Systematic transformations of the asymptotic aberration coefficients of round electrostatic lenses (1)

C. E. Kuyatt

National Bureau of Standards, Washington, D.C. 20234

(Received 12 December 1977)

In previous work we formulated the third-order asymptotic aberration coefficients of round (axially symmetric) electrostatic lenses in a form independent of object and aperture positions, and expressions for the six quantities which are sufficient to specify completely the aberration properties of the lenses were derived in the form of integrals involving derivatives of the axial potential through the fourth order. Because actual calculations involved numerical differentiation of the axial potentials, integrations by parts were used to transform the integrals to two new forms with axial derivatives of lower degree. Many other forms of the aberration integrals can be obtained by further integrations by parts, but the transformations are laborious and it is not easy to predict the forms which are possible nor to determine the sequence of operations which will yield a desired result. However, using a method originally developed by Seman and extended by Hawkes, a completely general formula has been derived from which all of the possible forms of the asymptotic integrals can be obtained simply. A few of these possible forms are derived and discussed.

PACS numbers: 41.80.−y, 07.77.+p, 07.80.+x

I. INTRODUCTION

In previous work[1,2] we formulated the third-order asymptotic aberration coefficients of round (axially symmetric) electrostatic lenses in a form independent of object and aperture positions. Six quantities are sufficient to specify completely the third-order aberration properties of round electrostatic lenses. Equations for these six quantities were derived in the form of integrals involving derivatives of the axial potential through the fourth order.

Because actual calculations of the aberration integrals involved numerical differentiation of computed axial potentials, we used successive integrations by parts to transform the integrals to two new forms; one form with axial derivatives no higher than the third, and a second form with axial derivatives no higher than the second. There are, however, many other possible forms of the aberration integrals which can be obtained through integrations by parts, but the complexity of the integrals makes the transformations laborious. Furthermore, it is not easy to predict the possible forms which may be attained nor to determine the sequence of operations which will yield a desired result.

In order to obtain integrals for the asymptotic aberration coefficients which do not contain contributions from the asymptotic (straight-line) portions of trajectories, it is necessary to obtain forms for the integrals which contain only derivatives of the axial potential. In this paper we use a method originally developed by Seman[3] for round magnetic and electrostatic lenses, to derive a formula from which all of the posible forms of the asymptotic aberration integrals for round electrostatic lenses can be obtained very simply. A few of these possible forms are discussed.

II. FORMULATION OF THE ABERRATION COEFFICIENTS

The incident asymptotic ray is specified by its slopes α_1 and γ_1, and by its coordinates x_1 and y_1 when projected onto some selected entrance plane A. Similarly, the emerging asymptotic ray is specified by its slopes α_2, γ_2, and by its coordinates x_2 and y_2 when projected onto a corresponding exit plane B. By asymptotic rays we mean rays outside of the effective field of the lens; hence real objects and images must be outside the lens field or they must be virtual.

Defining the dimensionless quantities $X_1 = x_1/D$, $Y_1 = y_1/D$, and $Z_1 = z_1/D$, where D is the diameter of the lens, the coordinates are grouped as system invariants,

$$r_1 = X_1{}^2 + Y_1{}^2, \quad s_1 = \alpha_1{}^2 + \gamma_1{}^2,$$
$$u_1 = X_1\alpha_1 + Y_1\gamma_1, \quad v_1 = X_1\gamma_1 - Y_1\alpha_1. \tag{1}$$

Aberration coefficients involving v_1 vanish for electrostatic lenses.[4]

Following Hawkes[4,5] we begin with Fermat's principle in the form

$$\delta \int_A^B m\, dZ = 0, \tag{2}$$

in which

$$m = \Phi^{1/2}(1 + X'^2 + Y'^2)^{1/2}, \tag{3}$$

for a purely electrostatic field with a potential distribution $\Phi(X,Y,Z)$. Here primes indicate differentiation with respect to Z. Introducing the vector $U = (X,Y)$ (i.e., $U = X_{\mathrm{i}} + Y_{\mathrm{j}}$, where i is a unit vector in the x direction, and j is a unit reactor in the y direction), m can be expressed as

