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Third-order aberration of soft X-ray optical systems with orthogonal and coplanar arrangement of the main planes of elements

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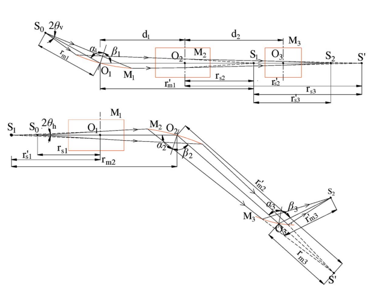
A third-order aberration analytical analysis method of soft X-ray optical systems with orthogonal and coplanar arrangement of the main planes of elements is proposed. Firstly, the transfer equations of the aperture ray and the principle ray are derived; then, based on the third-order aberration theory with the aperture-ray coordinates on the reference exit wavefront of a plane-symmetric optical system, the aberration expressions contributed by the wave aberration and defocus of this kind of optical system are studied in detail. Finally, the derived aberration calculation expressions are applied to calculate the aberration of two design examples of such types of optical systems; the images are compared with ray-tracing results obtained using the *Shadow* software to validate the aberration expressions. The study shows that the accuracy of the aberration expressions is satisfactory. The analytical analysis method of aberration is helpful in the design and optimization of the soft X-ray optical systems with orthogonal and coplanar arrangement of the main planes of optical elements.



1. Introduction

The imaging resolution of a soft X-ray optical system is a key factor determining the working performance of the large scientific apparatus applying the optical system, such as synchrotron radiation sources, soft X-ray microscopes, *etc.* (Veyrinas *et al.*, 2019; Fogelqvist *et al.*, 2017; Yang *et al.*, 2016). For soft X-ray optical systems, researchers need to adopt rays with a grazing-incidence impinged optical surface in order to gain a sufficiently high optical transmission. Consequently, the shape of the wavefront will significantly deviate from spherical, and the focusing geometry of a light beam in the meridional plane will differ from that in a sagittal one, thus determining the imaging performance of the plane-symmetric optical system (Lu, 2008). At synchrotron radiation facilities, in order to meet the design requirements of beam splitting and avoid space conflict with adjacent beamline facilities, an optical system with an orthogonal arrangement of the main planes of elements is usually used. However, beamline design often requires a number of optical elements to achieve high-resolution imaging, and the main plane of these optical elements may be orthogonal or coplanar.

To design a grazing-incidence optical system, like a soft X-ray optical system, the aberration analysis method is the key measure and is mainly as follows: light-path function (LPF) (Beutler, 1945; Noda *et al.*, 1974), analytic formulas of the ray-tracing spot diagram (SD) (Namioka *et al.*, 1994; Masui

& Namioka, 1999), Lie optics (Goto & Kurosaki, 1993; Palmer *et al.*, 1998*a*,*b*) and wavefront aberration (WFA) (Chrisp, 1983; Lu, 2008); the WFA method is a classical method for studying the ray aberration of a multi-element optical system. Recently, Lu (2008) adopted a toroidal surface as a reference wavefront to develop the fourth-order wave aberration theory with the aperture-ray coordinates on the optical surface of plane-symmetric optical systems based on the WFA method. The aberration theory was applicable to the aberration analysis of plane-symmetric optical systems of mirrors or gratings of different figures; but it is only suitable for analysing the aberrations of an optical system with a coplanar arrangement of the main planes of optical elements (Lu & Lin, 2010). In order to transfer the relationship of the aperture-ray coordinates to an orthogonal arrangement of optical elements, we used the aperture coordinates of the ray on the reference exit wavefront instead of those on the optical surface; then we derived the wave aberration expressions and studied the aberrations calculation method of soft X-ray and vacuum ultraviolet optical systems with orthogonal arrangement of double elements (Cao & Lu, 2017). However, for a soft X-ray optical system with orthogonal and coplanar arrangement of the main planes of elements, as yet there is still no aberration theory to analyse the aberration of such kinds of optical systems as a whole. Therefore, its imaging analysis and design relies mainly on the designer's experience and ray-tracing software.

According to the above discussions, based on the third-order aberration theory with the aperture-ray coordinates on the reference exit wavefront of the plane-symmetric optical system, here we propose an analytical analysis method of the third-order aberrations of a soft X-ray optical system with orthogonal and coplanar arrangements of the main planes of elements. In Section 2 we introduce the definition and the third-order aberration theory of plane-symmetric optical systems with the aperture-ray coordinates on the reference exit wavefront. In Section 3 we derive the transfer equations of the aperture ray and the principal ray, while Section 4 shows the aberration calculation method and the corresponding expressions in detail. Finally, we calculate the aberrations of two design examples, and the calculation results are compared with ones obtained using the ray-tracing software *Shadow* (Sanchez del Rio *et al.*, 2011) to validate the aberration expressions derived in this paper.

2. Third-order aberration theory of a plane-symmetric optical system

2.1. Definitions of a plane-symmetric optical system

Figs. 1 and 2 show a plane-symmetric optical system with an off-plane object point S_0 and its coordinate system on the meridional plane, respectively (Lu, 2008). The optical surface is symmetrical with respect to the plane $\chi O z'$, where O is the vertex of the optical surface. O_0OO_1, lying in the symmetry plane, is defined as the base ray; and its sign will be positive if rotation from the z' -axis to the ray is counterclockwise. The ray $S_0\overline{P}S_1$, emitted from source S_0 and passing through the centre of the entrance pupil, is the principle ray; it intersects the optical surface at $\overline{P}$, which is stipulated to be the common origin of the coordinate systems xyz, $x_0y_0z_0$ and $x_0'y_0'z_0'$, and they are represented as that of the optical surface, the entrance and exit wavefront. u and u' are the sagittal field angles in the object space and image space, respectively; and α and β denote the angles of incidence and diffraction, respectively.

