Third-order asymptotic aberration coefficients of electron lenses. III. Formulas and results for the two-tube electrostatic lens.

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The third-order asymptotic aberration coefficients of round electrostatic electron lenses are formulated, following Hawkes, in a form independent of object and aperture positions. Six quantities are sufficient to specify completely the third-order aberration properties of electrostatic electron lenses. Equations for these six quantities are derived in the form of integrals involving derivatives of the axial potential no higher than the second. Using these equations and our previously calculated potentials and first-order trajectories we have computed the six aberrations coefficients for the two-tube electrostatic lens for voltage ratios from 1.1 to 10 000. The results are believed accurate to better than 0.2%.

INTRODUCTION

In previous papers[1–3] we have discussed the deficiencies of the standard treatments of aberration coefficients of electron lenses and pointed out the lack of data on aberration coefficients other than for spherical aberration. We first adopted[1,2] a method due to Verster[4] in which the third-order aberrations of round electrostatic electron lenses for meridional trajectories are formulated in a way which does not depend on the positions of the object or aperture, and calculated all of the Verster aberration coefficients for the two-tube electrostatic lens for voltage ratios from 2 to 40. In this work, positions and slopes of accurately calculated trajectories were fitted to the aberration equations. The presence of some contributions from fifth-order aberrations limited the accuracy of the third-order coefficients to about 10%.

In later work,[3] we expanded our treatment to include nonmeridional (skew) trajectories by using the more general formulation of Hawkes,[5–7] and increased the accuracy of the aberration coefficients by calculating them from integrals involving the axial potential distribution and first-order trajectories. In this paper we give the detailed derivation of the aberration integrals and report results for the two-tube electrostatic lens at voltage ratios from 1.1 to 10 000. These results are estimated to be accurate to better than 0.2%.

DEFINITION OF THE ABERRATION COEFFICIENTS

In what follows, we treat only the asymptotic properties[8] of round electrostatic electron lenses. (The results are, of course, equally applicable to ion lenses.) By asymptotic we mean the properties of the lens as viewed from outside the lens field. Thus we treat only physical objects outside of the lens field; otherwise, the objects must be virtual. This is no real limitation since real objects cannot be placed in the field of an electrostatic lens without changing this field and thereby, the properties of the lens.

Following the formulation of Hawkes,[5–7] we specify the incident asymptotic ray by its slopes α_1, γ_1 and by its coordinates x_1, y_1 when projected onto the first focal plane of the lens. Similarly, the emerging asymptotic ray is specified by its slopes α_2, γ_2 and by its coordinates x_2, y_2 when projected onto the second focal plane of the lens. Defining the dimensionless quantities $X_1=x_1/f_2$ and $Y_1=y_1/f_2$, where f_1 and f_2 are the focal lengths of the lens, the coordinates are grouped as system invariants,

$$\begin{aligned} r_1&=X_1^2+Y_1^2 & s_1&=\alpha_1^2+\gamma_1^2 \\ u_1&=X_1\alpha_1+Y_1\gamma_1 & v_1&=X_1\gamma_1-Y_1\alpha_1. \end{aligned} \tag{1}$$

The coefficient of v_1 vanishes for electrostatic lenses.

The third-order properties are derived from a characteristic function V_F which is second order in r_1, s_1, u_1,

$$V_F=(r_1\,s_1\,u_1)\begin{pmatrix} F_{11} & F_{12} & F_{13} \\ 0 & F_{22} & F_{33} \\ 0 & 0 & F_{33} \end{pmatrix}\begin{pmatrix} r_1 \\ s_1 \\ u_1 \end{pmatrix}. \tag{2}$$

In distinction to Hawkes' formulation, we have defined the F's as dimensionless quantities. The aberration equations are given by[5]

$$\begin{aligned} \Delta X_2&=-\frac{\partial V_F}{\partial X_1}+\tfrac{1}{2}\alpha_1 s_1 \\ \Delta\alpha_2&=\frac{\partial V_F}{\partial \alpha_1}-\tfrac{1}{2}X_1 r_1, \end{aligned} \tag{3}$$

with similar equations for ΔY_2 and $\Delta\gamma_2$. Substituting Eq. (2) into Eq. (3) and adding in the first-order terms, we obtain equations valid to third order,

$$\begin{aligned} -X_2 &= \alpha_1+4F_{11}X_1r_1+2F_{12}X_1s_1+2F_{13}X_1u_1+F_{13}\alpha_1r_1 \\ &\quad +(F_{23}-\tfrac{1}{2})\alpha_1s_1+2F_{33}\alpha_1u_1 \\ \alpha_2 &= -X_1+(F_{13}-\tfrac{1}{2})X_1r_1+F_{23}X_1s_1+2F_{33}X_1u_1 \\ &\quad +2F_{12}\alpha_1r_1+4F_{22}\alpha_1s_1+2F_{23}\alpha_1u_1. \end{aligned} \tag{4}$$