 © 1978 American Vacuum Society

$$m = m^{(0)} + m^{(2)} + m^{(4)} + \dots, \tag{4}$$

where

$$m^{(0)} = \phi^{1/2},$$

$$m^{(2)} = -\tfrac{1}{8}(\phi''/\phi^{1/2})U^2 + (\tfrac{1}{2})\phi^{1/2}U'^2,$$

$$m^{(4)} = \tfrac{1}{128}\left(\frac{\phi^{iv}}{\phi^{1/2}} - \frac{\phi''^2}{\phi^{3/2}}\right)U^4 - \tfrac{1}{16}\frac{\phi''}{\phi^{1/2}}U^2U'^2 - \tfrac{1}{8}\phi^{1/2}U'^4, \tag{5}$$

$\phi(Z)$ is the axial potential, $U^2 = X^2 + Y^2$ and $U'^2 = \alpha^2 + \gamma^2$. In our previous work[1,2] the third-order aberration coefficients are obtained from a dimensionless characteristic function

$$V_F = (1/\phi_1^{1/2}) \int_A^B m^{(4)} dZ, \tag{6}$$

which is in second order in r_1, s_1, u_1 and can be expressed in matrix form as

$$V_F = (r_1 s_1 u_1)\begin{pmatrix} M_{11} & M_{12} & M_{13} \\ 0 & M_{22} & M_{23} \\ 0 & 0 & M_{33} \end{pmatrix}\begin{pmatrix} r_1 \\ s_1 \\ u_1 \end{pmatrix}. \tag{7}$$

Given two independent first-order trajectories $G(Z)$ and $H(Z)$ satisfying at plane A,

$$G_1 = 1, \quad H_1 = 0, \qquad G_1' = 0, \quad H_1' = 1, \tag{8}$$

the third-order aberration equations are obtained from

$$\Delta X_2 = H_2 \frac{\partial V_F}{\partial X_1} - G_2 \frac{\partial V_F}{\partial \alpha_1} - \tfrac{1}{2}H_2\alpha_1(\alpha_1^2 + \gamma_1^2)$$

$$\Delta \alpha_2 = H_2' \frac{\partial V_F}{\partial X_1} - G_2' \frac{\partial V_F}{\partial \alpha_1} - \tfrac{1}{2}H_2'\alpha_1(\alpha_1^2 + \gamma_1^2) + \tfrac{1}{2}\alpha_2(\alpha_2^2 + \gamma_2^2), \tag{9}$$

where the quantities α_2 and γ_2 are first-order projected values, and equations for ΔY_2 and $\Delta\gamma_2$ are obtained by replacing X_1, α_1, α_2 with Y_1, γ_1, γ_2. Previous work[1,2] should be consulted for concrete examples of the application of this formalism.

III. DERIVATION OF THE GENERAL FORM OF THE CHARACTERISTIC FUNCTION

The aberration integrals which result from differentiating Eq. (6) can be expressed in a multitude of different forms through transformations using integrations by parts. Often these transformations are carried out on each of the several aberration integrals. However, the labor involved can be considerably reduced by performing the transformation directly on the characteristic function V_F. Nevertheless, much labor is still involved. More importantly, it is difficult to predict the possible forms which may be obtained and to determine the sequence of operations which will yield a desired result.

An ingenious answer to this problem was originally developed by Seman[3] for round magnetic and electrostatic lenses, and extended by Hawkes[5,6] to quadrupole lenses. It consists of deriving a completely general formula from which all of the possible forms of the aberration integrals can be obtained simply, almost by inspection. In applying this method we follow Hawkes[5,6] closely.

Consider the function

$$V_F^* = \phi_1^{1/2} V_F = \int_A^B m^{(4)} dZ. \tag{10}$$

The integrand $m^{(4)}$, given in Eq. (4), consists of terms with the dimensions $[\partial]^4[\phi^{1/2}]^1[U^2]^2$, where $\partial \equiv d/dZ$. By applying the differentiation operator $[\partial]^4$ in all possible combinations, we find fourteen possible terms:

$$\begin{aligned}
T_1 &= \frac{\phi'^4}{\phi^{7/2}}U^4, & T_8 &= \frac{\phi'''}{\phi^{1/2}}U^2U^{2\prime}, \\
T_2 &= \frac{\phi'^2\phi''}{\phi^{5/2}}U^4, & T_9 &= \frac{\phi''}{\phi^{1/2}}U^2U'^2, \\
T_3 &= \frac{\phi''^2}{\phi^{3/2}}U^4, & T_{10} &= \frac{\phi'^2}{\phi^{3/2}}U^2U'^2, \\
T_4 &= \frac{\phi'''\phi'}{\phi^{3/2}}U^4, & T_{11} &= \frac{\phi'^2}{\phi^{3/2}}(U^{2\prime})^2, \\
T_5 &= \frac{\phi^{iv}}{\phi^{1/2}}U^4, & T_{12} &= \frac{\phi''}{\phi^{1/2}}(U^{2\prime})^2, \\
T_6 &= \frac{\phi'^3}{\phi^{5/2}}U^2U^{2\prime}, & T_{13} &= \frac{\phi'}{\phi^{1/2}}U^{2\prime}U'^2, \\
T_7 &= \frac{\phi''\phi'}{\phi^{3/2}}U^2U^{2\prime}, & T_{14} &= \phi^{1/2}U'^4.
\end{aligned} \tag{11}$$

