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Spline Function Representation For Transformation of Beam Phase Space With Arbitrary Contours

Mao Naifeng and Li Zenghai

(Institute of Atomic Energy, Beijing)

In order to study the transport of beams with arbitrary phase space contours, the spline function representation of the phase space contours is proposed in this paper. Having fitted the phase space contours with cubic spline functions, the phase space transformation is reduced to the spline function transformation, and the beam envelopes can be expressed with spline functions. The corresponding computer program is written and some typical examples are presented to illustrate the usefulness of this method.

1. INTRODUCTION

The theory of beam transport is widely used in the calculation and design of accelerators, beam transport systems, mass spectrometers, charged particle spectrographs, ion implanters and so on. In general, it is assumed in the theory[1] that the phase space contours are ellipsoids. However, measurements[2] have shown that the projections of practical phase space contours on each two-dimensional subspace are not exact ellipses, but very complex shapes. In recent years, the transport of beams with non-elliptic phase space contours (such as polygons and closed convex curves) has been studied by a few authors[3,4]. In their discussions the phase space contours are treated as the known analytical functions. The practical difficulty is that the measured phase space contours are in general composed of a series of discrete points and are hardly expressed as the analytical functions.

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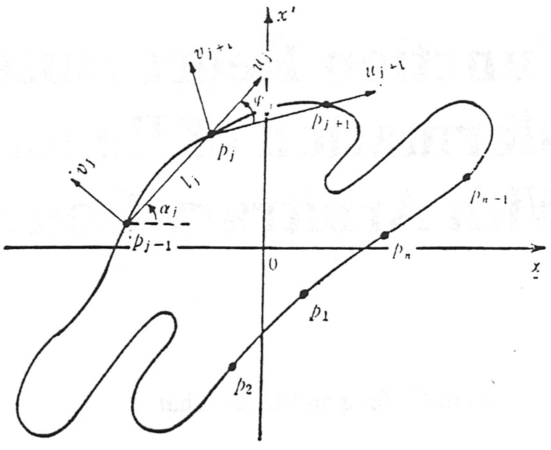

FIG.1 Arbitrary phase space contour and coordinate systems.

In this paper, the spline function representation of the beam phase space contours is proposed to study the transport of beams with arbitrary phase space contours. Firstly, the fitting procedure of the phase space contours with spline functions is described; secondly, the transformation expressions of spline functions during the transport of beams are derived, and the method for calculating the envelopes of beams with arbitrary phase space contours is given; finally, the corresponding program and some typical examples are presented.

2. SPLINE FUNCTION REPRESENTATION OF PHASE SPACE CONTOURS

The beam envelope is entirely determined by the transformation of beam phase space contours. Let us assume that a sequence of points $\{p_j(x_j(0),x_j'(0))\}$ $(j = 1,2,...,n)$ on an initial phase space contour in (x,x') phase plane is given (Fig.1). Generally speaking, the contour described by those n points is irregular or arbitrary. We try to use the spline functions to fit this contour and study its transformation. In such a case, the sequence of points are called sample points. It must be pointed out that the ordinary spline functions are not suitable on this occasion, because the contour is a closed curve which is multiple-valued and has vertical tangents. A preferable way to overcome the difficulty is to extend the spline functions in the ordinary coordinate system (x,x') to the spline functions in the local coordinate systems[5]. Thus the local coordinate systems should be set up at first. Taking the system (u_j,v_j) as an example. The abscissa u_j of the system coincides with the chord $\overline{p_{j-1}\,p_j}$ which connects the two adjacent points p_{j-1} and p_j, and the ordinate v_j is perpendicular to the chord as shown in Fig.1. Then fitting curvilinear equations are set up in each local coordinate system. In this way, the whole fitting curve has certain continuation properties at the sample points, and we can at once obtain the spline functions in the local coordinate systems.

The local cubic spline functions are used to fit the arbitrary phase space contour, which satisfy: (1) the fitting curve in each local coordinate system is a third order polynomial of u_j and passes through the two end points of the chord $\overline{p_{j-1}\,p_j}$; (2) the whole curve, its tangents and curvatures are contineous. Further considering the periodic end point condition determined by the closure property of the contour, we can immediately derive the local cubic spline functions.

