DOI 10.31489/2019Ph1/87-93

UDC 537.533.34

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Calculation of electron-optical characteristics of a quadrupole-cylindrical field

The article is devoted to the calculation and analysis of electron-optical characteristics of a electrostatic quadrupole-cylindrical field. The object of the research is the development of an energy analyzer based on a quadrupole-cylindrical field. The structure of electrostatic quadrupole-cylindrical fields is obtained on the basis of the superposition of a basic cylindrical field and axially symmetrical cylindrical quadrupoles. The calculation of electron-optical characteristics of a quadrupole-cylindrical field was fulfilled on the basis of the analytical method for calculating of trajectories of charged particles. The problem of integrating of differential equations of charged particle motion and the analytical description of the trajectory equation in a quadrupole-cylindrical field has been solved. A projection of charged particle trajectory from the source to its image has been calculated. The main aberration coefficients that determine the conditions of second-order angular focusing are calculated. The most optimal scheme of a quadrupole-cylindrical mirror for energy analysis has been found.

Keywords: electron spectroscopy, quadrupole-cylindrical field, quadrupole, energy analyzer, electron-optical characteristics, electron-optical scheme.

The implementation of electron spectroscopy methods is based on the use of complex equipment, one of the main elements of which is a dispersion energy analyzer of low and medium energy electrons. At present, the capabilities of the known energy analyzers used in the study of the solid surface are largely exhausted. Therefore, energy analysis of charged particles beams, as an effective method for studying nanostructures, requires the modernization of existing analyzing systems or the creation of qualitatively new analyzing systems based on the further development of the theory.

A new class of axially symmetric Laplace fields, built on the basis of the synthesis of multipoles and a cylindrical field, and of practical interest for solving the problem of energy analysis of charged particle beams, was first proposed in [1, 2]. The potential of a multipole-cylindrical field, built on the basis of the superposition of a cylindrical field and a various order circular multipole, has the following form

$$U(r,z) = \mu \ln r + U_m(r,z), \quad (1)$$

where $U_m(r,z)$ is a circular multipole; μ is coefficient that determines the weight contribution of a cylindrical field. Connecting multipole components of different order (quadrupole, hexapole, sextupole, etc.) to a basic cylindrical field leads to the synthesis of a wide class of various axially symmetric fields, among which variants of mirror analyzers schemes with improved quality of angular focusing can be found.

Earlier, the calculation of structures of electrostatic quadrupole-cylindrical fields (QCF), synthesized based on the sum of a basic cylindrical field and axially symmetric cylindrical quadrupoles of various types, was given in [3]. Equipotential portraits of quadrupole-cylindrical fields of various types are presented. The analysis of the obtained equipotential portraits of QCF was carried out. It is established that an electron mirror with QCF, having potential

$$U_q(r,z) = U_0(\mu + z)\ln r, \tag{2}$$

is more accessible for analytical study of its electron-optical properties and for building on its base a highluminosity energy analyzer. It is noted that this QCF at the value $\mu = 1$, coincides with the well-known Wannberg's field, proposed for the development of a device operating in a spectrograph mode [4]

$$U = \frac{V}{\ln(r_1/r_o)}(1 + Az)\ln\frac{r}{r_o}, \tag{3}$$

where A is a small dimensionless parameter. The presence of a small parameter A gives an additional degree of freedom in choosing the desired distribution of the electrostatic field and expands the ability to search for the most optimal analyzer scheme based on QCF.

The results of numerical modeling of electron-optical schemes of QCF-energy analyzer are presented in [5, 6]. Corpuscular-optical parameters of schemes with various parameters A are calculated.

The investigated QCF is formed in the space between two axially symmetric coaxial electrodes, the inner of which has a cylindrical shape (radius r_0) and is under the Earth potential, and deflecting potential U_0 is applied to an outer electrode having a curvilinear profile $r = r_0 \exp\left[\frac{\ln(r_1/r_0)}{1 + Az}\right]$ (Fig. 1).

