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High order aberrations calculation of a hexapole corrector using a differential algebra method

Yongfeng Kang[a], Xing Liu[a], Jingyi Zhao[b,*], Tiantong Tang[a]

[a] Key Laboratory for Physical Electronics and Devices of the Ministry of Education, Xi'an Jiaotong University, Xi'an 710049, People's Republic of China
[b] School of Science, Chang'an University, Xi'an 710064, People's Republic of China

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ABSTRACT

A differential algebraic (DA) method is proved as an unusual and effective tool in numerical analysis. It implements conveniently differentiation up to arbitrary high order, based on the nonstandard analysis. In this paper, the differential algebra (DA) method has been employed to compute the high order aberrations up to the fifth order of a practical hexapole corrector including round lenses and hexapole lenses. The program has been developed and tested as well. The electro-magnetic fields of arbitrary point are obtained by local analytic expressions, then field potentials are transformed into new forms which can be operated in the DA calculation. In this paper, the geometric and chromatic aberrations up to fifth order of a practical hexapole corrector system are calculated by the developed program.

1. Introduction

In 1990, Rose suggested [1] the imaging Cs corrector that provides two transfer doublets and two hexapoles alternately. Then, Haider et al. developed [2] the first practical Cs corrector for the TEM based on Rose's scheme and the successful results of this corrector were published in Ultramicroscopy [3], the Cs corrector for the TEM has attracted attention for application in high resolution microscopy. Recently, with the higher requirement of system resolution, the study in high-precision corrector is the focus of researchers [4–8]. Thus, computing high order aberration coefficients for such systems has become more important, especially for aberration correction systems in which the primary aberrations are eliminated, and the secondary aberrations become dominant.

In electron optics, aberration integral is a traditional and common method, where aberration coefficients are derived by solving aberration integrals with paraxial rays and axial potentials [9]. Using the aberration integral method, H. Liu et al. derived a set of formulae for computing geometrical aberration coefficients up to the third order, and the first order chromatic aberration coefficients for systems containing electrostatic and magnetic round, quadrupole, hexapole and octopole lenses and deflectors [10]. Due to the complexity of high order aberrations, it is very difficult to derive them with the aberration integral method. Yet another way of calculating the aberration coefficients numerically is the exact ray trace method. Via the method, the exact trajectory equations with very high accuracy are solved for a set of rays that leave the object planes at various distances from the axis with various gradients, including very small values in both cases. If the accuracy is good enough, the total aberration is simply the distance between the point of arrival of a paraxial electron and point of one far from the axis and with a non-negligible gradient. If enough rays are calculated, the aberration coefficients can be extracted from the resulting distances [11]. Recently, the aberrations of a new monochromator with multiple offset cylindrical up to the third rank are calculated by this method [12].

Differential algebraic (DA) method is a powerful and promising technique in computer numerical analysis. When applied to nonlinear dynamics systems, the arbitrary high-order transfer properties of the systems can be computed directly with high precision [13]. DA method presents a straightforward way to compute nonlinearity to arbitrary orders. Compared with the exact ray trace method, only by tracing a reference ray, the arbitrary order aberrations of an electron optics system can be obtained without analytic formulas derivatives; on the other hand, the method is always accurate, limited only by machine precision and algorithm error independent of the order of the aberrations, which is in sharp contrast to traditional numerical analysis methods. Radlička gives a helpful explanation of the procedure for obtaining aberration coefficients numerically [14]. Recently, H. Liu et al. compute aberrations up to the fifth order of multipole systems using the differential algebra (DA) method [15]. In this method, in order to achieve the axial field functions of optical elements differentiable to n-th order for applying the DA method, the axial field functions

* Corresponding author.
E-mail addresses: yfkang@mail.xjtu.edu.cn (Y. Kang), jingyi.zhao@foxmail.com (J. Zhao).

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are fitted by Hermite series in the form of Taylor series; Thus, the potential and field components at any off axis point can be computed with high accuracy [15,16]. In contrast to the method of the axial field functions fitted by Hermite series, in our previous work [17], a local analytical expression are constructed with high accuracy interpolation of the field calculated numerically for a given position of the reference electron ray independent of the axial field functions. The great advantage of this technique is that the DA method is extended to handle all electron optics systems with straight Axis or with curved Axis. Thus, Calculations of high order aberrations for a round electron lens and the combined focusing-deflection systems up to the fifth order have been solved effectively as well as time of flight (TOF) aberrations of a round lens [17–19].

A typical hexopole corrector for an objective lens consists of round lenses and hexapole lenses. Thus in this work, the hexapole fields are calculated by the finite element method (FEM) and the reduced hexapole potentials at mesh points are obtained [20,21]. Moreover, the DA theory, operation method and algorithm are investigated in detail, and a local analytical expression of the numerically computed hexapole field which can be adopted as DA extension numbers will be introduced into the up to the fifth order aberrations calculations. Only by tracing a reference ray, up to the fifth order aberrations of a hexapole corrector can be achieved. Finally, a practical hexapole corrector is analyzed and discussed as an example using the developed DA software in this paper.

2. The DA method for high order aberrations calculations of a hexapole corrector

The properties of a charged particle system can be described by a transfer map as follow:

$$r_f = \Re(r_0, \delta) \tag{1}$$

where r_f denotes the final positions and slopes of a charged particle, and r_0 denotes the initial positions and slopes of the charged particle. δ contains other systemic parameters of interest. Then $\partial R/\partial r_0$ denotes the geometric aberrations with respect to initial conditions, while $\partial R/\partial\delta$ is corresponding to the chromatic aberrations. Except for the most trivial cases, it is impossible to find a closed analytic solution for the map R. The calculation of aberrations will be based on the expansion of R along a reference trajectory by successive approximation. Then the complexity of the aberrations calculations increases dramatically with the order of the expansion coefficients. Therefore, this procedure is limited to lower orders. However, DA method presents a straightforward way to compute nonlinearity to arbitrary orders. Here no analytic formulas for derivatives must be derived; only by tracing a reference ray, the arbitrary order aberrations of an electron optics system can be obtained; on the other hand, the method is always accurate, limited only by machine precision and algorithm error independent of the order of the aberrations, which is in sharp contrast to traditional numerical analysis methods.