Assuming the length of the chord $\overline{p_{j-1}p_j}$ is l_j, and the rotational angle of the coordinate system (u_j,v_j) relative to the coordinate system (u_{j+1},v_{j+1}) is ϕ_j, the cubic spline function of the fitting curve in the local coordinate system (u_j,v_j) can be written as follows

$$v_j(u_j) = a_{0j} + a_{1j}u_j + a_{2j}u_j^2 + a_{3j}u_j^3, \quad (j = 1, 2, \cdots, n;\ 0 \leqslant u_j < l_j) \tag{1}$$

where $a_{ij}(i = 0,1,2,3)$ are the coefficients of the local spline function

$$\begin{aligned} a_{0j} &= 0, \\ a_{1j} &= m_{j-1}, \\ a_{2j} &= \frac{-1}{l_j}\left(2m_{j-1} + \frac{m_j - \operatorname{tg}\phi_j}{1 + m_j \operatorname{tg}\phi_j}\right), \\ a_{3j} &= \frac{1}{l_j^2}\left(m_{j-1} + \frac{m_j - \operatorname{tg}\phi_j}{1 + m_j \operatorname{tg}\phi_j}\right), \end{aligned} \tag{2}$$

and $m_j(j = 1,2,\ldots,n)$ are the first order derivatives at the sample points p_j in the local coordinate systems (u_{j+1},v_{j+1}), which satisfy the following simultaneous non-linear equations

$$\lambda_j m_{j-1} + 2m_j + \mu_j m_{j+1} = C_j + F_j, \quad (j = 1, 2, \cdots, n) \tag{3}$$

where

$$\lambda_j = \frac{l_{j+1}}{l_j + l_{j+1}}, \qquad \mu_j = \frac{l_j}{l_j + l_{j+1}}$$

$$C_j = 2\lambda_j \operatorname{tg}\phi_j + \mu_j \operatorname{tg}\phi_{j+1},$$

$$F_j = F_{1j} + F_{2j} + F_{3j}$$

$$F_{1j} = \frac{\mu_j m_{j+1}(m_{j+1} - \operatorname{tg}\phi_{j+1})\operatorname{tg}\phi_{j+1}}{1 + m_{j+1}\operatorname{tg}\phi_{j+1}},$$

$$F_{2j} = \frac{2\lambda_j m_j(m_j - \operatorname{tg}\phi_j)\operatorname{tg}\phi_j}{1 + m_j \operatorname{tg}\phi_j}(\cos\phi_j + m_j \sin\phi_j)^3,$$

$$F_{3j} = \lambda_j[m_{j-1} + 2(m_j - \operatorname{tg}\phi_j)][1 - (\cos\phi_j + m_j\sin\phi_j)^3].$$

Because of the periodicity of the end point condition, all variables in the equations mentioned above cycle periodically with the period of n, for instance $m_0 = m_n$, $m_1 = m_{n+1}$ and so on. The right side of Eq.(3) includes two parts: linear term C_j and non-linear term F_j. Both of them are related to the rotational angle ϕ_j, and F_j is a second order infinitesimal compared with C_j if ϕ_j is sufficiently small.

At this point, simultaneous Eq.(3) can be solved by an iteration method, such as the relaxation iteration. Substituting the solved m_j into Eq.(2), the coefficients of cubic spline functions in the local coordinate systems can be obtained.

By using coordinate transformation, we can further obtain the cubic spline functions x and x', which fit the arbitrary phase space contour in the ordinary coordinate system (x,x'), with the local coordinate u_j as parameter

$$\begin{aligned} x(0) &= A_{0j}(0) + A_{1j}(0)u_j + A_{2j}(0)u_j^2 + A_{3j}(0)u_j^3, \\ x'(0) &= A'_{0j}(0) + A'_{1j}(0)u_j + A'_{2j}(0)u_j^2 + A'_{3j}(0)u_j^3, \\ &(j = 1, 2, \cdots, n;\ 0 \leqslant u_j < l_j) \end{aligned} \tag{4}$$

where

$$\begin{aligned} A_{0j}(0) &= x_{j-1}(0), & A'_{0j}(0) &= x'_{j-1}(0) \\ A_{1j}(0) &= \cos\alpha_j - a_{1j}\sin\alpha_j, & A'_{1j}(0) &= \sin\alpha_j + a_{1j}\cos\alpha_j \\ A_{2j}(0) &= -a_{2j}\sin\alpha_j, & A'_{2j}(0) &= a_{2j}\cos\alpha_j \\ A_{3j}(0) &= -a_{3j}\sin\alpha_j, & A'_{3j}(0) &= a_{3j}\cos\alpha_j \end{aligned}$$

and α_j is the angle included between u_j and x axes, $x_0(0) = x'_n(0)$, $x'_0(0) = x_n(0)$. In order to show that the phase space contour discussed here is the initial one, we write $x(0)$ and $x'(0)$ for x and x' respectively, and similarly write $A_{ij}(0)$ and $A_{ij}(0)$ for A_{ij} and $A_{ij}(i = 0,1,2,3)$.