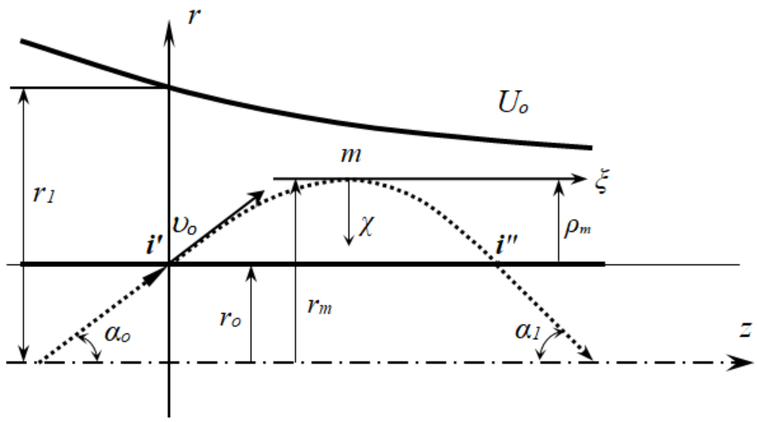

Figure 1. An electron-optical scheme of the QCF-mirror analyzer

Calculation of characteristics of QCF (3) is presented below, this calculation is performed on the basis of the analytical method for calculating of trajectories, proposed earlier in [7, 8], According to this method, the coordinate system x, ξ is located at the turning point m of the trajectory**,** and from this point the counting of the left and right branches of the trajectory, asymmetrical about the axis x , begins. Here and in the future, all linear dimensions will be kept in shares of the radius r_0 of the inner cylindrical electrode.

$$z = z_m\mu\xi, \quad \frac{r}{r_0} = \frac{(1+\rho_m)r_0}{r_0} - \frac{x \cdot r_0}{r_0} = R - x, \quad R = 1 + \rho_m. \tag{4}$$

The distribution of QCF (3) in coordinates x, ξ is as follows

$$U = U_{1,2}(x,\xi) = U_o\,\omega\,(1 \pm \mu A'\xi)\,ln(R - x), \tag{5}$$

where $R = \frac{r_m}{r_o} = 1 + \rho_m$, $\omega = (1 - A z_{m_1})/ln(r_1/r_o)$, $A' = \frac{A}{1 - Az_{m_1}}$.

The solution of equations of motion in the field leads to the following integro-differential equation of charged particlemotion in QCF (3), in which it is temporarily assumed that $A = \pm A'$ [7, 8].

$$\left(\xi'_{1,2}\right)^2 \left\{-\ln\left(1 - \frac{x}{R}\right) + A\left[\xi\ln(R - x) - \int_0^x ln(R - x)\,\xi' dx\right]\right\} = F_{m_{1,2}} + A\int_0^x ln(R - x)\,\xi' dx \tag{6}$$

and the condition of connection the left and right branches of the trajectory at the turning point m

$$P_1^2(A)\cot^2\alpha - A'f_{m_1} = P_2^2(A)\cot^2\alpha_1 + A'f_{m_2}, \tag{7}$$

where $f_{m_{1,2}} = \int_0^{\rho_m} \ln(R-x)\xi' dx$, $P_1^2(A) = \dfrac{P_o^2}{1-Az_m}$ is reflection parameter for the left branch; $P_2^2(A) = \dfrac{P_o^2}{1-Az_m}\dfrac{\sin^2\alpha_1}{\sin^2\alpha_o}$ is reflection parameter for the right branch and $P_o^2 = \dfrac{W}{qU} ln\left(\dfrac{r_1}{r_o}\right)\sin^2\alpha_o$ is the parameter connecting the geometric and energy characteristics of the reflection of a cylindrical mirror analyzer [8]. In these formulas, the number 1 in the subscript corresponds to the functions for the left branch; the number 2 corresponds to functions of the right branch of the trajectory.

The radial component $R = 1 + \rho_m$ of turning point of the trajectory is determined from the integro-differential equation (6) provided that $x = \rho_m, (\xi')^2 = \cot^2\alpha_{0,1}$ and is reduced to the following expression to determine R

$$\ln R = P_{1,2}^2(A)\cot^2\alpha_{0,1}\mu A'f_{m_{1,2}}. \tag{8}$$

The inclination angle of the trajectory at the exit from the field (3) is determined from the condition of connection of the trajectory branches at its vertex

$$\cot^2\alpha_1 = \frac{P_1^2(A)\cot^2\alpha_0 + A'\left(f_{m_1} + f_{m_2}\right)}{P_2^2(A)} = \frac{P_0^2\cot^2\alpha_0 + A\left(f_{m_1} + f_{m_2}\right)}{P_0^2 - A\left(f_{m_1} + f_{m_2}\right)}. \tag{9}$$