In the DA method, the analysis is carried out on a non- standard extension of the real space R, called ${}_nD_v$ [22]. For a given smooth function $f(x_1, x_2, \ldots, x_v,)$, its 0~n order derivatives are expressed by a ${}_nD_v$ structure in differential algebra. All the derivatives are arranged in a special sequence to form a differential algebraic vector sequence denoted by a differential algebraic super-number $a=(a_1, a_2, \ldots, a_N,)$. The collection of all such quantities is denoted by ${}_nD_v$. For a hexapole corrector, there is a replacement of the relative variables by differential algebraic variables when solving the electron trajectories; that is, the coordinate x, y, slope x′ , y′ and energy spread ΔΦ are set to be differential algebraic arguments. Using the available numerical arithmetic such as the fourth order Runge–Kutta method, a reference trajectory can be numerically traced in a hexapole corrector by numerical solving the trajectory Eq. (2) in the laboratory Cartesian coordinates (x, y, z).

$$\begin{cases} x'' = \frac{1}{2u}(1 + x'^2 + y'^2)\left(\frac{\partial u}{\partial x} - x'\frac{\partial u}{\partial z}\right) + \sqrt{\frac{-e}{2m_0\mu}}\sqrt{1 + x'^2 + y'^2} \\ \quad [x'(B_y x' - B_x y') - y'B_z + B_y] \\ y'' = \frac{1}{2u}(1 + x'^2 + y'^2)\left(\frac{\partial u}{\partial y} - y'\frac{\partial u}{\partial z}\right) + \sqrt{\frac{-e}{2m_0\mu}}\sqrt{1 + x'^2 + y'^2} \\ \quad [y'(B_y x' - B_x y') + x'B_z + B_x] \end{cases} \tag{2}$$

Obviously, in the trajectory Eq. (2) the coordinate x, y, slope x′, y′ are set to be differential algebraic arguments; In order to trace electron trajectories expressed in super-numbers, the electric and/or magnetic fields have to be transferred to differential algebraic arguments.

A typical hexopole corrector for an objective lens consists of three main parts: the objective lens whose spherical aberration we wish to reduce; a transfer lens to produce an image outside the objective lens; and the hexapole lens. DA calculations of high order aberrations for a round electron lens have been solved effectively in a previous work [17]. Thus, in this work, we focus on researching how to transform the numerically computed hexapole field into local analytical expressions which can be adopted as DA extension numbers. No matter how many lenses and hexapole lens are set in the system, for DA method, the complexity of the algorithm does not increase. The same approach can be used to transform every round lens and hexapole field into DA extension numbers. Then the DA extension numbers for arbitrary position on the electron trajectory in the entire system can be obtained. Only by tracing a referred ray, the Gaussian optical properties and high-order aberrations can be achieved.

Thus, a new version of DA software is developed aiming at engineering design of a hexapole corrector, and the key problem is to construct a local analytical expression for the electric and/or magnetic potentials values for a given position P(x, y, z) where an electron is passing by. These local analytical can be constructed by a suitable interpolation or a function fitting.

$$\begin{aligned} u_6 &= a_{60}x^3 - 3a_{60}xy^2 + a_{61}(x^5 - 2x^3y^2 - 3xy^4) \; or \; u_6 \\ &= (a_{60}r^3 + a_{61}r^5)\cos 3\theta \\ \frac{\partial u_6}{\partial x} &= 3a_{60}x^2 - 3a_{60}y^2 + 5a_{61}x^4 - 6a_{61}x^2y^2 - 3a_{61}y^4 \\ \frac{\partial u_6}{\partial y} &= -6a_{60}xy - 4a_{61}x^3y - 12a_{61}xy^3 \\ \frac{\partial u_6}{\partial z} &= b_{60}x^3 - 3b_{60}xy^2 + b_{61}(x^5 - 2x^3y^2 - 3xy^4) \; or \; \frac{\partial u_6}{\partial z} \\ &= (b_{60}r^3 + b_{61}r^5)\cos 3\theta \end{aligned} \tag{3}$$

The coefficients a_{ij} and b_{ij} of the Eq. (3) are obtained at the plane where the azimuth angle θ is zero by a suitable interpolation or a function fitting. Due to the finite element mesh is irregular and inconvenient to interpolation, we transfer the mesh to a regular one at first. Then, an efficient algorithm for interpolation is used to construct the local expression of the field variables, which is a 16-point interpolation shown as in Fig. 1. It is proved that the accuracy of the algorithm of interpolation meets completely the requirement of the calculation and the engineering design in the practical electron lenses [17].

The local expression of electric and/or magnetic potentials in round lenses has been present in the previous paper [17]. In this work, the local expression of electric and/or magnetic potentials including round lenses and hexapole lenses are achieved and transformed into DA super-number at arbitrary point with high accuracy. The complexity of the algorithm is independent of the number of round lenses and hexapole lenses in the corrector system.

Then, a reference ray is traced from the object plane to observation plane by numerical solving the trajectory Eq. (2) employing the fourth order Runge–Kutta method, with all the variables transformed to DA super-number. Then, the transfer properties at the final coordinates