3. SPLINE FUNCTION REPRESENTATION OF PHASE SPACE TRANSFORMATION

Having represented the initial phase space contours with spline functions, the transformation of phase space contours can be reduced to the transformation of spline functions. We express Eq.(4) in a matrix form as

$$\begin{aligned} x(0) &= [1,\ u_j^2]\begin{bmatrix} A_{0j}(0) & A_{1j}(0) \\ A_{2j}(0) & A_{3j}(0) \end{bmatrix}\begin{bmatrix} 1 \\ u_j \end{bmatrix} = [1,\ u_j^2]\,S_j(0)\begin{bmatrix} 1 \\ u_j \end{bmatrix}, \\ x'(0) &= [1,\ u_j^2]\begin{bmatrix} A'_{0j}(0) & A'_{1j}(0) \\ A'_{2j}(0) & A'_{3j}(0) \end{bmatrix}\begin{bmatrix} 1 \\ u_j \end{bmatrix} = [1,\ u_j^2]\,S'_j(0)\begin{bmatrix} 1 \\ u_j \end{bmatrix}, \\ &(j = 1, 2, \cdots, n;\ 0 \leqslant u_j < l_j) \end{aligned} \tag{5}$$

where $S_j = \begin{bmatrix} A_{0j}(0) & A_{1j}(0) \\ A_{2j}(0) & A_{3j}(0) \end{bmatrix}$ and $S'_j = \begin{bmatrix} A'_{0j}(0) & A'_{1j}(0) \\ A'_{2j}(0) & A'_{3j}(0) \end{bmatrix}$ are called coefficient matrices of spline functions of the initial phase space contour.

Through a transport section with the transport distance z and the transfer matrix R

$$R = \begin{bmatrix} R_{11} & R_{12} \\ R_{21} & R_{22} \end{bmatrix}, \tag{6}$$

the phase space contour of the beam is transformed into

$$\begin{bmatrix} x(z) \\ x'(z) \end{bmatrix} = \begin{bmatrix} R_{11} & R_{12} \\ R_{21} & R_{22} \end{bmatrix} \begin{bmatrix} x(0) \\ x'(0) \end{bmatrix}. \tag{7}$$

Substituting Eq.(5) into Eq.(7) and rearrange it, we can at once get

$$\begin{aligned} x(z) &= [1,\ u_j^2] S_j(z) \begin{bmatrix} 1 \\ u_j \end{bmatrix}, \\ x'(z) &= [1,\ u_j^2] S_j'(z) \begin{bmatrix} 1 \\ u_j \end{bmatrix}, \\ &(j = 1, 2, \cdots, n;\ 0 \leqslant u_j < l_j) \end{aligned} \tag{8}$$

where

$$\begin{aligned} S_j(z) &= \begin{bmatrix} A_{0j}(z) & A_{1j}(z) \\ A_{2j}(z) & A_{3j}(z) \end{bmatrix} = R_{11} S_j(0) + R_{12} S_j'(0), \\ S_j'(z) &= \begin{bmatrix} A_{0j}'(z) & A_{1j}'(z) \\ A_{2j}'(z) & A_{3j}'(z) \end{bmatrix} = R_{21} S_j(0) + R_{22} S_j'(0), \end{aligned} \tag{9}$$

Eq.(9) can also be expressed in the first order super-matrix form as

$$\begin{bmatrix} S_j(z) \\ S_j'(z) \end{bmatrix} = \begin{bmatrix} R_{11} & R_{12} \\ R_{21} & R_{22} \end{bmatrix} \begin{bmatrix} S_j(0) \\ S_j'(0) \end{bmatrix}. \tag{10}$$

Eq.(9) or (10) gives the transformation expressions for the coefficient matrices of spline functions. Obviously, at present we have reduced the transformation of the phase space contour to the transformation of the spline functions during the transport of the beam. The transformation of the arbitrary phase space contour can conveniently be calculated by using Eqs.(8)--(10).

4. BEAM ENVELOPES

Because of the arbitrariness of the phase space contour, the envelope equations of the beam, for instance the equations in (x,z) plane, should be studied for the left and right sides of the beam separately. By using the coefficient matrices of the spline functions, the envelope equations on both sides can be expressed as

$$x_l(z) = \min_{0 \le u_j < l_j} \left([1,\ u_j^3] S_j(z) \begin{bmatrix} 1 \\ u_j \end{bmatrix} \right),$$
$$(j = 1, 2, \cdots, n)$$
$$x_r(z) = \max_{0 \le u_j < l_j} \left([1,\ u_j^3] S_j(z) \begin{bmatrix} 1 \\ u_j \end{bmatrix} \right),$$
$$(j = 1, 2, \cdots, n) \tag{11}$$

It should be pointed out that the number of the extreme values of x on the phase space contour in the (x,x') phase plane are more than two in general. All of them satisfy the extreme value condition $dx/dx' = 0$. Assuming there are extreme values in the j-th local coordinate system $(0 \le u_j < l_j)$, it is not difficult to derive the extreme value condition of x with u_j as parameter

$$\frac{dx(z)}{du_j} = 3A_{3j}(z)u_j^2 + 2A_{2j}(z)u_j + A_{1j}(z) = 0,$$
$$(j = 1, 2, \cdots, n) \tag{12}$$

