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### **ANALYTICAL QUADRATURE FORMULAE FOR ELECTRIC FIELDS OF THE RF STRAIGHT-AXIS ION FUNNELS OF A GENERAL TYPE**

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**Abstract.** The article presents analytical quadrature expressions for electric field potentials that correspond to radio-frequency straight-axis ion funnels of a general type, specifically, the funnels with a curved channel profile, with multipole diaphragms, and with unequally spaced electrodes. When determining electric fields, the distribution of electric potential over the axis of the device was taken as a basis. The resulting formulae would be appropriate for use in quick, high-quality simulating of radio-frequency devices designed for isolation, conveying and focusing ions, as well as in solving some problems of mathematical physics.

**Keywords:** analytical solutions of the Laplace equation, analytical electric fields, electron-optical systems with periodic electrodes, ion guides, radiofrequency ion funnels

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### **АНАЛИТИЧЕСКИЕ КВАДРАТУРНЫЕ ФОРМУЛЫ ДЛЯ ЭЛЕКТРИЧЕСКИХ ПОЛЕЙ РАДИОЧАСТОТНЫХ ИОННЫХ ВОРОНОК ОБЩЕГО ВИДА С ПРЯМОЙ ОСЬЮ**

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**Аннотация.** В статье представлены аналитические формулы для потенциалов электрических полей, которые соответствуют радиочастотным воронкам с прямолинейным каналом транспортировки общего вида, в частности воронкам с криволинейным профилем канала, с мультипольными диафрагмами, с неравномерно расположенными

электродами. При определении электрических полей, за основу было взято распределение электрического потенциала на оси устройства. Полученные выражения целесообразно использовать для быстрого качественного моделирования радиочастотных устройств, предназначенных для изолирования, транспортировки и фокусировки ионов, а также при решении соответствующих задач математической физики.

**Ключевые слова:** аналитическое решение уравнения Лапласа, аналитическое электрическое поле, электронно-оптическая система

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## Introduction

This study is a direct continuation of the research started in [1–4], examining the analytical expressions for electric field potentials in cylindrical and conical radio frequency transport channels [5, 6]. Cylindrical RF traps with stacked ring ion guides (SRIG), first proposed in [7, 8] and studied in detail in [5, 9–11, 12], are a prototype of such devices. Conical RF funnels, which are the next generation of devices of this type, are considered in detail in [12–19]. However, the potential of RF ion funnels is not limited to these simplest cases.

In this paper, we obtained the analytical formulas for electric potentials; these expressions are convenient for fast qualitative simulation of ion funnels with a complex structure. Indeed, RF focusing funnels with profiles other than conical (see, for example, [17]), as well as quadrupole or segmented multipole electrodes (see [20]) offer benefits for design of ion-optical devices. Non-circular apertures can also be useful; in this case, the corresponding electrical potentials are an additive superposition of axisymmetric analytic potentials and multipole corrections, representing analytic solutions for segmented multipole electrodes. These solutions are obtained by expanding the boundary condition of a single aperture with the required shape in a Fourier series (with respect to the azimuthal angle) and satisfying this expansion at specific collocation points. Additionally, optimization of parameters of RF ion funnels with complex structure may require uneven spacing of apertures along the transport channel, with the corresponding analytic solutions.

Exact or approximate analytical models make it possible to analyze the properties of ion-optical devices, as well as to set and solve inverse problems of synthesis of ion-optical systems. In the latter case, the electric field providing the necessary functional characteristics is reconstructed from the behavior set for the charged particles. Subsequently, the electrode configuration required to construct the device is determined in accordance with this electric field. Yuri Golikov's studies (see, for example, books [21–23]) clearly demonstrate the advantages of this approach.

The quasi-static principle is used to construct electric potentials of high-frequency (HF) electric fields. The quasi-static model of a time-varying electric field assumes that the high-frequency potential of this field can be expressed as a function of time, setting the law of voltage variation on the electrodes multiplied by the potential of the electrostatic field corresponding to constant voltages on the electrodes.

The assumption about the quasi-static nature of a high-frequency electric field is valid when the characteristic time of voltage change at the electrodes significantly exceeds the propagation time of electromagnetic perturbation within the device. A time-dependent factor describes the time variation of electrical voltages, and a coordinate-dependent potential corresponds to



constant voltages at the electrodes, changing synchronously and proportionally to each other over time. Although this approach essentially neglects the electrodynamic effects of Maxwell's equations, it is still acceptable if the frequency of voltages applied to the electrodes is not too high (in the above sense).

Next, analytical expressions for electrostatic potentials are considered, corresponding to electrode configurations typical of RF ion funnels. Simulation of straight-axis RF ion funnels with the corresponding profile of the transport channel involves multiplying these electrostatic potentials by rapidly oscillating time functions that determine the law (in most cases sinusoidal) for variation of high-frequency voltages on the electrodes. RF voltages with a complex spectrum, in particular, pulse voltages with an arbitrary pulse shape, can be used within the framework of the quasi-static model of the electric field instead of sinusoidal RF voltages [24]. In addition, depending on the operating mode of the funnel, two- and four-phase RF voltages can be applied to the electrodes [12], as well as amplitude-, frequency-, and phase-modulated RF voltages [12], providing the *A*-wave mode during ion transport [25–37].

The goal of this study is to derive analytical quadrature formulas to quickly reconstruct the electric field over the entire required space from a given distribution of the electric potential on the axis of the device.

After reconstructing the electric field, we can essentially reconstruct the configuration of the electrodes responsible for generating the corresponding electric field.

The obtained analytic solutions of the three-dimensional Laplace equation are of not only practical, but also independent scientific interest, since they can be used to solve problems in mathematical physics that are not directly related to charged particle optics.

### Theoretical background

This section provides a brief overview of the mathematical framework used in subsequent mathematical calculations. We considered it appropriate to include a summary of these methods in the introduction to this article, since this material is largely unknown among specialists in charged particle optics, because the primary sources for reference are either rare editions and/or had very limited print runs, making them difficult to obtain [21–23].

**Planar fields.** Planar (two-dimensional) electrostatic fields are characterized by an electric potential  $U(x,y)$ , depending only on two Cartesian coordinates and satisfying the two-dimensional Laplace equation

$$\frac{\partial^2 U(x,y)}{\partial x^2} + \frac{\partial^2 U(x,y)}{\partial y^2} = 0. \quad (1)$$

It is well known that the real and imaginary parts of any analytic function of a complex variable, for example, taking the form

$$f(z) = f(x + iy) = u(x, y) + iv(x, y) \quad (2)$$

satisfy the two-dimensional Laplace equation because the Cauchy–Riemann conditions are satisfied for these functions [38]:

$$\frac{\partial u(x, y)}{\partial x} = \frac{\partial v(x, y)}{\partial y}, \quad \frac{\partial u(x, y)}{\partial y} = -\frac{\partial v(x, y)}{\partial x}. \quad (3)$$

If there are first-order partial derivatives for the real and imaginary parts of a complex-valued function of two real variables and the Cauchy-Riemann conditions (3) are satisfied, then such a function is an analytic function of a complex variable. This means that it is expanded into a convergent power series and is therefore infinitely differentiable in the neighborhood of any point where conditions (3) are satisfied.

While the converse statement is also true, it is less commonly recognized.

**Statement 1.** Any real function of two variables satisfying the two-dimensional Laplace equation can be regarded as the real (imaginary) part of some analytic function of a complex variable.

**Proof.** Let there be a function  $u(x,y)$  satisfying Eq. (1). Relations (3) can be considered as a system of first-order partial differential equations (PDEs) [38] given for an unknown function  $v(x,y)$  with a known function  $u(x,y)$ . The system of equations is solvable, the solution exists, and it is unique up to an additive constant, if the condition of equality of mixed derivatives is true for an unknown function  $v(x,y)$ :

$$\frac{\partial}{\partial y} \left( \frac{\partial v(x,y)}{\partial x} \right) \equiv \frac{\partial}{\partial x} \left( \frac{\partial v(x,y)}{\partial y} \right). \quad (4)$$

Since the function  $u(x,y)$  is harmonic, this condition is satisfied for system of equations (3) under consideration.

