DETERMINATION OF THE ION-OPTICAL PROPERTIES OF AN ELECTROSTATIC QUADRUPOLE LENS AS PART OF A COMPACT NUCLEAR MICROPROBE

V.V. Zhurakulov, H.E. Polojiy, O.G. Ponomarev Institute of Applied Physics, National Academy of Sciences of Ukraine, Sumy, Ukraine

The definition of the space of trajectory phase moments is introduced. The nonlinear differential equations of motion of a charged particle in the field of an electrostatic quadrupole lens in trajectory phase coordinates are transformed into a system of four linear ordinary differential equations in the third-order trajectory phase momentum space with 28 unknowns. The missing equations are obtained by applying a formal procedure of immersion of the original equations in the space of trajectory phase moments. The solution of the obtained complete system of equations is sought in the form of a matrizant, i.e., the matrix of phase moment transformation along the motion of a charged particle, which determines the ion-optical properties of an electrostatic quadrupole lens.

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1. INTRODUCTION

The Institute of Applied Physics of the National Academy of Sciences of Ukraine is developing the concept of a compact nuclear microprobe based on an immersion probe-forming system [1-3], which will significantly reduce the size of the microprobe installation and improve its resolution. The ion-optical scheme of such a probe-forming system includes (along the ion beam) a doublet of electrostatic quadrupole lenses (DEQL), an accelerating tube, an angular aperture, a scanner, and a doublet of magnetic quadrupole lenses for final beam focusing. The ionoptical properties of the accelerator tube and magnetic quadrupole lens including up to the third order were determined earlier using the matrizant method [2, 4]. The inclusion of the DEQL in the probe formation process will allow balancing the demagnifications in both transverse directions. Since it is assumed that the DEOL is located in front of the accelerator tube, this location is under high potential, which in turn determines the requirements for low power consumption for the doublet excitation, in contrast to magnetic quadrupole lenses. Similarly, the design of the DEQL is preferred due to the low beam energy in this region. In order to model the optics of such an immersion probeforming system, this paper considers the construction of a matrizant of an electrostatic quadrupole lens up to the third order in order to determine the physical and geometrical parameters of the ion-optic elements of the system. The fundamentals of the matrizant method are discussed in [5, 6], which are based on differential algebra and the matrix method for solving systems of linear ordinary differential equations.

2. CONSTRUCTION OF A SYSTEM OF DIFFERENTIAL EQUATIONS IN THE SPACE OF TRAJECTORY PHASE MOMENTS

The trajectory equations of motion of a charged particle in an electric field in a rectangular Cartesian coordinate system, which describe the ion optics of systems with a rectilinear axial trajectory, are as follows [7]

$$\begin{cases} x'' = \frac{qm}{p^2} (E_x - x'E_z)(x'^2 + y'^2 + 1) \\ y'' = \frac{qm}{p^2} (E_y - y'E_z)(x'^2 + y'^2 + 1) \end{cases}, (1)$$

where q,m,p – are the charge, mass and momentum of the particle, E_x , E_y , E_z – components of the electric field.

Equation (1) is a second-order nonlinear differential equation with respect to the trajectory phase coordinates (x, x', y, y'). Fig. 1 shows a schematic representation of an electrostatic quadrupole lens. Here, the poles are positioned in such a way that the ion beam is focused in the xOz plane, and the lens is defocused in the yOz plane.



Fig. 1. Schematic representation of an electrostatic quadrupole lens

For such poles, the electrostatic scalar potential can be represented as a series with the fourth order of coordinates x, y [7]

$$\varphi(x, y, z) = U_2(z)(x^2 - y^2) - \frac{U_2''(z)(x^4 - y^4)}{12}, \qquad (2)$$

where $U_2(z)$ – quadrupole component of the field. The quadrupole component can be represented as

$$U_2(z) = \frac{V\tau(z)}{r_a^2} \tag{3}$$

where V – potential at the pole of the lens; r_a – radius of the lens aperture;

 $\tau(z)$ – longitudinal field distribution profile (Fig. 2).



Fig. 2. Representation of the longitudinal distribution profile of the quadrupole field component: 1 - real field distribution; 2 – approximation of the field distribution with reduction to the effective length (rectangular model)

In Fig. 2 the effective field length $L_{eff} = l + (0.9...1.1)r_a$, where $l=z_2-z_1$ the physical length of the lens.

