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Determination of analytical expansion from numerical field data

Tomáš Radlička *, Bohumila Lencová

Institute of Scientific Instruments AS CR, Královopolská 147, 612 64 Brno, Czech Republic

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ABSTRACT

We introduce a method of calculation of the analytical expansion of the field near the axis that is based on an application of Green's theorem. The approach is demonstrated on an example of a round electrostatic unipotential lens with field computed by the finite-element method and results are compared to methods of Hermite polynomials and wavelet transformation which are used in electron optics. The work is motivated by application to calculations of aberration coefficients where the high order axial field derivatives must be known.

1. Introduction

Accurate calculations of the field and ray-tracing allow construction of better electron optical systems; moreover, the possibility of eliminating all primary aberrations [1] leads to the situation where the knowledge of the aberrations of the fifth order is necessary.

Several ways of calculating of the higher order aberrations exist. The results of ray-tracing in numerically computed field can be used for calculation of pairs of the object ray properties and the image ray properties, which are fitted on an assumed transition map [2]. The advantage of the method is simplicity of use. Only the values of the field at nodal points, which is interpolated at an arbitrary position, are required.

On the other hand, the methods based on the expression of aberration coefficients in the form of aberration integrals can be used. The results allow description of the influence of each optical element or the general properties of the aberration coefficient to establish, for example, Scherzer's theorem for spherical aberration of a round lens [3,4]. Nevertheless, the derivation of aberration integrals for general system is complicated even in the case of the third aberration order. The aberration integrals of the fifth order were calculated for a rotationally symmetric system with deflection field [5,6]. The form of aberration integrals of the higher orders is so complicated that the analysis gets impossible.

The method of differential algebra (DA) provides a connection between the two approaches. The results of calculations are only numerical values of the aberration coefficients. It can be easily applied to the calculation of higher order aberrations. However, the accuracy of the calculation is limited by the accuracy of the field.

The aberration integrals and the DA method use the field in the form of the analytical expansion into powers of the distance from the optical axis. For example, in the case of the rotationally symmetric electrostatic potential [7] this is

$$\Phi(z,r)=\sum_{n=0}^{\infty}\frac{1}{(n!)^2}\left(-\frac{r^2}{4}\right)^n\phi^{(2n)}(z), \tag{1}$$

where r is the distance from the axis and ϕ is the axial potential.

The finite-element method (FEM) is the most commonly used for numerical calculation of electrostatic and magnetic fields. The result is the electrostatic potential at the nodal points of the discretization mesh. Even if the potential is calculated very accurately, the determination of the analytical expansion is not a trivial task. Because the axial potential is known only at a discrete set of points (nodal points on the axis), calculation of its derivatives in (1) is not straightforward. Several methods are used to deal with the issue.

The first one implemented by Munro et al. was presented in [8,9]. It is based on the expansion of the axial function into a series of the Hermite functions [10]. The axial potential of a unipotential lens fulfils this condition; in the case of an acceleration or immersion lens a simple transformation must be done before the expansion [9]. When the form of the expansion is known, the derivatives of the axial function are computed by differentiation of each term of the series.

Another method proposed by Berz [11] was implemented in COSY INFINITY [12] and used, for example, by Liu [13]. It is based on the discrete wavelet transformation. The function values must

* Corresponding author. Tel.: +420 5 41514294; fax: +420 5 41514402.
E-mail address: radlicka@isibrno.cz (T. Radlička).

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be known at equidistant set of points z_k. The axial potential then takes the form

$$\phi(z)=\frac{1}{\sqrt{\pi}\sigma}\sum_{k=1}^{N}V_k\exp\left(-\frac{(z-z_k)^2}{(\Delta z\sigma)^2}\right), \tag{2}$$

where σ determines the width of Gaussian functions and Δz is a distance of two neighbours in the set of equidistant points. The structure of (2) shows the idea of the method. The value of the axial potential at any point on the axis is given mainly by the values at several surrounding points. The effect of the value of the potential at z_k on the value of the potential in z is determined by the distance of the point z_k from the point z. The procedure causes smoothing of the function which is controlled by the parameter σ. In other words, the level of smoothing grows with growing σ. Generally it can be said that the higher smoothing means better properties of derivatives but higher loss of details in the function dependence. The derivatives are calculated by differentiating the series (2).

These two approaches are simple but they can lead to inaccurate results. We will introduce methods utilizing the fact that the field satisfies the Laplace equation. We will compare the results of all methods mentioned on the example of a unipotential round electrostatic lens presented in paper [13].

2. The field in the vicinity of the optical axis

In a charge-free domain the electrostatic field is determined by the Laplace equation for the electrostatic potential and the magnetic field by the Laplace equation for the magnetic scalar potential [7,14].

Because the equations are equivalent, we will describe only the electrostatic case.

