

Nonlinear Analysis for the Electrostatic Analyzers with Lie Algebraic Methods

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Abstract With the Lie algebraic methods, the charged particle trajectories in electrostatic analyzers are analyzed and the third order solutions obtained. In this paper, we briefly describe the Lie algebraic methods and the procedures of calculating the nonlinear orbits. The procedures are: first, set up the Hamiltonian; then expand the Hamiltonian into a sum of homogeneous polynomials of different degrees; next, calculate the Lie map associating to the Hamiltonian; finally, apply the Lie map on the particle initial coordinates in the phase space, and obtain the particle nonlinear trajectories of the first order, the second order, and the third order approximations respectively. Higher orders solutions could be obtained if needed.

Key words Lie algebraic methods, nonlinear orbit, electrostatic analyzer, beam optics

1 Introduction

The electrostatic analyzers are often used for analyzing different ion species in accelerators. The linear particle orbits in the electrostatic analyzers are known. In order to get more accurate results, the nonlinear terms of the orbits should be taken into account. The conventional methods of solving the differential equations to obtain the nonlinear solutions are very complicated if we used the Lie algebraic methods, however, the procedures will become considerably simple.

2 Lie map

The motions of charged particle in a beam transport element are regarded as the coordinate transformations between the initial point ζ^{in} and the final point ζ^{fin} in the phase spaces. The transformation is called the Lie map \mathbf{M} , which is written as the integral of the Hamiltonian H :

$$\begin{aligned} \mathbf{M} = \exp\left[-\int_{z_0}^{z_f} H dz\right] &= \cdots \mathbf{M}_4 \mathbf{M}_3 \mathbf{M}_2 = \\ &\cdots (1 + :f_4: + \frac{1}{2} :f_4:^2 + \cdots) \times \\ &(1 + :f_3: + \frac{1}{2} :f_3:^2 + \cdots) \mathbf{M}_2 = \end{aligned}$$

$$\mathbf{M}_2 + :f_3: \mathbf{M}_2 + \left(:f_4: + \frac{1}{2} :f_3:^2\right) \mathbf{M}_2, \quad (1)$$

where z_0 is the value of the independent variable of the Hamiltonian H at the initial point ζ^{in} , and z_f is the value at the final point ζ^{fin} . And:

$$f_2 = -\int_{z_0}^{z_f} H_2 dz,$$

$$f_3 = -\int_{z_0}^{z_f} h_3^{\text{int}} dz,$$

$$f_4 = -\int_{z_0}^{z_f} h_4^{\text{int}} dz +$$

$$\frac{1}{2} \int_{z_0}^{z_f} dz_1 \int_{z_0}^{z_1} dz_2 [-h_3^{\text{int}}(z_2), -h_3^{\text{int}}(z_1)], \quad (2)$$

here

$$h_n^{\text{int}}(z) = \mathbf{M}_2 H_n. \quad (3)$$

where H_n is the n degree of homogeneous polynomial of the Taylor series of the Hamiltonian H .

In Eq. (1) the factorization theorem^[1,2] is used,

$$\mathbf{M}_2 = \exp(:f_2:), \mathbf{M}_3 = \exp(:f_3:), \mathbf{M}_4 = \exp(:f_4:), \quad (4)$$

and the symbol $:$ stands for the Poisson brackets expressed in the following:

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$$:f: g = [f, g] = \sum_i [\partial f / \partial q_i] (\partial g / \partial P_i) - (\partial g / \partial q_i) (\partial f / \partial P_i). \quad (5)$$

The Lie map \mathbf{M} of Eq. (1) is also called the Lie transformation, which can be expressed with a Taylor series^[3]:

$$\exp(:f:) g = g + [f, g] + [f, [f, g]]/2! + \dots \quad (6)$$

Let the map \mathbf{M} act on the canonical coordinate ζ^{in} , we obtain the particle orbits of different orders:

$$\begin{aligned} \zeta_1 &= \exp(:f_2:) \zeta^{\text{in}}, & (\text{first order}) \\ \zeta_2 &= :f_3: \zeta_1, & (\text{second order}) \\ \zeta_3 &= :f_4: \zeta_1 + \frac{1}{2} :f_3:^2 \zeta_1. & (\text{third order}) \end{aligned} \quad (7)$$

Here, the subscripts denote the order of the approximation.