Here $X_2=x_2/f_1$, and the corresponding equations for Y_2 and γ_2 are obtained by replacing X_1, α_1 with Y_1, γ_1. We use a sign convention in which f_1 is negative for weak lenses.[9]

DERIVATION OF THE ABERRATION INTEGRALS

To derive integrals for the quantities F_{ij}, it is necessary to obtain the terms of fourth degree in the expansion of

$$m=\sqrt{\phi}(1+x'^2+y'^2)^{\frac{1}{2}}, \tag{5}$$

where $\phi(z)$ is the axial potential distribution. The appropriate dimensionless characteristic function is then

$$V_F=\frac{1}{\sqrt{\phi_1}f_2}\int_{F_1}^{F_2} m^{(4)}dz, \tag{6}$$

where ϕ_1 is the initial axial potential of the lens, and F_1 and F_2 are the positions of the focal points with respect to some reference plane. The quantity m has been given, for example, by Grivet,[10] so that

$$V_F=\frac{1}{\sqrt{\phi_1}}\int_{F_1/f_2}^{F_2/f_2}\left[\sqrt{\phi}\left\{\frac{1}{128}\frac{\phi^{iv}}{\phi}-\left(\frac{\phi''}{\phi}\right)^2\right\}(X^2+Y^2)^2 -\frac{1}{16}\frac{\phi''}{\phi}(X^2+Y^2)(\alpha^2+\gamma^2)-\tfrac{1}{8}(\alpha^2+\gamma^2)^2\right]dZ, \tag{7}$$

where $Z=z/f_2$, and ϕ'', ϕ^{iv} are second and fourth derivatives of ϕ with respect to Z. Note also that because we are calculating asymptotic properties,

$$\int_{F_1/f_2}^{F_2/f_2} \equiv \int_{F_1/f_2}^{-\infty}+\int_{-\infty}^{\infty}+\int_{\infty}^{F_2/f_2}, \tag{8}$$

where the first and last integral on the right involve only straight-line (asymptotic) trajectories.

The integral in Eq. (7) must be evaluated for a general first-order trajectory. We choose the form

$$\begin{aligned} X&=X_1G+\alpha_1H \\ Y&=Y_1G+\gamma_1H, \end{aligned} \tag{9}$$

where G and H are first-order trajectories satisfying

$$\begin{aligned} &\lim_{Z\to-\infty} G(Z)=1 \\ &\lim_{Z\to-\infty} G'(Z)=0 \\ &\lim_{Z\to-\infty} H(Z)=Z-F_1f_2 \\ &\lim_{Z\to-\infty} H'(Z)=1 \end{aligned} \tag{10}$$

and

$$\begin{aligned} &\lim_{Z\to\infty} G(Z)=Z+\frac{F_2}{f_2} \\ &\lim_{Z\to\infty} G'(Z)=-1 \\ &\lim_{Z\to\infty} H(Z)=f_1/f_2 \\ &\lim_{Z\to\infty} H'(Z)=0. \end{aligned} \tag{11}$$

Note that

$$\begin{aligned} \alpha&=X_1G'+\alpha_1H' \\ \gamma&=Y_1G'+\gamma_1H'. \end{aligned} \tag{12}$$

Quantities appearing in the characteristic function V_F must now be expressed as functions of the invariants r_1, s_1, u_1.

$$\begin{aligned} X^2+Y^2&=X_1^2G^2+2X_1\alpha_1GH+\alpha_1^2H^2 \\ &\quad +Y_1^2G^2+2Y_1\gamma_1GH+\gamma_1^2H^2 \\ &=r_1G^2+2u_1GH+s_1H^2 \end{aligned} \tag{13}$$

$$\begin{aligned} X'^2+Y'^2&=\alpha^2+\gamma^2=(X_1G'+\alpha_1H')^2+(Y_1G'+\gamma_1H')^2 \\ &=X_1^2G'^2+2X_1\alpha_1G'H'+\alpha_1^2H'^2 \\ &\quad +Y_1^2G'^2+2Y_1\alpha_1G'H'+\gamma_1^2H'^2 \\ &=r_1G'^2+2u_1G'H'+s_1H'^2, \end{aligned} \tag{14}$$

$$\begin{aligned} (X^2+Y^2)'&=2X\alpha+2Y\gamma \\ &=2(X_1G+\alpha_1H)(X_1G'+\alpha_1H') \\ &\quad +2(Y_1G+\alpha_1H)(Y_1G'+\gamma_1H') \\ &=2r_1GG'+2u_1(G'H+GH')+2s_1HH'. \end{aligned} \tag{15}$$