Taking into account (2), the electrostatic field can be represented in the form with dependence on the coordinates x, y not higher than the third degree

$$\begin{cases} E_x(x, y, z) = -\frac{\partial \varphi}{\partial x} = -2U_2(z)x + \frac{U_2''(z)}{3}x^3 \\ E_y(x, y, z) = -\frac{\partial \varphi}{\partial x} = 2U_2(z)y - \frac{U_2''(z)}{3}y^3 \\ E_z(x, y, z) = -\frac{\partial \varphi}{\partial x} = -U_2'(z)(x^2 - y^2) \end{cases}$$
(4)

Taking into account the fact that the trajectory coordinates x, y and the momentum spread in the beam δ are small parameters, we can use a series expansion in small parameters

$$\frac{m}{p^2} = \frac{m}{p_o^2} \left[1 - 2\delta + \frac{2mq}{p_o^2} \varphi(x, y, z) \right], \quad (5)$$

where p_0 - is the average momentum of the ions in the beam.

Let's substitute the ratio (4) and (5) into (1), multiplying the factors, we leave only the third order of smallness terms in the trajectory phase coordinates x, x', y, y' and the second order of smallness terms containing δ , we obtain

$$\begin{cases} x'' = -\beta^{2}\tau x + 2\beta^{2}\tau x\delta + \beta^{2}\left(\frac{\tau''}{6} - \beta^{2}\tau^{2}\right)x^{3} + \frac{\beta^{2}}{2}\tau' x^{2}x' - \\ -\beta^{2}\tau xx'^{2} + \beta^{4}\tau^{2}xy^{2} - \beta^{2}\tau xy'^{2} - \frac{\beta^{2}}{2}\tau' x'y^{2} \end{cases}$$
(6)
$$y'' = +\beta^{2}\tau y - 2\beta^{2}\tau y\delta - \beta^{2}\left(\frac{\tau''}{6} + \beta^{2}\tau^{2}\right)y^{3} - \frac{\beta^{2}}{2}\tau' y^{2}y' + \\ +\beta^{2}\tau yy'^{2} + \beta^{4}\tau^{2}yx^{2} + \beta^{2}\tau yx'^{2} + \frac{\beta^{2}}{2}\tau' y'x^{2}, \\ \text{where } \frac{2mq}{p^{2}}U_{2}(z) = \frac{2mqV}{p^{2}r_{a}^{2}}\tau(z) = \beta^{2}\tau(z).$$
(7)

Let us introduce the generalised coordinates of the trajectory phase moments in the form

$$\vec{\Phi}_{x} = \|\Phi_{x,i}\|_{i=1\dots 14} =$$

$$= (x, x', x\delta, x'\delta, x^{3}, x^{2}x', xx'^{2}, x'^{3}, xy^{2}, xyy', xy'^{2}, x'yy', x'y'^{2})^{T};$$

$$\vec{\Phi}_{y} = \|\Phi_{y,i}\|_{i=1\dots 14} =$$

$$(8)$$

 $=(y, y', y\delta, y'\delta, y^3, y^2y', yy'^2, y'^3, yx^2, yxx', yx'^2, y'x^2, y'xx', y'x'^2)^T.$ Equation (6) in the generalised coordinates of

trajectory phase moments is written as $((\Phi))' = \Phi$

$$\begin{pmatrix} (\Phi_{x,1})' = \Phi_{x,2} \\ (\Phi_{x,2})' = -\beta^{2}\tau \Phi_{x,1} + 2\beta^{2}\tau \Phi_{x,3} + \beta^{2} \left(\frac{\tau''}{6} - \beta^{2}\tau^{2}\right) \Phi_{x,5} + \\ + \frac{\beta^{2}}{2}\tau' \Phi_{x,6} - \beta^{2}\tau \Phi_{x,7} + \beta^{4}\tau^{2} \Phi_{x,9} - \beta^{2}\tau \Phi_{x,11} - \frac{\beta^{2}}{2}\tau' \Phi_{x,12} \\ (\Phi_{y,1})' = \Phi_{y,2} \\ (\Phi_{y,2})' = \beta^{2}\tau \Phi_{y,1} - 2\beta^{2}\tau \Phi_{y,3} - \beta^{2} \left(\frac{\tau''}{6} + \beta^{2}\tau^{2}\right) \Phi_{y,5} - \\ - \frac{\beta^{2}}{2}\tau' \Phi_{y,6} + \beta^{2}\tau \Phi_{y,7} + \beta^{4}\tau^{2} \Phi_{y,9} + \beta^{2}\tau \Phi_{y,11} + \frac{\beta^{2}}{2}\tau' \Phi_{y,12}. \end{cases}$$
(9)

