A computer code for beam optics calculation —third order approximation*

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Abstract To calculate the beam transport in the ion optical systems accurately, a beam dynamics computer program of third order approximation is developed. Many conventional optical elements are incorporated in the program. Particle distributions of uniform type or Gaussian type in the (x, y, z) 3D ellipses can be selected by the users. The optimization procedures are provided to make the calculations reasonable and fast. The calculated results can be graphically displayed on the computer monitor.

Keywords: beam transport, computer program, third order approximation, Lie algebra.

Ion optical systems usually consist of electric and magnetic bending elements and focusing elements. Sometimes, the particle trajectories in these systems require nonlinear calculations, particularly in the systems which require high beam transmission, or precise beam spots. For this reason, we analyzed the particle nonlinear trajectories for a lot of beam optical elements with Lie algebraic method and designed a beam dynamics computer program based on program LEADS[1].

1 Theoretical analysis

The canonical coordinates $\zeta = (x, x', y, y', \Delta\phi, \Delta E)$ are used in the program. Here, $x' = p_x/p_s$, $y' = p_y/p_s$; $\Delta\varphi$, and ΔE are the phase difference and energy difference between the arbitrary particle and the reference particle, respectively; p_s is the momentum of the reference particle. The Lie algebraic method[2] is used in the analysis of nonlinear transport of particle trajectories in the beam optical elements. First, set up the Hamiltonian H of the particle motion in the phase space $\zeta = (x, x', y, y', \Delta\phi, \Delta E)$. Then, expand H into power series

$$H = \sum_{i=0}^{\infty} H_i. \tag{1}$$

Here, H_i is a homogeneous polynomial. Let ζ_0 be the initial point of a particle ray in the phase space $(x, x', y, y', \Delta\varphi, \Delta E)$, ζ is the final point of the ray, ζ_0 and ζ_0 can be connected by a Lie map $\mathscr{M}$:

$$\zeta = \mathscr{M}\zeta_0, \tag{2}$$

where $\mathscr{M}$ is a Lie map expressed as:

$$\mathscr{M} = \cdots\exp(:f_4:)\exp(:f_3:)\exp(:f_2:), \tag{3}$$

and

$$f_2 = -\int_{z_0}^{z_f} H_2 \mathrm{d}z, \quad f_3 = -\int_{z_0}^{z_f} h_3^{\mathrm{int}} \mathrm{d}z,$$

$$f_4 = -\int_{z_0}^{z_f} h_4^{\mathrm{int}} \mathrm{d}z + \frac{1}{2}\int_{z_0}^{z_f} \mathrm{d}z_1 \cdot \int_{z_0}^{z_1} \mathrm{d}z_2 [-h_3^{\mathrm{int}}(z_2), -h_3^{\mathrm{int}}(z_1)], \cdots \tag{4}$$

and

$$h_i^{\mathrm{int}}(z) = \mathscr{M}_2 H_i, \tag{5}$$

$$\mathscr{M}_2 = \exp(:f_2:). \tag{6}$$

The particle trajectories can be calculated by the following expressions:

$$\begin{aligned} &\zeta^{(1)} = \exp(:f_2:)\zeta_0, \\ &\text{first order approximation} \\ &\zeta^{(2)} = :f_3:\zeta^{(1)}, \\ &\text{second order aberrations} \\ &\zeta^{(3)} = :f_4:\zeta^{(1)} + \frac{1}{2}:f_3:^2\zeta^{(1)}, \\ &\text{third order aberrations} \\ &\cdots\cdots \end{aligned} \tag{7}$$

Higher order approximation could be extended if necessary.

Following the procedures expressed in Eqs. (1)—(7), we analyzed the particle trajectories of the third order approximation in the elements: magnetic quadrupoles, electrostatic quadrupoles, drift spaces, dipole magnets, solenoidal lenses, electrostatic ana-

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lyzers, $\boldsymbol{E}\times\boldsymbol{B}$ Wein filters, three-tube Einzel lenses, two-tube gap lenses, three-aperture Einzel lenses, and dc accelerating columns.

2 Optical elements

The program calculates the beam optics systems consisting of the elements: magnetic quadrupoles, electrostatic quadrupoles, drift spaces, dipole magnets, solenoidal lenses, electrostatic analyzers, $\boldsymbol{E}\times\boldsymbol{B}$ Wein filters, three-tube Einzel lenses, two-tube gap lenses, three-aperture Einzel lenses, dc accelerating columns, as well as QWR (quarter wave resonator) and SLR (split loop resonator) rf structures. Therefore, general beam transport lines, microprobe systems, ion optical systems of high voltage accelerators, and rf linear accelerators of QWR or SLR structures can also be calculated.