Putting Eqs. (12–14) into Eq. (7), we obtain

$$V_F=\frac{1}{\sqrt{\phi_1}}\int_{F_1/f_2}^{F_2/f_2}\sqrt{\phi}\left[\frac{1}{128}\left\{\frac{\phi^{iv}}{\phi}-\left(\frac{\phi''}{\phi}\right)^2\right\}(r_1G^2+2u_1GH+s_1H^2)^2 -\frac{1}{16}\frac{\phi''}{\phi}(r_1G^2+2u_1GH+s_1H^2)(r_1G'^2+2u_1G'H'+s_1H'^2) -\tfrac{1}{8}(r_1G'^2+2u_1G'H'+s_1H'^2)^2\right]dZ. \tag{16}$$

Before identifying the aberration coefficients, it is useful to divide the integral into parts involving only asymptotic trajectories and a part involving nonasymptotic trajectories. Assume that the lens field is bounded by $Z=L_1/f_2$ on the left and by $Z=L_2/f_2$ on the right. Then we can take

$$\int_{F_1/f_2}^{F_2/f_2}=\int_{F_1/f_2}^{L_1/f_2}+\int_{L_1/f_2}^{L_2/f_2}+\int_{L_2/f_2}^{F_2/f_2}. \tag{17}$$

Note that the derivatives of ϕ are zero in the first and last integral since the potential is constant outside of the lens field. Using Eqs. (10) and (11) to simplify the first and last integrals, respectively, we obtain

$$V_F=\frac{1}{\sqrt{\phi_1}}\int_{L_1/f_2}^{L_2/f_2}\sqrt{\phi}\Big[\quad\Big]dZ+\tfrac{1}{8}s_1^2\left(\frac{F_1}{f_2}-\frac{L_1}{f_2}\right) +\tfrac{1}{8}r_1^2\left(\frac{L_2}{f_1}-\frac{F_2}{f_1}\right), \tag{18}$$

where the relation $f_2/f_1=(\phi_2/\phi_1)^{\frac{1}{2}}$ has been used to simplify the last term. The term in brackets is the same as in Eq. (16). We could now substitute Eq. (18) into Eqs. (3) and identify the aberration coefficients F_{ij} by comparison with Eqs. (4). However, it is more efficient to identify the aberration coefficients directly from Eq. (18) by comparison with Eq. (2). There results

$$F_{11}=\frac{1}{\sqrt{\phi_1}}\int_{L_1/f_2}^{L_2/f_2}\sqrt{\phi}(LG^4+MG^2G'^2+NG'^4)dZ+\tfrac{1}{8}\left(\frac{L_2}{f_1}-\frac{F_2}{f_1}\right)$$

$$F_{12}=\frac{1}{\sqrt{\phi_1}}\int_{L_1/f_2}^{L_2/f_2}\sqrt{\phi}[2LG^2H^2+M(G^2H'^2+G'^2H^2)+2NG'^2H'^2]dZ$$

$$F_{13}=\frac{1}{\sqrt{\phi_1}}\int_{L_1/f_2}^{L_2/f_2}\sqrt{\phi}[4LG^3H+2M(G^2G'H'+GG'^2H)+4NG'^3H']dZ \qquad (19)$$

$$F_{22}=\frac{1}{\sqrt{\phi_1}}\int_{L_1/f_2}^{L_2/f_2}\sqrt{\phi}(LH^4+MH^2H'^2+NH'^4)dZ+\tfrac{1}{8}\left(\frac{F_1}{f_2}-\frac{L_1}{f_2}\right)$$

$$F_{23}=\frac{1}{\sqrt{\phi_1}}\int_{L_1/f_2}^{L_2/f_2}\sqrt{\phi}[4LGH^3+2M(GHH'^2+G'H'H^2)+4NG'H'^3]dZ$$

