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METHODS OF GEOMETRIC INTEGRATION IN ACCELERATOR PHYSICS

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In the paper, we consider a method of geometric integration for a long evolution of the particle beam in cyclic accelerators, based on the matrix representation of the operator of particles evolution. This method allows us to calculate the corresponding beam evolution in terms of two-dimensional matrices including the nonlinear effects. The ideology of the geometric integration introduces in appropriate computational algorithms the amendments which are necessary for preserving the qualitative properties of maps presented in the form of the truncated series generated by the operator of evolution. This formalism extends both to polarized and intense beams. Examples of practical applications are described.

Рассматривается метод геометрического интегрирования уравнений многооборотной эволюции пучка частиц в циклических ускорителях, основанный на матричном представлении оператора эволюции частиц. Этот метод позволяет вычислять эволюцию пучка частиц в терминах двумерных матриц, в том числе для нелинейных эффектов. Идеология геометрического интегрирования вводит в соответствующие вычислительные алгоритмы поправки, которые необходимы для сохранения качественных свойств отображений, представленных в виде усеченных рядов, порождаемых оператором эволюции. Этот формализм распространяется как на поляризованные, так и интенсивные пучки. Описаны примеры практического применения.

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INTRODUCTION

Numerical simulation of nonstationary processes in any field of science and technology, as a rule, can be reduced to the problem of solving systems of ordinary differential equations using appropriate methods. It is known that in many applications the exact solution (or stream) has a number of quality properties or the so-called "geometric" properties. For example, it is well known that the exact flow generated by the Hamiltonian system is symplectic, and the property of conservatism results in only to the constancy of energy along the exact solution, although the solution itself is changing with time. Z. Ge and J. Marsden demonstrated in [1] that the exact energy conservation should not follow, in general, from property symplecticity. Modern computer packages have a fairly good functionality (see, for example, [2–4]) and

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allow one to simulate the evolution of the particle beam in the nonlinear fields. However, the polarization of the beam is sufficiently fully included only into the COSY Infinity package. Moreover, these packages do not have "advanced" interface, that reduces the efficiency of their using. We also note that the COSY Infinity, MAD, and many other packages are based on the representation of the solution in the form of the Taylor series for the components of the phase vector

$$x_i(s) = \sum_{k_1=1}^{2n} T_{ik_1}(s|s_0)x_{k_1}(s_0) + \\ + \sum_{k_1=1}^{2n}\sum_{k_2=1}^{2n} T_{ik_1k_2}(s|s_0)x_{k_1}(s_0)x_{k_2}(s_0) + \ldots, i = \overline{1,2n}. \quad (1)$$

The "matrix" elements $T_{ik_1k_2\ldots k_n\ldots}(s|s_0)$ are generally calculated in numerical form, which greatly reduces the possibility of parametric optimization of beam control. Similar presentations are mainly used only for numerical calculations, thereby reducing the performance and accuracy of calculations. Indeed, numerical description does not allow realizing an effective parametric analysis of the impact of various factors on the characteristics of the beam. In addition, the representation of (1) is not very convenient for the implementation of computational procedures using parallel and distributed computing systems.

1. THE MATRIX FORMALISM FOR LIE ALGEBRAIC METHODS

The core of the matrix formalism is based on two well-known models of representation of nonlinear Taylor series. The first model is based on the traditional Taylor series in the tensor form, see [3]. The second model is based on the idea of presentation of an arbitrary power series using the basis of the Poincare–Witt [5]. Namely, this formalism gives us instead of coordinatewise equality (1) the required solution of nonlinear equations of evolution sought in the form

$$\mathbf{X}(s) = \sum_{k=1}^{\infty} \mathbb{R}^{1k}(s|s_0)\mathbf{X}_0^{[k]}, \quad (2)$$