For the calculations of electrostatic lenses, we take into account the total effective fields, i.e. thick lens calculations are performed. The procedure is: divide the total length of a lens into some small intervals, and each interval is considered to be a uniform accelerating field, and each dividing point is treated as a thin lens (Fig. 1).

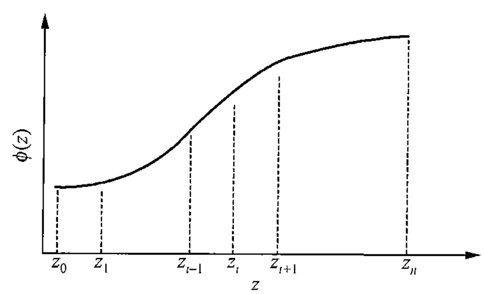

Fig. 1. Potential distribution.

Applying the Lie map Eq. (7) to each interval and dividing point, the third order particle trajectories can be obtained[3].

3 Optimization procedures

Powell nonlinear optimization subroutines[4] have been written in the codes. The goal of the optimization calculations is to find out the minimum values of the following object function

$$F = \sum_{i}^{n}[((f_i(x_1, x_2, \cdots, x_m) - f_{i0})/\varepsilon_i]^2, \quad (8)$$

where $f_i(i=1,2,\cdots,n)$ are the required optical conditions; f_{i0} are the given values for this conditions; $x_j(j=1,2,\cdots,m)$ are the variable parameters, such as magnetic field, voltage, element length and so on; ε_i is the tolerance for each condition (weight factor).

Some different optical conditions can be given, such as forming an image, making a beam waist, chromaticity, etc. If the transfer matrix of an element or a part of the beam line is $\boldsymbol{M}(i,j)$, $i,j=1,6$, the beam matrix is $\boldsymbol{\sigma}(i,j)$, $i,j=1,6$, the following optical conditions could be inserted into the input data file:

image in x-plane: $M(1,2)=0$;

image in y-plane: $M(3,4)=0$;

chromaticity: $M(1,6)=0$, or $M(2,6)=0$;

P-F image: $M(1,1)=0$;

F-P image: $M(2,2)=0$;

P-P image (telescope system): $M(2,1)=0$;

form a waist in x-plane: $\sigma(1,2)=0$;

beam size limit in x-plane: $\sigma(1,1)=$ given value;

form a waist in y-plane: $\sigma(3,4)=0$;

beam size limit in y-plane: $\sigma(3,3)=$ given value;

beam waist in the longitudinal direction: $\sigma(5,6)=0$.

4 Periodical structure calculation

In the linear particle accelerators consisting of QWRs or SLRs, or in some periodically arranged beam lines, the particle beams will pass through these periodic structures. In order to keep the particle motions stable, the program automatically adjusts the magnetic quadrupole fields to fit the following stability condition:

$$|\cos\mu| = |0.5\mathrm{Tr}(\boldsymbol{M})| \leqslant 1, \quad (9)$$

where μ is the phase shift per period, $\boldsymbol{M}$ is the Twiss matrix shown as:

$$\boldsymbol{M} = \begin{pmatrix} \cos\mu + \alpha\sin\mu & \beta\sin\mu \\ -\gamma\sin\mu & \cos\mu - \alpha\sin\mu \end{pmatrix}. \quad (10)$$

The periodic structures could be combined with the magnetic dipoles, quadrupoles, drift spaces and QWRs and SLRs.

5 Particle distributions

The particle distributions can be selected by the user. Two kinds of distributions are provided: uniform distribution and Gaussian distributions in the (x, y, z) 3D dimensional ellipses. The program generates the initial particle coordinates in the 3D ellipses randomly (Fig. 2 and Fig. 3).

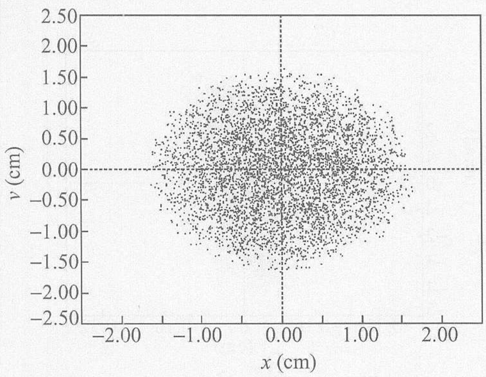

Fig. 2. Uniform distribution of particles.