The general form of a plane-symmetric surface can be expressed in the vertex coordinate system of $\chi\eta z'$ by the equation (Lu & Cao, 2017)

$$z' = \sum_{i=0}^{\infty}\sum_{j=0}^{\infty} c_{i,j}\,\chi^i\eta^j, \qquad c_{0,0} = c_{1,0} = 0; \quad j = \text{even}. \tag{1}$$

For the third-order aberration theory of plane-symmetric optical systems, the power series needs to be kept up to the fourth order; thus the figure equation is denoted by

$$z' = c_{2,0}\chi^2 + c_{0,2}\eta^2 + c_{3,0}\chi^3 + c_{1,2}\chi\eta^2 + c_{4,0}\chi^4 + c_{2,2}\chi^2\eta^2 + c_{0,4}\eta^4, \tag{2}$$

where the coefficient $c_{i,j}$ has been given for a toroid, ellipsoid and paraboloid by Peatman (1997). For a toroidal surface, $c_{i,j}$ is as follows,

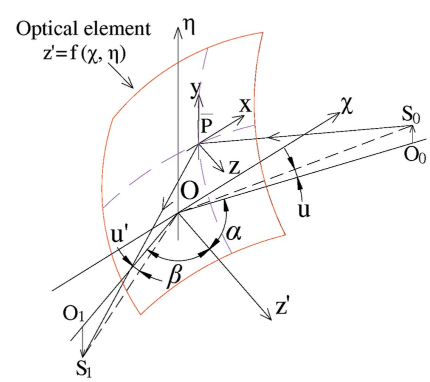


Figure 1
Optical scheme of a plane-symmetric optical system.

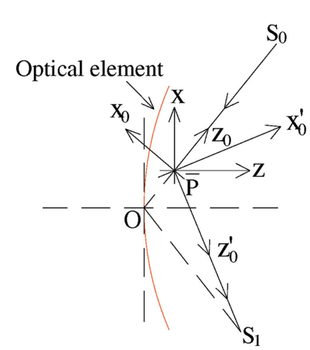


Figure 2
Coordinate systems of a plane-symmetric optical system on the meridional plane.

$$c_{2,0}=\frac{1}{2R},\quad c_{0,2}=\frac{1}{2\rho},\quad c_{3,0}=0,\quad c_{1,2}=0,$$
$$c_{4,0}=\frac{1}{8R^3},\quad c_{0,4}=\frac{1}{8\rho^3},\quad c_{2,2}=\frac{1}{4R^2\rho},\tag{3}$$

where R and ρ are major and minor curvature radii of the toroid. If $R = \rho$, equation (2) becomes a spherical equation.

2.2. Third-order aberration expressions with the aperture-ray coordinates on the reference exit wavefront

In order to make the transfer the relationship of the aperture-ray coordinates between the adjacent optical elements much simpler, for the two cases of orthogonal and coplanar arrangements of the main planes of elements, we use both the aperture-ray coordinates on the reference exit wavefront as the reference ones. Therefore, based on the fourth-order wave aberration expressions with the aperture-ray coordinates on the optical surface developed by Lu & Lin (2010), the wave aberration expressions are expressed with the aperture coordinates of the ray on the reference exit wavefront using the mapping relationships of aperture-ray coordinates between the optical surface and the reference exit wavefront; the corresponding expressions for $\tilde{w}_{ijk}$ are given by Cao & Lu (2017).

According to the above discussion, we firstly calculate the wave aberration with the aperture-ray coordinates on the optical surface; and the calculation expression of the wave aberration of a plane-symmetric optical system with the aperture-ray coordinates on the optical surface, x, y, and a sagittal field angle of u,

$$W=\sum_{ijk}^{4} w_{ijk}\, x^i y^j u^k,\qquad (i+j+k\le 4).\tag{4}$$

The wave aberration coefficients, w_{ijk}, are given by

$$w_{ijk}=M_{ijk}(\alpha,r_{\rm m},r_{\rm s},l_{\rm s})+(-1)^k M_{ijk}(\beta,r'_{\rm m},r'_{\rm s},l'_{\rm s})+\Lambda N_{ijk},\tag{5}$$

where $M_{ijk}(\alpha, r_m, r_s, l_s)$ and $M_{ijk}(\beta, r'_m, r'_s, l'_s)$ represent the wave aberration coefficients of the object and image beam pencil, r_m, r'_m, r_s, r'_s are the object and image distance in the meridional and sagittal plane, which means the respective curvature radius of the wavefront in the calculation of the wave aberration; l_s and l'_s are non-physical parameters and represent the position of the entrance and exit pupil on the sagittal plane. The last term of the above expression is the addition contribution of wave aberration when the optical element is a grating, and their expressions as well as N_{ijk} are given by Lu (2008) and $\Lambda = (m\lambda/\sigma)\Gamma$; otherwise, it should be zero.