where $\mathbf{X}_0^{[k]}$ is a vector consisting of all monomials of kth order built on the elements of an initial phase vector $\mathbf{X}_0$ [6]. The matrices $\mathbb{R}^{1k}(s|s_0)$ $\left(\dim \mathbb{R}^{1k} = (n \times d[n,k]),\ d[n,k] = \binom{n+k-1}{k}\right)$, $k \geqslant 1$, describe evolution changing of some initial phase vector $\mathbf{X}_0$ for kth order of nonlinearities. We write the equation of evolution in matrix form [6, 7]

$$\frac{d\mathbf{X}}{ds} = \sum_{k=1}^{\infty} \mathbb{P}^{1k}(s)\mathbf{X}^{[k]}, \quad \mathbf{X}(s_0) = \mathbf{X}_0, \quad (3)$$

where $\mathbb{P}^{1k}(s)$, $k \geqslant 1$, consist of coefficients of expansion of the evolution equation of the beam into power series in the neighborhood of the reference particle. Substituting (2) into (3), we can write the system of ODE for matrices $\mathbb{P}^{1k}$ in the form

$$\frac{d}{ds}\mathbb{R}^{1k} = \sum_{j=1}^{k} \mathbb{P}^{1j}(s)\mathbb{R}^{jk}(s|s_0), \quad \mathbb{R}^{kk} = (\mathbb{R}^{11})^{[k]}, \quad k \geqslant 1, \quad (4)$$

and introducing infinite matrices $\mathbb{P}^\infty$, $\mathbb{R}^\infty$ we can write

$$\frac{d}{ds}\mathbb{R}^\infty = \mathbb{P}^\infty\mathbb{R}^\infty, \quad \mathbb{R}^\infty = T\exp\left(\int\limits_{s_0}^{s}\mathbb{P}^\infty(\tau)\,d\tau\right), \quad k \geqslant 1, \tag{5}$$

where the symbol T indicates the chronologically ordered exponent according to the Volterra theory [8] or in the form of the Dayson operator [9]. It should be noted that the approach described above can be applied quite naturally in the case of high-intensity beams, for which we should take into account the effect of the self-field of the beam. In this case, one must use a method of constructing self-consistent solutions at every step of integration (see [7]). It should be noted that the matrix formalism naturally emerges both from the Taylor representation of the solution (1) and from the Lie formalism (see, e. g., [6, 10]). Each of these representations uses information representation of the beam using the coordinates of the beam. In the case of Taylor series, new coordinates are expressed in the form of a convergent Taylor series, in the neighborhood of the equilibrium path. In the case of Lie formalism, we use auxiliary homogeneous polynomials $h_k(\mathbf{X}, s)$, which can be written using the basis of the Poincare–Witt as $h_k(\mathbf{X}, s) = \mathbf{H}_k^T(s)\mathbf{X}^{[k]}$, $\mathbf{X} \in R^{2n}$. The use of phase coordinates reduces the flexibility of these methods, as it binds the process of building solutions to a particular trajectory. According to matrix formalism, one can build a map using a matrix $\mathbb{R}^{1k}(s|s_0)$, without regard for the specific coordinates of the particles. It should be noted that in the case of dense beams this approach is modified by using the concept of self-consistent evolution (see [7]).

Besides the usual description of a beam of particles as an ensemble of particles, we can use the following methods to describe the beam.

1. *A set of particles in phase space*. Suppose that at the initial time evolution the particles beam is described by some set in the phase space $G_0(\mathbf{X}) = G(\mathbf{X}, 0)$, which is being transformed into current one

$$G(\mathbf{X}, s) = G_0\left(\mathcal{M}^{-1}(s|s_0) \circ \mathbf{X}\right) = 0.$$