The solution of system of equations (3) is the following function:

$$\begin{aligned} v(x,y) &= - \int_{x_0}^x dt \left( \int_{y_0}^y \frac{\partial^2 u(t,s)}{\partial y^2} ds \right) - \int_{x_0}^x \frac{\partial u(t,y_0)}{\partial y} dt + \int_{y_0}^y \frac{\partial u(x_0,s)}{\partial x} ds + C = \\ &= + \int_{y_0}^y ds \left( \int_{x_0}^x \frac{\partial^2 u(t,s)}{\partial x^2} dt \right) + \int_{y_0}^y \frac{\partial u(x_0,s)}{\partial x} ds - \int_{x_0}^x \frac{\partial u(t,y_0)}{\partial y} dt + C, \end{aligned} \quad (5a)$$

which can also be transformed to

$$\begin{aligned} v(x,y) &= - \int_{x_0}^x \frac{\partial u(t,y)}{\partial y} dt + \int_{y_0}^y \frac{\partial u(x_0,s)}{\partial x} ds + C = \\ &= + \int_{y_0}^y \frac{\partial u(x,s)}{\partial x} ds - \int_{x_0}^x \frac{\partial u(t,y_0)}{\partial y} dt + C. \end{aligned} \quad (5b)$$

A function of forms (5a) and (5b) is uniquely defined up to the real additive constant  $C$ , setting the value of the function  $v(x_0,y_0)$ . Therefore, for any function  $u(x,y)$  satisfying Eq. (1), it is possible to reconstruct the missing imaginary part  $v(x,y)$ , which could ensure that the Cauchy–Riemann conditions (3) are satisfied. Thus, the analytic function of a complex variable (2) is determined, which is unique up to an additive imaginary constant.

The existing function  $v(x,y)$ , satisfying the two-dimensional Laplace equation, can always be supplemented in the same way with the missing real part  $u(x,y)$ , yielding the required analytic function of the complex variable.

Statement 1 is proved.

**Corollary to Statement 1.** If **only** harmonic functions of two variables derived from analytic functions of a complex variable are studied in the process of synthesizing two-dimensional electron and ion-optical systems, then no solution is omitted.

Let there be an arbitrary analytic function of a complex variable. It can be symmetrized by ensuring that the real part is even and the imaginary part is odd with respect to the second argument.

**Statement 2.** Any analytic function of a complex variable  $f(z) = f(x+iy)$  can be associated with a unique symmetrized (with respect to the variable  $y$ ) analytic function of a complex variable. This resulting function has a real part even with respect to the variable  $y$ , the imaginary part is odd with respect to the same variable, and the values of the real part on the axis  $y = 0$  coincide with those of the real part of the initial function.

**Proof.** Let us take an arbitrary analytic function of a complex variable  $f(z)$ , given by Eq. (2), where the real and imaginary parts satisfy the Cauchy–Riemann relations (3). Then, the real and imaginary parts of a complex-valued function (which, generally speaking, does not have to be an analytic function) of the form



$$\bar{f}(\bar{z}) = u(x, -y) - iv(x, -y)$$

satisfy the Cauchy–Riemann relations (3). Consequently, this function is also an analytic function of a complex variable. Therefore, the following function is an analytic function of a complex variable:

$$\begin{aligned} h(z) &= \frac{1}{2}[f(z) + \bar{f}(\bar{z})] = \\ &= \frac{1}{2}[u(x, y) + u(x, -y)] + \frac{i}{2}[v(x, y) - v(x, -y)], \end{aligned} \quad (6)$$

where the real and imaginary parts have the required parity with respect to  $y$ .

Similarly, an antisymmetric function of the form

$$\begin{aligned} g(z) &= \frac{1}{2}[f(z) - \bar{f}(\bar{z})] = \\ &= \frac{1}{2}[u(x, y) - u(x, -y)] + \frac{i}{2}[v(x, y) + v(x, -y)], \end{aligned} \quad (7)$$

whose real part is odd with respect to the variable  $y$  and identically equal to zero at  $y = 0$ , while the imaginary part is even with respect to the variable  $y$  and coincides with the imaginary part of the function  $f(z)$  on the axis  $y = 0$  is also an analytic function of a complex variable.

The value on the symmetry axis  $y = 0$  for the real part of the function  $f(z)$  and for the real part of the function  $h(z)$  given by Eq. (6) is the same. Similarly, the normal derivatives (derivatives with respect to the variable  $y$ ) of the imaginary parts of the functions  $f(z)$  and  $h(z)$  coincide on the symmetry axis  $y = 0$ .

The uniqueness of the symmetrized function of a complex variable follows from the uniqueness of the solution of the Cauchy problem (8) for a two-dimensional harmonic function, considered below, as well as from the uniqueness of the imaginary part of the analytic function of a complex variable (up to an additive constant, see Statement 1) for a given real part.

Statement 2 is proved.

Applying symmetrization (6) to an already symmetrized function does not change this function. The partial derivative of a symmetrized analytic function of a complex variable, taken with respect to the variable  $x$ , is also a symmetrized function of a complex variable. The partial derivative of a symmetrized function of a complex variable, taken with respect to the variable  $y$ , is a function of a complex variable, whose real part is odd and imaginary part is even with respect to the second argument, similarly to function (7). The components of the symmetrized (according to expression (6)) analytic function of a complex variable multiplied by an imaginary unit have the same parity properties. Similar statements are true for functions of a complex variable obtained by transformation (7). Successively applying transformations (6) and (7) yields an identical zero.

A Cauchy problem, namely, to determine the value of the function on the entire plane by its behavior on the symmetry axis, can be posed for a harmonic function  $U(x, y)$  that is even with respect to the variable  $y$  and satisfies the condition  $U(x, -y) = U(x, y)$ :

$$U(x, y) \Big|_{y=0} = G(x). \quad (8)$$

**Statement 3.** *A solution to the Cauchy problem (8) for a planar harmonic function even with respect to the variable  $y$  exists and is unique, at least in the neighborhood of the symmetry axis  $y = 0$ , if the function  $G(x)$  is infinitely differentiable and expands into a convergent power series at each point.*

**Proof.** If we take into account the requirements of parity with respect to  $y$ , then the two-dimensional harmonic function  $U(x, y)$  can be expanded into a series in even powers of the variable  $y$  in the neighborhood of the symmetry axis  $y = 0$ :

$$U(x, y) = U_0(x) - \frac{1}{2}y^2U_2(x) + \dots + (-1)^k \frac{y^{2k}}{(2k)!}U_{2k}(x) + \dots \quad (9)$$

The possibility of expansion into a power series follows from the analyticity of two-dimensional harmonic functions (see Bernstein's theorem on the analyticity of solutions of two-dimensional elliptic equations [39, 40]). Substituting expression (9) into Eq. (1) and combining the factors at identical powers of the variable  $y$ , we obtain the values of all coefficients of series (9) using the following recurrence relations:

$$U_0(x) = G(x), \quad U_{2k+2}(x) = \frac{d^2U_{2k}(x)}{dx^2}. \quad (10)$$

Series (9) converges absolutely for the function  $U(x, y)$ , since the power series for the function  $G(x)$  converges, which can be used as a majorant for series (9).

Statement 3 is proved.

Series of form (9), functional with respect to one variable and power-law with respect to the other, are called Scherzer series<sup>1</sup>. They are used in ion optics to describe symmetric electric and magnetic fields in analysis of paraxial trajectories in the neighborhood of the symmetry plane or the symmetry axis.