The calculation of wave aberration coefficients requires knowing the parameters of the base ray and principle ray, α, β, r_m, r'_m, r_s, r'_s, l_s, l'_s of each optical element. Firstly, the direction of the base ray is determined by $w_{100} = 0$,

$$\sin\alpha+\sin\beta=m\lambda/\sigma.\tag{6}$$

To determine the direction of the principal ray, an additional condition, $w_{011} = 0$, should be satisfied,

$$l_{\rm s}\left(2c_{0,2}\cos\alpha-\frac{1}{r_{\rm s}}\right)-l'_{\rm s}\left(2c_{0,2}\cos\beta-\frac{1}{r'_{\rm s}}\right)=n_{02}\Lambda l_{\rm s}.\tag{7}$$

In addition, the positions of the image along the base ray on the meridional and the sagittal plane are determined by $w_{200} = 0$ and $w_{020} = 0$, respectively,

$$2c_{2,0}(\cos\alpha+\cos\beta)-\left(\frac{\cos^2\alpha}{r_{\rm m}}+\frac{\cos^2\beta}{r'_{\rm m}}\right)=n_{20}\Lambda,\tag{8}$$

$$2c_{0,2}(\cos\alpha+\cos\beta)-\left(\frac{1}{r_{\rm s}}+\frac{1}{r'_{\rm s}}\right)=n_{02}\Lambda.\tag{9}$$

Once α, β, r_m, r'_m, r_s, r'_s, l_s and l'_s are determined, the third- and fourth-order wave aberration coefficients with the aperture-ray coordinates on the optical surface, w_{ijk}, can be calculated. Then, by applying the relationship between w_{ijk} and the wave aberration coefficient with the aperture-ray coordiantes on the reference exit wavefront, $\tilde{w}_{ijk}$, given in equations (11)–(26) of Cao & Lu (2017), $\tilde{w}_{ijk}$ can be obtained. Therefore, the imaging aberration is contributed by the remaining third- and fourth-order wave aberration,

$$\begin{aligned}\tilde{W}=\;&\tilde{w}_{300}\,x_0'^3+\tilde{w}_{120}\,x'_0y_0'^2+\tilde{w}_{400}\,x_0'^4+\tilde{w}_{040}\,y_0'^4+\tilde{w}_{220}\,x_0'^2y_0'^2\\&+\tilde{w}_{102}\,x'_0u^2+\tilde{w}_{111}\,x'_0y'_0u+\tilde{w}_{031}\,y_0'^3u+\tilde{w}_{022}\,y_0'^2u^2\\&+\tilde{w}_{211}\,x_0'^2y'_0u+\tilde{w}_{202}\,x_0'^2u^2+\tilde{w}_{013}\,y'_0u^3.\end{aligned}\tag{10}$$

Since equation (10) is derived with respect to the aperture-ray coordinates on the reference exit wavefront, x'_0, y'_0, the angular deviation of the actual ray from the reference ray can be obtained; then the aberration yield by the wave aberration contribution on the image plane at a distance r'_0 from the final element of the optical system will be

$$\begin{aligned}\tilde{X}'=\;&\tilde{d}_{200}\,x_0'^2+\tilde{d}_{020}\,y_0'^2+\tilde{d}_{300}\,x_0'^3+\tilde{d}_{120}\,x'_0y_0'^2+\tilde{d}_{002}\,u^2\\&+\tilde{d}_{011}\,y'_0u+\tilde{d}_{111}\,x'_0y'_0u+\tilde{d}_{102}\,x'_0u^2,\\ \tilde{Y}'=\;&\tilde{h}_{110}\,x'_0y'_0+\tilde{h}_{030}\,y_0'^3+\tilde{h}_{210}\,x_0'^2y'_0+\tilde{h}_{101}\,x'_0u+\tilde{h}_{021}\,y_0'^2u\\&+\tilde{h}_{012}\,y'_0u^2+\tilde{h}_{201}\,x_0'^2u+\tilde{h}_{003}\,u^3.\end{aligned}\tag{11}$$

where

$$\tilde{d}_{ijk}=(i+1)\,r'_0\tilde{w}_{(i+1)jk},\quad \tilde{h}_{ijk}=(j+1)\,r'_0\tilde{w}_{i(j+1)k}\qquad (i+j+k\le 3).\tag{12}$$

In the above discussions, equation (11) denotes the aberrations on the arbitrary image plane without defocus; however, if the image plane is displaced from the focal plane, the defocus aberration occurs. The defocus aberration calculation expressions with the aperture-ray coordinates on the reference exit wavefront are given by equation (49) of Cao & Lu (2017).

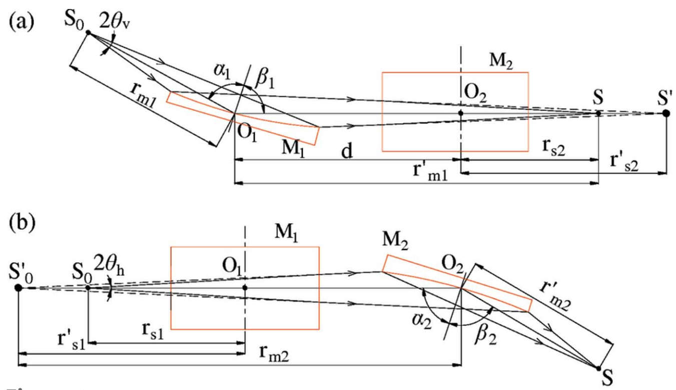


Figure 3
Optical scheme of an optical system with an orthogonal arrangement of the main planes of double elements.