$$F_{33}=\frac{1}{\sqrt{\phi_1}}\int_{L_1/f_2}^{L_2/f_2}\sqrt{\phi}(4LG^2H^2+4MGG'HH'+4NG'^2H'^2)dZ,$$

where

$$L=\frac{1}{128}\left[\frac{\phi^{iv}}{\phi}-\left(\frac{\phi''}{\phi}\right)^2\right]$$

$$M=-\frac{1}{16}\frac{\phi''}{\phi} \qquad (20)$$

$$N=-\tfrac{1}{8}.$$

TRANSFORMATION OF THE ABERRATION INTEGRALS

Since calculations of the aberration integrals in Eqs. (19) involve numerical differentiation of the axial potential ϕ, it is advantageous to transform the term in V_F involving the fourth derivative to a term involving lower-ordered derivatives. It is, in fact, always possible to obtain a form involving derivatives of order no higher than the second.[11]

The term we want to reduce is of the form

$$\int\frac{\phi^{iv}}{\phi^{\frac{1}{2}}}f(Z)dZ. \qquad (21)$$

Integration by parts gives

$$\int\frac{\phi^{iv}}{\phi^{\frac{1}{2}}}f(Z)dZ=\frac{\phi'''}{\phi^{\frac{1}{2}}}f(Z)+\int\left[\frac{1}{2}\frac{\phi'''\phi'}{\phi^{\frac{3}{2}}}f(Z)-\frac{\phi'''}{\phi^{\frac{1}{2}}}f'(Z)\right]dZ. \qquad (22)$$

Since the integral is taken between regions of constant potential, the integrated term vanishes. Using Eq. (22) with $f(Z)=(r_1G^2+2u_1GH+s_1H^2)^2$, there results

$$V_F=\frac{1}{\phi_1^{\frac{1}{2}}}\int_{L_1/f_2}^{L_2/f_2}\phi^{\frac{1}{2}}[K_1(r_1G^2+2u_1GH+s_1H^2)^2+L_1(r_1G^2+2u_1GH+s_1H^2)^2\{r_1GG'+u_1(GH'+G'H)+s_1HH'\}+M_1(r_1G^2+2u_1GH+s_1H^2)(r_1G'^2+2u_1G'H'+s_1H^2)+N_1(r_1G'^2+2u_1G'H'+H'^2)^2]dZ+\tfrac{1}{8}r_1^2\left(\frac{L_2}{f_1}-\frac{F_2}{f_1}\right)+\tfrac{1}{8}s_1^2\left(\frac{F_1}{f_2}-\frac{L_1}{f_2}\right), \qquad (23)$$

where

$$K_1=\frac{1}{256}\left\{\frac{\phi'''\phi'}{\phi^2}-2\left(\frac{\phi''}{\phi}\right)^2\right\}$$

$$L_1=-\frac{1}{32}\frac{\phi'''}{\phi} \qquad (24)$$

$$M_1=-\frac{1}{16}\frac{\phi''}{\phi}$$

$$N_1=-\tfrac{1}{8}.$$

The aberration coefficients are again picked out by comparison with Eq. (2), with the following results:

$$F_{11}=\frac{1}{\phi_1^{\frac{1}{2}}}\int_{L_1/f_2}^{L_2/f_2}\phi^{\frac{1}{2}}(K_1G^4+L_1G^3G'+M_1G^2G'^2+N_1G'^4)dZ+\tfrac{1}{8}\left(\frac{L_2}{f_1}-\frac{F_2}{f_1}\right)$$

$$F_{12}=\frac{1}{\phi_1^{\frac{1}{2}}}\int_{L_1/f_2}^{L_2/f_2}\phi^{\frac{1}{2}}[2K_1G^2H^2+L_1(G^2HH'+GG'H^2)+M_1(G^2H'^2+G'^2H^2)+2N_1G'^2H'^2]dZ$$

$$F_{13}=\frac{1}{\phi_1^{\frac{1}{2}}}\int_{L_1/f_2}^{L_2/f_2}\phi^{\frac{1}{2}}[4K_1G^3H+L_1(G^3H'+3G^2G'H)+2M_1(G^2G'H'+GG'^2H)+4N_1G'^3H']dZ \qquad (25)$$

$$F_{22}=\frac{1}{\phi_1^{\frac{1}{2}}}\int_{L_1/f_2}^{L_2/f_2}\phi^{\frac{1}{2}}(K_1H^4+L_1H^3H'+M_1H^2H'^2+N_1H'^4)dZ+\tfrac{1}{8}\left(\frac{F_1}{f_2}-\frac{L_1}{f_2}\right)$$

