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Computer program TRIO 2.0
for calculation and visualization of ion trajectories

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Abstract

The computer program TRIO 2.0 was developed for the design and evaluation of ion optical systems. The program has many functions with useful graphical user interfaces. The program can handle systems including the following ion optical components: drift spaces, electrostatic sectors, magnetic sectors, electric or magnetic quadrupole lenses, and multipole lenses. The program supplies functions for evaluating the ion optical properties of a system. The following properties can be simulated and visualized: the ion trajectory, the image of the beam profile, the beam envelope and the ion transmission, the peak shape of time-of-flight, and the energy and angular focal planes. All the programs of TRIO 2.0 are written in the modern object oriented language of Java, which makes the code highly expandable, flexible and easy to maintain.

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1. Introduction

When designing any mass spectrometer, it is essential to investigate the ion optics. In magnetic sector type instruments and time-of-flight (TOF) mass spectrometers, the spatial or time aberrations have a direct influence on the performance of the ion optical system. Therefore, the aberration theory for the mass spectrograph or mass spectrometer has been investigated since the late 1910s.

Aston constructed his first mass spectrograph which achieved energy focusing in 1919 [1]. Dempster designed the first 180° mass spectrograph which achieved angular focusing in 1918 [2]. Regarding the magnetic sector type instrument, Mattauch and Herzog investigated the first-order double-focusing ion optics in 1930s [3]. The second-order calculation of an ion trajectory was reported in the late 1950s by Hintenberger [4] and by Ewald [5]. To calculate the aberration coefficients of an ion optical system, the transfer matrix method was introduced by Penner in 1961[6]. The effect of the fringing field on the focusing properties of the magnetic sector was first investigated by
Enge [7]. Wollnik and Ewald discussed it in the second-order [8]. Matsuda and Wollnik calculated it in the third-order [9]. Matsuo calculated the third-order aberration coefficients of the magnetic sector field [10] and electric sector field [11]. Toyoda et al. calculated the transfer matrix for crossed electric and magnetic fields up to the third-order both in the horizontal and vertical directions [12].

Regarding the TOF mass spectrometer, Poschenrieder proposed isochronous focusing and space focusing by electrostatic sectors [13]. Sakurai et al. calculated the time aberration coefficients for a toroidal electrostatic sector and an electrostatic quadrupole lens up to the third-order considering the influence of the fringing fields [14].

In order to calculate these aberrations, the equation of motion for ions in the ion optical system must be solved theoretically or numerically. Computational calculations have played an important role for this purpose in recent years. There are two general methods to solve the equation of motion, i.e., to calculate an ion trajectory: one is the transfer matrix method, and the other is the ray tracing method. If the aberration coefficients for each part of the ion optical system have already been determined in an available form by theoretical investigation, then the transfer matrix method is simpler and faster than the ray tracing method. Several computer programs employing the transfer matrix method have already been developed, such as TRANSPORT [15], TRIO [16] and GIOS [17]. GIOS can calculate the aberration coefficients and the ion density distribution at any profile plane with the space-charge effect. The computer program TRIO can calculate the image aberration coefficients including the influence of the fringing fields up to the third-order in the horizontal direction and up to the second-order in the vertical direction. The computer program BEIS was developed to simulate the image shape and scanned peak shape at the detecting position [18]. Sakurai and Matsuo developed the computer program TRIO-TOF to calculate the time aberration coefficients for an ion optical system consisting of electrostatic sectors and quadrupole lenses [19]. Toyoda and Matsuo developed the computer program TRIO-DRAW [20] by combining the functions of TRIO, TRIO-TOF and BEIS. The computer program TRIO-DRAW can calculate the spatial and time aberration coefficients using the transfer matrix method and output drawings of the ion trajectories as postscript files. The program was written in FORTRAN and C languages.

Although TRIO-DRAW has several useful functions, it does not have a graphical user interface (GUI). Moreover, several languages of FORTRAN, C and Postscript are employed in the program, making it troublesome or time-consuming to expand or add functions in the program. Therefore, the computer program TRIO 2.0 with GUIs was developed as an improved version of TRIO-DRAW, and offers the following features:

1. TRIO 2.0 can calculate spatial and time aberration coefficients of an ion optical system up to the third-order both in the horizontal and vertical directions by the transfer matrix method. Note that the third-order aberration coefficients in the vertical direction are calculated without considering the fringing field.