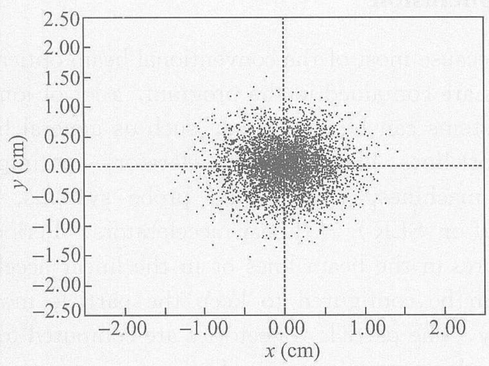

Fig. 3. Gaussian distribution of particles.

6 Calculation procedures

First, the program reads the input data line by line from the input data file provided by the users. Then, the particle initial coordinates in the phase spaces will be generated randomly. After that, the program checks if there are periodic structures in the system. If yes, the fields of the magnetic quadrupoles contained in the periodic modules are adjusted automatically to keep the particle moving in the stable area. After that, the program checks the input data again to find out if there are some sections of the beam line to be optimized. If yes, the optimization procedures will run to adjust variable parameters of the optics elements to fit the given optical conditions. Meanwhile, the linear transfer matrix of each optics element and the beam $\boldsymbol{\sigma}$ matrices are used. When the optimization calculations are finished, the program will calculate the particle trajectories of the first order approximation in the system based on the parameters obtained from the periodic stability and/or optimization calculations from the beginning to the end, and the linear phase space diagrams and beam envelopes will be displayed. Next step, the program will calculate the nonlinear particle trajectories in the system without restarting the program and displaying the nonlinear phase space diagrams and beam envelopes.

7 Graphical display

The particle scattergrams in the x-x', y-y', $\Delta\varphi$-ΔE phase spaces or x-y plane after each element can be displayed on the screen without the need of additional post-processing (Figs. 4—7).

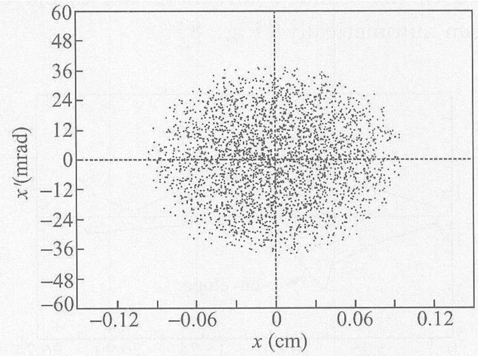

Fig. 4. Phase diagram in x-x' space.

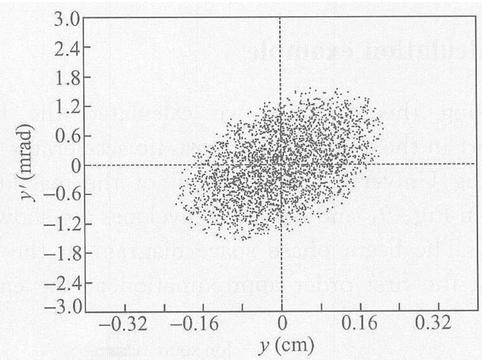

Fig. 5. Phase diagram in y-y' space.

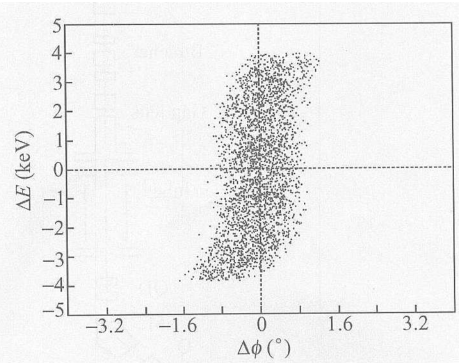

Fig. 6. Phase diagram in $\Delta\phi$-ΔE space.