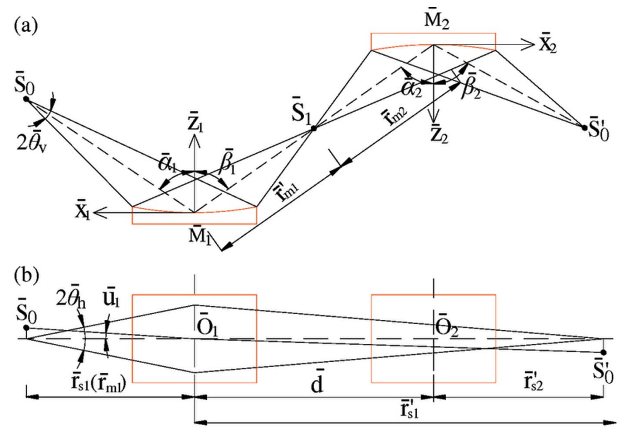


Figure 4
Optical scheme of an optical system with coplanar arrangement of the main planes of double elements.

3. Transfer equations of the aperture ray and the principal ray

For a soft X-ray optical system with orthogonal and coplanar arrangements of the main planes of elements, it is possible for the main planes of the optical elements to have an orthogonal arrangement or a coplanar arrangement. Therefore, the transfer equations of the aperture ray and the principal ray will also be different in the two cases.

3.1. Case of orthogonal arrangement of the main planes of the optical elements

Fig. 3 shows the optical scheme of an optical system with orthogonal arrangement of the main planes of double elements. The optical elements M_1, M_2 are arranged orthogonally to each other, and the distance between them is d; $2\theta_v$ and $2\theta_h$ are the vertical and horizontal acceptance angles of the light beam, r_{mi}, r'_{mi}, r_{si}, r'_{si} are the object and image distances in the meridional and sagittal plane of the ith (i = 1, 2) optical element. For an optical system, the transfer equations of the aperture ray and the principal ray have been derived by Cao & Lu (2017), and are as follows,

$$x'_{01} = A_1 y'_{02}, \quad y'_{01} = B_1 x'_{02}, \tag{13}$$

$$u_2 = C_1 v_1, \quad v_2 = D_1 u_1, \tag{14}$$

$$l_{m1} = C_1^2 \left(l_{s2} - \frac{d}{A_1} \right), \quad l_{s1} = D_1 (D_1 l_{m2} - d), \tag{15}$$

where u_i and v_i (i = 1, 2) are the sagittal and meridional field angle in the object space of the ith optical element; l_{mi} and l_{si} represent the position of the meridional and sagittal pupil in the object space of the ith optical element; $A_1 = r'_{m1}/r_{s2}$, $B_1 = r'_{s1}\cos\alpha_2/(r_{m2}\cos\beta_2)$, $C_1 = r'_{m1}\cos\alpha_1/(r_{s2}\cos\beta_1)$, $D_1 = r'_{s1}/r_{m2}$.

3.2. Case of coplanar arrangement of the main planes of optical elements

Fig. 4 shows the optical scheme of an optical system with a coplanar arrangement of the main planes of double elements, $\bar{M}_1$, $\bar{M}_2$. According to the geometry of the ray, the transfer equations of the aperture ray and the principal ray between $\bar{M}_1$ and $\bar{M}_2$ can be obtained, respectively,

$$\bar{x}'_{01} = \bar{A}_1 \bar{x}'_{02}, \quad \bar{y}'_{01} = \bar{B}_1 \bar{y}'_{02}, \tag{16}$$

$$\bar{u}_2 = \bar{B}_1 \bar{u}_1, \quad \bar{v}_2 = \bar{C}_1 \bar{v}_1, \tag{17}$$

$$\bar{l}_{m1} = \bar{C}_1 \left[\bar{C}_1 \bar{l}_{m2} - \left(\frac{\bar{r}_{m3}}{\bar{r}'_{m2}} \right) \bar{d} \right], \quad \bar{l}_{s1} = \bar{B}_1 (\bar{B}_1 \bar{l}_{s2} + \bar{d}), \tag{18}$$

where a bar above a parameter distinguishes it from the case of the orthogonal arrangement of the main planes of elements, $\bar{A}_1 = \bar{r}'_{m1}\cos\bar{\alpha}_2/(\bar{r}_{m2}\cos\bar{\beta}_2)$, $\bar{B}_1 = -\bar{r}'_{s1}/\bar{r}_{s2}$, $\bar{C}_1 = \bar{r}'_{m1}\cos\bar{\alpha}_1/(\bar{r}_{m2}\cos\bar{\beta}_1)$.