2. Ion optical systems including the following components can be calculated: cylindrical or toroidal electrostatic sectors, homogeneous or inhomogeneous magnetic sectors, electric and magnetic quadrupole lenses, and multipole lenses.

3. TRIO 2.0 has many useful functions for evaluating ion optical systems and all of these functions have GUIs.

4. TRIO 2.0 employs the modern object oriented language of Java, and all the programs are written in only Java, making the coding more expandable, flexible and easy to maintain. Moreover, it has high platform compatibility, running on Mac OS X, Linux and Windows.

2. Functions of TRIO 2.0 computer program

2.1. Transfer matrix method

The computer program TRIO 2.0 employs the transfer matrix method to calculate aberration coefficients. In this method, the geometrical trajectory of an arbitrary particle is expressed as an ion optical position vector \( \mathbf{P}(x, \alpha, y, \beta, \chi, \delta, \lambda) \) in a curvilinear coordinate system as shown in Fig. 1. Here \( x \) and \( \alpha \) denote the positional and angular...
deviations of the arbitrary trajectories in the horizontal direction, and \( y \) and \( \beta \) denote those in the vertical direction. They are defined with respect to the optic axis that corresponds to the trajectory of the reference ion. The plane perpendicular to the optic axis is called the profile plane, and the \( x \)-axis and \( y \)-axis are on the profile plane. The mass and energy deviations, \( \gamma \) and \( \delta \), are defined as

\[
\frac{m}{e} = \left( \frac{m}{e_0} \right) (1 + \gamma), \quad \frac{U}{e} = \left( \frac{U}{e_0} \right) (1 + \delta)
\]

where \( m \), \( e \), and \( U \) are the mass, charge, and energy of an arbitrary ion and \( m_0 \), \( e_0 \), and \( U_0 \) are those of the reference ion. The parameter \( l \) expresses the path length deviation defined relative to the path length of the reference ion [14].

The relation between the position vector \( \mathbf{P}(x, \alpha, y, \beta, \gamma, \delta, l) \) at an arbitrary profile plane and an initial position vector \( \mathbf{P}_0(x_0, \alpha_0, y_0, \beta_0, \gamma, \delta, l_0) \) is expressed in the first-order approximation by the transfer matrix method as follows:

\[
\begin{pmatrix}
    x \\
    \alpha \\
    y \\
    \beta \\
    \gamma \\
    \delta \\
    l
\end{pmatrix} =
\begin{pmatrix}
    (x \mid x) & (x \mid \alpha) & 0 & 0 & (x \mid \gamma) & (x \mid \delta) & 0 & x_0 \\
    (\alpha \mid x) & (\alpha \mid \alpha) & 0 & 0 & (\alpha \mid \gamma) & (\alpha \mid \delta) & 0 & \alpha_0 \\
    0 & 0 & (y \mid y) & (y \mid \beta) & 0 & 0 & y_0 \\
    0 & 0 & (\beta \mid y) & (\beta \mid \beta) & 0 & 0 & \beta_0 \\
    0 & 0 & 0 & 0 & 1 & 0 & 0 & \gamma \\
    0 & 0 & 0 & 0 & 0 & 1 & 0 & \delta \\
    0 & 0 & 0 & 0 & 0 & 0 & 1 & l_0
\end{pmatrix}
\begin{pmatrix}
    x_0 \\
    \alpha_0 \\
    y_0 \\
    \beta_0 \\
    \gamma \\
    \delta \\
    l_0
\end{pmatrix}
\]

(2)

The ion optical characteristics of the system can be investigated from the total transfer matrix. The focusing conditions of the ion optical system will be discussed in relation to the corresponding aberration coefficients of the total transfer matrix.

