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Lie algebraic analysis for the beam transport in the spherical electrostatic analyser*

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This paper uses the Lie algebraic method to analyse the charged particle trajectories in the spherical electrostatic analyser, and obtains the nonlinear solutions. The results show that the focusing abilities both in the x and y directions of the analyser are almost the same. Moreover, there exist dispersion effects in the x direction, and no dispersion effects in the y direction.

Keywords: Lie algebraic method, spherical electrostatic analyser, optical properties, nonlinearity
PACC: 2921

1. Introduction

In the electrostatic accelerators, ion implantation machines and other electron or ion beam systems, the spherical electrostatic analysers are often used to measure the particle energy and angular distributions.[1−3] To calculate the particle motions more accurately in this kind of analysers, we analysed the particle trajectories with the Lie algebraic method[4] up to third order approximation.

2. Potential distribution

Suppose that the outer electrode of the analyser has the radius ρ_2, and the voltage V_2, the inner electrode radius is ρ_1, the potential is V_1, the radius of the central orbit is ρ_0 (see Fig.1).

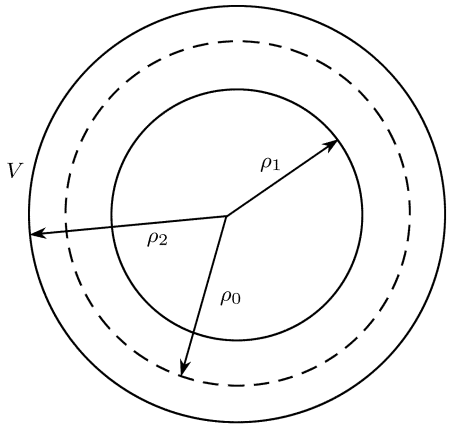


Fig.1. Radius and voltage of the spherical electrodes.

Ignoring the fringe field effects, we can easily obtain the potential function Ψ by solving the Laplace equation in the spherical coordinates (ρ, θ, ϕ):

$$\Psi = \frac{V_2\rho_2 - V_1\rho_1}{\rho_2 - \rho_1} + \frac{1}{\rho}\frac{\rho_1\rho_2(V_1 - V_2)}{\rho_2 - \rho_1}. \tag{1}$$

Let the radius of the central orbit be

$$\rho_0 = \frac{1}{2}(\rho_1 + \rho_2),$$

and $\rho_2 = \rho_0 + d, \rho_1 = \rho_0 - d, V_2 = V$, one obtains

$$\begin{aligned} V_1\rho_1 &= -V_2\rho_2, \\ \Psi &= \frac{V}{d}(\rho_0 + d)\left(1 - \frac{\rho_0}{\rho}\right). \end{aligned} \tag{2}$$

The electric field between two electrodes is

$$E = E_{\rm r} = -\frac{\partial\Psi}{\partial\rho} = -\frac{V(\rho_0 + d)}{d}\frac{\rho_0}{\rho^2}.$$

The electric field on the circle of radius ρ_0 is

$$E_0 = E|_{\rho=\rho_0} = -\frac{V(\rho_0 + d)}{d}\frac{1}{\rho_0}.$$

The force applied on the reference particle moving along the central orbit is

$$qE_0 = -\frac{qV(\rho_0 + d)}{d}\frac{1}{\rho_0} = \frac{m_0\gamma_0 v_0^2}{\rho_0}.$$

Where m_0 is the rest mass of the reference particle, $\gamma_0 = 1/\sqrt{1-\beta_0^2}$, $\beta_0 = v_0/c$, v_0 is the velocity of reference particle, c is the light velocity. From the above equation we have

$$\frac{\rho_0 + d}{d} = \frac{m_0\gamma_0 v_0^2}{qV}.$$

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Substituting the above equation into Eq.(2), we obtain

$$\Psi = \frac{m_0\gamma_0 v_0^2}{q}\left(1 - \frac{\rho_0}{\rho}\right). \tag{3}$$

3. Hamiltonian and its expansion

In the phase space (x, p_x, y, p_y, z, p_z), the Hamiltonian with time t as the independent variable is

$$H_t = \left[(\boldsymbol{p} - q\boldsymbol{A})^2c^2 + m_0^2c^4\right]^{1/2} + q\,\Psi. \tag{4}$$

where $\boldsymbol{p}$ is the canonical momentum, $\boldsymbol{A}$ is the magnetic vector potential ($\boldsymbol{A} = 0$ for the electrostatic field), ψ is the electric potential function.