Using the method of separation of variables, we can find the multipole expansion of the electrostatic potential in the form

$$\Phi=\sum_{m=0}^{\infty}\Phi_m(r,z,\varphi)=\sum_{m=0}^{\infty}\Phi_{m,s}(r,z)\sin(m\varphi)+\Phi_{m,c}(r,z)\cos(m\varphi), \tag{3}$$

where Φ_0 is a rotationally symmetric field, Φ_1 a dipole field, Φ_2 a quadrupole field, etc. Let us note that r, z, and φ are standard cylindrical coordinates. For each $\Phi_{m,c}$ and $\Phi_{m,s}$ it can be shown that [15]

$$\Phi_{m,\alpha}=\sum_{n=0}^{\infty}\frac{(-1)^n c_{m,\alpha}^{(2n)}(z)}{n!(n+m)!2^{2n}}r^{2n+m}, \tag{4}$$

where the analytical functions $c_{m,\alpha}$—*the generalized gradients*—were introduced. Their meaning can be seen from (4):

$$c_{m,\alpha}(z)=\hat{D}_m\Phi_{m,\alpha}(r,z)=m!\left.\frac{\Phi_{m,\alpha}}{r^m}\right|_{r=0}, \tag{5}$$

where the differential operator $\hat{D}_m=\partial^m/\partial r^m|_{r=0}$ was defined. The value of $\Phi_{m,\alpha}/r^m$ can be computed directly using FEM [16].

The derivatives of generalized gradients must be known for the complete determination of the analytical expansion, that is, the derivatives of $c_{m,\alpha}$ must be computed from a set of discrete points. The methods based on Hermite functions or Gaussian wavelet interpolation were shortly summarized in the Introduction, now we describe the methods based on the fact that in the charge free domain the electrostatic and magnetic fields satisfy the Laplace equation.

3. The method of infinite cylinder

The first method for calculating the derivatives of generalized gradients that uses the fact that the field is a solution of Laplace equation was introduced by Venturini and Dragt [15]. Let us suppose that we know the field on an infinite cylinder with the axis that coincides with the axis z, that is, the potential is known on the surface $r=R$. Moreover, we consider that the Laplace equation is satisfied inside the cylinder or, in the region where it is not satisfied, the field vanishes. These requirements are satisfied in case of lenses where the field smoothly vanishes with the distance from the center of the lens. In such a case the nth derivative of the generalized gradients can be found in the form [15]

$$c_{m,\alpha}^{(n)}(z)=\frac{\mathrm{i}^n}{\sqrt{2\pi}2^m}\int_{-\infty}^{\infty}\mathrm{d}k e^{\mathrm{i}kz}k^{m+n}\frac{\tilde{\Phi}_{m,\alpha}(k)}{I_m(kR)}, \tag{6}$$

where $\tilde{\Phi}_{m,\alpha}(k)$ is the Fourier image of $\Phi_{m,\alpha}(R,z)$ and I_m is the modified Bessel function [10]. If the function $\Phi_{m,\alpha}(R,z)$ is known at equidistant set of points $\{z_i\}$, the speed of calculation can be increased by the FFT algorithm.

Accuracy of the method depends on the accuracy of potential computed by the FEM. The errors of the method consist of two parts. The first one is the *random error* of solution of algebraic equations in the FEM algorithm. This error can be very small (10^{-12} in order of magnitude) and it has random character. The second one, the *discretization error*, is due to the nature of a mesh method. This error is much larger (10^{-4} in order of magnitude) and it does not have random properties. It can be estimated by comparing the results using the original mesh and a mesh that is twice as denser in both directions [17].

The random error influences mainly the high frequencies in the Fourier image $\tilde{\Phi}_{m,\alpha}$, which is multiplied by $k^{m+n}/I_m(kR)$ in Eq. (6). It tends to zero for large k; however, small values of the cylinder radius R may slow down the rate of the convergence. To avoid the possible inaccuracy in high order derivatives we can simply estimate the error. Let us consider the perturbation of $\Phi_{m,\alpha}$ in the form $\Delta\Phi_{m,\alpha}(z)=\varepsilon(z)\Phi_{m,\alpha}(z)$, where $\varepsilon(z)$ represents uniformly distributed random numbers in the range $[-\varepsilon_0,\varepsilon_0]$. Using the linearity of the Fourier transform, the error of generalized gradients takes a form analogous to (6),

$$\Delta c_{m,\alpha}^{(n)}(z)=\frac{\mathrm{i}^n}{\sqrt{2\pi}2^m}\int_{-\infty}^{\infty}\mathrm{d}k e^{\mathrm{i}kz}k^{m+n}\frac{\Delta\tilde{\Phi}_{m,\alpha}(k)}{I_m(kR)}. \tag{7}$$

On the other hand, the influence of the discretization error is mainly in the low frequency range. It can also be compensated by the rapidly increasing denominator $I_m(kR)$, except for the case of zero derivative of the rotationally symmetric field, in which the denominator is $I_0(0)=1$ for $k=0$ and thus for any R. Hence the effect of zero frequency in Fourier decomposition is not eliminated with growing radius of the cylinder and the method is not suitable for interpolation of the zero derivative of the axial potential ϕ. However, this deficiency is already eliminated for the first derivative by multiplicative factor k. On the other hand, the potential values are often most accurate on the axis and errors grow in the direction to electrodes [17]. In practical calculation it is necessary to analyze, whether the increasing radius of the cylinder compensates the growing error of potential.

Until now, we computed the generalized gradients from potential values on one cylinder; however, we can combine the results from many cylinders. The final generalized gradient values can be computed as weighted averages, in which the weights are determined from errors of the method for individual radii of the cylinders (the lower the error, the higher the weight). This can improve the results and make the method more stable.