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High order aberration calculations of a quadrupole–octupole corrector using a differential algebra method

Kang Yongfeng*, Wei Momo, Zhao Jingyi

Key Laboratory for Physical Electronics and Devices of the Ministry of Education, Department of Electronic Science and Technology, Xi'an Jiaotong University, Xi'an 710049, People's Republic of China

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ABSTRACT

A Differential algebraic method is of an effective technique in computer 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 electron lenses with quadrupole and octupole corrector whose electric/magnetic fields are in the forms of discrete arrays, for example, the files computed by FEM or FDM method. The quadrupole and octupole electromagnetic fields of arbitrary point are obtained by local analytic expressions, and then field potentials are transformed into new forms which can be operated in the DA calculation. The program has been developed and tested as well. The geometric and chromatic aberrations coefficients up to fifth order of electron lenses with quadrupole and octupole corrector are calculated by the developed program.

1. Introduction

The resolution limiting spherical and chromatic aberrations of static rotationally symmetric electron lenses are unavoidable in the absence of space charge and flight reversal [1]. To improve the resolution of electron microscopes, quadrupole–octupole correctors are necessary to compensate for both the chromatic and the spherical aberrations, while a hexapole corrector suffices to eliminate the spherical aberration which is the dominant resolution-limiting aberration at accelerating voltages larger than about 100 kV [2]. By employing the quadrupole–octupole correctors, the aberration correction of round electron lenses is proven successful [3, 4]. With the successful correction of the primary aberration, the high order aberration calculation of round lenses with quadrupole–octupole correctors become dominant. Due to the complexity of such systems, it is very difficult to calculate the high aberration coefficients with the Aberration Integrals methods.

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 octupole lenses and deflectors [5]. As well the fifth and even higher order geometrical aberrations and the chromatic aberrations of third order were analyzed and a full list of formulae for the fifth order aberration coefficients of round lenses in reasonably usable form at last became available [6–8]. Lencová extended exact ray tracing to cover the new requirements of aberration-corrected instruments [9].

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 [10]. DA method presents a straightforward way to compute nonlinearity to arbitrary orders, only by tracing a reference ray. Furthermore, the DA method is always accurate, limited only by machine precision and algorithm error independent of the order of the aberrations. In the previous work of our group, DA methods have been introduced into the electron optics [11–12]. Further a local analytical expression has been constructed with high accuracy interpolation of the field, which is calculated numerically for a given position of the reference electron ray. An advantage of such a way of the built-in interpolation method is that it is relatively easy to use, in comparison with the expansion of the axial function into a series of the Hermite functions [13, 14]; this method that is independent of the axial field functions, can directly use the potential values of nodal points which are surrounding the given point. Thus, up to the fifth order aberrations for a round electron lens, the combined focusing-deflection systems and hexapole correctors have been solved effectively [15–17].

In this work, the quadrupole and octupole fields are calculated by the finite element method (FEM) and the reduced quadrupole and

* Corresponding author.
E-mail address: yfkang@mail.xjtu.edu.cn (Y. Kang).

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octupole potentials at mesh points are obtained [18, 19]. Moreover, the DA theory, operation method and algorithm are investigated in detail and a local analytical expression of the numerically computed quadrupole–octupole 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 quadrupole–octupole corrector are achieved. Finally, a practical quadrupole–octupole corrector is analyzed and discussed as an example using the developed DA software in this paper.

2. DA methods for high order aberrations calculations of a quadrupole–octupole 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 interesting parameters such as energy spread. Thus $\partial\Re/\partial r_0$ denotes the geometric aberrations with respect to initial conditions, while $\partial\Re/\partial\delta$ is corresponding to the chromatic aberrations. 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. In addition, 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.

For a quadrupole–octupole 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. By employing the available numerical arithmetic such as the fourth order Runge–Kutta method, a reference trajectory can be numerically traced in a quadrupole–octupole corrector by numerical solving the trajectory Eq. (2) in the laboratory Cartesian coordinates (x, y, z).

$$\begin{cases} x'' = \frac{1}{2u}(1 + x'^2 + y'^2)\left(\frac{\partial u}{\partial x} - x'\frac{\partial u}{\partial z}\right) \\ \quad + \sqrt{\frac{-e}{2m_0u}}\sqrt{1 + x'^2 + y'^2}\,[x'(B_yx' - B_xy') - y'B_z + B_y] \\ y'' = \frac{1}{2u}(1 + x'^2 + y'^2)\left(\frac{\partial u}{\partial y} - y'\frac{\partial u}{\partial z}\right) \\ \quad + \sqrt{\frac{-e}{2m_0u}}\sqrt{1 + x'^2 + y'^2}\,[y'(B_yx' - B_xy') + x'B_z + B_x] \end{cases} \tag{2}$$

Obviously in the trajectory Eq. (2), the coordinate (x, y), slope (x', y') and energy spread ΔΦ 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 quadrupole–octupole corrector for an objective lens will consist of two main parts: the electron lenses whose spherical aberration and chromatic aberration expected to be corrected; and the quadrupole–octupole lenses. DA calculations of high order aberrations for a round electron lens have been solved effectively in a previous work [13]. Thus in this work, we focus on researching how to transform the numerically computed quadrupole–octupole field into local analytical expressions which can be adopted as DA extension numbers. No matter how many lenses and quadrupole–octupole 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 quadrupole–octupole field into DA extension numbers. And then the DA extension numbers at arbitrary position in the entire system can be obtained. Only by tracing a referred ray, the optical properties including high-order aberrations will be achieved.