Now, we are going to set up the natural coordinate system (r, y, s). Suppose that the reference particle moves along the circle C (see Fig.2).

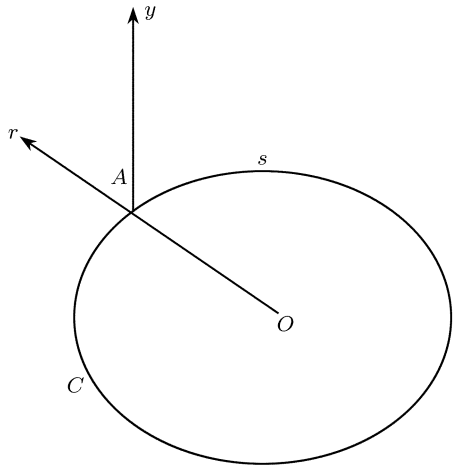


Fig.2. Natural coordinate system.

At a point A on the circle C, the line connecting the centre O of C and the point A is r axis; the line perpendicular to the circle C and passing through the point A is y axis; the path length along the circle is s axis. The coordinate system (r, y, s) moves along with the reference particle. To get the Hamiltonian in the natural coordinate system (r, y, s), we should write the Lagrangian first. In the cylindrical coordinate system (r, θ, y), the Lagrangian is

$$L = -m_0c^2\left(1 - \frac{1}{c^2}(\dot{r}^2 + r^2\dot{\theta}^2 + y^2)\right)^{1/2} - q\,\Psi. \tag{5}$$

Here the magnetic vector potential $\boldsymbol{A}$ is ignored. The canonical momentum can be derived from $p_{\rm i} = \partial L/\partial\dot{x}$:

$$p_{\rm r} = m_0\gamma\dot{r} = p_{r\rm m},$$
$$p_\theta = m_0\gamma r^2\dot{\theta} = rp_{\vartheta\rm m},$$
$$p_y = m_0\gamma\dot{y} = p_{y\rm m}.$$

Here the subscript "m" stands for the mechanical momentum. Substituting the above expressions into Eq.(4), we have

$$H_t = \left[(p_r^2 + p_\theta^2/r^2 + p_y^2)c^2 + m_0^2c^4\right]^{1/2} + q\,\Psi. \tag{6}$$

In the natural coordinate system, the electrical potential ψ can be expressed as

$$\Psi = \frac{m_0\gamma_0 v_0^2}{q}\left(1 - \frac{r_0}{\sqrt{r^2 + y^2}}\right). \tag{7}$$

Let

$$p_t = -H_t. \tag{8}$$

Solving Eq.(8) for p_θ, one obtains

$$p_\theta = r\left[(p_t + q\psi)^2/c^2 - p_r^2 - p_y^2 - m_0^2c^2\right]^{1/2}. \tag{9}$$

Here, p_θ is the canonical momentum in the θ direction. Because the particle bending angle ϕ is in the opposite direction of the angle θ, the particle bending canonical momentum is $p_\phi = -p_\theta$. Therefore, the Hamiltonian with ϕ as the independent variable is

$$\begin{aligned} K = -p_\vartheta = \; & -r\left[(p_t + q\psi)^2/c^2 - p_r^2\right. \\ & \left. -p_y^2 - m_0^2c^2\right]^{1/2}. \end{aligned} \tag{10}$$

The function K is valid in the phase space (r, p_r, y, p_y, t, p_t). Introducing a new canonical phase space $\zeta = (x, p_x, y, p_y, \tau, p_\tau)$, we have

$$\begin{aligned} & x = r - r_0, \quad p_x = p_r, \quad y = y, \quad p_y = p_y, \\ & \tau = t - \phi/\omega_0, \quad p_\tau = p_t - p_t^0, \end{aligned} \tag{11}$$

where ω_0 is the particle bending angle frequency, p_t^0 is the value of p_t for the reference particle, i.e.

$$p_t^0 = H_t| = -m_0\gamma_0c^2.$$

In fact, Eq.(11) is a canonical transformation, the corresponding generating function is

$$F_3 = xp_x + yp_y + (t - \phi/\omega_0)(p_\tau + p_t^0).$$

Therefore, the new Hamiltonian in ζ phase space is

$$H = K + \partial F_3/\partial\phi = -(r_0 + x)\left[(p_\tau + p_t^0 + q\psi)^2/c^2 - p_x^2 - p_y^2 - m_0^2c^2\right]^{1/2} - (p_\tau + p_t^0)/\omega_0. \tag{12}$$