The Cauchy problem on reconstructing a harmonic function, odd with respect to the variable  $y$ , from its normal derivative on the symmetry axis is formulated similarly:

$$\left. \frac{\partial U(x, y)}{\partial y} \right|_{y=0} = H(x). \quad (11)$$

Searching for a solution as an antisymmetric series

$$U(x, y) = yU_1(x) - \frac{1}{6}y^3U_3(x) + \dots + (-1)^k \frac{y^{2k+1}}{(2k+1)!}U_{2k+1}(x) + \dots \quad (12)$$

yields recurrence relations of the form

$$U_{2k+1}(x) = \frac{d^2U_{2k-1}(x)}{dx^2} \quad (13)$$

to express all terms of the series in terms of derivatives of the function  $H(x)$ . Thus, the unique solution can be found, valid at least in some neighborhood of the symmetry axis  $y = 0$  where this series converges.

Scherzer series (9) with coefficients (10) does not contain information about the behavior of the function  $U(x, y)$ , which is a solution to Cauchy problem (8) away from the symmetry axis. The integral formula using Green's function for the Dirichlet problem of the two-dimensional Laplace equation on the upper half-plane [42] is free from this drawback and takes the following form:

$$U(x, y) = \frac{y}{\pi} \int_{-\infty}^{+\infty} \frac{G(t)}{(x-t)^2 + y^2} dt. \quad (14)$$

It can be directly verified that if the integral in Eq. (14) converges, then the function  $U(x, y)$  satisfies the two-dimensional Laplace equation at  $y > 0$ , and satisfies condition (8) at  $y \rightarrow 0$ . If function (14) must satisfy the given Laplace equation, including on the boundary  $y = 0$ , then differentiability (analyticity) of the function  $G(t)$  is required.

<sup>1</sup> Apparently, this term was introduced in monograph [41].



Eq. (14) should be used for direct calculations only for  $y > 0$ . However, function (14) satisfies the condition  $\partial U(x,y)/\partial y = 0$  for  $y = 0+$  and therefore can be smoothly extended onto the half-plane  $y < 0$  in a symmetrical manner, thus generating an even function with respect to the variable  $y$ .

Similarly, Green's function for the Neumann problem (11), which is considered on the upper half-plane  $y > 0$  for the harmonic function  $U(x,y)$  odd with respect to  $y$  (see book [42]), leads to the following formula:

$$U(x, y) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} H(t) \ln \left[ (x-t)^2 + y^2 \right] dt. \tag{15}$$

This formula provides the unique solution for the antisymmetric Cauchy problem (11) if the function  $H(t)$  tends to zero at infinity sufficiently rapidly.

Unfortunately, Eq. (14) for the symmetric Cauchy problem (8) is applicable only when the modulus of the function  $G(t)$  grows at infinity slower than a linear function. An even more stringent condition for tending to zero at infinity is imposed on the function  $H(t)$ , used in integral (15). Furthermore, calculating integrals in expressions (14) and (15) requires either a high level of skill and experience in analytic calculation of integrals or access to reliable mathematical handbooks (of considerable volume) on function integration.

However, the function  $G(t)$  is generally a superposition of well-known elementary functions, and then the problem is solved more simply. Indeed, for any elementary function of a real variable, its counterpart on the complex plane is known (the result of analytic continuation from the real axis to the entire complex plane). All that is required in this case is to construct a similar superposition, including the known analytic functions of a complex variable, and separate its real or imaginary part from the obtained result. If necessary, it may be necessary to perform symmetrization or antisymmetrization of the resulting solution, in accordance with Eqs. (6) or (7).

**Axisymmetric fields.** The electric potential of axisymmetric electrostatic fields has the form

$$U(x, y, z) = V\left(z, \sqrt{x^2 + y^2}\right),$$

where the function  $V(z,r)$  satisfies the axisymmetric Laplace equation of the form

$$\frac{\partial^2 V(z, r)}{\partial z^2} + \frac{\partial^2 V(z, r)}{\partial r^2} + \frac{1}{r} \frac{\partial V(z, r)}{\partial r} = 0. \tag{16}$$

As in the case of planar fields, the Cauchy problem on reconstructing the function  $V(z,r)$  from its value on the symmetry axis can be posed for an axisymmetric potential:

$$V(z, r) \Big|_{r=0} = F(z) \tag{17}$$

**Statement 4.** *A solution to Cauchy problem (17) for an axisymmetric harmonic function in the neighborhood of the symmetry axis exists and is unique if the function  $F(z)$  is infinitely differentiable and expands into a convergent power series at each point.*

**Proof.** Searching for a solution as a Scherzer series

$$V(z, r) = V_0(z) - \frac{1}{2} r^2 V_2(z) + \dots + (-1)^k \frac{r^{2k}}{(2k)!} V_{2k}(z) + \dots \tag{18}$$

after substituting this series into Eq. (16) and taking into account the initial value (17) yields the following recurrence relations:

$$V_0(z) = F(z), \quad V_{2k+2}(z) = \frac{(2k+1)}{2(k+1)} V_{2k}''(z). \tag{19}$$

If we use recurrence relations (19), we can uniquely reconstruct the unknown coefficients of series (18). The absolute convergence of series (18) with these coefficients follows from the convergence of the power series for the function  $F(z)$ , which can serve as a majorant.

Statement 4 is proved.

As in the planar case, the axisymmetric Scherzer series (18) makes it possible to study the behavior of the axisymmetric electric potential only in a certain neighborhood of the symmetry axis  $r \approx 0$ . The axisymmetric electric potential on the entire plane  $(z, r)$  can be reconstructed by the following effective method. The tools discussed above should be used to analytically continue the real function  $F(x)$  onto the complex plane; this yields a two-dimensional harmonic function  $u(x, y)$  with the required behavior on the axis  $y = 0$ :

$$F(x) \rightarrow f(x + iy) = u(x, y) + iv(x, y), \quad u(x, 0) = F(x).$$

We can then apply the Whittaker–Watson formula<sup>2</sup>

$$V(z, r) = \frac{1}{\pi} \int_0^\pi u(z, r \cos \varphi) d\varphi, \quad (20)$$

calculating the axisymmetric potential  $V(z, r)$  when the integrand is a two-dimensional harmonic function  $u(x, y)$ .

In the case when the function  $u(x, y)$  is even with respect to  $y$ , i.e., satisfies the condition  $u(x, -y) = u(x, y)$ , Eq. (20) is reduced to the form

$$V(z, r) = \frac{2}{\pi} \int_0^{\pi/2} u(z, r \cos \varphi) d\varphi. \quad (21)$$

**Statement 5.** *Eq. (20) establishes a one-to-one correspondence between solutions  $V(z, r)$  of Cauchy problem (17) for axisymmetric harmonic functions and solutions  $u(x, y)$  of Cauchy problem (8) for planar harmonic functions, even with respect to the second argument, which are characterized by the same behavior on the symmetry axis.*

**Proof.** The function  $V(z, r)$  given by Eq. (20) satisfies the axisymmetric equation (16) when the function  $u(x, y)$  satisfies the planar Laplace equation (1). This can be verified by direct substitution after changing the integration variable  $\varphi$  to the variable  $y$ , in accordance with the formulas

$$y = r \cos \varphi, \quad dy = -\sqrt{r^2 - y^2} d\varphi, \quad x = z.$$

We obtain the following equality:

$$\begin{aligned} & \frac{\partial^2 V(z, r)}{\partial z^2} + \frac{\partial^2 V(z, r)}{\partial r^2} + \frac{1}{r} \frac{\partial V(z, r)}{\partial r} = \frac{1}{\pi} \int_0^\pi \left( \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \cos^2 \varphi + \frac{\cos \varphi}{r} \frac{\partial u}{\partial y} \right) d\varphi = \\ & = \frac{1}{\pi} \int_{-r}^r \left( \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \frac{y^2}{r^2} + \frac{y}{r^2} \frac{\partial u}{\partial y} \right) \frac{dy}{\sqrt{r^2 - y^2}} = \frac{1}{\pi r^2} \int_{-r}^r \left( -\frac{\partial^2 u}{\partial y^2} (r^2 - y^2) + y \frac{\partial u}{\partial y} \right) \frac{dy}{\sqrt{r^2 - y^2}} = \\ & = \frac{1}{\pi r^2} \left( -\frac{\partial u}{\partial y} \sqrt{r^2 - y^2} \right) \Big|_{y=-r}^{y=+r} = 0. \end{aligned}$$

Provided that  $r = 0$ , the following condition is satisfied:

<sup>2</sup> This formula is given in monograph [43]. Its author is unknown to us, but it was presumably derived by one of the monograph's authors as a particular case of a general formula for a three-dimensional harmonic function, derived and examined in Chapter 18. The name 'Whittaker formula', introduced by Golikov, is gradually gaining recognition.



$$V(z, 0) = \frac{1}{\pi} \int_0^\pi u(z, 0) d\varphi = u(z, 0) = F(z),$$

therefore, the behavior of the functions  $V(z, r)$  and  $u(z, r)$  must coincide on the symmetry axis  $r = 0$ .