Assuming k extreme points $U_i(i = 1,2,...k)$ have been obtained in all by solving Eq.(12), the envelope equations Eq.(11) are reduced to

$$x_l(z) = \min_{i=1,2,\cdots,k} \left([1,\ U_i^3] S_j(z) \begin{bmatrix} 1 \\ U_i \end{bmatrix} \right),$$
$$x_r(z) = \max_{i=1,2,\cdots,k} \left([1, U_i^3] S_j(z) \begin{bmatrix} 1 \\ U_i \end{bmatrix} \right), \tag{13}$$

If the beam phase space contour is centrosymmetric, we have $x_l(z) = -x_r(z)$.

5. COMPUTER PROGRAM AND APPLIED EXAMPLES

Based on the spline function method for the transport of beams with arbitrary phase space contours, a computer program called TAPSC (Transformation of Arbitrary Phase Space Contours) has been developed.

The program has many entries, such as the entries for arbitrary, elliptic and polygonal phase space contours. The elliptic phase space contour is a regular case. At this point, only the major and minor axes, and the angle included between the major or minor axis and the abscissa axis x need to be input for any oblique ellipse. The sample points on the circumference of the ellipse are generated automatically by the program. The polygonal phase space contour is a special case of the arbitrary phase space contours. On this occasion, the cubic spline function reduces to a linear one.

The program TAPSC can make not only the transformation of (x,x') phase space related to the horizontal motion of the beam, but also the transformation of the (y,y') phase space related to the vertical motion of the beam.

The elements calculated by the program TAPSC may include all the first order magnetic elements involved in the program TRANSPORT[6].

A series of numerical tests have been made for the program TAPSC and the results are satisfactory. Here we take the transformation of an elliptic phase space contour in a double focusing mass spectrometer as an example. The beam envelope obtained by the program TAPSC (the spline function method, sample points $n = 16$) is in good agreement with the result obtained by

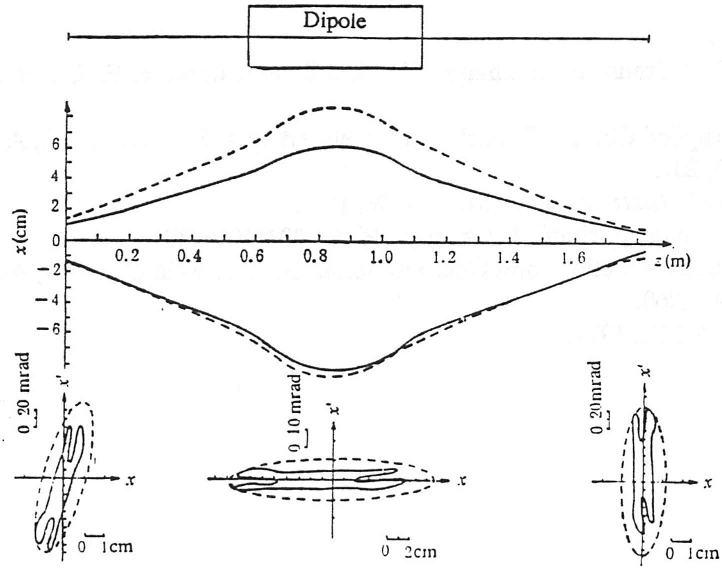

FIG.2 Beam envelopes and transformation of phase space in a magnetic analyzer. Solid lines are for arbitrary phase space contours; and dotted lines for circumscribed elliptic phase space contours.

TRANSPORT (traditional σ matrix method) with a relative deviation less than 1×10^{-4}. The CPU execution time taken by TAPSC on computer CYBER 170/825 is 2.96 seconds as against 2.51 seconds by TRANSPORT.

As another example, we discuss the transport of the beam with a very complex initial phase space contour passing through a magnetic analyzer. The envelope of the beam in the horizontal plane and the phase space contours at different positions along the beam line are shown in Fig.2 (solid lines). In comparison, the beam envelope of the centrosymmetric ellipses circumscribing the practical phase space contours, which have to be taken in the σ matrix method as an approximation, as well as the contours themself at different positions are also shown in Fig.2 (the dotted lines).

6. CONCLUSION

The spline function representation for the beam phase space proposed in this paper can realistically describe the transformation of the practical complex phase space contours and exactly calculate the beam envelopes. This method provides a new approach to the optimal design of the charged particle optical systems, and it is very easy to be programmed. Compared with the traditional σ matrix method, the additional CPU execution time taken by using the spline function method is just brief.

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