To calculate the particle trajectories with the Lie algebraic method, it is necessary to expand the function H into the power series, the results are

$$H = \sum_{n=0}^{\infty} H_n. \tag{13}$$

The first five terms are listed as follows:

$$\begin{aligned}
H_0 =\ & \frac{r_0 m_0 c}{\beta_0\gamma_0},\\
H_1 =\ & 0,\\
H_2 =\ & x^2\frac{m_0c\beta_0}{2r_0\gamma_0} + xp_\tau\frac{1+\gamma_0^2}{c\beta_0\gamma_0^2} + p_x^2\frac{r_0}{2m_0c\beta_0\gamma_0} + y^2\frac{m_0c\beta_0\gamma_0}{2r_0} + p_y^2\frac{r_0}{2m_0c\beta_0\gamma_0} + p_\tau^2\frac{r_0}{2m_0c^3\beta_0^3\gamma_0^3},\\
H_3 =\ & x^2p_\tau\frac{3}{2cr_0\beta_0\gamma_0^2} + xp_x^2\frac{1}{m_0c\beta_0\gamma_0} - xy^2\frac{m_0c\beta_0(-1+2\gamma_0^2)}{2r_0^2\gamma_0} + xp_y^2\frac{1}{m_0c\beta_0\gamma_0} + xp_\tau^2\frac{2}{m_0c^3\beta_0^3\gamma_0^3}\\
& + p_x^2p_\tau\frac{r_0}{2m_0^2c^3\beta_0^3\gamma_0^2} + y^2p_\tau\frac{1}{2cr_0\beta_0\gamma_0^2} + p_y^2p_\tau\frac{r_0}{2m_0^2c^3\beta_0^3\gamma_0^2} + p_\tau^3\frac{r_0}{2m_0^2c^5\beta_0^5\gamma_0^4},\\
H_4 =\ & x^4\frac{m_0c[8+(-8+8\beta_0^2+\beta_0^4)r_0^2]}{8r_0^3\beta_0^3\gamma_0^5} + x^3p_\tau\frac{1+\gamma_0^2}{2r_0^2c\beta_0\gamma_0^4} + x^2p_x^2\frac{1+2\gamma_0^2}{4r_0m_0c\beta_0\gamma_0^3}\\
& + x^2y^2\frac{3m_0c[2-(4+\beta_0^4)\gamma_0^2+2\gamma_0^4]}{4r_0^3\beta_0^3\gamma_0^3} + x^2p_y^2\frac{1+2\gamma_0^2}{4r_0m_0c\beta_0\gamma_0^3} + x^2p_\tau^2\frac{3(1+4\gamma_0^2)}{4r_0m_0c^3\beta_0^3\gamma_0^5}\\
& + xp_x^2p_\tau\frac{1+3\gamma_0^2}{2m_0^2c^3\beta_0^3\gamma_0^4} + xy^2p_\tau\frac{1}{2r_0^2c\beta_0\gamma_0^2} + xp_y^2p_\tau\frac{1+3\gamma_0^2}{2m_0^2c^3\beta_0^3\gamma_0^4} + xp_\tau^3\frac{1+5\gamma_0^2}{2m_0^2c^5\beta_0^5\gamma_0^6}\\
& + p_x^4\frac{r_0}{8m_0^3c^3\beta_0^3\gamma_0^3} + p_x^2y^2\frac{1}{4r_0m_0c\beta_0\gamma_0} + p_x^2p_y^2\frac{1}{4m_0^3c^3\beta_0^3\gamma_0^3} + p_x^2p_\tau^2\frac{r_0(1+2\gamma_0^2)}{4m_0^3c^5\beta_0^5\gamma_0^5}\\
& - y^4\frac{m_0c\beta_0(-1+3\gamma_0^2)}{8r_0^3\gamma_0} + y^2p_y^2\frac{1}{4r_0m_0c\beta_0\gamma_0} + y^2p_\tau^2\frac{3}{4r_0m_0c^3\beta_0^3\gamma_0^3} + p_y^4\frac{r_0}{8m_0^3c^3\beta_0^3\gamma_0^3}\\
& + p_y^2p_\tau^2\frac{r_0(1+2\gamma_0^2)}{4m_0^3c^5\beta_0^5\gamma_0^5} + p_\tau^4\frac{r_0(1+4\gamma_0^2)}{8m_0^3c^7\beta_0^7\gamma_0^7}.
\end{aligned} \tag{14}$$