Similarly, V_F^* has the dimensions $[\partial]^3[\phi^{1/2}]^1[U^2]^2$, and eight possible terms are generated:

$$\begin{aligned}
t_1 &= \phi^{1/2}U^{2\prime}U'^2 & t_5 &= \frac{\phi'^2}{\phi^{3/2}}U^2U^{2\prime} \\
t_2 &= \frac{\phi'}{\phi^{1/2}}(U^{2\prime})^2 & t_6 &= \frac{\phi'''}{\phi^{1/2}}U^4 \\
t_3 &= \frac{\phi'}{\phi^{1/2}}U^2U'^2 & t_7 &= \frac{\phi''\phi'}{\phi^{3/2}}U^4 \\
t_4 &= \frac{\phi''}{\phi^{1/2}}U^2U^{2\prime} & t_8 &= \frac{\phi'^3}{\phi^{3/2}}U^4.
\end{aligned} \tag{12}$$

The function V_F^* can be altered in form without affecting its value by adding to it expressions which vanish; suitable expressions are obtained by differentiating each of the terms t_i and eliminating U'' with the aid of the paraxial equation of motion wherever it occurs:

$$\phi^{1/2}U'' + \frac{1}{2}\frac{\phi'}{\phi^{1/2}}U' + \frac{1}{4}\frac{\phi''}{\phi^{1/2}}U = 0. \tag{13}$$

The expressions which result are:

$$\begin{aligned}
\Gamma_1 &\equiv t_1' + \tfrac{1}{2}T_9 + \tfrac{1}{4}T_{12} + T_{13} - 2T_{14} = 0 \\
\Gamma_2 &\equiv t_2' + T_7 + \tfrac{3}{2}T_{11} - T_{12} - 4T_{13} = 0 \\
\Gamma_3 &\equiv t_3' + \tfrac{1}{4}T_7 - T_9 + \tfrac{3}{2}T_{10} - T_{13} = 0 \\
\Gamma_4 &\equiv t_4' + \tfrac{1}{2}T_3 + T_7 - T_8 - 2T_9 - T_{12} = 0 \\
\Gamma_5 &\equiv t_5' + \tfrac{1}{2}T_2 + 2T_6 - 2T_7 - 2T_{10} - T_{11} = 0
\end{aligned} \tag{14}$$

$$\Gamma_6 \equiv t_6' + \tfrac{1}{2}T_4 - T_5 - 2T_8 = 0$$
$$\Gamma_7 \equiv t_7' + \tfrac{3}{2}T_2 - T_3 - T_4 - 2T_7 = 0$$
$$\Gamma_8 \equiv t_8' + \tfrac{5}{2}T_1 - 3T_2 - 2T_6 = 0.$$

The function $V_F{}^*$ has the form

$$128V_F{}^* = \int_A^B (-T_3 + T_5 - 8T_9 - 16T_{14})\,dZ. \quad (15)$$

We now add

$$\sum_{i=1}^{8} \tau_i\Gamma_i = 0, \quad (16)$$

where the quantities τ_i are arbitrary parameters, giving

$$\begin{aligned}128V_F{}^* = {} & \left(\sum_{i=1}^{8} \tau_i t_i\right)_A^B \\ & + \int_A^B [\tfrac{5}{2}\tau_8 T_1 + (\tfrac{1}{2}\tau_5 + \tfrac{3}{2}\tau_7 - 3\tau_8)T_2 \\ & + (-1 + \tfrac{1}{2}\tau_4 - \tau_7)T_3 + (\tfrac{1}{2}\tau_6 - \tau_7)T_4 \\ & + (1 - \tau_6)T_5 + 2(\tau_5 - \tau_8)T_6 \\ & + (\tau_2 + \tfrac{1}{4}\tau_3 + \tau_4 - 2\tau_5 - 2\tau_7)T_7 + (-\tau_4 - 2\tau_6)T_8 \\ & + (-8 + \tfrac{1}{2}\tau_1 - \tau_3 - 2\tau_4)T_9 + (\tfrac{3}{2}\tau_3 - 2\tau_5)T_{10} \\ & + (\tfrac{3}{2}\tau_2 - \tau_5)T_{11} + (\tfrac{1}{4}\tau_1 - \tau_2 - \tau_4)T_{12} \\ & + (\tau_1 - 4\tau_2 - \tau_3)T_{13} + (-16 - 2\tau_1)T_{14}]\,dZ. \quad (17)\end{aligned}$$