Integrating equation (6) by an approximate-analytical method of decomposing a quantity ξ into a fractional-power series $\xi = \sqrt{x}\sum_{n=0}^{\infty} c_n x^n + \sum_{n=1}^{\infty} a_n x^n$ [4, 5], using the method of successive approximations for determining R, we obtain the equations for the basic electron-optical characteristics of QCF. The parameter $R_0 = \exp\left(P^2\right)$ of a cylindrical mirror analyzer [9] is used as a zero approximation in the determination R. Final results of the calculation of characteristics $\rho_m = R - 1$ and ξ_n, obtained as a series expansion by the magnitude of reflection parameter P up to order 12 inclusiveare presented below:

$$\rho_m = \left(1 + p^2 + \frac{1}{2}p^4 + \frac{1}{6}p^6 + \frac{1}{24}p^8 + ...\right) - \left(\frac{2}{3}p^4 + \frac{14}{15}p^6 + \frac{71}{105}p^8 + ...\right)\times$$
$$\times\cot\alpha_o \cdot A + \left[\left(\frac{1}{18}p^6 + \frac{11}{90}p^8 + ...\right) + \left(p^6 + \frac{101}{45}p^8 + ...\right)\cot^2\alpha_o\right]\cdot A^2 \tag{10}$$

is the radial coordinate of the trajectory vertex in the field (3);

$$\xi_i = \left(4p^2 - \frac{8}{3}p^4 - \frac{16}{15}p^6 - \frac{32}{105}p^8 + ...\right)\cdot\cot\alpha_o -$$
$$-\left[\left(\frac{8}{3}p^4 + \frac{176}{45}p^6 + \frac{64}{21}p^8 + ...\right) + \left(\frac{16}{3}p^4 + \frac{128}{15}p^6 + \frac{2176}{315}p^8 + ...\right)\cot^2\alpha_o\right]\cdot A + \tag{11}$$
$$+\left[\left(\frac{32}{3}p^6 + \frac{7744}{315}p^8 + ...\right)\cdot\cot\alpha_o + \left(\frac{128}{9}p^6 + \frac{512}{15}p^8 + ...\right)\cdot\cot^3\alpha_o\right]\cdot A^2$$

is the projection of the trajectory on the symmetry axis z of the mirror in the area from i' to i'';

$$\cot\alpha_1 = \cot\alpha_o - \left(\frac{4}{3}p^2 + \frac{16}{15}p^4 + \frac{16}{35}p^6 + ...\right)\cdot\left[1 + \cot^2\alpha_o\right]\cdot A +$$
$$+\left[\left(\frac{16}{3}p^4 + \frac{128}{15}p^6 + \frac{869}{126}p^8 + ...\right)\cdot\left[\cot\alpha_o + \cot^3\alpha_o\right]\right]\cdot A^2 \tag{12}$$

is the inclination angle of the trajectory at the exit from QCF.

The total projection of the trajectory on the symmetry axis of a quadrupole-cylindrical mirror from the source to its image is the sum of the projections of the trajectory in the mirror field and in the region of the inner cylindrical electrode

$$l=\frac{L}{r_o}=\Delta_1\cot\alpha_o+\xi_i+\Delta_2\cot\alpha_1, \qquad (13)$$

where Δ_1, Δ_2 are values of distance of the source and its image from the surface of the inner cylindrical electrode, which are considered positive in direction from the radius r_0.

For the analysis of characteristics of an electrostatic QCF-energy analyzer, aberration coefficients of spatial focusing of the 1st, 2nd and 3rd orders were determined: $\frac{dl}{d\alpha},\frac{d^2l}{d\alpha^2},\frac{d^3l}{d\alpha^3}$:

$$\frac{dl}{d\alpha}=\Delta_1\left[1+\cot^2\alpha_o\right]+\frac{d\xi_i}{d\alpha}+\Delta_2\frac{d}{d\alpha}\left(\cot\alpha_1\right); \qquad (14)$$

$$\frac{d^2l}{d\alpha^2}=2\Delta\cot\alpha_0\left[1+\cot^2\alpha_o\right]+\frac{d^2\xi_i}{d\alpha^2}+\Delta\frac{d^2}{d\alpha^2}\left(\cot\alpha_1\right); \qquad (15)$$

$$/\frac{d^3l}{d\alpha^3}=-2\Delta\left[1+4\cot^2\alpha_o+3\cot^4\alpha_o\right]+\frac{d^3\xi_i}{d\alpha^3}+\Delta\frac{d^3}{d\alpha^3}\left(\cot\alpha_1\right). \qquad (16)$$