$$F_{23}=\frac{1}{\phi_1^{\frac{1}{2}}}\int_{L_1/f_2}^{L_2/f_2}\phi^{\frac{1}{2}}[4K_1GH^3+L_1(3GH^2H'+G'H^3)+2M_1(G'H^2H'+GHH'^2)+4N_1G'H'^3]dZ$$

$$F_{33}=\frac{1}{\phi_1^{\frac{1}{2}}}\int_{L_1/f_2}^{L_2/f_2}\phi^{\frac{1}{2}}[4K_1G^2H^2+2L_1(G^2HH'+GG'H^2)+4M_1GG'HH'+4N_1G'^2H'^2]dZ.$$

TABLE I. Aberration coefficients of two-tube lens (accelerating).*

V_2/V_1	F_{11}	F_{12}	F_{13}	F_{22}	F_{23}	F_{33}
1.1	−2.8211 +5	−5.3797 +5	−1.1019 +6	−2.5647 +5	−1.0506 +6	−1.0759 +6
1.3	−5.3566 +3	−9.3971 +3	−2.0067 +4	−4.1212 +3	−1.7601 +4	−1.8793 +4
1.5	−1.0132 +3	−1.6555 +3	−3.6625 +3	−6.7612 +2	−2.9919 +3	−3.3100 +3
2	−1.3889 +2	−1.9715 +2	−4.6739 +2	−6.9851 +1	−3.3143 +2	−3.9328 +2
5	−8.2480 +0	−7.7991 +0	−2.1897 +1	−1.7603 +0	−1.0056 +1	−1.4530 +1
10	−3.1576 +0	−2.3520 +0	−6.7540 +0	−3.6436 −1	−2.2267 +0	−3.5569 +0
20	−1.9197 +0	−1.1931 +0	−3.0810 +0	−1.1719 −1	−6.8744 −1	−1.1177 +0
40	−1.6314 +0	−8.5962 −1	−1.7450 +0	−4.8876 −2	−2.1992 −1	−2.6840 −1
100	−2.0277 +0	−8.0334 −1	−8.8208 −1	−2.0757 −2	+8.8890 −3	+2.3513 −1
250	−3.9950 +0	−1.0223 +0	+2.0568 −1	−1.3734 −2	+1.2958 −1	+5.0646 −1
500	−9.2559 +0	−1.5135 +0	+2.8104 +0	−1.5468 −2	+2.4529 −1	+5.0210 −1
1 000	−3.0556 +1	−2.9398 +0	+1.3866 +1	−2.6986 −2	+5.4952 −1	−4.8604 −1
2 000	−1.7583 +2	−9.6927 +0	+9.0082 +1	−8.4491 −2	+2.1116 +0	−9.5788 +0
5 000	−3.3341 +4	−1.0053 +3	+1.6188 +4	−7.4081 +0	+2.4142 +2	−1.9536 +3
6 600	+2.1750 +7	+5.7857 +5	−1.0032 +7	+3.8462 +3	−1.3340 +5	+1.1566 +6
9 000	+2.0129 +4	+4.8056 +2	−8.6175 +3	+2.7548 +0	−1.0069 +2	+9.1277 +2
10 000	+9.8006 +3	+2.2699 +2	−4.0742 +3	+1.2281 +0	−4.5490 +1	+4.1591 +2

*Last part of each number gives the power of 10.

A further integration by parts of Eq. (22) gives

$$\int \frac{\phi^{iv}}{\phi^{1/2}} f(Z)dZ = \int \left[\frac{\phi''}{\phi^{1/2}} f''(Z) - \frac{\phi''\phi'}{\phi^{3/2}} f'(Z) - \frac{1}{2}\frac{\phi''^2}{\phi^{3/2}} f(Z) + \frac{3}{4}\frac{\phi''\phi'^2}{\phi^{5/2}} f(Z)\right] dZ, \quad (26)$$

where again the integrated terms vanish at the limits of integration. Using Eq. (26) with $f(Z)=(r_1G^2+2u_1GH+s_1H^2)^2$ and using the paraxial ray equation for G and H,

$$G''+\frac{1}{2}\frac{\phi'}{\phi}G'+\frac{1}{4}\frac{\phi''}{\phi}G=0$$
$$H''+\frac{1}{2}\frac{\phi'}{\phi}H'+\frac{1}{4}\frac{\phi''}{\phi}H=0 \quad (27)$$