As shown in Statement 3, reconstruction of a planar harmonic function  $u(z, r)$ , even with respect to the variable  $r$ , from its value  $u(z, 0)$  on the symmetry axis  $r = 0$  (as given by Eq. (8)) is a solvable problem. This solution not only exists but is also unique, at least in some neighborhood of the axis  $r = 0$ . Substituting the resulting solution  $u(z, r)$  into Eq. (20), we obtain an axisymmetric harmonic function  $V(z, r)$  with the required behavior on the symmetry axis (generally speaking, it is just one of many such functions). However, it follows from analysis of Scherzer series (18) that such an axisymmetric harmonic function is unique and, consequently, there are no other solutions to the problem except the one expressed by Eq. (20).

Statement 5 is proved.

If we represent the function  $u(z, r)$  as the sum of a planar harmonic function even with respect to  $r$

$$u_+(z, r) = [u(z, r) + u(z, -r)]/2$$

and planar harmonic function odd with respect to  $r$

$$u_-(z, r) = [u(z, r) - u(z, -r)]/2,$$

it is easy to see that integral (20) vanishes for an odd function, and replacing the harmonic function  $u(z, r)$  with the symmetrized harmonic function  $u_+(z, r)$  leaves the value of this integral unchanged. Therefore, only planar harmonic functions even with respect to  $r$  are important for practical application of Eq. (20). Notice that although there may be many planar harmonic prototypes  $u(z, r)$  for Eq. (20) for the existing function  $V(z, r)$ , the symmetrized planar harmonic prototype is unique.

An important conclusion to the subsection on axisymmetric fields is that in the analysis and synthesis of charged particle optics systems, integral formula (20) can generate all possible axisymmetric potentials that have no singularities on the symmetry axis, without omitting any.

**Multipole fields.** In the general case, the potentials of multipole electrostatic fields have the form

$$U(x, y, z) = \left(\sqrt{x^2 + y^2}\right)^m \cos(m \arg(x + iy) + \gamma) W\left(z, \sqrt{x^2 + y^2}\right), \quad (22)$$

where  $m$  is a positive integer determining the order of multipole<sup>3</sup>;  $\arg(x, y)$  here and below is a function returning the argument of the complex number  $x + iy$ , lying in the range from  $-\pi$  to  $+\pi$ .

When the function  $U(x, y, z)$  satisfies the three-dimensional Laplace equation, the function  $W(z, r)$  satisfies the multipole Laplace equation:

$$\frac{\partial^2 W(z, r)}{\partial z^2} + \frac{\partial^2 W(z, r)}{\partial r^2} + \frac{(2m+1)}{r} \frac{\partial W(z, r)}{\partial r} = 0. \quad (23)$$

Multipole symmetry is determined by multipole factors

$$\begin{aligned} R_m(x, y) &= \left(\sqrt{x^2 + y^2}\right)^m \cos(m \arg(x + iy) + \gamma) = \\ &= c_p P_m(x, y) + c_q Q_m(x, y), \\ P_m(x, y) &= \left(\sqrt{x^2 + y^2}\right)^m \cos(m \arg(x + iy)), \\ Q_m(x, y) &= \left(\sqrt{x^2 + y^2}\right)^m \sin(m \arg(x + iy)), \end{aligned} \quad (24)$$

for which the planar Laplace equation (1) holds true.

<sup>3</sup> Strictly speaking, it is not necessary for subsequent mathematical calculations that the index  $m$  be positive or an integer.

If the index  $m$  takes positive integer values, factors (24) are homogeneous harmonic polynomials of degree  $m$ , as follows from the recurrence relations

$$\begin{aligned} P_0(x, y) &= 1, \quad Q_0(x, y) = 0, \\ P_{m+1}(x, y) &= xP_m(x, y) - yQ_m(x, y), \\ Q_{m+1}(x, y) &= yP_m(x, y) + xQ_m(x, y), \end{aligned}$$

Consider the Cauchy problem on reconstructing the function  $W(z, r)$  from its value on the symmetry axis:

$$W(z, r)|_{r=0} = F(z). \tag{25}$$

**Statement 6.** *A solution to the Cauchy problem (25) for the factor of a multipole harmonic function (22) in the neighborhood of the symmetry axis exists and is unique if the function  $F(z)$  is infinitely differentiable and expands into a convergent power series at each point.*

*Proof.* Searching for a solution as a Scherzer series

$$W(z, r) = W_0(z) - \frac{1}{2}r^2W_2(z) + \dots + (-1)^k \frac{r^{2k}}{(2k)!}W_{2k}(z) + \dots \tag{26}$$

yields, after substituting series (26) into Eq. (23), taking into account the initial value (25), the following recurrence relations:

$$W_0(z) = F(z), \quad W_{2k+2}(z) = \frac{(2k+1)}{2(k+m+1)}W_{2k}''(z), \quad \dots \tag{27}$$

The unknown coefficients of series (26) can be uniquely reconstructed from recurrence relations (27). Its absolute convergence with coefficients (27) follows from convergence of the power series for  $F(z)$ , if this series is used as a majorant for series (26).

Statement 6 is proved.

Scherzer series (26) does not make it possible to study the behavior of the multipole electric potential (22) away from the symmetry axis  $r = 0$ . As in the case of the axisymmetric electric potential, to determine the values of the factor  $W(z, r)$  away from the symmetry axis, the real function  $F(x)$  is analytically continued onto the complex plane. We then define a two-dimensional harmonic function  $u(x, y)$  with the given behavior on the symmetry axis:

$$F(x) \rightarrow f(x + iy) = u(x, y) + iv(x, y), \quad u(x, 0) = F(x),$$

after that, it becomes possible to apply the Dougall formula (28).

The Dougall formula<sup>4</sup>, whose particular case at  $m = 0$  is the Whittaker–Watson equation (20), is used to construct multipole potentials with the arbitrary 2D harmonic functions  $u(x, y)$  as a basis:

$$W(z, r) = \frac{m!/\sqrt{\pi}}{\Gamma(m+1/2)} \int_0^\pi u(z, r \cos \varphi) \sin^{2m}(\varphi) d\varphi. \tag{28}$$

In the case when the harmonic function  $u(x, y)$  is even with respect to the variable  $y$  and satisfies the condition  $u(x, -y) = u(x, y)$ , Eq. (28) is reduced to the form

<sup>4</sup> The formula is given in the monograph [43] (see Chapter 18, example 2 at the end of the chapter) with reference to John Dougall as the author of this result. John Dougall (1867–1960) was an outstanding Scottish mathematician, a member of the Edinburgh Mathematical Society and the Royal Society of Edinburgh. We were unable to uncover the original publication deriving this formula.



$$W(z, r) = \frac{2m!/\sqrt{\pi}}{\Gamma(m+1/2)} \int_0^{\pi/2} u(z, r \cos \varphi) \sin^{2m}(\varphi) d\varphi. \quad (29)$$

The normalizing factor in front of the integral sign in Eqs. (28) or (29) is not necessary and does not affect the form of the required multipole potential. However, it is necessary for normalizing the value of the function along the multipole symmetry axis  $r = 0$  to ensure its coincidence with the function  $u(z, 0)$ .

