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Third-rank chromatic aberrations of electron lenses

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ABSTRACT

In this paper the third-rank chromatic aberration coefficients of round electron lenses are analytically derived and numerically calculated by *Mathematica*. Furthermore, the numerical results are cross-checked by the differential algebraic (DA) method, which verifies that all the formulas for the third-rank chromatic aberration coefficients are completely correct. It is hoped that this work would be helpful for further chromatic aberration correction in electron microscopy.

1. Introduction

The first successful geometric and chromatic aberration correction system for a low-voltage scanning electron microscope (LVSEM) was realized by Zach and Haider [1]. Since then, the aberration correction for electron microscopy (EM) has made great progress [2–5]. In 2011 Leary and Brydson published an article entitled by "Chromatic aberration correction: the next step in electron microscopy" [6] to elucidate the importance of chromatic aberration correction in the future although C_c correction faces competition from other techniques, such as improved electron sources, beam monochromators, energy filters, and so on. Recently, owing to the application of combined chromatic and spherical aberration correction in high-resolution transmission electron microscopy (HRTEM), a huge step has been made forward in the aberration correction in EM. Now we can achieve the spatial resolution down to 50 pm at 200 kV [7] and a resolution better than 140 pm at 20 kV [8].

In theory, it was as early as 2002 that Rose [9] and Plies [10] did investigate up to the third-rank chromatic aberration in detail. Afterwards, Liu [11] analytically derived the third-order (fourth-rank) chromatic aberration coefficients of round electron lenses in terms of *Mathematica* [12]. However, the expressions of third-rank chromatic aberration coefficients of round electron lenses were not published in the literature until the present work. They were also analytically derived and numerically calculated by *Mathematica* and cross-checked by the differential algebraic method [13]. It is hoped that this work would be helpful for further chromatic aberration correction in EM.

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2. Second-degree perturbation of variational function

2.1. In fixed coordinates

In the analytical derivation of third-rank chromatic aberration coefficients of round electron lenses we start from the second-order variational function of the rotationally symmetric electromagnetic field in a fixed coordinate system [14],

$$F_2 = -\frac{V''}{8\sqrt{V}}(\boldsymbol{R}\cdot\boldsymbol{R}) + \frac{1}{2}\sqrt{V}\left(\boldsymbol{R}'\cdot\boldsymbol{R}'\right) - \frac{1}{2}\eta B\left(\boldsymbol{R}^{*}\cdot\boldsymbol{R}'\right), \tag{1}$$

where $\boldsymbol{R} = (X, Y)$, $\boldsymbol{R}' = (X', Y')$, and $\boldsymbol{R}^{*} = (-Y, X)$ are two-dimensional vectors in the fixed coordinate system. $V = V(X, Y, z)$ is the axial electric potential distribution, $B = B_0 b(z)$ the axial magnetic field distribution [14], and $\eta = \sqrt{e/2m}$, respectively. Its up to the second-degree perturbation of the variational function caused by the fluctuation of both electric (or electron initial energy) and magnetic field is written as

$$\Delta F_2 = F_V\left(\frac{\Delta V_o}{V_o}\right) + F_B\left(\frac{\Delta B_0}{B_0}\right) + F_{V2}\left(\frac{\Delta V_o}{V_o}\right)^2 + F_{B2}\left(\frac{\Delta B_0}{B_0}\right)^2 + F_{VB}\left(\frac{\Delta V_o}{V_o}\right)\left(\frac{\Delta B_0}{B_0}\right), \tag{2}$$

In Eq. (2) we have

$$F_V = V_o\left[\frac{V'' + \eta^2 B^2}{16V^{3/2}}(\boldsymbol{R}\cdot\boldsymbol{R}) + \frac{1}{4\sqrt{V}}\left(\boldsymbol{R}'\cdot\boldsymbol{R}'\right) + \frac{\eta B}{4V}\left(\boldsymbol{R}^{*}\cdot\boldsymbol{R}'\right)\right],$$

$$F_B = -\frac{\eta^2 B^2}{4\sqrt{V}}(\boldsymbol{R}\cdot\boldsymbol{R}) - \frac{1}{2}\eta B\left(\boldsymbol{R}^{*}\cdot\boldsymbol{R}'\right),$$

$$F_{V2} = -V_o^2\left[\frac{V''+\eta^2B^2}{64V^{5/2}}(\boldsymbol{R}\cdot\boldsymbol{R}) - \frac{\eta B}{16V^2}\left(\boldsymbol{R}^*\cdot\boldsymbol{R}'\right)\right],$$
$$F_{B2} = 0,$$
$$F_{VB} = 0. \tag{3}$$

Note that the subscript in V_o is letter "o" meaning the object side and the subscript in B_0 is zero. Below we will use the corresponding rotational coordinate system (x, y, z) to discuss the third-rank chromatic aberration.

