Nuclear Inst. and Methods in Physics Research, A 885 (2018) 124–133

Contents lists available at ScienceDirect

Nuclear Inst. and Methods in Physics Research, A

journal homepage: www.elsevier.com/locate/nima

Transfer matrix calculation for ion optical elements using real fields

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ARTICLE INFO

Keywords:
Transfer matrix
Ion-optics simulation

ABSTRACT

With the increasing importance of ion storage rings and traps in low energy physics experiments, an efficient transport of ion species from the ion source area to the experimental setup becomes essential. Some available, powerful software packages rely on transfer matrix calculations in order to compute the ion trajectory through the ion-optical beamline systems of high complexity. With analytical approaches, so far the transfer matrices are documented only for a few ideal ion optical elements. Here we describe an approach (using beam tracking calculations) to determine the transfer matrix for any individual electrostatic or magnetostatic ion optical element. We verify the procedure by considering the well-known cases and then apply it to derive the transfer matrix of a 90-degree electrostatic quadrupole deflector including its realistic geometry and fringe fields. A transfer line consisting of a quadrupole deflector and a quadrupole doublet is considered, where the results from the standard first order transfer matrix based ion optical simulation program implementing the derived transfer matrix is compared with the real field beam tracking simulations.

1. Introduction

Precision spectroscopy experiments on atomic, molecular and cluster ions have become active research areas among others in fundamental physics, medical science, and astrophysics. These measurements often take advantage of the excellent experimental conditions offered by storage rings [1–5] and traps [6–10]. Especially the large-scale storage ring devices are usually separated from the ion source area for beam production and preparation. Hence, the ions have to be transferred efficiently to the experimental setup. A typical beamline system consists of electrostatic and magnetostatic ion optical elements. The beamline design requires detailed ion trajectory simulations and beam property calculations for an efficient ion transport. Therefore the field characteristics of the ion optical elements have to be optimized. Ion trajectory computations are performed either using real fields or employing transfer matrices of the ion optical elements. The latter are derived by solving the equation of motion for a charged particle passing through the element. They are first order calculations based on sharp cuts of the fields at the boundary of the device. Furthermore, the transfer matrix can only be derived if the central particle follows a straight or a circular path inside the element.

However, there are ion optical elements such as an electrostatic quadrupole deflector or an electrostatic energy analyzer made of parallel plates, where the central orbit of the charged particle moving inside the element is neither a straight line nor a circle. In this case the transfer matrix cannot be derived analytically. So far such ion optical elements cannot be used in simulation programs such as MAD8 [11] and MIRKO [12], which are based on transfer matrices.

The advantage of a quadrupole deflector compared to cylindrical or spherical deflectors is that the beam can be optionally directed 90 degree to the left, to the right, or even guided straightforward. Such quadrupole deflectors are implemented, e.g., in the SAPHIRA storage ring [13]. Furthermore, the two-dimensional quadrupole field has properties not only as an ion beam deflector, but also as energy analyzer and beam merger [14]. Therefore, the transfer matrix is essential to use the quadrupole deflector in first order ion optics simulation programs. To our knowledge only the work of Zeman [14], deriving the transfer matrix of an ideal hyperbolic electrostatic quadrupole deflector neglecting any fringe field effects at the entrance and the exit of the device, is available in this field of research. This is not sufficient for real beam simulations, where fringe fields exist and crucially affect the ion motion. In extended beamline systems these errors add up becoming unacceptably large. Here, the real field simulations are advantageous. But the computing power is increasing with the number of involved ion optical elements and real field simulations become impractical for larger beamline systems. Instead, employing transfer matrices for beamline simulations is a promising approach.

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https://doi.org/10.1016/j.nima.2017.11.057
Received 24 August 2017; Received in revised form 30 October 2017; Accepted 16 November 2017
Available online 24 December 2017
0168-9002/

In this article we describe a method calculating the transfer matrices of complex ion optical elements for which analytical calculations are not possible. As an example we will discuss an electrostatic quadrupole deflector. Such a deflector is foreseen to be used in the low energy beamline of the cryogenic storage ring (CSR) [15] ion injector presently under construction at the Max-Planck-Institut für Kernphysik in Heidelberg. Unlike previous studies, the real field simulations of a single ion optical element are employed in order to derive its transfer matrix. Therefore the Twiss parameters [16] describing the phase space ellipse of the ion beam under test are calculated at the entrance and the exit of the ion optical element by tracking ions through the real field. The matrix elements are extracted from fits to the relations between the initial and the final Twiss parameters. Important to note is that the higher order terms and the coupling between the horizontal and vertical motions are still neglected in the first order approach considered here. Hence, the results are valid for ion optical elements whose apertures are significantly larger than the beam diameter.

The article is structured as follows: In Section 2 the procedure to derive the matrix elements from tracking calculations is described. The transfer matrix calculation of an electrostatic cylindrical deflector, an electrostatic spherical deflector, and a magnetic quadrupole lens are discussed as case studies in Section 3. These case-study elements are well understood and the derived transfer matrices can be compared to analytical solutions. Furthermore, employing the present method, the theoretically derived matrix elements of an ideal hyperbolic electrostatic quadrupole deflector excluding the fringe field by Zeman [14] is also reproduced. Finally, in Section 4, an electrostatic quadrupole deflector geometry consisting of circular electrodes including fringe fields at the entrance and the exit of the deflector field is discussed for a real situation. The derived matrix elements are compared to the phase space ellipse obtained from beam tracking simulations using real fields demonstrating the applicability of the method to arbitrary ion optical elements. Henceforth, in order to show the use of such matrix calculation in a first order ion optical simulation program like MAD8 [11], a transfer line with quadrupole deflector and quadrupole doublet is simulated in MAD8 using the derived matrix of the quadrupole deflector. These results are compared with the beam tracking simulations using real field.