4. Calculation of third-order transverse aberration

For a multi-element optical system, the total wave aberration is the sum of that of each optical element. In this paper, we discuss the aberration of an optical system of three elements. The main plane of the first and second element is orthogonal while that of the second and third element is coplanar; its optical scheme is shown in Fig. 5. Although an aberration calculation method of soft X-ray optical systems with orthogonal and coplanar arrangement of the main planes of three elements is given in the following discussion, this method can

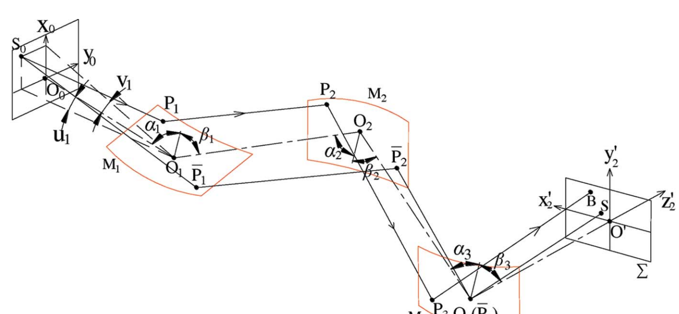


Figure 5
Optical scheme of an optical system of three elements; the main plane of the first and second elements is orthogonal while that of the second and third elements is coplanar.

be extended to any case of multi-element optical systems. Therefore, the total wave aberration of the optical system is

$$\tilde{W} = \tilde{W}_{(1)} + \tilde{W}_{(2)} + \tilde{W}_{(3)} = \sum_{ijk}^{4} \tilde{w}_{ijk(1)} x_{01}^{\prime i} y_{01}^{\prime j} u_1^k + \sum_{ijk}^{4} \tilde{w}_{ijk(2)} x_{02}^{\prime i} y_{02}^{\prime j} u_2^k + \sum_{ijk}^{4} \tilde{w}_{ijk(3)} x_{03}^{\prime i} y_{03}^{\prime j} u_3^k. \quad (19)$$

For convenience of calculation of the wave aberration and aberration of multi-element optical systems, the aperture-ray coordinates on the reference exit wavefront of the final optical element and the field angles of the first optical element are assumed to be the reference ones of the optical system. With the transfer equations (13)–(14), and (16)–(17), the relation of the aperture-ray coordinates and the field angles between each optical element and the reference one can be obtained,

$$x_{01}' = A_1 \bar{B}_1 y_{03}', \quad y_{01}' = \bar{A}_1 B_1 x_{03}', \quad x_{02}' = \bar{A}_1 x_{03}', \quad y_{02}' = \bar{B}_1 y_{03}'. \quad (20)$$

$$u_2 = C_1 v_1, \quad v_2 = D_1 u_1, \quad u_3 = \bar{B}_1 C_1 v_1, \quad v_3 = \bar{C}_1 D_1 u_1. \quad (21)$$

Combining (20) and (21), the wave aberration of equation (19) can be transformed into

$$\tilde{W} = \sum_{ijk}^{4} (A_1 \bar{B}_1)^i (\bar{A}_1 B_1)^j \tilde{w}_{ijk(1)} x_{03}^{\prime j} y_{03}^{\prime i} u_1^k + \sum_{ijk}^{4} \bar{A}_1^i \bar{B}_1^j C_1^k \tilde{w}_{ijk(2)} x_{03}^{\prime i} y_{03}^{\prime j} v_1^k + \sum_{ijk}^{4} (\bar{B}_1 C_1)^k \tilde{w}_{ijk(3)} x_{03}^{\prime i} y_{03}^{\prime j} v_1^k. \quad (22)$$

Similar to the conversion relationship from equations (10) to (11), the third-order transverse aberration from the wave aberration contribution of the optical system are derived,

$$\bar{x}' = \bar{d}_{2000} x_{03}^{\prime 2} + \bar{d}_{1100} x_{03}' y_{03}' + \bar{d}_{0200} y_{03}^{\prime 2} + + \bar{d}_{1200} x_{03}' y_{03}^{\prime 2} + \bar{d}_{3000} x_{03}^{\prime 3} + \bar{d}_{0110} y_{03}' u_1 + \bar{d}_{2010} x_{03}^{\prime 2} u_1 + \bar{d}_{1020} x_{03}' u_1^2 + \bar{d}_{0210} y_{03}^{\prime 2} u_1 + \bar{d}_{0030} u_1^3 + \bar{d}_{0002} v_1^2 + \bar{d}_{0101} y_{03}' v_1 + \bar{d}_{1101} x_{03}' y_{03}' v_1 + \bar{d}_{1002} x_{03}' v_1^2,$$

$$\bar{y}' = \bar{h}_{0200} y_{03}^{\prime 2} + \bar{h}_{2000} x_{03}^{\prime 2} + \bar{h}_{1100} x_{03}' y_{03}' + \bar{h}_{0300} y_{03}^{\prime 3} + \bar{h}_{2100} x_{03}^{\prime 2} y_{03}' + \bar{h}_{0020} u_1^2 + \bar{h}_{1010} x_{03}' u_1 + \bar{h}_{1110} x_{03}' y_{03}' u_1 + \bar{h}_{0120} y_{03}' u_1^2 + \bar{h}_{1001} x_{03}' v_1 + \bar{h}_{0201} y_{03}^{\prime 2} v_1 + \bar{h}_{0102} y_{03}' v_1^2 + \bar{h}_{2001} x_{03}^{\prime 2} v_1 + \bar{h}_{0003} v_1^3, \quad (23)$$

where the expressions of the aberration coefficients, $\bar{d}_{ijkh}$ and $\bar{h}_{ijkh}$ are given as follows:

$$\bar{d}_{2000} = 3r_0' (\bar{A}_1^3 \tilde{w}_{300(2)} + \tilde{w}_{300(3)}), \quad (24)$$

$$\bar{d}_{1100} = 2r_0' A_1 \bar{B}_1 (\bar{A}_1 B_1)^2 \tilde{w}_{120(1)}, \quad (25)$$