3 Hamiltonian and its expanded homogeneous polynomial

The electrostatic analyzer consists of a pair of coaxial cylindrical electrodes. In the cylindrical coordinates (r, θ, γ) (see Fig. 1), r is the radius of the arbitrary particle trajectory, r_0 is the radius of the reference particle trajectory, a, b are the radius of the inner and outer electrodes respectively, and θ is the bending angle of the analyzer.

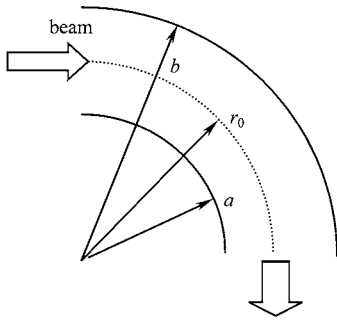


Fig. 1

Suppose the voltage along the reference trajectory is zero,

$$H = -(r_0 + x) \sqrt{[p_\tau - m_0 \gamma_0 c^2 + m_0 \gamma_0 v_0^2 \ln(1 + x/r_0)]^2 / c^2 - p_x^2 - p_y^2 - (m_0 c)^2} - (p_\tau - m_0 \gamma_0 c^2) r_0 / v_0. \quad (15)$$

Expand the function H into Taylor series, we have:

$$H = \sum_{n=0}^{\infty} H_n. \quad (16)$$

where H_n is the homogeneous polynomial of n -th order. The first five items are:

$$H_0 = r_0 p_0 (\beta_0^{-2} - 1), \quad (\text{here } p_0 = m_0 \gamma_0 v_0)$$

$$H_1 = 0,$$

$$H_2 = \frac{p_0 k^2}{2r_0} x^2 + \frac{r_0}{2p_0} (p_x^2 + p_y^2) + \frac{r_0}{2p_0 v_0^2 \gamma_0^2} p_\tau^2 + \frac{k^2}{v_0} x p_\tau,$$

the electric potential is

$$\psi = \frac{m_0 \gamma_0 v_0^2}{q} \ln(x/r_0 + 1). \quad (8)$$

where, v_0 is the velocity of the reference particle, and

$$x = r - r_0. \quad (9)$$

The Hamiltonian with time t as the independent variable is:

$$H_t = \sqrt{m_0^2 c^4 + p_x^2 c^2 + p_y^2 c^2 + [p_\theta / (r_0 + x)]^2 c^2} + m_0 \gamma_0 v_0^2 \ln(1 + x/r_0). \quad (10)$$

Let $p_t = -H_t$, and solve p_θ from p_t , we have:

$$p_\theta = (r_0 + x) \times \sqrt{[p_t + m_0 \gamma_0 v_0^2 \ln(1 + x/r_0)]^2 / c^2 - p_x^2 - p_y^2 - m_0^2 c^2}. \quad (11)$$

Eq. (11) is the Hamiltonian in the phase space (x, p_x, y, p_y, t, p_t) with θ as the independent variable. Let

$$\begin{aligned} x &= x, p_x = p_x, y = y, p_y = p_y, \\ \tau &= t - r_0 \theta / v_0, p_\tau = p_t - p_t^0. \end{aligned} \quad (12)$$

where p_t^0 is the value of p_t of the reference particle. We can see from Eq. (12) that the coordinates of the reference particle always keeps zero in the new phase space $\zeta = (x, p_x, y, p_y, \tau, p_\tau)$. According to Eq. (10), we have:

$$\begin{aligned} p_t^0 &= -H_t |_{\text{reference particle}} = \\ &= -\sqrt{m_0^2 c^4 + p_0^2 c^2} = \\ &= -m_0 \gamma_0 c^2. \end{aligned} \quad (13)$$

Here p_0 is the momentum of the reference particle,

$$\gamma_0 = 1 / \sqrt{1 - (v_0/c)^2}.$$

Under the canonical transformation given by Eq. (12), the generating function is:

$$\begin{aligned} F_2 &= \sum_{i=1}^3 Q_i p_i = \\ &= x p_x + y p_y + \tau p_\tau = \\ &= x p_x + y p_y + (t - r_0 \theta / v_0) p_t. \end{aligned} \quad (14)$$