4. Calculations of particle trajectories

4.1. First order approximation

The particle trajectories of first order approximation can be calculated from the function H_2. First, calculate the function f_2 according to the following expression[5,6]:

$$f_2 = -\int_0^\mu H_2 \mathrm{d}\mu. \tag{15}$$

Let the subscript '1' stand for the particle trajectories of first order. Using the formula

$$\zeta_1 = \mathcal{M}_2\zeta = \exp(:f_2:)\zeta = \sum_{n=0}^{\infty}\frac{1}{n!}:f_2:^n\zeta, \tag{16}$$

we have

$$\begin{aligned}
x_1 =\ & x\cos(\phi/\gamma_0) + \frac{p_xr_0\gamma_0}{p_0}\sin(\phi/\gamma_0)\\
& - p_\tau\frac{r_0(1+\gamma_0^2)}{p_0c\beta_0\gamma_0}[1-\cos(\phi/\gamma_0)],\\
p_{x1} =\ & -x\frac{p_0}{r_0\gamma_0}\sin(\phi/\gamma_0) + p_x\cos(\phi/\gamma_0)\\
& - p_\tau\frac{1+\gamma_0^2}{\beta_0c\gamma_0}(\phi/\gamma_0),\\
y_1 =\ & y\cos(\phi) + \frac{p_yr_0}{p_0}\sin(\phi),\\
p_{y1} =\ & -y\frac{p_0}{r_0}\sin(\phi) + p_y\cos(\phi),\\
\tau_1 =\ & x\frac{1+\gamma_0^2}{\beta_0c\gamma_0}\sin(\phi/\gamma_0) + p_x\frac{r_0(1+\gamma_0^2)}{p_0\beta_0c}\\
& \times[1-\cos(\phi/\gamma_0)] + \tau + p_\tau\frac{r_0}{p_0\beta_0^2c^2\gamma_0}\sin(\phi/\gamma_0)
\end{aligned}$$

$$+p_\tau\frac{r_0\gamma_0(2+\gamma_0^2)}{p_0\beta_0^2c^2}[\sin(\phi/\gamma_0)-\phi/\gamma_0],$$

$$p_{\tau 1}= p_\tau. \tag{17}$$

Where ϕ is the bending angle of the reference particle.

4.2. Second order terms of the trajectories

Let the subscript '2' stand for the second order terms of the trajectories. Using the following formula

$$\zeta_2 =: f_3 : \zeta_1, \tag{18}$$

where

$$f_3 = -\int_0^\phi h_3^{\rm int}\mathrm{d}\phi, \tag{19}$$

$$h_3^{\rm int} = \mathcal{M}_2 H_3(\zeta), \tag{20}$$

we obtain the second order terms of the trajectories listed as the follows:

$$\begin{aligned}
x_2 = {} & -\frac{x^2}{r_0}\sin^2(\phi/\gamma_0)+\frac{xp_x}{m_0c\beta_0}\sin(2\phi/\gamma_0)+\frac{xp_\tau}{m_0c^2\beta_0^2\gamma_0}[\phi\beta_0^2\gamma_0-2(1+\gamma_0^2)\sin(\phi/\gamma_0)]\sin(\phi/\gamma_0)\\
& +\frac{p_x^2r_0}{m_0^2c^2\beta_0^2}[1-\cos(\phi/\gamma_0)]\cos(\phi/\gamma_0)+\frac{p_xp_\tau r_0}{m_0^2c^3\beta_0^3\gamma_0}[-\phi\beta_0^2\gamma_0\cos(\phi/\gamma_0)-((2+\gamma_0^2)\sin(\phi/\gamma_0)\\
& -(1+\gamma_0^2)\sin(2\phi/\gamma_0))]+\frac{y^2}{2r_0}[\cos(\phi/\gamma_0)-\cos^2(\phi)]-\frac{yp_y}{p_0}[\gamma_0\sin(\phi/\gamma_0)-\cos(\phi)\sin(\phi)]\\
& -\frac{p_y^2r_0}{2p_0^2}\sin^2(\phi)+\frac{p_\tau^2r_0}{2p_0^2c^2\beta_0^2}\{(1-\cos(\phi/\gamma_0))[-2\beta_0^2\gamma_0^4+(-3-2\gamma_0^2+(-3+\beta_0^4)\gamma_0^4)\cos(\phi/\gamma_0)]\\
& +2\phi\beta_0^2\gamma_0(1+\gamma_0^2)\sin(\phi/\gamma_0)\},\\
p_{x2} = {} & \frac{xp_\tau}{r_0c\beta_0\gamma_0}[\phi\beta_0^2\gamma_0\cos(\phi/\gamma_0)-(2+\gamma_0^2)\sin(\phi/\gamma_0)]-\frac{p_x^2}{m_0c\beta_0}\sin(\phi/\gamma_0)+\frac{p_xp_\tau\phi}{m_0c^2}\sin(\phi/\gamma_0)\\
& -\frac{y^2m_0c\beta_0}{2r_0^2}[\sin(\phi/\gamma_0)-\gamma_0\sin(2\phi)]+\frac{yp_y}{r_0}[\cos(\phi/\gamma_0)-\cos(2\phi)]-\frac{p_y^2}{p_0}\cos(\phi)\sin(\phi)\\
& +\frac{p_\tau^2}{2m_0c^3\beta_0^3\gamma_0^2}[2\phi\beta_0^2\gamma_0(1+\gamma_0^2)\cos(\phi/\gamma_0)-(1+2\gamma_0^2+(1+\beta_0^4)\gamma_0^4)\sin(\phi/\gamma_0)],\\
y_2 = {} & \frac{xy}{r_0}(\cos(\phi/\gamma_0)-1)\cos(\phi)+\frac{xp_y}{p_0}(\cos(\phi/\gamma_0)+1)\sin(\phi)+\frac{p_xy}{p_0}[\gamma_0\cos(\phi)\sin(\phi/\gamma_0)-\sin(\phi)]\\
& +\frac{p_xp_yr_0}{m_0^2c^2\beta_0^2\gamma_0}\sin(\phi)\sin(\phi/\gamma_0)-\frac{yp_\tau(1+\gamma_0^2)}{m_0c^2\beta_0^2\gamma_0}\cos(\phi)(1-\cos(\phi/\gamma_0))\\
& +\frac{p_yp_zr_0}{m_0^2c^3\beta_0^3\gamma_0^2}[(1+\gamma_0^2)\cos(\phi/\gamma_0)-\gamma_0^2]\sin(\phi),\\
p_{y2} = {} & \frac{xym_0c\beta_0}{r_0^2}[\gamma_0(1+\cos(\phi/\gamma_0))\sin(\phi)-\cos(\phi)\sin(\phi/\gamma_0)]+\frac{xp_y}{r_0\gamma_0}[\gamma_0\cos(\phi)(1-\cos(\phi/\gamma_0))\\
& -\sin(\phi)\sin(\phi/\gamma_0)]+\frac{p_xy}{r_0}[-\cos(\phi)(1-\cos(\phi/\gamma_0))+\gamma_0\sin(\phi)\sin(\phi/\gamma_0)]+\frac{p_xp_y}{p_0}[\cos(\phi/\gamma_0)\sin(\phi)\\
& -\gamma_0\cos(\phi)\sin(\phi/\gamma_0)]+\frac{yp_\tau}{cr_0\beta_0\gamma_0}[\gamma_0(-\gamma_0^2+(1+\gamma_0^2)\cos(\phi/\gamma_0))\sin(\phi)-(1+\gamma_0^2)\cos(\phi)\sin(\phi/\gamma_0)]\\
& -\frac{p_yp_\tau(1+\gamma_0^2)}{m_0c^2\beta_0^2\gamma_0^2}[\gamma_0\cos(\phi)(\cos(\phi/\gamma_0)-1)+\sin(\phi)\sin(\phi/\gamma_0)],\\
\tau_2 = {} & \frac{x^2}{4r_0c\beta_0\gamma_0}[-2\phi\beta_0^2\gamma_0+(2+\gamma_0^2)\sin(2\phi/\gamma_0)]+\frac{xp_x}{m_0c^2\beta_0^2\gamma_0}(2+\gamma_0^2)\sin^2(\phi/\gamma_0)\\
& +\frac{xp_\tau}{2m_0c^3\beta_0^3\gamma_0^2}[-2\phi\beta_0^2\gamma_0(1+\gamma_0^2)(\cos(\phi/\gamma_0)+1)+2\gamma_0^2(-3+\gamma_0^2)\sin(\phi/\gamma_0)+(2+3\gamma_0^2+\gamma_0^4)\sin(2\phi/\gamma_0)]\\
& -\frac{p_x^2r_0}{4m_0^2c^3\beta_0^3\gamma_0}[2\phi\beta_0^2\gamma_0-4(1+\gamma_0^2)\sin(\phi/\gamma_0)+(2+\gamma_0^2)\sin(2\phi/\gamma_0)]\\
& +\frac{p_xp_\tau r_0}{2m_0^2c^4\beta_0^4\gamma_0^2}[-\phi\beta_0^2\gamma_0(1+\gamma_0^2)\sin(\phi/\gamma_0)+(-1-\gamma_0^2+\beta_0^4\gamma_0^4+(2+3\gamma_0^2+\gamma_0^4)\cos(\phi/\gamma_0))(1-\cos(\phi/\gamma_0))]\\
& +\frac{y^2}{2r_0c\beta_0\gamma_0}[(1+\gamma_0^2)\sin(\phi/\gamma_0)-\gamma_0\cos(\phi)\sin(\phi)]+\frac{p_yy}{2m_0c^2\beta_0^2\gamma_0}[1+2\gamma_0^2+\cos(2\phi)-2(1+\gamma_0^2)\cos(\phi/\gamma_0)]
\end{aligned}$$

