{T}} \varphi(t) dt$, where $\|\mathbb{P}^{ij}(t)\| \leq \varphi(t)/(j-1)!$, and

$$J_i(L, M) = \begin{cases} \prod\limits_{k=3}^{i} \left\{ \frac{(k-1) L^{k-1} M}{(k-2)!} + 1 \right\}, i \geq 3, \\ 1, i = 2 \end{cases}$$

CONCLUSION

The above described estimations allow a researcher to evaluate truncated matrix expansion up to necessary order. If it is necessary, the corresponding matrices can be corrected for symplecticity property guarantee without loss of accuracy.

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