As can be seen, equations (9) are linear with respect to the coordinates of the trajectory phase moments (8). However, in (9) there are 28 unknown functions and 4 equations. The expansion of equations (9) to 28 is carried out according to the formal procedure of immersion in the phase momentum space.

$$(\Phi_{x,3})' = (x\delta)' = x'\delta = \Phi_{x,4},$$
...
$$(\Phi_{x,8})' = (x'^3)' = 3x'^2 x'' =$$

$$= -3\beta^2 \tau x x'^2 + o_5 = -3\beta^2 \tau \Phi_{x,7},$$
...
$$(\Phi_{x,14})' = (x'y'^2)' = x''y'^2 + 2x'y'y'' =$$

$$= -\beta^2 \tau x y'^2 + 2\beta^2 \tau x' y y' + o_5 =$$

$$= -\beta^2 \tau \Phi_{x,11} + 2\beta^2 \tau \Phi_{x,13}.$$
(10)

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A similar procedure is used for unknown functions $\Phi_{v,i}$, *i*=3...14. Functions o_5 and o_4 contain terms with 5th i 4-th order by trajectory phase coordinates and momentum spread, respectively.

In this way, we obtained two systems of linear ordinary differential equations with respect to the trajectory phase moment coordinates that approximate the original nonlinear differential equations (5) in the domain of trajectory phase coordinates with the 4-th and 5-th order of smallness in terms of the spread in momentum and trajectory phase coordinates. The resulting equations can be written in matrix form

$$\frac{d\vec{\Phi}_x}{dz} = \mathbf{P}_x \cdot \vec{\Phi}_x, \qquad \frac{d\vec{\Phi}_y}{dz} = \mathbf{P}_y \cdot \vec{\Phi}_y, \qquad (11)$$

where the matrices \mathbf{P}_{x} and \mathbf{P}_{y} have a block form

$$\mathbf{P}_{x} = \begin{bmatrix} T_{1,1} & T_{1,2} & T_{1,3} & T_{1,4} \\ 0 & T_{2,2} & 0 & 0 \\ 0 & 0 & T_{3,3} & 0 \\ 0 & 0 & 0 & T_{4,4} \end{bmatrix},$$
(12)
$$\mathbf{P}_{y} = \begin{bmatrix} H_{1,1} & H_{1,2} & H_{1,3} & H_{1,4} \\ 0 & H_{2,2} & 0 & 0 \\ 0 & 0 & H_{3,3} & 0 \\ 0 & 0 & 0 & H_{4,4} \end{bmatrix},$$

where blocks can be written in the form

3. ELECTROSTATIC QUADRUPOLE LENS MATRIZANT

For equations (11), we introduce the concepts of the matrizant $\mathbf{R}_x(z,z_0)$ and $\mathbf{R}_y(z,z_0)$ respectively, which are defined as the matrix of transformation of coordinates of trajectory phase moments from the z_0 plane to the z plane in the form

$$\vec{\Phi}_{x}(z) = \mathbf{R}_{x}(z, z_{0})\vec{\Phi}_{x}(z_{0}),$$

$$\vec{\Phi}_{y}(z) = \mathbf{R}_{y}(z, z_{0})\vec{\Phi}_{y}(z_{0}).$$
(13)

It is worth noting the properties of the matrizant

 $\mathbf{R}_{x(y)}(z_{3},z_{1}) = \mathbf{R}_{x(y)}(z_{3},z_{2}) \mathbf{R}_{x(y)}(z_{2},z_{1}).$ (14) Substituting (13) into (11), we obtain

$$\frac{d\mathbf{R}_{x}(z,z_{0})}{dz} = \mathbf{P}_{x}(z) \cdot \mathbf{R}_{x}(z,z_{0}),$$

$$\frac{d\mathbf{R}_{y}(z,z_{0})}{dz} = \mathbf{P}_{y}(z) \cdot \mathbf{R}_{y}(z,z_{0}),$$
(15)

with initial conditions

$$\mathbf{R}_{x(y)}(z_0, z_0) = \mathbf{E},\tag{16}$$

where \mathbf{E} – unit matrix.