Thus a new version of the DA software is to be developed aimed to engineering design of a quadrupole–octupole corrector and the key problem is to construct a local analytical expression for the electric and/or magnetic potentials at a given position $P(x, y, z)$ of reference trajectory. In order to calculate up to the 5th order aberrations, these local analytical expressions are as follows which are constructed by a suitable interpolation.

$$\begin{aligned}
u_4 &= [a_{40}(x^2 - y^2) + a_{41}(x^2 + y^2)(x^2 - y^2) \\
&\quad + a_{42}(x^2 - y^2)(x^2 + y^2)^2]\cos 2\beta_2 \\
&\quad + 2[a_{40}xy + a_{41}(x^2 + y^2)xy + a_{42}(x^2 + y^2)^2xy]\sin 2\beta_2 \\
&\quad \times \frac{\partial u_4}{\partial x} = [2a_{40}x + 4a_{41}x^3 + 2a_{42}(3x^5 + 2x^3y^2 - xy^4)]\cos 2\beta_2 \\
&\quad + 2[a_{40}y + a_{41}(3x^2y + y^3) + a_{42}(5x^4y + 6x^2y^3 + y^5)]\sin 2\beta_2 \\
&\quad \times \frac{\partial u_4}{\partial y} = [-2a_{40}y - 4a_{41}y^3 + 2a_{42}(-2x^2y^3 + x^4y - 3y^5)]\cos 2\beta_2 \\
&\quad + 2[a_{40}x + a_{41}(x^3 + 3xy^2) + a_{42}(x^5 + 6x^3y^2 + 5xy^4)]\sin 2\beta_2 \\
&\quad \times \frac{\partial u_4}{\partial z} = [b_{40}(x^2 - y^2) + b_{41}(x^2 + y^2)(x^2 - y^2) \\
&\qquad + b_{42}(x^2 - y^2)(x^2 + y^2)^2]\cos 2\beta_2 \\
&\quad + 2[b_{40}xy + b_{41}(x^2 + y^2)xy + b_{42}(x^2 + y^2)^2xy]\sin 2\beta_2 \\
u_8 &= [a_{80}(x^4 + y^4 - 6x^2y^2) + a_{81}(x^4 + y^4 - 6x^2y^2)(x^2 + y^2)]\cos 4\beta_4 \\
&\quad + [4a_{80}xy(x^2 - y^2) + 4a_{81}xy(x^2 - y^2)(x^2 + y^2)]\sin 4\beta_4 \\
&\quad \times \frac{\partial u_8}{\partial x} = [4a_{80}(x^3 - 3xy^2) + 2a_{81}(3x^5 - 10x^3y^2 - 5xy^4)]\cos 4\beta_4 \\
&\quad + [4a_{80}(3x^2y - y^3) + 4a_{81}(5x^4y - y^5)]\sin 4\beta_4 \\
&\quad \times \frac{\partial u_8}{\partial y} = [4a_{80}(y^3 - 3x^2y) + 2a_{81}(-5x^4y - 10x^2y^3 + 3y^5)]\cos 4\beta_4 \\
&\quad + [4a_{80}(x^3 - 3xy^2) + 4a_{81}(x^5 - 5xy^4)]\sin 4\beta_4 \\
u_8 &= [b_{80}(x^4 + y^4 - 6x^2y^2) + b_{81}(x^4 + y^4 - 6x^2y^2)(x^2 + y^2)]\cos 4\beta_4 \\
&\quad + [4b_{80}xy(x^2 - y^2) + 4b_{81}xy(x^2 - y^2)(x^2 + y^2)]\sin 4\beta_4
\end{aligned} \tag{3}$$

The coefficients a_{ij} and b_{ij} of the Eq. (3) are obtained at the fixed reference plane (r, z) by a suitable interpolation using the reduced quadrupole and octupole potentials at the finite element mesh points. β_2 and β_4 are the rotation angles of the quadrupole and octupole lenses relative to the fixed reference plane respectively. For the convenience of interpolation, the rectangular finite element mesh are adopted in the vicinity of optical axis where the reference trajectory will be trace, but mesh size is not necessarily equivalence. Then, an efficient algorithm for the interpolation is used to construct the local expression of the field variables, which is a 16-point interpolation shown as in Fig. 1. Compared with our previous methods in which the potentials at irregular mesh points are firstly interpolated into the potentials at rectangular mesh points with the equivalent mesh size and then construct the local expression by 16 points interpolation, the present methods constructing

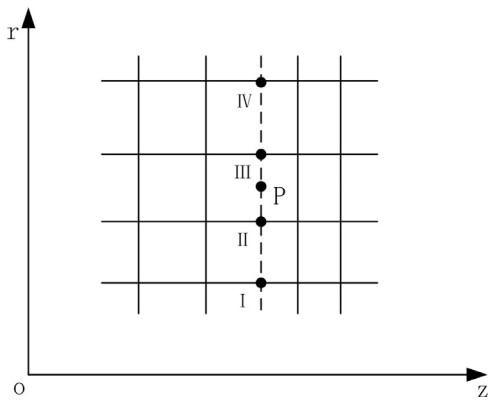

Fig. 1. The interpolation using the potentials at 16 points.