Putting in the trajectory U and the functions T,

$$\begin{aligned}128V_F{}^* = {} & [\tau_1\phi^{1/2}U^{2\prime}U'^2]_A^B \\ & + \int_A^B \Big\{U^4\Big[\tfrac{5}{2}\tau_8\frac{\phi'^4}{\phi^{7/2}} + (\tfrac{1}{2}\tau_5 + \tfrac{3}{2}\tau_7 - 3\tau_8)\frac{\phi'^2\phi''}{\phi^{5/2}} \\ & + (-1 + \tfrac{1}{2}\tau_4 - \tau_7)\frac{\phi''^2}{\phi^{3/2}} + (\tfrac{1}{2}\tau_6 - \tau_7)\frac{\phi'''\phi'}{\phi^{3/2}} \\ & + (1 - \tau_6)\frac{\phi^{iv}}{\phi^{1/2}}\Big] + U^2U^{2\prime}\Big[2(\tau_5 - \tau_8)\frac{\phi'^3}{\phi^{5/2}} \\ & + (\tau_2 + \tfrac{1}{4}\tau_3 + \tau_4 - 2\tau_5 - 2\tau_7)\frac{\phi''\phi'}{\phi^{3/2}} + (-\tau_4 - 2\tau_6)\frac{\phi'''}{\phi^{1/2}}\Big] \\ & + U^2U'^2\Big[(-8 + \tfrac{1}{2}\tau_1 - \tau_3 - 2\tau_4)\frac{\phi''}{\phi^{1/2}} \\ & + (\tfrac{3}{2}\tau_3 - 2\tau_5)\frac{\phi'^2}{\phi^{3/2}}\Big] + (U^{2\prime})^2\Big[(\tfrac{3}{2}\tau_2 - \tau_5)\frac{\phi'^2}{\phi^{3/2}} \\ & + (\tfrac{1}{4}\tau_1 - \tau_2 - \tau_4)\frac{\phi''}{\phi^{1/2}}\Big] \\ & + U^{2\prime}U'^2\Big[(\tau_1 - 4\tau_2 - \tau_3)\frac{\phi'}{\phi^{1/2}}\Big] \\ & + U'^4[(-16 - 2\tau_1)\phi^{1/2}]\Big\}\,dZ. \quad (18)\end{aligned}$$

IV. SOME SPECIAL FORMS

Because planes A and B are both effectively in regions of constant ϕ, all the integrated terms, with the exception of the term in τ_1, contain derivatives of ϕ and hence vanish. Similarly, all but the last term in the integrand contain derivatives of the potential and vanish along the asymptotic (straight-line) portions of trajectories. To eliminate such contributions it is necessary only to set $\tau_1 = -8$. An expression which we derived previously[1,2] with derivatives of ϕ up to the third order corresponds to

$$\tau_1 = 0,\ \tau_2 = 0,\ \tau_3 = 0,\ \tau_4 = 0,\ \tau_5 = 0,\ \tau_6 = 1,\ \tau_7 = 0,\ \tau_8 = 0,$$

and one with derivatives of ϕ up to the second order to

$$\tau_1 = 0,\ \tau_2 = 0,\ \tau_3 = 0,\ \tau_4 = -2,\ \tau_5 = 0,\ \tau_6 = 1,\ \tau_7 = \tfrac{1}{2},\ \tau_8 = 0.$$