Matrizants $\mathbf{R}_x(z,z_0)$ and $\mathbf{R}_y(z,z_0)$ have the same block structure as the matrices $\mathbf{P}_{x(y)}(z)$

$$\mathbf{R}_{x}(z, z_{0}) = \begin{bmatrix} R_{x}^{1,1} & R_{x}^{1,2} & R_{x}^{1,3} & R_{x}^{1,4} \\ 0 & R_{x}^{2,2} & 0 & 0 \\ 0 & 0 & R_{x}^{3,3} & 0 \\ 0 & 0 & 0 & R_{x}^{4,4} \end{bmatrix},$$
(17)
$$\mathbf{R}_{y}(z, z_{0}) = \begin{bmatrix} R_{y}^{1,1} & R_{y}^{1,2} & R_{y}^{1,3} & R_{y}^{1,4} \\ 0 & R_{y}^{2,2} & 0 & 0 \\ 0 & 0 & R_{y}^{3,3} & 0 \\ 0 & 0 & 0 & R_{y}^{4,4} \end{bmatrix}$$

From the form (15) and (17) we can write $\frac{1}{1000}$

$$\frac{dR_x^{1,1}(z,z_0)}{dz} = T_{1,1}(z) \cdot R_x^{1,1}(z,z_0),$$

$$\frac{dR_y^{1,1}(z,z_0)}{dz} = H_{1,1}(z) \cdot R_y^{1,1}(z,z_0).$$
(18)

Let us consider the so-called rectangular field model, when the smooth longitudinal field distribution is replaced by a rectangular distribution with the effective field length L_{eff} (see Fig. 2). This distribution can be written as a superposition of two step functions [8]

$$\tau(z) = [\theta(z - z_0) - \theta(z - z_0 - L_{eff})], \quad (19)$$

where $\theta(z)$ single asymmetric step function

For the rectangular model of the longitudinal field distribution (19), we have the solution of equations (18) in the form

$$R_{x}^{1,1}(z,z_{0}) = \begin{bmatrix} r_{1,1} & r_{1,2} \\ r_{2,1} & r_{2,2} \end{bmatrix} = \begin{bmatrix} \cos[\beta(z-z_{0})] & \frac{1}{\beta}\sin[\beta(z-z_{0})] \\ -\beta\sin[\beta(z-z_{0})] & \cos[\beta(z-z_{0})] \end{bmatrix}.$$
(20)

$$R_{y}^{1,1}(z, z_{0}) = \begin{bmatrix} q_{1,1} & q_{1,2} \\ q_{2,1} & q_{2,2} \end{bmatrix} = \begin{bmatrix} \cosh[\beta(z-z_{0})] & \frac{1}{\beta} \sinh[\beta(z-z_{0})] \\ \beta \sinh[\beta(z-z_{0})] & \cosh[\beta(z-z_{0})] \end{bmatrix}.$$
(21)

Once the elements of the matrizants are defined

$$R_{x}^{1,1}(z, z_{0}) \text{ and } R_{y}^{1,1}(z, z_{0}) \text{ the equations can be written}$$

$$\Phi_{x,1}(z) = x(z) =$$

$$= r_{1,1}(z, z_{0})x_{0} + r_{1,2}(z, z_{0})x'_{0} + o_{2} + o_{3},$$

$$\Phi_{x,2}(z) = x'(z) =$$

$$= r_{2,1}(z, z_{0})x_{0} + r_{2,2}(z, z_{0})x'_{0} + o_{2} + o_{3},$$

$$\Phi_{y,1}(z) = y(z) =$$

$$= q_{1,1}(z, z_{0})y_{0} + q_{1,2}(z, z_{0})y'_{0} + o_{2} + o_{3},$$

$$\Phi_{x,2}(z) = y'(z) =$$

$$= q_{2,1}(z, z_{0})y_{0} + q_{2,2}(z, z_{0})y'_{0} + o_{2} + o_{3},$$
(22)

where $x(z_0) = x_0$, $x'(z_0) = x'_0$, $y(z_0) = y_0$, $y'(z_0) = y'_0$, o_2 and o_3 – functions of the second and third order of smallness in terms of momentum spread and trajectory phase coordinates, respectively.