![Fig. 1. Coordinate system of the transfer matrix method. The optic axis corresponds to the trajectory of the reference ion.](image)

2.2. Main frame

For the design of an ion optical system, first, each component of the ion optical system and its physical parameters, e.g., the length of a drift space, the mean radius and the deflection angle of an electric or magnetic sector, the field strength of a quadrupole lens, etc., must be determined. In TRIO 2.0, the selection of the ion optical component and the setting of its physical parameters are easily carried out via the main frame. The calculated transfer matrix is shown in a window as text data. A screenshot of the main frame and the output window is shown in Fig. 2. In the main frame, an ion optical component can be selected from the pull-down menu. Then, its physical parameters are set through a dialog box. The parameters setting dialog box for an electric sector is also shown in Fig. 2. The physical parameters for each ion optical component are the same as those of TRIO. The definitions of the parameters are presented in Ref. 15. In the pull-down menu, a menu of simplex supplies a function for
optimizing the parameters by the simplex method. In many cases of designing an ion optical system, the system must satisfy several focusing conditions. For this purpose, arbitrary physical parameters of ion optical components will be optimized to fulfill the required focusing conditions by the parameter search function. The program MSPLEX employing the simplex method has already been developed by Ishihara [21], and has been transported to TRIO 2.0. The parameters being optimized for required focusing conditions can be chosen in the parameter-setting dialog. Moreover, the buttons in the upper side of the main frame supply each function to evaluate the ion optical system.

Fig. 2. Screenshot of the main frame of TRIO 2.0.

2.3. Simulation and visualization of ion trajectories

Ion trajectories in an ion optical system can be simulated and visualized for different initial conditions in the first-order approximation. When the “Trajectory” button in the main frame is clicked, a window will appear for setting the initial conditions and the parameters for drawing. Ion trajectories are visualized in several display modes the same as TRIO-DRAW, i.e., top view, x-direction, y-direction, and path length deviation mode. The top view mode shows a plane view of ion trajectories. The display modes of x-direction and y-direction represent ion trajectories in the x- and y-directions as the optic axis will be drawn in a straight line. Ion trajectories are drawn with different colors for each initial condition of x₀, α₀, y₀, β₀, and δ. Although TRIO 2.0 can calculate the transfer matrix up to the third-order, ion trajectories are simulated in the first-order because the first-order focusing conditions are the most interesting features for an ion optical system. The third-order calculation of ion trajectories is supplied by another function in TRIO 2.0. The visualization of ion trajectories enables the focusing properties of an ion optical system to be clearly grasped. As an example, ion trajectories of the multi-turn time-of-flight mass spectrometer MULTUM II [22] are shown in Figs. 3(a)-(c). For a TOF mass spectrometer, the path length deviation can be calculated for each initial condition. The path length deviation at an arbitrary profile plane is expressed by the hue for each trajectory. Advanced and retarded trajectories are colored red and blue, respectively. If the color of a trajectory is green at the final profile plane, it indicates that the trajectory is focusing in time. Here, ion trajectories of MULTUM II using the path length deviation mode are shown in Fig. 3(d).

2.4. Simulation and visualization of beam profile

Although the peak shape in only the x-direction was calculated by TRIO-DRAW, the divergence of the ion beam in the y-direction and the two-dimensional image of the beam profile are significant information to estimate the acceptability of the beam and the required detector size. In TRIO 2.0, the two-dimensional image of the beam profile can be simulated in the third-order. When the “Beam profile” or the “Star shape” button in the main frame is
clicked, a window will appear for the simulation and the visualization of the beam profile. Two types of initial beam shape can be simulated: a normal rectangular slit and a star-shaped slit. The initial parameters of $x_0$, $\alpha_0$, $y_0$, $\beta_0$, and $\delta$ are generated by a random number in the range of the specified maximal. In addition, the angle between the detecting plane and the optic axis can be varied for a mass spectrograph. The simulated image of the beam profile and the peak shape are shown in a window. The peak width (10% valley) and the mass resolution are also calculated. Here, a simulation result of the CQH-type mass spectrometer is shown in Fig. 4.

Fig. 3. Ion trajectories of each visualization mode for MULTUM II. (a) Top view, (b) x-direction, (c) y-direction, (d) path length deviation mode.