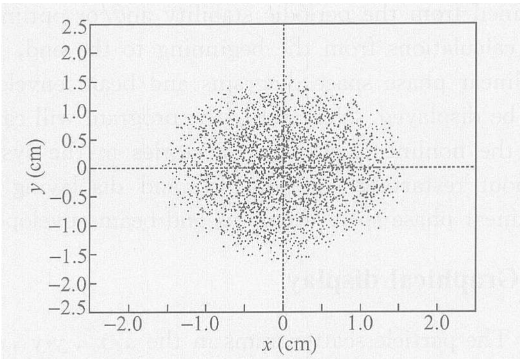

Fig. 7. Particle distribution in x-y plane.

When the calculations are finished, beam envelopes both in x and y directions are displayed on the screen automatically (Fig. 8).

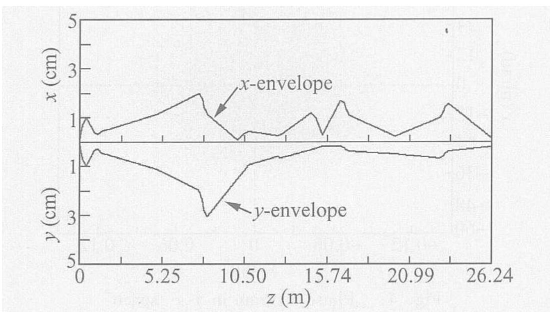

Fig. 8. Beam envelopes of 4.5 MV electrostatic accelerator.

8 Calculation example

Using this program we calculated the beam transport in the 4.5 MV electrostatic accelerator built at Peking University. The layout of the machine is shown in Fig. 9, and its beam envelopes are shown in Fig. 8. The beam phase space diagram in the y-y' plane in the first order approximation at the end of the system is already shown in Fig. 5. When taking the nonlinear terms of the particle trajectories into account, the phase diagram at the same point is shown in Fig. 10. Comparing Fig. 5 with Fig. 10, we can see that the difference between the linear approximation and the nonlinear approximation is not too small.

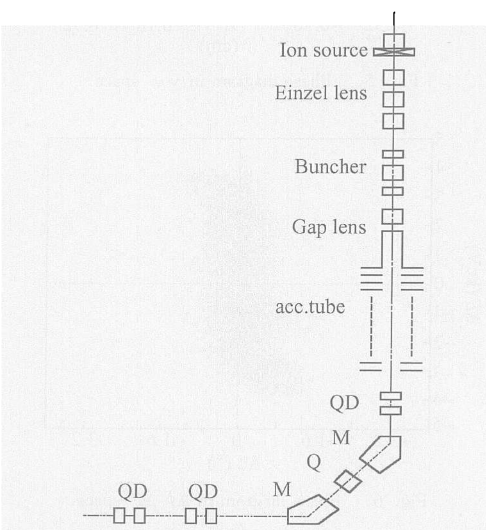

Fig. 9. Layout of the 4.5 MV electrostatic accelerator.

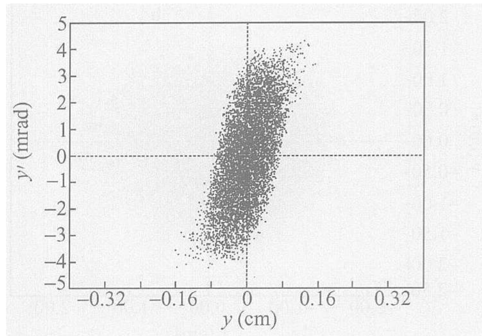

Fig. 10. Phase space diagram of nonlinear orbits.

9 Conclusion

Because most of the conventional beam optical elements are contained in the program, a lot of ion optics systems can be calculated, such as general beam transport lines, electrostatic accelerators, ion implantation machines, micro beam probe systems, and QWR (or SLR) rf linear accelerators. Periodical structures in the beam lines or in the linear accelerators can be configured to keep the particle moving steadily. The particle trajectories are computed to the third order approximation. The optimization procedures ensure that the calculations are reasonable and fast. In addition, the calculated results can be visually seen on the screen.

References

1 Lü J. Q. Leads: A graphical display computer program for linear and electrostatic accelerator beam dynamics simulation. Nucl. Instru. & Methods, 1995, A 355: 253—257.

2 Dragt A. J. Lecture notes on nonlinear orbit dynamics. AIP Conf. Proc. 1982, 87: 147—269.

3 Lü J. Q. The applications of Lie map in the analysis of pulsed beam transport in electrostatic lenses. Nucl. Instrum. & Methods 1998, A 416: 229—235.

4 Himmelblau D. M. Applied Nonlinear Programming. New York: MC Graw-Hill, 1972, 102—126.