**Statement 7.** *Eq. (28) provides a one-to-one correspondence between solutions of Cauchy problem (25) for factors of multipole harmonic functions (22) and solutions of Cauchy problem (8) for planar harmonic functions even with respect to the second argument with the same behavior on the symmetry axis.*

**Proof.** The function  $W(z, r)$  given by Eq. (28) satisfies the multipole equation (23) when the function  $u(x, y)$  satisfies the planar Laplace equation (1). This is verified by direct substitution after changing the integration variable  $\varphi$  to the variable  $y$  in accordance with the formulas

$$y = r \cos \varphi, \quad dy = -\sqrt{r^2 - y^2} d\varphi, \quad x = z:$$

$$\begin{aligned} & \frac{\partial^2 W(z, r)}{\partial z^2} + \frac{\partial^2 W(z, r)}{\partial r^2} + \frac{(2m+1)}{r} \frac{\partial W(z, r)}{\partial r} = \\ & = \frac{m!/\sqrt{\pi}}{\Gamma(m+1/2)} \int_0^{\pi} \left( \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \cos^2 \varphi + \frac{(2m+1) \cos \varphi}{r} \frac{\partial u}{\partial y} \right) \sin^{2m} \varphi d\varphi = \\ & = \frac{m!/\sqrt{\pi}}{\Gamma(m+1/2)} \int_{-r}^r \left( \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \frac{y^2}{r^2} + \frac{(2m+1)y}{r^2} \frac{\partial u}{\partial y} \right) \left( \frac{r^2 - y^2}{r^2} \right)^m \frac{dy}{\sqrt{r^2 - y^2}} = \\ & = \frac{1}{r^{2m+2}} \frac{m!/\sqrt{\pi}}{\Gamma(m+1/2)} \int_{-r}^r \left( -\frac{\partial^2 u}{\partial y^2} (r^2 - y^2) + (2m+1)y \frac{\partial u}{\partial y} \right) \left( \sqrt{r^2 - y^2} \right)^{2m-1} dy = \\ & = \frac{1}{r^{2m+2}} \frac{m!/\sqrt{\pi}}{\Gamma(m+1/2)} \left( -\frac{\partial u}{\partial y} \left( \sqrt{r^2 - y^2} \right)^{2m+1} \right) \Bigg|_{y=-r}^{y=+r} = 0. \end{aligned}$$

Provided that  $r = 0$ , the following condition is satisfied:

$$W(z, 0) = \frac{m!/\sqrt{\pi}}{\Gamma(m+1/2)} \int_0^{\pi} u(z, 0) \sin^{2m} \varphi d\varphi = u(z, 0) = F(z),$$

therefore, the behavior of the functions  $W(z, r)$  and  $u(z, r)$  must coincide on the symmetry axis  $r = 0$ .

As shown in Statement 3, Cauchy problem (8) on reconstruction of a planar harmonic function  $u(z, r)$ , even with respect to  $r$ , from its value on the symmetry axis is always solvable, and its solution not only exists, but is unique. Substituting this prototype  $u(z, r)$  with the given behavior on the symmetry axis into Eq. (28), we obtain the sought multiplier  $W(z, r)$  of the multipole harmonic function (22) with the required behavior on the symmetry axis (generally speaking, this multiplier is one of the many possible). It follows from analysis of Scherzer series (26) carried out earlier for solutions of Eq. (23) that such a factor is unique and, consequently, there are no other solutions for Cauchy problem (25), except for the function given by Eq. (28).

Statement 7 is proved.

Representing the function  $u(z, r)$  as a sum consisting of a planar harmonic function even with respect to  $r$

$$u_+(z, r) = [u(z, r) + u(z, -r)]/2$$

and planar harmonic function odd with respect to  $r$

$$u_-(z, r) = [u(z, r) - u(z, -r)]/2,$$

it is easy to see that integral (28) vanishes for an odd function, and replacing the harmonic function  $u(z, r)$  with the symmetrized harmonic function  $u_+(z, r)$  leaves the value of this integral unchanged. In other words, only even planar harmonic functions are relevant for using Eq. (28). Moreover, while there are many suitable planar harmonic prototypes  $u(z, r)$ , there exists a unique symmetrized planar harmonic prototype for any given function  $W(z, r)$ .

Thus, in the analysis and synthesis of charged particle optics systems, integral formula (28) can be used to generate all possible multipole potentials that have no singularities on the symmetry axis, without omitting any.

### General-type RF funnels with evenly spaced electrodes

This section discusses analytical formulas for planar, axisymmetric, and multipole electrostatic fields providing potentials of the following form on the  $OZ$  axis of the device:

$$U_C(x, y, z) \Big|_{\substack{x=0, \\ y=0}} = U_C^0(z) = f(z) \cos(\lambda z), \quad (30)$$

$$U_S(x, y, z) \Big|_{\substack{x=0, \\ y=0}} = U_S^0(z) = f(z) \sin(\lambda z). \quad (31)$$

where  $\lambda$  is the parameter determining the geometric scale of the transport device.

In this case, the function  $f(z)$  varies slowly along the axis of the device, compared with the rapidly oscillating functions  $\cos(\lambda z)$  and  $\sin(\lambda z)$ .

Analysis of planar, axisymmetric, or multipole Scherzer series applied to Cauchy conditions (30), (31) suggests that the solution (which exists and is unique, at least in the neighborhood of the axis  $r = 0$ ) should be sought in the form

$$\begin{aligned} U_C(z, r) &= F(z, r) \cos(\lambda z) + G(z, r) \sin(\lambda z), \\ U_S(z, r) &= F(z, r) \sin(\lambda z) - G(z, r) \cos(\lambda z), \\ F(z, 0) &= f(z), \\ G(z, 0) &= 0. \end{aligned} \quad (32)$$

Importantly, the change of variables  $x \rightarrow z, y \rightarrow r$  is performed for consistency of notation for the planar Laplace equation (1).

A solution of form (32), in particular, can be used to consider modified Scherzer series for the functions  $U_C(z, r)$  and  $U_S(z, r)$ :

$$\begin{aligned} U_C(z, r) &= (\cos(\lambda z) F_0(z) + \sin(\lambda z) G_0(z)) - \\ &\quad - \frac{1}{2} r^2 (\cos(\lambda z) F_2(z) + \sin(\lambda z) G_2(z)) + \dots \\ &\quad + (-1)^k \frac{r^{2k}}{(2k)!} (\cos(\lambda z) F_k(z) + \sin(\lambda z) G_k(z)) + \dots, \end{aligned} \quad (33)$$

$$\begin{aligned} U_S(z, r) &= (\sin(\lambda z) F_0(z) - \cos(\lambda z) G_0(z)) - \\ &\quad - \frac{1}{2} r^2 (\sin(\lambda z) F_2(z) - \cos(\lambda z) G_2(z)) + \dots \\ &\quad + (-1)^k \frac{r^{2k}}{(2k)!} (\sin(\lambda z) F_k(z) - \cos(\lambda z) G_k(z)) + \dots, \end{aligned} \quad (34)$$

Substituting expressions (33) and (34) into the corresponding Laplace equations shows that the coefficients of Scherzer series (33) and (34) are the same and satisfy the same recurrence relations:

a) for the planar Laplace equation (1)

$$\begin{cases} F_0(z) = f(z), \quad G_0(z) = 0, \\ F_{k+1}(z) = \frac{1}{2(k+1)(2k+1)} (F_k''(z) + 2\lambda G_k'(z) - \lambda^2 F_k(z)), \\ G_{k+1}(z) = \frac{1}{2(k+1)(2k+1)} (G_k''(z) - 2\lambda F_k'(z) - \lambda^2 G_k(z)), \end{cases} \quad (35)$$

b) for the axisymmetric Laplace equation (16)

$$\begin{cases} F_0(z) = f(z), \quad G_0(z) = 0, \\ F_{k+1}(z) = \frac{1}{4(k+1)^2} (F_k''(z) + 2\lambda G_k'(z) - \lambda^2 F_k(z)), \\ G_{k+1}(z) = \frac{1}{4(k+1)^2} (G_k''(z) - 2\lambda F_k'(z) - \lambda^2 G_k(z)), \end{cases} \quad (36)$$

c) for the multipole Laplace equation (23)

$$\begin{cases} F_0(z) = f(z), \quad G_0(z) = 0, \\ F_{k+1}(z) = \frac{1}{4(k+1)(k+m+1)} (F_k''(z) + 2\lambda G_k'(z) - \lambda^2 F_k(z)), \\ G_{k+1}(z) = \frac{1}{4(k+1)(k+m+1)} (G_k''(z) - 2\lambda F_k'(z) - \lambda^2 G_k(z)), \end{cases} \quad (37)$$