to eliminate G'' and H'', there results

$$V_F=\frac{1}{\phi_1^{1/2}}\int_{L_1/f_2}^{L_2/f_2} \phi^{1/2}\{K^*(r_1G^2+2u_1GH+s_1H^2)^2 + L^*[r_1GG'+u_1(GH'+G'H)+s_1HH'](r_1G^2+2u_1GH + s_1H^2) + M^*\langle 2[r_1GG'+u_1(GH'+G'H)+s_1HH']^2 - (r_1G'^2+2u_1G'H'+s_1H'^2)(r_1G^2+2u_1GH+s_1H^2)\rangle + N^*(r_1G'^2+2u_1G'H'+s_1H'^2)^2\}dZ + \tfrac{1}{8}r_1^2\left(\frac{L_2}{f_1}-\frac{F_2}{f_1}\right) + \tfrac{1}{8}s_1^2\left(\frac{F_1}{f_2}-\frac{L_1}{f_2}\right), \quad (28)$$

where

$$K^*=\frac{1}{512}\left(3\frac{\phi''\phi'^2}{\phi^3}-10\frac{\phi''^2}{\phi^2}\right)$$
$$L^*=-\frac{3}{64}\frac{\phi''\phi'}{\phi^2}$$
$$M^*=-\frac{1}{32}\frac{\phi''}{\phi} \quad (29)$$
$$N^*=-\tfrac{1}{8}.$$

Again the aberration coefficients are picked by comparison with Eq. (2), with the following results:

$$F_{11}=\frac{1}{\phi_1^{1/2}}\int_{L_1/f_2}^{L_2/f_2}\phi^{1/2}(K^*G^4+L^*G^3G'+M^*G^2G'^2+N^*G'^4)dZ + \tfrac{1}{8}\left(\frac{L_2}{f_1}-\frac{F_2}{f_1}\right)$$

$$F_{12}=\frac{1}{\phi_1^{1/2}}\int_{L_1/f_2}^{L_2/f_2}\phi^{1/2}\{2K^*G^2H^2+L^*(G^2HH'+GG'H^2) + M^*(4GG'HH'-G^2H'^2-G'^2H^2)+2N^*G'^2H'^2\}dZ$$

$$F_{13}=\frac{1}{\phi_1^{1/2}}\int_{L_1/f_2}^{L_2/f_2}\phi^{1/2}\{4K^*G^3H+L^*(G^3H'+3G^2G'H) + 2M^*(G^2G'H'+GG'^2H)+4N^*G'^3H'\}dZ \quad (30)$$

$$F_{22}=\frac{1}{\phi_1^{1/2}}\int_{L_1/f_2}^{L_2/f_2}\phi^{1/2}(K^*H^4+L^*H^3H'+M^*H^2H'^2+N^*H'^4)dZ + \tfrac{1}{8}\left(\frac{F_1}{f_2}-\frac{L_1}{f_2}\right)$$

$$F_{23}=\frac{1}{\phi_1^{1/2}}\int_{L_1/f_2}^{L_2/f_2}\phi^{1/2}\{4K^*GH^3+L^*(3GH^2H'+G'H^3) + 2M^*(GHH'^2+G'H^2H')+4N^*G'H'^3\}dZ$$

$$F_{33}=\frac{1}{\phi_1^{1/2}}\int_{L_1/f_2}^{L_2/f_2}\phi^{1/2}\{4K^*G^2H^2+2L^*(G^2HH'+GG'H^2) + 2M^*(G^2H'^2+G'^2H^2)+4N^*G'^2H'^2\}dZ.$$

ABERRATION COEFFICIENTS FOR A REVERSED LENS

Assuming now that we have carried out the calculation of the aberration coefficients F_{ij} for an accelerating lens we would like to obtain the aberration coefficients of the inverted (decelerating) lens. The aberration integrals for the inverted lens can be written very quickly by interchanging everywhere the subscripts 1 and 2, being careful also to change appropriately the definitions of G, H, Z, and remembering that derivatives should be taken with respect to the transformed Z. Comparison of the new and old aberration integrals gives

$$\begin{aligned} F_{11}^{\mathrm{inv}}&=F_{22} \quad F_{22}^{\mathrm{inv}}=F_{11}\\ F_{12}^{\mathrm{inv}}&=F_{12} \quad F_{23}^{\mathrm{inv}}=F_{13}\\ F_{13}^{\mathrm{inv}}&=F_{23} \quad F_{33}^{\mathrm{inv}}=F_{33}. \end{aligned} \tag{31}$$

Hence the aberration coefficients for the reversed lens are also given simply by interchanging the subscripts 1 and 2. This simple relationship follows directly from our definition of the aberration coefficients as dimensionless quantities. Otherwise, powers of focal lengths would appear.