The new Hamiltonian in the phase space ζ is:

$$\begin{aligned} H_3 &= \frac{p_0(3 - \gamma_0^2)}{6r_0^2 \gamma_0^2} x^3 + \frac{1}{p_0} x (p_x^2 + p_y^2) + \frac{2}{\gamma_0^2 v_0 r_0} x^2 p_\tau + \\ &= \frac{2}{p_0 \gamma_0^2 v_0^2} x p_\tau^2 + \frac{r_0}{2p_0^2 \gamma_0^2 v_0^3} p_\tau^3 + \frac{r_0}{2p_0^2 v_0} (p_x^2 + p_y^2) p_\tau, \\ H_4 &= \left(\frac{8 - 3\beta_0^2}{\gamma_0^2} + 2 \right) \frac{p_0 x^4}{24r_0^3} + (4 - \beta_0^2) \frac{x^2 (p_x^2 + p_y^2)}{4p_0 r_0} + \end{aligned}$$

$$\frac{r_0}{4p_0^3} p_x^2 p_y^2 + (14 - 3\beta_0^2) \frac{x^3 p_\tau}{6v_0 \gamma_0^2 r_0} +$$

$$\frac{3 - \beta_0^2}{4p_0^3 v_0^2} r_0 (p_x^2 + p_y^2) p_\tau^2 + (6 - \beta_0^2) \frac{3x^2 p_\tau^2}{4p_0 v_0^2 \gamma_0^2 r_0} + \frac{(4 - \beta_0^2)}{2p_0^2 v_0} x p_\tau (p_x^2 + p_y^2) + \frac{r_0}{8p_0^3} (p_x^4 + p_y^4). \quad (17)$$

$$(6 - \beta_0^2) \frac{x p_\tau^3}{2p_0^2 v_0^3 \gamma_0^2} + (5 - \beta_0^2) \frac{r_0 p_\tau^4}{8p_0^3 v_0^4 \gamma_0^2} + \text{where:} \quad k^2 = \frac{1 + \gamma_0^2}{\gamma_0^2}. \quad (18)$$

4 Particle trajectory calculations

4.1 First order

From H_2 , solving the equation of the motion, we can get the first order approximation:

$$\begin{bmatrix} x \\ p_x \\ y \\ p_y \\ \tau \\ p_\tau \end{bmatrix} = \begin{bmatrix} \cos(k\theta) & \frac{r_0}{kp_0} \sin(k\theta) & 0 & 0 & 0 & \frac{r_0}{p_0 v_0} (\cos(k\theta) - 1) \\ -\frac{kp_0}{r_0} \sin(k\theta) & \cos(k\theta) & 0 & 0 & 0 & -\frac{k}{v_0} \sin(k\theta) \\ 0 & 0 & 1 & \frac{r_0 \theta}{p_0} & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ \frac{k}{v_0} \sin(k\theta) & \frac{-r_0}{p_0 v_0} (\cos(k\theta) - 1) & 0 & 0 & 1 & \frac{kr_0}{p_0 v_0^2} \sin(k\theta) - \frac{r_0 \theta}{p_0 v_0^2} \\ 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x_0 \\ p_{x_0} \\ y_0 \\ p_{y_0} \\ \tau \\ p_{\tau_0} \end{bmatrix}. \quad (19)$$

4.2 Second order

According to Eq. (2) and the second expression of Eq. (3), we have:

$$f_3 = - \int_0^\theta h_3^{\text{int}}(\zeta, \theta) d\theta = - \int_0^\theta M_2 H_3(\zeta, \theta) d\theta. \quad (20)$$

According to the second expression of Eq. (7), and the fourth expression of Eq. (17), Eq. (19) and Eq. (20), the second order terms of the trajectories are obtained:

$$\begin{aligned} x_2 = & \left[-3(5 + \gamma_0^2) - 2(\gamma_0^2 - 3) \cos(k\theta) + (9 + 5\gamma_0^2) \cos(2k\theta) \right] \frac{x^2}{12r_0 k^2 \gamma_0^2} + \\ & \left[2(\gamma_0^2 - 3) \sin(k\theta) + (9 + 5\gamma_0^2) \sin(2k\theta) \right] \frac{x p_x}{6k^3 p_0 \gamma_0^2} - \\ & \left[3(5 + \gamma_0^2) - 2(3 - \gamma_0^2) \cos(k\theta) - (9 + 5\gamma_0^2) \cos(2k\theta) \right] \frac{x p_\tau}{6k^2 p_0 v_0 \gamma_0^2} - \\ & \left[3(5 + \gamma_0^2) - 8(3 + \gamma_0^2) \cos(k\theta) + (9 + 5\gamma_0^2) \cos(2k\theta) \right] \frac{r_0 p_x^2}{12k^4 p_0^2 \gamma_0^2} - \\ & \left[4(3 + \gamma_0^2) \sin(k\theta) - (9 + 5\gamma_0^2) \sin(2k\theta) \right] \frac{r_0 p_x p_\tau}{6k^3 p_0^2 v_0 \gamma_0^2} - \\ & (1 - \cos(k\theta)) \frac{r_0 p_y^2}{k^2 p_0^2} - \left[3(3 - \gamma_0^2) + 8\gamma_0^2 \cos(k\theta) - (9 + 5\gamma_0^2) \cos(2k\theta) \right] \frac{r_0 p_\tau^2}{12k^2 p_0^2 v_0^2 \gamma_0^2}, \quad (21) \end{aligned}$$

$$\begin{aligned} p_{x_2} = & \left[\sin(k\theta) + \sin(2k\theta) \right] \frac{p_0 (\gamma_0^2 - 3) x^2}{6kr_0^2 \gamma_0^2} - \left[\cos(k\theta) - \cos(2k\theta) \right] \frac{(3 - \gamma_0^2) x p_x}{3k^2 r_0 \gamma_0^2} - \\ & \left[2(3 + \gamma_0^2) \sin(k\theta) + (3 - \gamma_0^2) \sin(2k\theta) \right] \frac{x p_\tau}{3kr_0 v_0 \gamma_0^2} - \left[4(3 + \gamma_0^2) \sin(k\theta) - (3 - \gamma_0^2) \sin(2k\theta) \right] \frac{p_x^2}{6k^3 p_0 \gamma_0^2} - \\ & \left[\cos(k\theta) - \cos(2k\theta) \right] \frac{(3 - \gamma_0^2) p_x p_\tau}{3k^2 p_0 v_0 \gamma_0^2} - \frac{\sin(k\theta) p_y^2}{kp_0} - \\ & \left[2(3 + \gamma_0^2) \sin(k\theta) + (3 - \gamma_0^2) \sin(2k\theta) \right] \frac{p_\tau^2}{6kp_0 v_0^2 \gamma_0^2}, \quad (22) \end{aligned}$$

$$y_2 = \frac{2xp_y \sin(k\theta)}{kp_0} + \frac{2p_x p_y r_0(1 - \cos(k\theta))}{k^2 p_0^2} + \frac{(2\sin(k\theta) - k\theta) r_0 p_y p_\tau}{kp_0^2 v_0}, \quad (23)$$

$$p_{y_2} = 0, \quad (24)$$

$$\begin{aligned} \tau_2 = & [2(3 - \gamma_0^2) \sin(k\theta) + (9 + \gamma_0^2) \sin(2k\theta)] \frac{x^2}{12kr_0 v_0 \gamma_0^2} + \\ & [3 + 3\gamma_0^2 + 2(3 - \gamma_0^2) \cos(k\theta) - (9 + \gamma_0^2) \cos(2k\theta)] \frac{xp_x}{6k^2 p_0 v_0 \gamma_0^2} + \\ & [2(3 - \gamma_0^2) \sin(k\theta) + (9 + \gamma_0^2) \sin(2k\theta)] \frac{xp_\tau}{6kp_0 v_0^2 \gamma_0^2} + \\ & [8(\gamma_0^2 + 3) \sin(k\theta) - (9 + \gamma_0^2) \sin(2k\theta)] \frac{r_0 p_x^2}{12k^3 p_0^2 v_0 \gamma_0^2} - \\ & [3 + 3\gamma_0^2 - 4(3 + \gamma_0^2) \cos(k\theta) + (9 + \gamma_0^2) \cos(2k\theta)] \frac{r_0 p_x p_\tau}{6k^2 p_0^2 v_0^2 \gamma_0^2} + \\ & \frac{r_0 p_\tau^2 (2\sin(k\theta) - k\theta)}{2kp_0^2 v_0} + [6k\theta\gamma_0^2 - 8\gamma_0^2 \sin(k\theta) + (9 + \gamma_0^2) \sin(2k\theta)] \frac{r_0 p_\tau^2}{12kp_0^2 v_0^3 \gamma_0^2}, \quad (25) \end{aligned}$$