Due to the awkwardness expressions for aberration coefficients, here only formulas defining the magnitude of first order aberrations $\frac{dl}{d\alpha}$ are given.

$$\begin{gathered}\frac{d\xi_i}{d\alpha}=\left(-4P^2-\frac{8}{3}P^4-\frac{16}{15}P^6-\frac{32}{105}P^8-\ldots\right)+\left(8P^4+\frac{16}{3}P^6+\frac{32}{15}P^8\right)\cot^2\alpha_0-\\ -\left[\left(\frac{32}{5}P^6+\frac{3328}{315}P^8+\ldots\right)\cot\alpha_0+\left(\frac{32}{3}P^4+\frac{512}{15}P^6+\frac{4352}{105}P^8+\ldots\right)\cot^3\alpha_0\right]A+\\ +\left[\left(-\frac{32}{3}P^6-\frac{7744}{315}P^8+\ldots\right)+\left(\frac{32}{3}P^6+\frac{3136}{45}P^8+\ldots\right)\cot^2\alpha_0+\left(\frac{128}{3}P^6+\frac{512}{3}P^8+\ldots\right)\cot^4\alpha\right]A^2;\end{gathered} \qquad (17)$$

$$\begin{gathered}\frac{d}{d\alpha}\left(\cot\alpha_1\right)=-\left[1+\cot^2\alpha_0\right]-\left(\frac{32}{15}P^4+\frac{64}{35}P^6+\frac{256}{315}P^8\right)\left[\cot\alpha_0+\cot^3\alpha_0\right]A+\\ +\left[\begin{array}{l}\left(-\frac{16}{3}P^4-\frac{128}{15}P^6-\frac{869}{126}P^8\ldots\right)+\left(\frac{256}{15}P^6+\frac{1738}{63}P^8+\ldots\right)\cot^2\alpha_0+\\ +\left(\frac{16}{3}P^4+\frac{128}{15}P^6+\frac{4345}{126}P^8\ldots\right)\cot^4\alpha\end{array}\right]A^2.\end{gathered} \qquad (18)$$

The magnitude of the linear dispersion in energy $D=\frac{dl}{d\varepsilon}$ (where $\varepsilon=\frac{\Delta\omega}{\omega}$ is the value of the relative energy spread in the particle beam) is determined by following expressions

$$D=\frac{dl}{d\varepsilon}=\frac{d\xi_i}{d\varepsilon}+\Delta\frac{d}{d\varepsilon}\left(\cot\alpha_1\right), \qquad (19)$$

where

$$\begin{gathered}\frac{d\xi_i}{d\varepsilon}=\left(4P^2+\frac{16}{3}P^4+\frac{16}{5}P^6+\frac{128}{105}P^8-\ldots\right)\cot\alpha_0+\left(8P^4+\frac{16}{3}P^6+\frac{32}{15}P^8\right)\cot^2\alpha_0-\\ -\left[\left(\frac{16}{3}P^6+\frac{176}{15}P^6+\frac{256}{21}P^8+\ldots\right)+\left(\frac{32}{3}P^4+\frac{128}{5}P^6+\frac{8704}{315}P^8+\ldots\right)\cot^2\alpha_0\right]A+\\ +\left[\left(32P^6+\frac{30976}{315}P^8+\ldots\right)\cot\alpha_0+\left(\frac{128}{3}P^6+\frac{2048}{15}P^8+\ldots\right)\cot^3\alpha\right]A^2.\end{gathered} \qquad (20)$$

$$\frac{d}{d\varepsilon}\left(\cot\alpha_1\right) = -\left(\frac{4}{3}P^2 + \frac{32}{15}P^4 + \frac{48}{35}P^6 + \frac{512}{945}P^8 + \dots\right)\left[1+\cot^2\alpha_0\right]A +$$
$$+\left[\begin{array}{l}\left(-\frac{16}{3}P^4 - \frac{128}{15}P^6 - \frac{869}{126}P^8 - \dots\right) + \left(\frac{256}{15}P^6 + \frac{1738}{63}P^8 + \dots\right)\cot^2\alpha_0 + \\ +\left(\frac{32}{3}P^4 + \frac{128}{5}P^6 + \frac{1738}{63}P^8 + \dots\right)\left[\cot\alpha_0 + \cot^3\alpha_0\right]\end{array}\right]A^2. \quad (21)$$

Table shows the basic electron-optical characteristics of QCF-energy analyzers for schemes with $A = -0.01$, $A = +0.01$, $A = 0$, calculated depending on the entering angle α_0 and reflection parameter P, and satisfying the conditions of second-order angular focusing $\frac{dl}{d\alpha} = \frac{d^2 l}{d\alpha^2} = 0$.