$$\bar{d}_{0200} = r_0' (\bar{A}_1 \bar{B}_1^2 \tilde{w}_{120(2)} + \tilde{w}_{120(3)}), \quad (26)$$

$$\bar{d}_{1200} = 2r_0' \left[(A_1 \bar{B}_1)^2 (\bar{A}_1 B_1)^2 \tilde{w}_{220(1)} + (\bar{A}_1 \bar{B}_1)^2 \tilde{w}_{220(2)} + \tilde{w}_{220(3)} \right], \quad (27)$$

$$\bar{d}_{3000} = 4r_0' \left[(\bar{A}_1 B_1)^4 \tilde{w}_{040(1)} + \bar{A}_1^4 \tilde{w}_{400(2)} + \tilde{w}_{400(3)} \right], \quad (28)$$

$$\bar{d}_{0110} = r_0' (A_1 \bar{B}_1)(\bar{A}_1 B_1) \tilde{w}_{111(1)}, \quad (29)$$

$$\bar{d}_{2010} = 3r_0' (\bar{A}_1 B_1)^3 \tilde{w}_{031(1)}, \quad (30)$$

$$\bar{d}_{1020} = 2r_0' (\bar{A}_1 B_1)^2 \tilde{w}_{022(1)}, \quad (31)$$

$$\bar{d}_{0210} = r_0' (A_1 \bar{B}_1)^2 (\bar{A}_1 B_1) \tilde{w}_{211(1)}, \quad (32)$$

$$\bar{d}_{0030} = r_0' (\bar{A}_1 B_1) \tilde{w}_{013(1)}, \quad (33)$$

$$\bar{d}_{0002} = r_0' [\bar{A}_1 C_1^2 \tilde{w}_{102(2)} + (\bar{B}_1 C_1) \tilde{w}_{102(3)}], \quad (34)$$

$$\bar{d}_{0101} = r_0' [\bar{A}_1 \bar{B}_1 C_1 \tilde{w}_{111(2)} + (\bar{B}_1 C_1) \tilde{w}_{111(3)}], \quad (35)$$

$$\bar{d}_{1101} = 2r_0' [\bar{A}_1^2 \bar{B}_1 C_1 \tilde{w}_{211(2)} + (\bar{B}_1 C_1) \tilde{w}_{211(3)}], \quad (36)$$

$$\bar{d}_{1002} = 2r_0' \left[\bar{A}_1^2 C_1^2 \tilde{w}_{202(2)} + (\bar{B}_1 C_1)^2 \tilde{w}_{202(3)} \right], \quad (37)$$

$$\bar{h}_{0200} = 3r_0' (A_1 \bar{B}_1)^3 \tilde{w}_{300(1)}, \quad (38)$$

$$\bar{h}_{2000} = r_0' (A_1 \bar{B}_1)(\bar{A}_1 B_1)^2 \tilde{w}_{120(1)}, \quad (39)$$

$$\bar{h}_{1100} = 2r_0' (\bar{A}_1 \bar{B}_1^2 \tilde{w}_{120(2)} + \tilde{w}_{120(3)}), \quad (40)$$

$$\bar{h}_{0300} = 4r_0' \left[(A_1 \bar{B}_1)^4 \tilde{w}_{400(1)} + \bar{B}_1^4 \tilde{w}_{040(2)} + \tilde{w}_{040(3)} \right], \quad (41)$$

$$\bar{h}_{2100} = 2r_0' \left[(A_1 \bar{B}_1)^2 (\bar{A}_1 B_1)^2 \tilde{w}_{220(1)} + \bar{A}_1^2 \bar{B}_1^2 \tilde{w}_{220(2)} + \tilde{w}_{220(3)} \right], \quad (42)$$

$$\bar{h}_{0020} = r_0' (A_1 \bar{B}_1) \tilde{w}_{102(1)}, \quad (43)$$

$$\bar{h}_{1010} = r_0' (A_1 \bar{B}_1)(\bar{A}_1 B_1) \tilde{w}_{111(1)}, \quad (44)$$

$$\bar{h}_{1110} = 2r_0' (A_1 \bar{B}_1)^2 (\bar{A}_1 B_1) \tilde{w}_{211(1)}, \quad (45)$$

$$\bar{h}_{0120} = 2r_0' (A_1 \bar{B}_1)^2 \tilde{w}_{202(1)}, \quad (46)$$

$$\bar{h}_{1001} = r_0' [\bar{A}_1 \bar{B}_1 C_1 \tilde{w}_{111(2)} + (\bar{B}_1 C_1) \tilde{w}_{111(3)}], \quad (47)$$

$$\bar{h}_{0201} = 3r_0' [\bar{B}_1^3 C_1 \tilde{w}_{031(2)} + (\bar{B}_1 C_1) \tilde{w}_{031(3)}], \quad (48)$$

$$\bar{h}_{0102} = 2r_0' \left[\bar{B}_1^2 C_1^2 \tilde{w}_{022(2)} + (\bar{B}_1 C_1)^2 \tilde{w}_{022(3)} \right], \quad (49)$$

$$\bar{h}_{2001} = 2r_0' [\bar{A}_1^2 \bar{B}_1 C_1 \tilde{w}_{211(2)} + (\bar{B}_1 C_1) \tilde{w}_{211(3)}], \quad (50)$$

$$\bar{h}_{0003} = r'_0\Big[\bar{B}_1 C_1^3 \tilde{w}_{013(2)} + \big(\bar{B}_1 C_1\big)^3 \tilde{w}_{013(3)}\Big]. \quad (51)$$