The aberration coefficients F_{ij}^{inv} are used by substituting them for the F_{ij} in Eq. (4) with subscripts 1 and 2 interchanged on the quantities X, α, r, s, and u.

PETZVAL'S THEOREM

There is a simple relationship between the coefficients F_{12} and F_{33}, in direct analogy with a similar relationship between the coefficients of field curvature and astigmatism in the standard treatment of aberrations. Glaser[12] has called this relationship "Petzval's Theorem" in analogy with a similar relationship in light optics and has shown how to obtain Petzval's Theorem from the aberration integrals.

Consider the quantity $2F_{12}-F_{33}$,

$$\begin{aligned} 2F_{12}-F_{33}&=\frac{4}{\phi_1^{\frac{1}{2}}}\int_{L_1/f_2}^{L_2/f_2}\phi^{\frac{1}{2}}M^*(G^2H'^2-2GG'HH'+G'^2H^2)dZ\\ &=\frac{4}{\phi_1^{\frac{1}{2}}}\int_{L_1/f_2}^{L_2/f_2}\phi^{\frac{1}{2}}M^*(GH'-G'H)^2dZ. \end{aligned} \tag{32}$$

From the Helmholtz–Lagrange Law[13] and Eqs. (10), we have

$$\phi^{\frac{1}{2}}(GH'-G'H)=\mathrm{const}=\phi_1^{\frac{1}{2}}(GH'-G'H)_{L_1/f_2}=\phi_1^{\frac{1}{2}}, \tag{33}$$

and we obtain

$$2F_{12}-F_{33}=-4\phi_1^{\frac{1}{2}}\int_{L_1/f_2}^{L_2/f_2}\frac{M^*}{\phi^{\frac{1}{2}}}dZ=-\frac{\phi_1^{\frac{1}{2}}}{8}\int_{L_1/f_2}^{L_2/f_2}\frac{\phi''}{\phi^{\frac{1}{2}}}dZ. \tag{34}$$

Petzval's Theorem is useful to check the precision with which the aberration integrals are calculated.

EVALUATION OF THE ABERRATION INTEGRALS

The aberration integrals of Eqs. (30) were evaluated for the two-tube electrostatic lens for voltage ratios from 1.1 to 10 000. Results for voltage ratios from 2 to 40 have already been published.[3] Potentials were calculated with a precision of 1 in 10^5 using overrelaxation on a 593×81 network covering the entire lens. Trajectories were calculated using the predictor-corrector method. Details of these methods have already been given.[14] These methods have been used successfully to determine first-order focal properties[9,15,16] and matrix elements[17] to an accuracy of about 0.1%.

Paraxial trajectories G and H were already available from the previous calculations of focal properties,[9,15,16] needing only to be suitably scaled to satisfy Eqs. (10). Axial potentials were calculated using five-point Lagrange interpolation between the five closest mesh points. Derivatives of the axial potential were then obtained from the interpolating polynomial.

The integrals giving the six aberration coefficients were calculated using the Romberg iterative method.[18] This method uses "cautious extrapolation" from results on two or more intervals and gives error estimates. In our calculations, the integrals were required to converge to a precision of 0.1% which required division of each mesh interval into 16 points ($\Delta z=D/1080$, where D is the diameter of the lens).

For some voltage ratios the integrals of both Eqs. (30) and (25) were evaluated and found to give results in agreement to better than 0.1%. The final results were all calculated from Eqs. (30) involving derivatives of the axial potential up to the second order.

RESULTS AND DISCUSSION

Results for the six aberration coefficients for accelerating lenses with voltage ratios from 1.1 to 10 000 are given in Table I. Aberration coefficients for decelerating lenses can be found by using Eqs. (31). Calculations were carried out so as to give a precision of the calculated values of the order of 0.1%. A demonstration of the precision of the calculations is given in Table II, where our values are tested against Petzval's Theorem. For all lenses, with the exception of the weakest lens, Petzval's Theorem is verified to a precision of 0.04% or better. It should be pointed out that, for the weakest lens, calculation of the quantity $2F_{12}-F_{33}$ involves subtracting two numbers of order 10^6 to get a number of order unity. The result is nevertheless accurate to better than 0.3%.