Substituting expressions (32) directly into the corresponding Laplace equations and separately vanishing each of the grouped factors at sines and cosines leads to the Cauchy problem on the axis  $r = 0$  for a system of two linear elliptic PDEs given with respect to two unknown functions ( $F(z, r)$  and  $G(z, r)$ ):

a) for the planar Laplace equation (1)

$$\begin{cases} \frac{\partial^2 F}{\partial z^2} + \frac{\partial^2 F}{\partial r^2} - \lambda^2 F + 2\lambda \frac{\partial G}{\partial z} = 0, \\ \frac{\partial^2 G}{\partial z^2} + \frac{\partial^2 G}{\partial r^2} - \lambda^2 G - 2\lambda \frac{\partial F}{\partial z} = 0, \\ F(z, 0) = f(z), \quad \frac{\partial F(z, 0)}{\partial r} = 0, \\ G(z, 0) = 0, \quad \frac{\partial G(z, 0)}{\partial r} = 0, \end{cases} \quad (38)$$

b) for the axisymmetric Laplace equation (16)

$$\begin{cases} \frac{\partial^2 F}{\partial z^2} + \frac{\partial^2 F}{\partial r^2} + \frac{1}{r} \frac{\partial F}{\partial r} - \lambda^2 F + 2\lambda \frac{\partial G}{\partial z} = 0, \\ \frac{\partial^2 G}{\partial z^2} + \frac{\partial^2 G}{\partial r^2} + \frac{1}{r} \frac{\partial G}{\partial r} - \lambda^2 G - 2\lambda \frac{\partial F}{\partial z} = 0, \\ F(z, 0) = f(z), \frac{\partial F(z, 0)}{\partial r} = 0, \\ G(z, 0) = 0, \frac{\partial G(z, 0)}{\partial r} = 0, \end{cases} \quad (39)$$

c) for the multipole Laplace equation (23)

$$\begin{cases} \frac{\partial^2 F}{\partial z^2} + \frac{\partial^2 F}{\partial r^2} + \frac{(2m+1)}{r} \frac{\partial F}{\partial r} - \lambda^2 F + 2\lambda \frac{\partial G}{\partial z} = 0, \\ \frac{\partial^2 G}{\partial z^2} + \frac{\partial^2 G}{\partial r^2} + \frac{(2m+1)}{r} \frac{\partial G}{\partial r} - \lambda^2 G - 2\lambda \frac{\partial F}{\partial z} = 0, \\ F(z, 0) = f(z), \frac{\partial F(z, 0)}{\partial r} = 0, \\ G(z, 0) = 0, \frac{\partial G(z, 0)}{\partial r} = 0. \end{cases} \quad (40)$$

Let the real function  $f(z)$  be analytically continued onto the complex plane, resulting in a symmetrized function of a complex variable:

$$\begin{aligned} f(z) &\rightarrow f(x+iy) = u(x, y) + iv(x, y), \\ \frac{\partial u}{\partial x} &= \frac{\partial v}{\partial y}, \quad \frac{\partial u}{\partial y} = -\frac{\partial v}{\partial x}, \\ u(z, 0) &= f(z), \quad v(z, 0) = 0, \\ u(z, -r) &= u(z, r), \quad v(z, -r) = -v(z, r). \end{aligned} \quad (41)$$

For the planar Laplace equation, using direct substitution, we can verify that the solution

$$\begin{cases} F(z, r) = u(z, r) \operatorname{ch}(\lambda r), \\ G(z, r) = v(z, r) \operatorname{sh}(\lambda r) \end{cases} \quad (42)$$

satisfies system of equations (38), including the initial conditions.

If we apply the Whittaker–Watson formula (20), taking into account parity of the functions  $u(z, r)$  and  $v(z, r)$  with respect to  $r$ , we obtain that the solutions of Cauchy problem (39) for the axisymmetric Laplace equation (16), written in the form (32), follow the expressions

$$\begin{cases} F(z, r) = \frac{2}{\pi} \int_0^{\pi/2} u(z, r \cos \varphi) \operatorname{ch}(r \cos \varphi) d\varphi, \\ G(z, r) = \frac{2}{\pi} \int_0^{\pi/2} v(z, r \cos \varphi) \operatorname{sh}(r \cos \varphi) d\varphi. \end{cases} \quad (43)$$



Similarly, after applying the Dougall formula (28), taking into account parity of the functions  $u(z, r)$  and  $v(z, r)$  with respect to  $r$ , we obtain that solutions (32) for Cauchy problem (40) (derived for the multipole Laplace equation (23)) after substituting (32) can be expressed as

$$\begin{cases} F(z, r) = \frac{2m!/\sqrt{\pi}}{\Gamma(m+1/2)} \int_0^{\pi/2} u(z, r \cos \varphi) \operatorname{ch}(r \cos \varphi) \sin^{2m}(\varphi) d\varphi, \\ G(z, r) = \frac{2m!/\sqrt{\pi}}{\Gamma(m+1/2)} \int_0^{\pi/2} v(z, r \cos \varphi) \operatorname{sh}(r \cos \varphi) \sin^{2m}(\varphi) d\varphi. \end{cases} \quad (44)$$

**Positioning of main and auxiliary apertures for ion funnel with uniformly spaced electrodes.**

Let there be a planar, axisymmetric, or multipole electric potential  $U_c(z, r)$ , defined by the first formula in (32) for the appropriately calculated functions  $F(z, r)$  and  $G(z, r)$ , and this potential behaves as follows along the axis  $r = 0$ :

$$U_c(z, 0) = f(z) \cdot \cos(\lambda z).$$

Thin apertures (planar, axisymmetric, or multipole) should be located at points of local minima and maxima of the axial distribution, i.e., at points  $z_k = \pi k / \lambda$ .

The sizes of the apertures  $r_k$  for planar and axisymmetric systems are determined from the conditions

$$U_c(z_k, r_k) = \pm U_R$$

or, which is the same, from the conditions

$$F(z_k, r_k) = U_R$$

(segmented multipole apertures are discussed below).

Additional apertures with zero or almost zero potential can be positioned at points  $z_{k+1/2} = \pi(k + 1/2) / \lambda$ , where the oscillating function  $\cos(\lambda z)$  vanishes. The sizes  $r_{k+1/2}$  of the additional apertures can be conveniently determined from the conditions

$$G(z_{k+1/2}, r_{k+1/2}) = U_R,$$

providing a smooth profile of the transport channel and making it possible to combine the potentials  $U_c(z, r)$  and  $U_s(z, r)$  within a single electrode system.

Consider a planar, axisymmetric, or multipole electric potential  $U_s(z, r)$ , defined by the second formula in (32) and providing an axial distribution

$$U_s(z, 0) = f(z) \sin(\lambda z)$$

along the axis  $r = 0$ .

Now the thin apertures generating the given electric field should be positioned at the points

$$z_{k+1/2} = \pi(k + 1/2) / \lambda,$$

that is, at the points of local minima and maxima of the axial distribution.