Diagonal blocks of matrizants $R_x^{3,3}$, $R_x^{4,4}$, $R_y^{3,3}$, $R_y^{4,4}$ can be obtained by the following formal procedure

$$\begin{split} \Phi_{x,5}(z) &= x^3(z) = (r_{1,1}x_0 + r_{1,2}x_0')^3 = \\ &= r_{1,1}^3 x_0^3 + 3r_{1,1}^2 r_{1,2} x_0^2 x_0' + 3r_{1,1}r_{1,2}^2 x_0 x_0'^2 + r_{1,2}^3 x_0'^3 = \\ &= r_{1,1}^3 \Phi_{0x,5} + 3r_{1,1}^2 r_{1,2} \Phi_{0x,6} + 3r_{1,1}r_{1,2}^2 \Phi_{0x,7} + r_{1,2}^3 \Phi_{0x,7}, \\ & \cdots \\ \Phi_{x,8}(z) &= x'^3(z) = (r_{2,1}x_0 + r_{2,2}x_0')^3 = \\ &= r_{2,1}^3 x_0^3 + 3r_{2,1}^2 r_{2,2} x_0^2 x_0' + 3r_{2,1}r_{2,2}^2 x_0 x_0'^2 + r_{2,2}^3 x_0'^3 = \\ &= r_{2,1}^3 \Phi_{0x,5} + 3r_{2,1}^2 r_{2,2} \Phi_{0x,6} + 3r_{2,1}r_{2,2}^2 \Phi_{0x,7} + r_{2,2}^3 \Phi_{0x,7}, \\ & \cdots \\ \Phi_{x,14}(z) &= x'(z)y'^2(z) = \\ &= (r_{2,1}x_0 + r_{2,2}x_0')(q_{2,1}y_0 + q_{2,2}y_0')^2 = \dots = \\ &= r_{2,1}q_{2,1}^2 \Phi_{0x,9} + \dots + r_{2,2}q_{22}^2 \Phi_{0x,14}. \end{split}$$

The same procedure is used for $\Phi_{v,i}$, where i=5...14.

As can be seen from (12), the elements of the square matrices $\mathbf{P}_x(z)$ and $\mathbf{P}_y(z)$ include not only the profile function $\tau(z)$, but also its derivatives, which are expressed through the asymmetric impulse function $\phi(z)$ [8], known in physics as the Dirac function and its derivatives

$$\frac{d^{(k)}\theta(z+a)}{dz^{(k)}} = \frac{d^{(k-1)}\phi(z+a)}{dz^{(k-1)}}.$$
 (24)

Given the equality of (12), (20), (21), (23) and (24), the off-diagonal blocks of matrizants $R_x^{1,2}$, $R_x^{1,3}$, $R_x^{1,4}$, $R_y^{1,2}$, $R_y^{1,3}$, $R_y^{1,4}$ are calculated according to the formula [6]

$$R_{x(y)}^{i,k}(z,z_0) =$$

$$= \sum_{j=1+i}^{k} \int_{z_0}^{z} R_{x(y)}^{i,i}(z,t) P_{x(y)}^{i,j}(t) R_{x(y)}^{j,k}(t,z_0) dt.$$
(25)

4. CONCLUSIONS

Based on the introduction of the definition of the trajectory phase momentum space, a system of linear ordinary differential equations is obtained that approximates the original nonlinear differential equations of motion of a charged particle in the field of an electrostatic quadrupole lens with the third order of trajectory phase coordinates. The resulting system of differential equations is solved by the matrix method by introducing the concept of matrizant. For a rectangular model of the longitudinal distribution of the electric field in a quadrupole lens, a matrizant is obtained that determines the third-order ion-optical properties of the lens. Taking into account the fact that the matrizants of the electrostatic accelerating structure (accelerator tube) and the magnetic quadrupole lens were obtained earlier, it is possible to simulate the motion of the ion beam in a compact nuclear microprobe in order to determine the geometric and physical parameters of the immersion probe-forming system.

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