Assuming now that we take $\tau_1 = -8$ to eliminate asymptotic contributions to the integral, how can we eliminate as many of the higher derivatives of ϕ as possible? We must have $\tau_6 = 1$ to eliminate ϕ^{iv} and $\tau_6 = 2\tau_7$ and $\tau_4 = -2\tau_6 = -4\tau_7$ to eliminate ϕ'''. So we have $\tau_1 = -8$, $\tau_4 = -2$, $\tau_7 = \tfrac{1}{2}$, and $\tau_6 = 1$. The terms in ϕ'' remaining are:

$$(\tfrac{1}{2}\tau_5 + \tfrac{3}{4} - 3\tau_8)\frac{\phi'^2\phi''}{\phi^{5/2}}, \quad (-\tfrac{5}{2})\frac{\phi''^2}{\phi^{3/2}},$$
$$(\tau_2 + \tfrac{1}{4}\tau_3 - 2\tau_5 - 3)\frac{\phi''\phi'}{\phi^{3/2}},$$
$$(-\tau_3 - 8)\frac{\phi''}{\phi^{1/2}}, \quad (-\tau_2)\frac{\phi''}{\phi^{1/2}}.$$

One easily sees that four of these five terms can be eliminated by choosing $\tau_2 = 0$, $\tau_3 = -8$, $\tau_5 = -\tfrac{5}{2}$, and $\tau_8 = -\tfrac{1}{6}$. We now have

$$\mathrm{T}_1 = -8,\ \tau_2 = 0,\ \tau_3 = -8,\ \tau_4 = -2,\ \tau_5 = -\tfrac{5}{2},\ \tau_6 = 1,\ \tau_7 = \tfrac{1}{2},\ \tau_8 = -\tfrac{1}{6}$$

giving

$$\begin{aligned}128V_F{}^* = {} & [\tau_1\phi^{1/2}U^{2\prime}U'^2]_A^B \\ & + \int_A^B \Big\{U^4\Big[-\tfrac{5}{12}\frac{\phi'^4}{\phi^{7/2}} - \tfrac{5}{2}\frac{\phi''^2}{\phi^{3/2}}\Big] \\ & + U^2U^{2\prime}\Big[-\tfrac{14}{3}\frac{\phi'^3}{\phi^{5/2}}\Big] + U^2U'^2\Big[-7\frac{\phi'^2}{\phi^{3/2}}\Big] \\ & + (U^{2\prime})^2\Big[\tfrac{5}{2}\frac{\phi'^2}{\phi^{3/2}}\Big]\Big\}\,dZ. \quad (19)\end{aligned}$$

It is interesting that this form of the integral leads to aberration coefficients in a form originally derived by Scherzer.[7] We further find that in order to obtain another form derived by Scherzer to demonstrate that the spherical aberration coefficient is always negative it is only necessary to substitute $\tau_5 = -\tfrac{5}{4}$ and $\tau_8 = -\tfrac{13}{8}$ in the above set of values.

According to Hawkes,[8] the aberration integrals given by Sturrock[9] can be obtained by setting

$$\tau_1 = -8,\ \tau_2 = 0,\ \tau_3 = -8,\ \tau_4 = -2,\ \tau_5 = -\tfrac{5}{2},\ \tau_6 = 1,\ \tau_7 = \tfrac{1}{2},\ \tau_8 = -\tfrac{23}{8},$$

that is, changing only the value of τ_8 from those which give Eq. (19). However, using these values does not reproduce the appropriate nonrelativistic limit of Sturrock's formulas. In fact, since Sturrock's formulas do not contain a term in ϕ'^3 it is necessary that $\tau_8 = \tau_5$. By changing τ_8 to $-\tfrac{5}{2}$, one gets formulas with the same form as Sturrock but with somewhat different coefficients, leading to the conclusion that Sturrock's formulas are in error. We do not have space in this paper to present the detailed equations. However, it is clear that it is easier to investigate the possible forms of the aberration integrals using the general Eq. (18) than in any other way.

[1]C. E. Kuyatt, D. CiChio, and S. V. Natali, Rev. Sci. Instrum. **45**, 1275 (1974).

[2]D. DiChio, S. V. Natali, and C. E. Kuyatt, Rev. Sci. Instrum. **46**, 71 (1975).

[3]P. W. Hawkes, Optik **24**, 252 (1966), footnote.

[4]P. W. Hawkes, Optik **27**, 287 (1968).

[5]P. W. Hawkes, Optik **24**, 252 (1966), Optik **24**, 275 (1967).

[6]P. W. Hawkes, J. Microscopie **6**, 917 (1967).

[7]This form is attributed to Scherzer by P. Grivet, *Electron Optics* (Pergamon, Oxford, 1965), p. 126, and the aberration integrals are given. However, the cited references do not give the complete set of equations.

[8]P. W. Hawkes, in *Focusing of Charged Particles*, edited by A. Septier (Academic, New York, 1967), p. 411.

[9]P. A. Sturrock, *Static and Dynamic Electron Optics* (Cambridge Univ., 1955), pp. 105–106.