Table

Electron-optical characteristics of QCF

	α_0, degree	P	r_m	$\Delta = \frac{\Delta_1 + \Delta_2}{2}$	α_1, degree	$l = \frac{L}{r_0}$	$D = \frac{dl}{d\varepsilon}$	$\frac{d^3 l}{d\alpha^3}$
A=+0,01	35	0.4315	0.2042	0.2131	35.1638	1.8068	1.3430	-4.5463
	36	0.4825	0.2615	0.2770	36.2123	2.2503	1.7140	-5.5699
	37	0.5324	0.3266	0.3519	37.2686	2.7382	2.1391	-6.7186
	38	0.5817	0.4011	0.4409	38.3345	3.2815	2.6317	-8.0431
	39	0.6312	0.4871	0.5478	39.4123	3.8955	3.2104	-9.6113
	40	0.6812	0.5871	0.6779	40.5050	4.5983	3.8980	-11.5073
	41	0.7322	0.7047	0.8382	41.6166	5.4151	4.7267	-13.8498
	42	0.7848	0.8446	1.0391	42.7529	6.3806	5.7410	-16.8080
	43	0.8394	1.0135	1.2952	43.9216	7.5437	7.0046	-20.6319
A= 0	35	0.4249	0.1979	0.2069	35	1.7560	1.7560	-4.3979
	36	0.4743	0.2522	0.2677	36	2.1787	2.1787	-5.3537
	37	0.5221	0.3133	0.3382	37	2.6383	2.6383	-6.4048
	38	0.5690	0.3823	0.4207	38	3.1430	3.1430	-7.5887
	39	0.6154	0.4605	0.5179	39	3.7025	3.7025	-8.9484
	40	0.6618	0.5496	0.6339	40	4.3289	4.3289	-10.5368
	41	0.7083	0.6516	0.7718	41	5.0366	5.0366	12.4187
	42	0.7552	0.7690	0.9389	42	5.8440	5.8440	-14.6779
	43	0.8028	0.9049	1.1424	43	6.7740	6.7740	-17.4230
A= - 0,01	35	0.4187	0.1920	0.2012	34.8446	1.7091	1.2765	-4.2629
	36	0.4665	0.2437	0.2592	35.8001	2.1128	1.6186	-5.1590
	37	0.5126	0.3014	0.3260	36.7491	2.5487	2.0047	-6.1321
	38	0.5575	0.3658	0.4031	37.6908	3.0216	2.4424	-7.2061
	39	0.6016	0.4378	0.4929	38.6239	3.5392	2.9429	-8.4146
	40	0.6452	0.5188	0.5979	39.5466	4.1102	3.5193	-9.7950
	41	0.6885	0.6098	0.7215	40.4572	4.7442	4.1873	-11.3896
	42	0.7317	0.7127	0.8677	41.3534	5.4534	4.9669	-13.2524
	43	0.7749	0.8291	1.0416	42.2323	6.2517	5.8820	-15.4467

Here the following parameters are presented: r_m is the radial coordinate of the trajectory vertex in the mirror field; $\Delta = \frac{\Delta_1 + \Delta_2}{2}$ is the value of the average total distance of the source and its image from the surface of the inner cylindrical electrode, which is determined from the condition of first order angular focusing: $\frac{dl}{d\alpha} = 0$,

$$\Delta = \frac{d\xi_i}{d\alpha} \Big/ \left[1 + \cot\alpha_0 - \frac{d}{d\alpha}\left(\cot\alpha_1\right) \right]. \qquad (22)$$

Table also presents: α_1 is the exit angle of the trajectory from the mirror field; $l = \frac{L}{r_0}$ is focal length and $D = \frac{dl}{d\varepsilon}$ is the value of the relative linear dispersion in energy, $\frac{d^3 l}{d\alpha^3}$ is cubic angular aberration.