2. Determination of the transfer matrix

A charged particle at any position s with respect to the central orbit inside an electrostatic or magnetostatic beamline system is described by the vector $X(s) = [x, x', y, y', l, \Delta p/p]$. x, y denote the horizontal and vertical displacements while x', y' are the corresponding angles of the ion trajectory with respect to the central orbit [16]. l is the deviation in longitudinal displacement of the particle with respect to the central particle (which moves along the central orbit). $\Delta p/p$ is the relative momentum deviation of an ion compared to the central particle with momentum p.

The ion transit through each ion optical element from the initial ($s = 0$) to the final position s can be described by [16,17]:

$$X(s) = R(s)X(0). \tag{1}$$

If the horizontal and vertical motions are decoupled and any temporal evolution is neglected, then the transfer matrix $R(s)$ is given by:

$$R(s) = \begin{pmatrix} M_{11} & M_{12} & 0 & 0 & M_{15} \\ M_{21} & M_{22} & 0 & 0 & M_{25} \\ 0 & 0 & M_{33} & M_{34} & M_{35} \\ 0 & 0 & M_{43} & M_{44} & M_{45} \\ M_{51} & M_{52} & M_{53} & M_{54} & M_{55} \end{pmatrix}, \tag{2}$$

with

$$M_{hor} = \begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix} \tag{3}$$

and

$$M_{ver} = \begin{pmatrix} M_{33} & M_{34} \\ M_{43} & M_{44} \end{pmatrix}. \tag{4}$$

Eqs. (3) and (4) give the horizontal and vertical transfer matrices. M_{15} and M_{25} in Eq. (2) describe the dispersive elements in horizontal direction, while M_{35} and M_{45} are zero considering no dispersion in vertical direction. For the constant $\Delta p/p$, all matrix elements in the fifth row of Eq. (2) are zero except M_{55}, which is equal to 1 [16].

In first order, a beam of charged particles can be described by a two-dimensional phase space ellipse in horizontal and vertical direction, given by the coordinates x, y and the slopes x', y' of each trajectory with respect to the central orbit. The root mean square (RMS) emittance (ε_{RMS}) of the ion beam is thus a measure of the average spread of transverse particle coordinates and is defined [18] in horizontal direction by:

$$\varepsilon_{x,RMS} = \sqrt{\langle x^2\rangle\langle x'^2\rangle - \langle xx'\rangle^2}, \tag{5}$$

where $\langle x^2\rangle$, $\langle x'^2\rangle$ and $\langle xx'\rangle$ represent the averages of x^2, x'^2, and xx', respectively, over all particles in the beam. Respectively, the vertical RMS emittance is defined.

The beam emittance is related to the three Twiss or Courant–Snyder parameters α, β, and γ [17,19] by:

$$\varepsilon_{x,RMS} = \gamma_x x^2 + 2\alpha_x xx' + \beta_x x'^2. \tag{6}$$

The Twiss parameters α_x and β_x can be determined by:

$$\alpha_x = -\frac{\langle xx'\rangle}{\varepsilon_{x,RMS}} \tag{7}$$

and

$$\beta_x = \frac{\langle x^2\rangle}{\varepsilon_{x,RMS}}. \tag{8}$$

β_x is related to the beam width and α_x describes the orientation of the phase space ellipse. A beam can be converging ($\alpha_x > 0$), diverging ($\alpha_x < 0$), or being at waist ($\alpha_x = 0$).
γ_x is determined using α_x and β_x:

$$\gamma_x = \frac{1+\alpha_x^2}{\beta_x} = \frac{\langle x'^2\rangle}{\varepsilon_{x,RMS}}. \tag{9}$$

It characterizes the divergence of the ion beam.

2.1. Twiss parameters determination

Beam tracking calculations through the real field are used to determine the phase space coordinates (x, x') of each ion in front and after the ion optical element. For this, various initial beam sizes (β_i) with zero momentum deviation are considered under the condition that the emittance is conserved. The momentum deviation has to be zero enabling the transfer matrix elements calculations of M_{hor} and M_{ver}. The Twiss parameters at the exit (α_f, β_f) of the element as well as the final RMS emittance are obtained using Eqs. (5)–(8). Furthermore, they are determined along the beam trajectory at positions outside the ion optical element, where the fringe fields of the element can be neglected. The relation between the initial (α_i, β_i) and final (α_f, β_f) Twiss parameters allows reconstructing the matrix elements of M_{hor} and M_{ver} (see Section 2.2).

2.2. Determination of the matrix elements of M_{hor} and M_{ver}

The transformation of Twiss parameters (α, β and γ) from initial ($s = 0$) to final position s can be described by [17]:

$$\begin{pmatrix} \beta_f \\ \alpha_f \\ \gamma_f \end{pmatrix} = \begin{pmatrix} {M_{11}}^2 & -2M_{11}M_{12} & {M_{12}}^2 \\ -M_{11}M_{21} & (M_{11}M_{22} + M_{21}M_{12}) & -M_{12}M_{22} \\ {M_{21}}^2 & -2M_{21}M_{22} & {M_{22}}^2 \end{pmatrix} \begin{pmatrix} \beta_i \\ \alpha_i \\ \gamma_i \end{pmatrix}, \tag{10}$$