2.2. In rotational coordinates

According to Eqs. (2) and (3) and the rotational transform in electron optics, up to the second-degree perturbation of the variational function in rotational coordinates is

$$\Delta f_2 = f_V\left(\frac{\Delta V_o}{V_o}\right) + f_B\left(\frac{\Delta B_0}{B_0}\right) + f_{V2}\left(\frac{\Delta V_o}{V_o}\right)^2,$$
$$f_V = A_V(\boldsymbol{r}\cdot\boldsymbol{r}) + B_V\left(\boldsymbol{r}'\cdot\boldsymbol{r}'\right) + C_V\left(\boldsymbol{r}^*\cdot\boldsymbol{r}'\right),$$
$$f_B = A_B(\boldsymbol{r}\cdot\boldsymbol{r}) + B_B\left(\boldsymbol{r}'\cdot\boldsymbol{r}'\right) + C_B\left(\boldsymbol{r}^*\cdot\boldsymbol{r}'\right),$$
$$f_{V2} = A_{V2}(\boldsymbol{r}\cdot\boldsymbol{r}) + B_{V2}\left(\boldsymbol{r}'\cdot\boldsymbol{r}'\right) + C_{V2}\left(\boldsymbol{r}^*\cdot\boldsymbol{r}'\right), \tag{4}$$

where all coefficients are

$$A_V = \frac{V_o\left(\eta^2B^2+V''\right)}{16V^{3/2}},$$
$$B_V = \frac{V_o}{4\sqrt{V}},$$
$$C_V = \frac{\eta BV_o}{4\sqrt{V}}, \tag{5}$$

$$A_B = -\frac{\eta^2B^2}{4\sqrt{V}},$$
$$B_B = 0,$$
$$C_B = -\frac{\eta B}{2}, \tag{6}$$

$$A_{V2} = -\frac{V_o^2(3V''+\eta^2B^2)}{64V^{5/2}},$$
$$B_{V2} = -\frac{V_o^2}{16V^{3/2}},$$
$$C_{V2} = -\frac{V_o^2\eta B}{16V^2}. \tag{7}$$

2.3. Gaussian values of f_V, f_B, and f_{V2}

Now we substitute the Gaussian trajectory,

$$\boldsymbol{r}_g = \boldsymbol{r}'_o r_\alpha + \boldsymbol{r}_o r_\beta,$$
$$\boldsymbol{r}'_g = \boldsymbol{r}'_o r'_\alpha + \boldsymbol{r}_o r'_\beta,$$
$$\boldsymbol{r}^*_g = \boldsymbol{r}'^*_o r_\alpha + \boldsymbol{r}^*_o r_\beta, \tag{8}$$

for $\boldsymbol{r}$, $\boldsymbol{r}'$, and $\boldsymbol{r}^*$ in Eq. (4) to obtain the Gaussian values of f_V, f_B, and f_{V2}. Their unified forms are

$$f_{Xg} = f_{X,100}(\boldsymbol{r}_o\cdot\boldsymbol{r}_o) + f_{X,010}\left(\boldsymbol{r}'_o\cdot\boldsymbol{r}'_o\right) + f_{X,001}\left(\boldsymbol{r}_o\cdot\boldsymbol{r}'_o\right) + f^*_{X,000}\left(\boldsymbol{r}^*_o\cdot\boldsymbol{r}'_o\right),$$
$$f_{X,100} = A_X r_\beta^2 + B_X r'^2_\beta,$$
$$f_{X,010} = A_X r_\alpha^2 + B_X r'^2_\alpha,$$
$$f_{X,001} = 2A_X r_\alpha r_\beta + 2B_X r'_\alpha r'_\beta,$$
$$f^*_{X,000} = C_X\left(\frac{V_o}{V}\right)^{1/2}, \tag{9}$$

where subscript X stands for V, B, or V2, respectively. These Gaussian values play an important role in aberration analysis and will be involved in the third-rank chromatic aberration coefficients.