There is no definitive way to estimate the accuracy of the aberration coefficients and there are no previous data available for direct comparison. The axial potentials and first-order trajectories are believed to be accurate to about 0.1%,[9] and as discussed above, the integrals were evaluated

TABLE II. Check of Petzval's theorem.

V_2/V_1	$2F_{12}-F_{33}$	Petzval integral	Relative Difference
1.1	−1.004	−1.00125	2.8×10^{-3}
1.3	−1.00304	−1.00293	1.1×10^{-4}
1.5	−1.00538	−1.005324	5.6×10^{-5}
2	−1.01330	−1.013258	4.1×10^{-5}
5	−1.06857	−1.068557	1.2×10^{-5}
10	−1.147101	−1.147123	1.9×10^{-5}
20	−1.26850	−1.26858	6.3×10^{-5}
40	−1.45084	−1.45084	0
100	−1.841816	−1.841771	2.4×10^{-5}
250	−2.551149	−2.551088	2.4×10^{-5}
500	−3.529150	−3.529047	2.9×10^{-5}
1 000	−5.39356	−5.39575	4.1×10^{-4}
2 000	−9.80653	−9.8057	8.5×10^{-5}
5 000	−56.940	−56.930	1.8×10^{-4}
6 600	494.95	494.87	1.6×10^{-4}
9 000	48.343	48.330	2.7×10^{-4}
10 000	38.0576	38.0463	3.0×10^{-4}

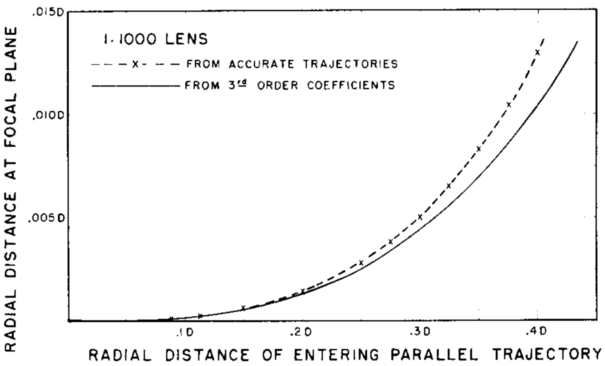

FIG. 1. Radial distance at the second focal plane of a 1:1000 lens for trajectories entering parallel to the axis as a function of the distance of the parallel trajectory from the axis. The smooth curve is calculated from the third-order aberration coefficients. The points are from a full trajectory calculation. Differences are due to fifth and higher order aberrations.

to a precision of better than 0.1%. Since aberration coefficients calculated from the integrals of Eqs. (25) and (30) agreed to better than 0.1% and since these integrals involve derivatives of the axial potential of different orders, we believe that the numerical calculation of derivatives of the axial potential does not introduce an error greater than 0.1%. Over-all, we believe that a conservative estimate of the accuracy of the aberration coefficients is 0.2%. In any case, the aberration coefficients are sufficiently accurate for any practical calculations.

In a previous paper,[3] we calculated spherical aberration coefficients from our coefficients F_{11} and F_{22} for voltage ratios from 2 to 40 and compared them with calculations by Read, Adams, and Soto-Montiel.[19] Agreement was within 0.5% in almost all cases.

Using the aberration coefficients, predictions for uniquely third-order effects can be compared to results obtained from precise trajectories calculated as previously described[14] which contain, in addition, all of the higher order aberrations. Figure 1 shows such a comparison for the lens with a voltage ratio of 1000. Radial distances at the second focal plane are plotted for trajectories entering parallel to the axis at various distances from the axis. For trajectories very close to the axis, the agreement between the third-order deviations and the total deviations is very good. As the distance from the axis increases, the effect of fifth and higher order aberrations is apparent. It should be emphasized that we have presented here a complete set of third-order aberration coefficients for the two-tube electrostatic lens. From these coefficients it is possible to calculate the position and slope to third order of the exit trajectory which corresponds to any incident ray. Since skew trajectories are included, it would be possible to calculate spot diagrams for electrostatic lenses, in analogy with similar calculations in light optics.[20]

From the equations of Verster[21] and of Hawkes,[6] it is possible to calculate the more usual coefficients of spherical aberration, coma, astigmatism, curvature of field, and distortion for any position of the object and aperture.

Finally, we have presented a complete set of aberration integrals with which it is possible to calculate all of the aberrations of an electrostatic lens, given only the axial potential and two independent first-order trajectories. It is hoped that the availability of these integrals will encourage similar calculations for other electrostatic lenses.

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