Fig. 4. Image of the beam profile and the peak shape for the CQH-type mass spectrometer.
From the simulation of the star-shaped slit, the deformation of the beam profile after passing through the system can be clearly found. A simulated image of the star-shaped slit in MULTUM II is shown in Fig. 5. The size of the star-shaped slit is 1 mm. Since the ion optical system of MULTUM II satisfies perfect focusing [23], the initial star-shaped image is conserved after one cycle of the ion optical system. The final image is inverse in both the $x$- and $y$-directions relative to the initial image because of the image magnification values of $(\alpha|x|) = -1$ and $(\beta|y|) = -1$.

2.5. Simulation and visualization of beam envelope and ion transmission

For any mass analyzer, the sensitivity is an important property. Accordingly, the ion transmission or the beam acceptance should be evaluated in the design of the system. The program BEIS and TRIO-DRAW could visualize the beam envelope from a few ion trajectories with different initial conditions. In TRIO 2.0, the function to visualize the beam envelope is improved and a function to calculate the ion transmission is newly added. When the “Envelope” button in the main frame is clicked, a window to set the parameters will appear for these functions. The program TRIO 2.0 can calculate ion trajectories in the third-order for many particles with each initial condition generated by the random number. In addition, the collision with ion optical components, e.g., electric and magnetic sectors, quadrupole lenses, etc., is judged for each ion trajectory every determined step. For example, the collision when an ion is passing through an electric sector is judged as follows: if the deviation $x$ of the ion trajectory becomes larger than the half gap width of the electric sector, it is judged that the ion collides with the electric sector. The ion transmission is defined as the ratio of the number of ions passing through the whole system without the collision to the total number of ions.

Furthermore, TRIO 2.0 can accept multi-turn ion optical systems. In recent years, several types of multi-turn TOF mass spectrometers have been developed and high performance has been achieved [24]. For a multi-turn ion optical system, the beam envelope for the overall flight path should be evaluated to estimate its ion transmission. By specifying the cycle number in the parameter-setting window, the beam envelope in a multi-turn ion optical system can be simulated and visualized. As an example, the beam envelopes in MULTUM II are shown in Fig. 6. The ion trajectories of 1,000 particles are simulated. Figs. 6(a) and (b) show beam envelopes for 5 cycles in the $x$- and $y$-directions, respectively. From this function, the beam envelope for the overall flight path can be easily simulated and visualized. In addition, the ion transmission can be calculated simultaneously. These evaluations are necessary for the design of any mass analyzer.

2.6. Simulation and visualization of peak shape of time-of-flight

For TOF mass spectrometers, the peak shape of TOF can be simulated and visualized in the third-order. This simulation also accepts multi-turn ion optical systems. A peak shape of TOF in MULTUM II after 5 cycles is shown
in Fig. 7. The total number of ions is 100,000, and these initial conditions are generated by a random number. The peak width (FWHM) and the mass resolution are also calculated and shown simultaneously.

2.7. Simulation and visualization of energy and angular focusing planes

The configurations of the energy and angular focal planes are the principal ion optical properties for a double-focusing mass spectrograph. The energy and angular focal planes can be simulated in third-order. When the “Focal planes” button in the main frame is clicked, a window to set the parameters for simulating the focal planes will appear. In this function, the energy and angular focusing points are calculated for the ion trajectories of each value of the mass deviation $\gamma$. A simulation result of the energy and angular focal planes of the CQH-type mass spectrometer is shown in Fig. 8. In this ion optical system, it is found that the energy and angular focal planes are not consistent with each other, and the double-focusing is satisfied at only one point.

Fig. 6. Beam envelope in (a) $x$- and (b) $y$-directions for 5 cycles in MULTUM II.

Fig. 7. Peak shape of TOF after 5 cycles in MULTUM II.

Fig. 8. Energy and angular focal planes for the CQH-type mass spectrometer. The numbers shown along the plots mean the mass deviation $\gamma$. 
3. Conclusion

The computer program TRIO 2.0 with GUIs was developed for the design of ion optical systems. The program has many useful functions for evaluating the ion optical properties of a system. In TRIO 2.0, the following information can be simulated and visualized: the ion trajectory, the image of the beam profile, the beam envelope and the ion transmission, the TOF peak, and the energy and angular focal planes. This program enables us to design a high-resolution, high-sensitivity mass analyzer.

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