Equation (23) represents the displacement of the actual ray from the reference ray of the optical system; however, the final coordinates of the ray on the arbitrary image plane should also consider that of the reference ray from the principal ray, and the principal ray from the base ray. The former applies equation (49) of Cao & Lu (2017), and the latter can be calculated by using the first-order approximation (Lu & Zhu, 2012),

$$\Delta x'_3 = \left\{ -\frac{r'_0 \cos\alpha_3}{\cos\beta_3} + \frac{\left[1-(r'_0/r'_{m3})\right] l_{m3}\cos\beta_3}{\cos\alpha_3} \right\} \big(\bar{C}_1 D_1\big) u_1,$$
$$\Delta y'_3 = \left[l_{s3} - r'_0\left(1+\frac{l_{s3}}{r'_{s3}}\right)\right]\big(\bar{B}_1 C_1\big) v_1. \quad (52)$$

In this paper, we apply the third-order aberration theory with the aperture-ray coordinates of the reference exit wavefront with a one-dimensional source to study the aberration of the optical system with a two-dimensional source. However, in this case, for a source point with a meridional field angle of v_1, the meridional field angle will cause the angles of incidence and diffraction of the principal ray on the optical surface of each element to change by an amount, and thus they should actually be

$$\alpha'_i = \alpha_i + v_i, \qquad \beta'_i = \beta_i + v'_i, \quad (53)$$

where $v'_i = -(\cos\alpha_i / \cos\beta_i)\, v_i$.

The meridional field angle v_1 is usually small, and thus the variation of the angles of incidence and diffraction of the principal ray on the optical surface of each element is also very small. However, for a grazing-incidence optical system (α and β are usually larger than 80°, even near to 89°), the object and image distance in the meridional and sagittal plane of each optical element, r_{mi}, r'_{mi}, r_{si}, r'_{si}, will change quite significantly. For a multi-element optical system, the calculation expressions of their variables are too complex because the object and image distance in the meridional and sagittal plane of the latter optical element are determined by that of its preceding ones; therefore, with substitution of the corresponding parameters of equations (8) and (9), $\alpha_i \to \alpha'_i$, $\beta_i \to \beta'_i$, the actual value of r_{mi}, r'_{mi}, r_{si}, r'_{si} of each optical element of the optical system with two-dimensional source, $\tilde{r}_{mi}$, $\tilde{r}'_{mi}$, $\tilde{r}_{si}$, $\tilde{r}'_{si}$, can be calculated. Therefore, in applying the wave aberration and aberration expressions as discussed above in this paper, the parameters α_i, β_i, r_{mi}, r'_{mi}, r_{si}, r'_{si} should be replaced by α'_i, β'_i, $\tilde{r}_{mi}$, $\tilde{r}'_{mi}$, $\tilde{r}_{si}$, $\tilde{r}'_{si}$.

5. Numerical validation

To validate the third-order aberration calculation method discussed above in this paper, we now apply the aberration expressions to calculate the imaging of two design examples of a soft X-ray optical system with orthogonal and coplanar arrangement of the main planes of three elements and compare them with the ray-tracing results from the *Shadow* software. Optical system I is a modified design of the Kirkpatrick–Baez (KB) microscope system with two spherical mirrors (Gu *et al.*, 2005), and adds a spherical mirror after it; the main planes of the third spherical mirror and the second optical element of the KB microscope system are coplanar, as shown in Fig. 6. The optical system accepts from the source a light beam with a diverging angle of $2\theta_v \times 2\theta_h$ = 4 mrad × 4 mrad, and works at a wavelength of 4.4 nm. Its optical parameters are listed in Table 1. In addition, in order to further verify that the aberration calculation method proposed in this paper is suitable for the case of the aspherical surface, optical system II is thus a modified design of the third optical element of optical system I. The structure of the optical element to be modified is a toroidal mirror, and its major and minor curvature radius are R_3 = 20000 mm, ρ_3 = 490.442 mm, and its other optical parameters are consistent with that of optical system I. In the following imaging calculations of the optical systems discussed above, the field angles are assumed to be u_1 = 0.01°, v_1 = 0.01°; and u_1 = 0.03°, v_1 = 0.03°.

Fig. 7 shows ray spot diagrams. Rays from row 1 to row 2 are the aberration distributions at an image plane of r'_0 = 400 mm

Table 1
Optical parameters of the optical system [units: mm (unless otherwise stated)].