The sizes of the apertures  $r_{k+1/2}$  for planar and axisymmetric systems are determined from the conditions

$$U_s(z_{k+1/2}, r_{k+1/2}) = \pm U_R, \text{ i.e., } G(z_{k+1/2}, r_{k+1/2}) = U_R.$$

Additional apertures with zero or almost zero potential can be positioned at points  $z_k = \pi k / \lambda$ , at which the oscillating function  $\sin(\lambda z)$  vanishes. The sizes  $r_k$  of the additional apertures are conveniently determined from the conditions  $F(z_k, r_k) = U_R$ , ensuring a smooth profile of the transport channel and making it possible to combine the potentials  $U_c(z, r)$  and  $U_s(z, r)$  within a single electrode system.

It should be noted that a combined set of apertures located at points  $(z_k, r_k)$  and  $(z_{k+1/2}, r_{k+1/2})$  can be used to construct both an electric field with an electric potential  $U_c(z, r)$  (or  $U_s(z, r)$ ) and an arbitrary linear combination of these potentials within a single electrode system. For this purpose, the voltages applied to the apertures should be changed.

To calculate the sizes of apertures for multipole systems, we should bear in mind that the three-dimensional multipole electric potential is related to the multipole factor  $W(z, r) = U_c(z, r)$

by Eq. (22). Additionally, instead of curved multipole apertures whose shape is defined by the cross-sections of equipotential surfaces at corresponding points on the axis, segmented multipole circular apertures can be used for analytical electric potentials  $U_C(z, r)$  or  $U_S(z, r)$ .

The conditions for determining the radius of the apertures take the form

$$r_k^m F(z_k, r_k) = \gamma U_R \quad \text{and} \quad r_{k+1/2}^m F(z_{k+1/2}, r_{k+1/2}) = \gamma U_R,$$

where  $\gamma$  is the normalized first harmonic in the expansion of the boundary condition for a segmented multipole circular aperture into a Fourier series.

The contribution of the higher harmonics into the expansion of the boundary condition into a Fourier series in the neighborhood of the symmetry axis away from the edges of the electrodes is insignificant and can be neglected.

### General-type RF funnels with non-uniformly spaced electrodes

This section discusses analytical formulas for planar, axisymmetric, and multipole electrostatic fields providing potentials of the following form on the  $OZ$  axis of the device:

$$U_C(x, y, z) \Big|_{\substack{x=0, \\ y=0}} = U_C^0(z) = f(z) \cos(h(z)), \quad (45)$$

$$U_S(x, y, z) \Big|_{\substack{x=0, \\ y=0}} = U_S^0(z) = f(z) \sin(h(z)), \quad (46)$$

where  $h(z)$  is a monotonic function determining the points where the electrodes are positioned, and the function  $f(z)$  varies slowly along the axis of the device, compared with the rapidly oscillating functions  $\cos[h(z)]$  and  $\sin[h(z)]$ .

The study of planar, axisymmetric, or multipole Scherzer series applied to Cauchy conditions (45), (46) suggests that the solution (which exists and is unique) should be sought in the form

$$\begin{aligned} U_C(z, r) &= F(z, r) \cos(h(z)) + G(z, r) \sin(h(z)), \\ U_S(z, r) &= F(z, r) \sin(h(z)) - G(z, r) \cos(h(z)), \\ F(z, 0) &= f(z), \\ G(z, 0) &= 0. \end{aligned} \quad (47)$$

Indeed, let us consider the modified Scherzer series adapted to Eqs. (47):

$$U_C(z, r) = \sum_{k=0, \infty} (-1)^k \frac{r^{2k}}{(2k)!} [\cos(h(z)) F_k(z) + \sin(h(z)) G_k(z)], \quad (48)$$

$$U_S(z, r) = \sum_{k=0, \infty} (-1)^k \frac{r^{2k}}{(2k)!} [\sin(h(z)) F_k(z) - \cos(h(z)) G_k(z)]. \quad (49)$$

Substituting expressions (48) and (49) into the corresponding Laplace equations shows that the coefficients of Scherzer series (48) and (49) are the same and satisfy the same recurrence relations. These recurrence relations have the following form for the multipole Laplace equation (23):

$$\begin{cases} F_0(z) = f(z), \quad G_0(z) = 0, \\ F_{k+1}(z) = \frac{1}{4(k+1)(k+m+1)} (F_k''(z) - h'(z)^2 F_k(z) + 2h'(z) G_k'(z) + h''(z) G_k(z)), \\ G_{k+1}(z) = \frac{1}{4(k+1)(k+m+1)} (G_k''(z) - h'(z)^2 G_k(z) - 2h'(z) F_k'(z) - h''(z) F_k(z)), \end{cases} \quad (50)$$

The required recurrence relations for the planar Laplace equation (1) are obtained from Eqs. (50) as a particular case  $m = -1/2$ . The required recurrence relations for the axisymmetric Laplace equation (17) are obtained from Eqs. (50) as a particular case  $m = 0$ .

Substituting expressions (47) directly into the corresponding Laplace equations and separately vanishing each of the grouped factors at sines and cosines leads to the Cauchy problem on the axis  $r = 0$  for a system of two linear elliptic PDEs given with respect to two unknown functions:  $F(z, r)$  and  $G(z, r)$ . For the multipole Laplace equation (23), this system of equations has the form:

$$\left\{ \begin{array}{l} \frac{\partial^2 F}{\partial z^2} + \frac{\partial^2 F}{\partial r^2} + \frac{(2m+1)}{r} \frac{\partial F}{\partial r} - h'(z)^2 F + 2h'(z) \frac{\partial G}{\partial z} + h''(z) G = 0, \\ \frac{\partial^2 G}{\partial z^2} + \frac{\partial^2 G}{\partial r^2} + \frac{(2m+1)}{r} \frac{\partial G}{\partial r} - h'(z)^2 G - 2h'(z) \frac{\partial F}{\partial z} - h''(z) F = 0, \\ F(z, 0) = f(z), \frac{\partial F(z, 0)}{\partial r} = 0, \\ G(z, 0) = 0, \frac{\partial G(z, 0)}{\partial r} = 0. \end{array} \right. \quad (51)$$

The system of equations for the planar Laplace equation (1) is obtained from Eqs. (51) as a particular case  $m = -1/2$ . The system of equations for the axisymmetric Laplace equation (17) is obtained from Eqs. (51) as a particular case  $m = 0$ .

Let the real functions  $f(z)$  and  $h(z)$  be analytically continued onto the complex plane, resulting in symmetrized functions of a complex variable:

$$\begin{aligned} f(z) &\rightarrow f(x+iy) = u(x, y) + iv(x, y), \\ \frac{\partial u}{\partial x} &= \frac{\partial v}{\partial y}, \quad \frac{\partial u}{\partial y} = -\frac{\partial v}{\partial x}, \end{aligned} \quad (52)$$

$$u(z, 0) = f(z), \quad v(z, 0) = 0, \quad u(z, -r) = u(z, r), \quad v(z, -r) = -v(z, r),$$

$$\begin{aligned} h(z) &\rightarrow h(x+iy) = p(x, y) + iq(x, y), \\ \frac{\partial p}{\partial x} &= \frac{\partial q}{\partial y}, \quad \frac{\partial p}{\partial y} = -\frac{\partial q}{\partial x}, \end{aligned} \quad (53)$$

$$p(z, 0) = h(z), \quad q(z, 0) = 0, \quad p(z, -r) = p(z, r), \quad q(z, -r) = -q(z, r).$$

Using direct substitution, we can verify that, taking into account relations (52) and (53) for pairs of functions of the form

$$\left\{ \begin{array}{l} U_C(x, y) = u(x, y) \cos(p(x, y)) \operatorname{ch}(q(x, y)) + v(x, y) \sin(p(x, y)) \operatorname{sh}(q(x, y)), \\ V_C(z, r) = v(x, y) \cos(p(x, y)) \operatorname{ch}(q(x, y)) - u(x, y) \sin(p(x, y)) \operatorname{sh}(q(x, y)), \end{array} \right. \quad (54)$$

$$\left\{ \begin{array}{l} U_S(x, y) = u(x, y) \sin(p(x, y)) \operatorname{ch}(q(x, y)) - v(x, y) \cos(p(x, y)) \operatorname{sh}(q(x, y)), \\ V_S(z, r) = v(x, y) \sin(p(x, y)) \operatorname{ch}(q(x, y)) + u(x, y) \cos(p(x, y)) \operatorname{sh}(q(x, y)), \end{array} \right. \quad (55)$$

the Cauchy–Riemann relations are satisfied.