2. *The density function in phase space* $f(\mathbf{X}, s)$:

$$f(\mathbf{X}, s) = f_0\left(\left(\mathcal{M}^{-1} \circ \mathbf{X}\right)\right),$$

which satisfies the Vlasov equation. The above description of the particle density function of the beam can be used in terms of matrix formalism. In particular, at the initial time for the ellipsoidal beam we can write $G_0(\mathbf{X}, \varepsilon) = \mathbf{X}^T\mathbb{A}_0\mathbf{X} - \varepsilon$, $0 < \varepsilon \leqslant 1$. Next, using the properties of the Kronecker product, we can calculate the current value $G(\mathbf{X}, s)$:

$$G(\mathbf{X}, s) = \sum_{k=1}^{\infty}\sum_{j=1}^{\infty}\left(\mathbf{X}^{[k]}\right)^T\mathbb{A}_{kj}\mathbf{X}^{[j]} - \varepsilon, \quad \mathbb{A}_{kj} = \left(\mathbb{T}^{1k}\right)^T\mathbb{A}_0\mathbb{T}^{1j},$$

where the matrices $\mathbb{T}^{1k}$ can be evaluated according to the generalized Gauss method [7]:

$$\left(\mathcal{M}^{-1} \circ \mathbf{X}\right)^{[k]} = \sum_{l=k}^{\infty}\mathbb{T}^{kl}\mathbf{X}^{[l]}, \quad \mathbb{T}^{kk} = \left(\mathbb{M}^{kk}\right)^{-1} = \left(\mathbb{M}^{11}\right)^{-[k]},$$

$$\mathbb{T}^{ik} = -\mathbb{T}^{ii}\sum_{j=i+1}^{k}\mathbb{M}^{ij}\mathbb{T}^{jk}, \quad i < k, \quad \mathbb{T}^{ik} \equiv 0, \quad \forall j > k.$$

In particular, listed equalities and property of Kronecker products (see, e.g., [11]) for envelope matrices $\mathbb{S}^{11}$ taking into account nonlinear effects, we get $\mathbb{S}^{11}(s) = \sum\limits_{l=1,k=1}^{\infty} \mathbb{R}^{1l}(s|s_0)\mathbb{S}^{lk}(s_0) \times \left(\mathbb{R}^{1k}(s \mid s_0)\right)^T$, where

$$\mathbb{S}^{ik}(t) = \int\limits_{R^{2n}} f(\mathbf{X}, t)\mathbf{X}^{[i]} \left(\mathbf{X}^{[k]}\right)^T d\mathbf{X}.$$

For distribution functions we obtain

$$f(\mathbf{X}, s) = \sum_{k=0}^{\infty} \mathbb{F}_k^T \mathbf{X}^{[k]}, \quad \mathbb{F}_0 = \mathbb{F}_0^0, \quad \mathbb{F}_k = \sum_{l=1}^{k} \left(\mathbb{T}^{kl}\right)^T \mathbb{F}_l^0, \quad \forall\, k > l,$$

where $f_0(\mathbf{X}) = \sum\limits_{k=0}^{\infty} \left(\mathbb{F}_k^0\right)^T \mathbf{X}^{[k]}$ is the initial distribution function.

2. GEOMETRIZATION OF TRUNCATED SERIES

In Introduction, we briefly mentioned that the representation of the solution in the form of power series (COSY Infinity, MAD, and so on) or using formalism by A. Dragt conserve the qualitative properties inherent to the considered dynamical system. It is well known that the equations of evolution of particles can be described in the Hamiltonian form

$$\frac{d\mathbf{X}}{ds} = \mathbb{J}\frac{\partial \mathcal{H}(\mathbf{X}, s)}{\partial s}, \tag{6}$$

where $\mathbb{J} = \mathbb{J}(\mathbf{X}, s)$ is the Jacobi matrix consisting of the structural functions of Poisson manifolds respect to a local coordinate system $\mathbf{X} = = (x_1, \ldots; p_1, \ldots)^T$, and $\mathcal{H}(\mathbf{X}, s)$ is the Hamiltonian of the system. In the case of the canonical Poisson brackets we have $\mathbb{J}(\mathbf{X}) = \mathbb{J}_0 = \begin{pmatrix} \mathbb{O} & \mathbb{E} \\ -\mathbb{E} & \mathbb{O} \end{pmatrix}$. Let us introduce the Jacobi matrix $\mathbb{M}(\mathbf{X}; s|s_0) = \partial\left(\mathcal{M}(s|s_0; \mathcal{H}) \circ \mathbf{X}\right)/\partial \mathbf{X}^T$, then the requirement of conservation of the canonical Poisson bracket, defining the symplectic structure in phase space, leads to the identity, that is, for the canonical Jacobi matrix has the form:

$$\mathbb{M}^*(\mathbf{X}; s|s_0)\, \mathbb{J}_0 \mathbb{M}(\mathbf{X}; s|s_0) = \mathbb{J}_0, \quad \det \mathbb{M}(\mathbf{X}; s|s_0) \equiv 1, \quad \forall\, \mathbf{X} \in R^{2n}, \quad \forall\, s, s_0. \tag{7}$$

However, the property of symplecticity in practical calculations is violated, for example, due to truncation of the series or when using the approximate numerical schemes. Namely, the introduction of corrective amendments into the appropriate scheme that returns the property of symplecticity is called by symplectification (or geometrization) of used computational schemes. In particular, the COSY Infinity package uses a specially developed scheme symplectification [12]. The process of symplectification in the MaryLie package is realized using the other approach [10]. In the case of the matrix formalism for the return of properties symplecticity for a certain order of nonlinearity, we must impose the requirements of symplecticity to the corresponding matrices $\mathbb{R}^{1k}$, included in the corresponding expansion. To do this, we must substitute the appropriate series in the identity (7), and after some series of transformations, we obtain the chain of algebraic equalities. The first equation is satisfied

identically, and the rest should be considered as equations connecting the elements of the corresponding matrices. In the case of restricting up to some order nonlinearity, one can obtain a chain of simple linear algebraic equations with integer coefficients which can be easily solved in symbolic form [7]. For example, for the case of nonlinear second-order equations we obtain simple equalities

$$\mathbb{M}^{12} = \mathbb{M}^{11} \cdot \begin{pmatrix} q_{11} & q_{12} & q_{13} \\ q_{21} & -2q_{11} & -\dfrac{1}{2}q_{12} \end{pmatrix},$$

where the elements of q_{ik} are calculated according to the approach which can be realized in symbolic form and can be stored in a special database.

3. MULTITURN PROBLEM

In the long process of evolution, the beam passes through a series of identical sections in a single revolution and repeats this procedure many times (more than millions of revolutions). In other words, it is necessary to construct a map that is the Nth degree of the map for one revolution. We note that in the exponential representation of the operator Scaling and Squaring method is used, which is currently being actively discussed in the literature (see, for example, [10]). A similar approach has also been implemented in terms of the matrix formalism, the essence of which can be summarized as the following steps [7].

1. We determine the type and dimension of the matrix $\mathbb{R}^N$ according to (5) for this problem.

2. We build $\mathbb{R}^N$ in degree K (see [7]) symbolically according to the iterative exponentiation $\left(\left(\mathbb{R}^N\right)^m\right)^n$, where the total number of revolutions is equal to $K = m \cdot n$.

3. For the problem under study, we calculate a particular type of matrix $\mathbb{R}^N$.

4. We substitute the resulting matrix in the general solution $\mathbb{R}^N$.

Note that the third phase may be realized in multiple exponentiations, for example, $((2^2)^2 \ldots)^2$. Selection of the basis for the degree of multiplicity depends on the concrete model of the accelerator. We also note that the iterative exponentiation significantly reduces the computation time because we use the symbolic representation of the respective degrees of matrices. Despite the cumbersome form of these matrices, the process of calculation does not take a lot of time and memory is due to the interactivity of exponentiation process.

CONCLUSIONS

All of the approaches and algorithms described above are checked and implemented within the scope of JEDI collaboration for the problem of evolution of the polarized beam.

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