$$+\frac{p_y^2 r_0}{2m_0^2c^3\beta_0^3\gamma_0^2}\cos(\phi)\sin(\phi)+\frac{p_\tau^2 r_0}{4m_0^2c^5\beta_0^5\gamma_0^4}\{2\phi[3+\gamma_0^2(1+\gamma_0^2)(-3(-3+\gamma_0^2)+2\beta_0^2(1+\gamma_0^2))$$
$$-2\beta_0^2\gamma_0^2(1+\gamma_0^2)^2\cos(\phi/\gamma_0)]-2\gamma_0(1+\gamma_0^2)[3+10\gamma_0^2-(1+\beta_0^4)\gamma_0^4$$
$$+(-3-\gamma_0^2+(-2+\beta_0^4)\gamma_0^4)\cos(\phi/\gamma_0)]\sin(\phi/\gamma_0)\},$$
$$p_{\tau 2}= 0. \tag{21}$$

5. Summary

The nonlinear transport of the charged particle beams in the spherical electrostatic analysers was calculated with the Lie algebraic method. We can see from the particle trajectories of linear approximation that the focusing abilities both in the x and y directions are almost the same. The difference is that there exist the momentum dispersion effects only in the x direction.

Besides, comparing the spherical analysers with the cylindrical analysers,[7] we can see that the cylindrical analysers have the focusing function only in the x direction, and for the same bending radius r_0 the spherical analysers have stronger focusing ability than the cylindrical analysers. This can be seen from their focusing lengths: $f=\dfrac{\gamma_0 r_0}{\sin(\phi/\gamma_0)}$ for the spherical analysers and $f=\dfrac{\sqrt{2}r_0}{\sin(\phi/\sqrt{2})}$ for the cylindrical ones. It is obvious that, in the low energy situations the focusing length is shorter than that of the cylindrical analysers. Moreover, the energy dispersion effect of the spherical analyser, $D_{\text{spherical}}=-\dfrac{r_0(1+\gamma_0^2)}{p_0c\beta_0\gamma_0}[\cos(\phi/\gamma_0)-1]$, is stronger than that, $D_{\text{cylindrical}}=-\dfrac{r_0}{p_0c\beta_0}[\cos(\sqrt{2}\phi)-1]$, of the cylindrical analyser. For example: for the same radius r_0, same beam momentum p_0, if the bending angles both of spherical and cylindrical analysers are all 90°, the dispersion effect of the spherical analyser is $\sim$1.25 times of that of the cylindrical analyser.

The analytical results can be coded to calculate the practical particle motions in the electron or ion optical systems containing these elements. The phase space variables used in our analysis can be converted into the variables $(x,x',y,y',\Delta t,\Delta w)$ frequently used by the accelerator physicists: $x'=p_x/p_0, y'=p_y/p_0, \Delta t=\tau, \Delta w=-p_\tau$.

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