This means that the functions

$$U_C(x, y) + iV_C(x, y) \quad \text{and} \quad U_S(x, y) + iV_S(x, y) \quad (55a)$$

are symmetrized analytic functions of a complex variable.

We should note that if the functions

$$u(x,y) + iv(x,y) \text{ and } p(x,y) + iq(x,y)$$

are symmetric, the symmetrized behavior of functions (54) and (55) can be verified directly.

Due to symmetrization of functions (55a), the functions  $U_c(z,r)$  and  $U_s(z,r)$  are symmetrized solutions of the two-dimensional Laplace equation (1), providing the required behavior of potentials (45), (46) on the symmetry axis  $r = 0$ .

We obtain the solution of Cauchy problem (51) for  $m = -1/2$ , which corresponds to the planar Laplace equation (1), from equalities (47), after substituting functions (54), (55) into them:

$$\begin{cases} F(z,r) = u(z,r) \cos[h(z) - p(z,r)] \operatorname{ch}[q(z,r)] - \\ \quad - v(z,r) \sin[h(z) - p(z,r)] \operatorname{sh}[q(z,r)], \\ G(z,r) = u(z,r) \sin[h(z) - p(z,r)] \operatorname{ch}[q(z,r)] + \\ \quad + v(z,r) \cos[h(z) - p(z,r)] \operatorname{sh}[q(z,r)]. \end{cases} \quad (56)$$

Using the Whittaker–Watson formula (20), we obtain a solution to Cauchy problem (51) at  $m = 0$ , which corresponds to the axisymmetric Laplace equation (17):

$$\begin{cases} F(z,r) = \frac{2}{\pi} \int_0^{\pi/2} [u(z, r \cos \varphi) \cos[h(z) - p(z, r \cos \varphi)] \operatorname{ch}[q(z, r \cos \varphi)] - \\ \quad - v(z, r \cos \varphi) \sin[h(z) - p(z, r \cos \varphi)] \operatorname{sh}[q(z, r \cos \varphi)]] d\varphi, \\ G(z,r) = \frac{2}{\pi} \int_0^{\pi/2} [u(z, r \cos \varphi) \sin[h(z) - p(z, r \cos \varphi)] \operatorname{ch}[q(z, r \cos \varphi)] + \\ \quad + v(z, r \cos \varphi) \cos[h(z) - p(z, r \cos \varphi)] \operatorname{sh}[q(z, r \cos \varphi)]] d\varphi. \end{cases} \quad (57)$$

After applying the Dougall formula (28), we obtain exactly the same solution to Cauchy problem (51) with an arbitrary index  $m > 0$ , which corresponds to the multipole Laplace equation (23):

$$\begin{cases} F(z,r) = \frac{2m!/\sqrt{\pi}}{\Gamma(m+1/2)} \int_0^{\pi/2} [u(z, r \cos \varphi) \cos[h(z) - p(z, r \cos \varphi)] \operatorname{ch}[q(z, r \cos \varphi)] - \\ \quad - v(z, r \cos \varphi) \sin[h(z) - p(z, r \cos \varphi)] \operatorname{sh}[q(z, r \cos \varphi)]] \sin^{2m}(\varphi) d\varphi, \\ G(z,r) = \frac{2m!/\sqrt{\pi}}{\Gamma(m+1/2)} \int_0^{\pi/2} [u(z, r \cos \varphi) \sin[h(z) - p(z, r \cos \varphi)] \operatorname{ch}[q(z, r \cos \varphi)] + \\ \quad + v(z, r \cos \varphi) \cos[h(z) - p(z, r \cos \varphi)] \operatorname{sh}[q(z, r \cos \varphi)]] \sin^{2m}(\varphi) d\varphi. \end{cases} \quad (58)$$

**Positioning of main and auxiliary apertures for ion funnel with non-uniformly spaced electrodes.**

By analogy with the case of uniformly spaced electrodes for a planar, axisymmetric, or multipole electric potential  $U_c(z,r)$ , defined using the first formula in (47), its distribution along the axis  $r = 0$  is determined by the formula



$$U_C(z,0) = f(z) \cdot \cos[h(z)],$$

where the function  $h(z)$  is monotonic and has a sufficiently large range of values.

Thin apertures should be positioned at points of local minima and maxima of the axial distribution, i.e., at points  $z_k$ , representing solutions of algebraic equations  $h(z_k) = \pi k/\lambda$ . In view of the assumptions made about the properties of the function  $h(z)$ , such solutions exist and are unique for any values of the subscript  $k$  that we are interested in.

The sizes of planar and axisymmetric apertures  $r_k$  are determined from the conditions

$$U_C(z_k, r_k) = \pm U_R, \text{ i.e., } F(z_k, r_k) = U_R;$$

additional apertures with zero (or almost zero) potential can be positioned at points  $z_{k+1/2}$ , which are solutions to algebraic equations.

$$h(z_{k+1/2}) = \pi(k + 1/2)/\lambda;$$

the oscillating function  $\cos[h(z)]$  vanishes at them.

The following distribution is provided along the axis  $r = 0$  for a planar, axisymmetric, or multipole electric potential  $U_S(z,r)$ , defined by the second formula in (47):

$$U_S(z,0) = f(z) \cdot \sin[h(z)].$$

The thin apertures generating the given electric field should be positioned at the points  $z_{k+1/2}$ , for which the following conditions are satisfied:

$$h(z_{k+1/2}) = \pi(k + 1/2)/\lambda,$$

that is, at the points of local minima and maxima of the axial distribution.

The sizes of the apertures of planar and axisymmetric systems  $r_{k+1/2}$  are determined from the conditions

$$U_S(z_{k+1/2}, r_{k+1/2}) = \pm U_R, \text{ i.e., } G(z_{k+1/2}, r_{k+1/2}) = U_R.$$

Additional apertures with zero (or almost zero) potential can be positioned at points  $z_k$ , determined by the equations  $h(z_k) = \pi k/\lambda$ , where the function  $\sin[h(z)]$  vanishes. The sizes  $r_k$  of the additional apertures are determined from the conditions  $F(z_k, r_k) = U_R$ , providing a smooth profile of the transport channel and making it possible to combine the potentials  $U_C(z,r)$  and  $U_S(z,r)$  within a single electrode system.

Using a combined set of apertures located at points  $(z_k, r_k)$  and  $(z_{k+1/2}, r_{k+1/2})$  makes it possible to construct both an electric field with an electric potential  $U_C(z,r)$  or  $U_S(z,r)$ , and an arbitrary linear combination of these potentials within the framework of a single electrode system. For this purpose, the voltages applied to the apertures should be changed.

The sizes of the apertures for multipole systems are calculated in exactly the same way as in the case of uniformly spaced electrodes.

### Conclusion

In this paper, we obtained analytical quadrature expressions for electrical potentials, which can be recommended for analyzing the ion motion in RF traps and straight-axis RF funnels, formed by planar, circular or multipole apertures with a rectilinear transport channel characterized by a complex radial profile. The profile of the transport channel is uniquely determined by the axial distribution of the electric potential used as the initial data for the Cauchy problem to calculate the electric potentials in the entire space under consideration. Weighted sums of analytical expressions corresponding to circular and segmented multipole apertures make it possible to synthesize electric potentials for RF funnels with non-circular apertures.

Using the analytical expressions obtained, it is possible to quickly investigate and optimize the behavior of ions in the corresponding RF ion funnels with the help of a pseudopotential model of ion motion in high-frequency electric fields [44–46, 6, 12].

The obtained analytical expressions for three-dimensional harmonic functions with oscillating behavior on the axis can also be useful in solving a number of problems in mathematical physics.

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The calculations were performed using the Wolfram Mathematica version 11 (Home Edition) program [47].

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