$$p_{\tau_2} = 0. \quad (26)$$

4.3 Third order

In the similar way, according to Eq. (3), Eqs. (19)—(26), the third expression of Eq. (2), Eq. (7), and the fifth expression of Eq. (17), we obtain the function f_4 first, and then the third order terms of the trajectories. Because the results are too long, only the terms of x_3 are listed here:

$$\begin{aligned} x_3 = & [12k\theta(6\beta_0^2 + 6\gamma_0^2 + \gamma_0^4 - 3) \sin(k\theta) - 12(15 - 2\gamma_0^2 - \gamma_0^4) - (15 + 144\gamma_0^2 + 13\gamma_0^4) \cos(k\theta) + \\ & 4(27 + 6\gamma_0^2 - 5\gamma_0^4) \cos(2k\theta) + 3(29 + 32\gamma_0^2 + 7\gamma_0^4) \cos(3k\theta)] \frac{x_0}{144k^4 r_0^2 \gamma_0^4} - \\ & [12k\theta(3 - 6\beta_0^2 - 6\gamma_0^2 - \gamma_0^4) \cos(k\theta) + (99 + 384\gamma_0^2 + 25\gamma_0^4) \sin(k\theta) + 4(27 + 6\gamma_0^2 - 5\gamma_0^4) \sin(2k\theta) - \\ & 9(29 + 32\gamma_0^2 + 7\gamma_0^4) \sin(3k\theta)] \frac{x^2 p_x}{144k^5 p_0 r_0 \gamma_0^4} + \\ & [12k\theta(6\beta_0^2 + 6\gamma_0^2 + \gamma_0^4 - 3) \sin(k\theta) - 48(5 + \gamma_0^2) + (9 - 128\gamma_0^2 - 21\gamma_0^4) \cos(k\theta) + \\ & 16(9 + 5\gamma_0^2) \cos(2k\theta) + 3(29 + 32\gamma_0^2 + 7\gamma_0^4) \cos(3k\theta)] \frac{x^2 p_\tau}{48k^4 p_0 r_0 v_0 \gamma_0^4} + \\ & [12k\theta(3 - 6\beta_0^2 - 6\gamma_0^2 - \gamma_0^4) \sin(k\theta) - 72(5 + 6\gamma_0^2 + \gamma_0^4) - (27 - 288\gamma_0^2 - 95\gamma_0^4) \cos(k\theta) + \\ & 8(81 + 54\gamma_0^2 + 5\gamma_0^4) \cos(2k\theta) - 9(29 + 32\gamma_0^2 + 7\gamma_0^4) \cos(3k\theta)] \frac{xp_x^2}{144k^6 p_0^2 \gamma_0^4} + \\ & [12k\theta(6\beta_0^2 + 6\gamma_0^2 + \gamma_0^4 - 3) \cos(k\theta) - (99 + 384\gamma_0^2 + 25\gamma_0^4) \sin(k\theta) - \\ & 4(27 + 6\gamma_0^2 - 5\gamma_0^4) \sin(2k\theta) + 9(29 + 32\gamma_0^2 + 7\gamma_0^4) \sin(3k\theta)] \frac{xp_x p_\tau}{72k^5 p_0^2 v_0 \gamma_0^4} - \\ & [3k\theta\beta_0^4 \gamma_0^2 \sin(k\theta) + 3(5 + \gamma_0^2) - 2(3 - \gamma_0^2) \cos(k\theta) - (9 + 5\gamma_0^2) \cos(2k\theta)] \frac{xp_y^2}{6k^4 p_0^2 \gamma_0^2} + \\ & [(9 - 128\gamma_0^2 - 21\gamma_0^4) \cos(k\theta) + 16(9 + 5\gamma_0^2) \cos(2k\theta) + 3(29 + 32\gamma_0^2 + 7\gamma_0^4) \cos(3k\theta) - \\ & 48(5 + \gamma_0^2) - 12k\theta(6\beta_0^2 + 6\gamma_0^2 + \gamma_0^4 - 3) \sin(k\theta)] \frac{xp_\tau^2}{48k^4 p_0^2 v_0^2 \gamma_0^4} - \\ & [12k\theta(3 - 6\beta_0^2 - 6\gamma_0^2 - \gamma_0^4) \cos(k\theta) + (279 + 336\gamma_0^2 + 37\gamma_0^4) \sin(k\theta) - 16(27 + 24\gamma_0^2 + 5\gamma_0^4) \sin(2k\theta) + \\ & 3(29 + 32\gamma_0^2 + 7\gamma_0^4) \sin(3k\theta)] \frac{r_0 p_x^3}{144k^7 p_0^3 \gamma_0^4} - \\ & [12k\theta(6\beta_0^2 + 6\gamma_0^2 + \gamma_0^4 - 3) \sin(k\theta) + 36(5 + 6\gamma_0^2 + \gamma_0^4) + (315 + 96\gamma_0^2 + \gamma_0^4) \cos(k\theta) - \\ & 4(189 + 150\gamma_0^2 + 25\gamma_0^4) \cos(2k\theta) + 9(29 + 32\gamma_0^2 + 7\gamma_0^4) \cos(3k\theta)] \frac{r_0 p_x^2 p_\tau}{144k^6 p_0^3 v_0 \gamma_0^4} + \end{aligned}$$