Furthermore, for the later use in this context [15], we introduce ε_{Xg} and $\varepsilon_{X,ijk}$ that are defined as

$$\varepsilon_{Xg}(z) = \int_{z_o}^{z} f_{Xg}\mathrm{d}z$$
$$\varepsilon_{X,ijk}(z) = \int_{z_o}^{z} f_{X,ijk}\mathrm{d}z. \tag{10}$$

3. Third-rank chromatic aberration

It is well known that the electron trajectory including the third-rank chromatic aberration is expressed as

$$\boldsymbol{r}_c = \boldsymbol{r}_g + \Delta\boldsymbol{r}_{c1} + \Delta\boldsymbol{r}_{c2}, \tag{11}$$

where $\boldsymbol{r}_g$ is the Gaussian trajectory, $\Delta\boldsymbol{r}_{c1}$ the second-rank (first-order plus first-degree) chromatic aberration, and $\Delta\boldsymbol{r}_{c2}$ the third-rank (first-order plus second-degree) chromatic aberration, respectively. Therefore, the corresponding trajectory equation is written as

$$\boldsymbol{r}''_c + \frac{V'}{2V}\boldsymbol{r}'_c + \frac{V''+\eta^2B^2}{4V}\boldsymbol{r}_c = \frac{1}{V^{1/2}}\left[\left(-\frac{d}{dz}\frac{\partial}{\partial\boldsymbol{r}'} + \frac{\partial}{\partial\boldsymbol{r}}\right)\Delta f_2\right],$$
$$\boldsymbol{r}_c(z_o) = r_o \quad\text{and}\quad \boldsymbol{r}'_c(z_o) = r'_o. \tag{12}$$

Considering the Gaussian trajectory equation and the second-rank chromatic aberration equation, we immediately obtain the equation for the third-rank chromatic aberration as follows:

$$\Delta\boldsymbol{r}''_{c2} + \frac{V'}{2V}\Delta\boldsymbol{r}'_{c2} + \frac{V''+\eta^2B^2}{4V}\Delta\boldsymbol{r}_{c2}$$
$$= \frac{1}{V^{1/2}}\left(\frac{\Delta V_o}{V_o}\right)^2\left[\left(-\frac{d}{dz}\frac{\partial}{\partial\boldsymbol{r}'} + \frac{\partial}{\partial\boldsymbol{r}}\right)f_{V2}\right]_g$$
$$+\frac{1}{V^{1/2}}\left(\frac{\Delta V_o}{V_o}\right)\left[\left(-\frac{d}{dz}\frac{\partial}{\partial\boldsymbol{r}'} + \frac{\partial}{\partial\boldsymbol{r}}\right)f_V\right]_{c1}$$
$$+\frac{1}{V^{1/2}}\left(\frac{\Delta B_0}{B_0}\right)\left[\left(-\frac{d}{dz}\frac{\partial}{\partial\boldsymbol{r}'} + \frac{\partial}{\partial\boldsymbol{r}}\right)f_B\right]_{c1}$$
$$+\Delta\boldsymbol{r}_{c2}(z_o) = 0 \quad\text{and}\quad \Delta\boldsymbol{r}'_{c2}(z_o) = 0. \tag{13}$$

where subscripts "g" and "c1" stand for $(\boldsymbol{r} = \boldsymbol{r}_g, \boldsymbol{r}' = \boldsymbol{r}'_g, \boldsymbol{r}^* = \boldsymbol{r}^*_g, \boldsymbol{r}'^* = \boldsymbol{r}'^*_g)$ and $(\boldsymbol{r} = \Delta\boldsymbol{r}_{c1}, \boldsymbol{r}' = \Delta\boldsymbol{r}'_{c1}, \boldsymbol{r}^* = \Delta\boldsymbol{r}^*_{c1}, \boldsymbol{r}'^* = \Delta\boldsymbol{r}'^*_{c1})$, respectively.

In order to solve Eq. (13) concisely, we divide the third-rank chromatic aberration into two components, i. e. $\Delta\boldsymbol{r}_{c2} = \Delta\boldsymbol{r}_{c2i} + \Delta\boldsymbol{r}_{c2c}$, in which $\Delta\boldsymbol{r}_{c2i}$ and $\Delta\boldsymbol{r}_{c2c}$ are respectively called the intrinsic and combined chromatic aberration.

3.1. Intrinsic chromatic aberration

From Eq. (13) the third-rank intrinsic chromatic aberration satisfies the following equation:

$$\Delta\boldsymbol{r}''_{c2i} + \frac{V'}{2V}\Delta\boldsymbol{r}'_{c2i} + \frac{V''+\eta^2B^2}{4V}\Delta\boldsymbol{r}_{c2i}$$
$$= \frac{1}{V^{1/2}}\left(\frac{\Delta V_o}{V_o}\right)^2\left[\left(-\frac{d}{dz}\frac{\partial}{\partial\boldsymbol{r}'} + \frac{\partial}{\partial\boldsymbol{r}}\right)f_{V2}\right]_g,$$
$$\Delta\boldsymbol{r}_{c2i}(z_o) = 0 \quad\text{and}\quad \Delta\boldsymbol{r}'_{c2i}(z_o) = 0. \tag{14}$$

It is clear that the perturbation caused by the magnetic field has no contribution to the third-rank intrinsic chromatic aberration. By