Parameters	Value
R_1	9700
R_2	9700
R_3	9700
α_1	88.948°
β_1	−88.948°
α_2	−88.857°
β_2	88.857°
α_3	81°
β_3	−81°
r_{m1} (r_{s1})	100
d_1	10
d_2	10

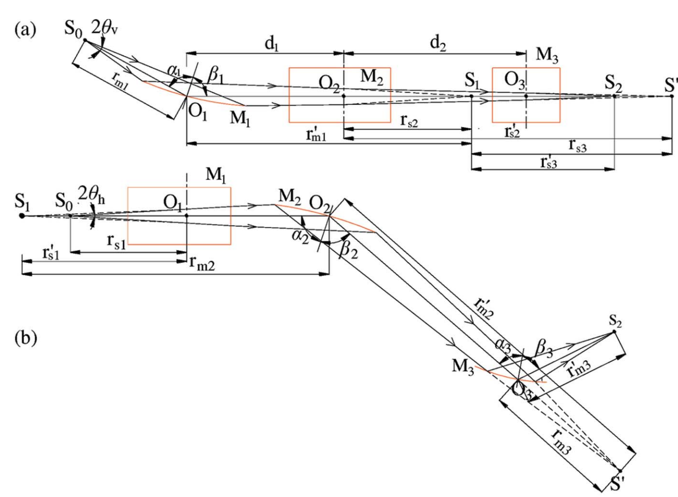


Figure 6
Optical scheme of an optical system of three elements; the main planes of the first and second elements is orthogonal while that of the second and third elements is coplanar.

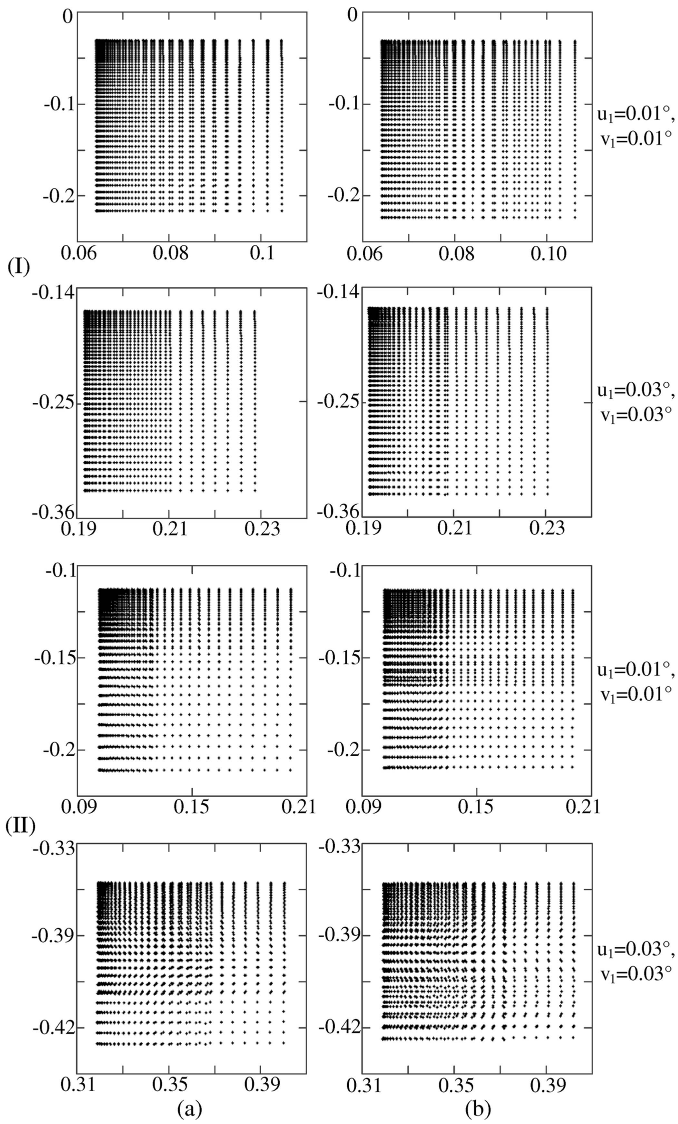


Figure 7
Ray spot diagrams (I) and (II) corresponding to the images of optical system I with an image plane of $r_0' = 400$ mm and optical system II with an image plane of $r_0' = 668$ mm, respectively (axis units: mm). Panels (*a*) and (*b*) are obtained using the ray-tracing software *Shadow* and the aberration expressions derived in this paper, respectively. The field angles are shown on the right-hand side of each row.

of optical system I, whereas those from row 3 to row 4 are the calculation results of optical system II with an image plane of $r_0' = 668$ mm. The field angles are shown on the right-hand side of each row. Fig. 7(*a*) shows the the ray-tracing results obtained using the *Shadow* software, whereas Fig. 7(*b*) shows the aberration calculation results using the aberration expressions derived in this paper.

As shown in Fig. 7, compared with the calculation result obtained with the ray-tracing software *Shadow*, the calculation accuracy of the aberration expressions derived in this paper is satisfactory both in the size and shape of the spot diagrams. However, there is a small deviation between them, mainly because of the contribution of the high-order aberration (including the intrinsic aberration and extrinsic aberration) and high-order coordinate components in the transfer of the aperture-ray coordinates.

6. Conclusions

In this paper, we have proposed an aberration calculation method for a multi-element optical system using the third-order aberration theory with the aperture-ray coordinates on the reference exit wavefront of a plane-symmetric optical system, and derived the corresponding calculation expressions; the main planes of the adjacent optical element of the optical system are likely to be orthogonal or coplanar arrangements. The resultant aberration expressions are applied to calculate the aberration of one design example of such kind of optical systems to compare the results with those obtained from the ray-tracing software *Shadow*, and they have satisfactory calculation accuracy.

Compared with the ray-tracing software *Shadow*, this aberration analytical analysis method discussed in this paper has some advantages, as follows: analysing the contribution of different types of aberration, determining of initial structural parameters, the relationship between the optical structures and parameters and the imaging performance, and so on. It will give us some insight into the optimization and design of these kinds of optical systems.

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