$$\begin{aligned}
& [3k\theta\beta_0^4\gamma_0^2\cos(k\theta) - 2(3+5\gamma_0^2)\sin(k\theta) + (9+5\gamma_0^2)\sin(2k\theta)] \frac{r_0 p_x p_y^2}{6k^5 p_0^3 \gamma_0^2} + \\
& [12k\theta(6\beta_0^2 + 6\gamma_0^2 + \gamma_0^4 - 3)\cos(k\theta) + (45 - 192\gamma_0^2 + 23\gamma_0^4)\sin(k\theta) - \\
& 8(27 + 24\gamma_0^2 + 5\gamma_0^4)\sin(2k\theta) + 9(29 + 32\gamma_0^2 + 7\gamma_0^4)\sin(3k\theta)] \frac{r_0 p_x p_z^2}{144k^5 p_0^3 v_0^2 \gamma_0^4} - \\
& [3(3 - \gamma_0^2) + 8\gamma_0^2\cos(k\theta) - (9 + 5\gamma_0^2)\cos(2k\theta) + 3k\theta\beta_0^4\gamma_0^2\sin(k\theta)] \frac{r_0 p_z^2 p_x}{6k^4 p_0^3 v_0 \gamma_0^2} - \\
& [12(17 + 2\gamma_0^2 + \gamma_0^4) - (9 - 96\gamma_0^2 + 11\gamma_0^4)\cos(k\theta) - 4(27 + 6\gamma_0^2 - 5\gamma_0^4)\cos(2k\theta) - \\
& 3(29 + 32\gamma_0^2 - 7\gamma_0^4)\cos(3k\theta) + 12k\theta(6\beta_0^2 + 6\gamma_0^2 + \gamma_0^4 - 3)\sin(k\theta)] \frac{r_0 p_z^3}{144k^4 p_0^3 v_0^3 \gamma_0^4}. \quad (27)
\end{aligned}$$

5 Conclusion

Now the nonlinear charged particle trajectories in the electrostatic analyzers are obtained. In some cases, one wants to calculate the nonlinear particle transport in an ion optical system. To do so, it is necessary to know the nonlinear trans-

port in each single optical element, although in a single element the nonlinear part of the trajectories is not quite big compared with the linear part. To calculate the nonlinear particle orbits in the ion optical systems including the electrostatic analyzers, the analytical results will be put into a computer program^[4].

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静电分析器非线性轨迹的 Lie 代数分析

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摘要 介绍了 Lie 代数的方法, 用 Lie 代数方法分析了静电分析器对束流传输过程的非线性影响, 其计算结果分析到三级近似. 首先给出了静电分析器的哈密顿函数, 然后将哈密顿函数展开为齐次多项式的和, 再求 Lie 映射, 最后得到粒子轨迹各级近似解.

关键词 Lie 代数 非线性 静电分析器 束流光学