The analysis of the data of the Table shows that in the mirror energy analyzers based on QCF in a wide range of parameter values P and α_0, the second order angular focusing regime is implemented. With an increase of P and α_0 parameters, an increase of the cubic angular aberration $\frac{d^3 l}{d\alpha^3}$ is observed, which leads to a decrease of the resolution of the analyzer.

Comparing of parameters of the schemes with different values A shows that the angular aberrations of the analyzers with $A < 0$, the outer electrode of which has an increasing exponential profile, are smaller than those of QCF-analyzers with $A > 0$ and less than those of the mirror analyzer corresponding to the schemes with $A = 0$. This means that mirror analyzers based on QCF with improved electron-optical characteristics must be chosen among the schemes with $A < 0$.

At small values of the parameter A, the profile of the generator of the outer electrode is approximated by a sloping straight line, which allows replacing the outer exponential electrode by conical one. In the scheme of the most optimal energy analyzer based on QCF, presented in Figure 1, the improving of resolution by 30 % is achieved by using an outer deflecting electrode in the cone form with a small angle of inclination of the generator line.

Thus, equations for the trajectories of charged particle motion in an electrostatic QCF are determined. The general parameters that determine the electron-optical properties of quadrupole-cylindrical analyzers are calculated. It has been established that for all the QCF schemes with $A = 0.01$, $A = 0$, $A = -0.01$ a second-order angular focusing regime is performed, and the best focusing schemes correspond to analyzers with $A = -0.01$, in which an outer electrode has an increasing exponential profile at a small inclination angle of the generatrix.

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Квадрупольді-цилиндрлік өрістің электронды-оптикалық сипаттамаларын есептеу

Мақала электрстатикалық квадрупольді-цилиндрлік өрістің электронды-оптикалық сипаттамаларын есептеу мен талдауға арналған. Зерттеу нысаны квадрупольді-цилиндрлік өріс негізінде энергия талдағышты құрастыру болып табылады. Электрстатикалық квадрупольді-цилиндрлік өрістердің құрылымы базалық цилиндрлік өріс пен осьтік симметриялық цилиндрлік квадрупольдердің суперпозициясы негізінде алынған. Квадрупольді-цилиндрлік өрістің электронды-оптикалық сипаттамаларын есептеу зарядталған бөлшектердің қозғалыс траекторияларын есептеудің аналитикалық әдісі негізінде жүргізілген. Квадрупольді-цилиндрлік өрісте зарядталған бөлшектер қозғалысының дифференциалдық теңдеулерін интегралдау және траектория теңдеуінің аналитикалық сипаттау есебі шешілген. Зарядталған бөлшектің көзден оның кескініне дейінгі қозғалыс траектория проекциясының есептелуі жүргізілген. Екінші ретті бұрыштық тоғыстау шарттарын анықтайтын негізгі аберрациялық коэффициенттер есептелген. Энергия талдау үшін квадрупольді-цилиндрлік айнаның ең тиімді сұлбасы анықталды.

Кілт сөздер: электрондық спектроскопия, квадрупольді-цилиндрлік өріс, квадруполь, энергия талдағышы, электронды-оптикалық сипаттамалар, электронды-оптикалық сұлба.

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Расчет электронно-оптических характеристик квадрупольно-цилиндрического поля

Статья посвящена расчету и анализу электронно-оптических характеристик электростатического квадрупольно-цилиндрического поля. Объектом исследования является разработка энергоанализатора на основе квадрупольно-цилиндрического поля. Структура электростатических квадрупольно-цилиндрических полей получена на основе суперпозиции базового цилиндрического поля и осесимметричных цилиндрических квадруполей. Расчет электронно-оптических характеристик квадрупольно-цилиндрического поля выполнен на основе аналитического метода расчета траекторий движения заряженных частиц. Решена задача интегрирования дифференциальных уравнений движения заряженных частиц и аналитического описания траекторного уравнения в квадрупольно-цилиндрическом поле. Выполнен расчет проекции траектории движения заряженной частицы от источника до его изображения. Рассчитаны основные аберрационные коэффициенты, определяющие условия угловой фокусировки второго порядка. Найдена наиболее оптимальная для энергоанализа схема квадрупольно-цилиндрического зеркала.

Ключевые слова: электронная спектроскопия, квадрупольно-цилиндрическое поле, квадруполь, энергоанализатор, электронно-оптические характеристики, электронно-оптическая схема.

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