Angular Aberrations in Sector Shaped Electromagnetic Lenses for Focusing Beams of Charged Particles

EDGAR G. JOHNSON* AND ALFRED O. NIER
Department of Physics, University of Minnesota, Minneapolis, Minnesota
(Received March 13, 1953)

The general expression for the second-order angular aberration of sector shaped electromagnetic lenses consisting of superimposed uniform magnetic and radial electric fields used for the plane focusing of diverging beams of charged particles is derived. The result is applied to the special cases of pure magnetic and pure electric field lenses. The ion optics of a mass spectrometer employing sector electric and magnetic lenses in tandem and which has first-order velocity focusing and second-order angular focusing is obtained.

THE development of electronic techniques and the successful application of mass spectrometers to the measurement of isotopic abundances and gas analyses suggests that a mass spectrometer might be employed advantageously for the precision measurement of atomic masses. A properly designed instrument would have certain immediate advantages over existing mass spectrographs and could in time be developed to the point where it might far surpass these instruments.

An instrument employing magnetic deflection only cannot be employed for the precision determination of atomic masses. The spread in energy of ions from the ion sources limits the resolution. Also, the distribution in the energy spread depends upon the type of ion studied with ion fragments formed from molecules usually having an initial energy obtained in the dissociation process; thus they will be focused in the instrument with lower accelerating voltages than are the molecular ions, and a measurement of their position in the mass spectrum will not be an accurate measure of their mass. Hence, it is customary to employ combinations of electric and magnetic fields which will give double-focusing, i.e., which will focus ions having both a spread in energy and angle as they leave the ion source.

In a mass spectrograph a photographic plate is employed for detecting the ions. Compromises in design are often necessary in order to achieve approximate focusing over a region of the spectrum. Since in a mass spectrometer focusing is required at only one point, it should be possible to achieve a more exact focus.

The sector-shaped electromagnetic lenses usually used in the construction of mass spectrometers are those in which the mean ion beam enters and exits perpendicular to the field boundaries. The first-order ion optical properties of such lenses have been worked out by Herzog[1] and others. In the derivations, variations of the ion beam in mass, energy, distance from optical axis, and angular divergence are limited to sufficiently small percentages of the mean values so that squares, cross products, and higher order terms can be neglected in the treatment. The resolution of systems employing the optical properties is then limited by the effect of these second-order terms, chief of which is the second-order angular aberration. A completely general expression for this aberration is not available in the literature, although formulas applicable to a number of special cases are given by Henneberg,[2] Bruche and Scherzer,[3] and by Hutter.[4] These include all arrangements for pure magnetic lenses; but for pure electric lenses, or for combinations, only cases in which object and image distances are both zero are covered. In none of these special cases, nor in any of the double-focusing systems employing two of them in tandem, can the final second-order angular aberration be reduced to zero. In the next section we shall derive a more general expression for the second-order angular aberration, and in a following section we shall show that arrangements can be constructed in which the second-order angular aberration vanishes. An instrument having this property could employ a relatively large divergence angle and hence have good intensity without a loss in resolution.

DERIVATION OF SECOND-ORDER ANGULAR ABERRATION

To derive the expression for second-order angular aberration we shall, as Herzog did, write the equation of motion of a given charged particle as it approaches, passes through, and leaves an electromagnetic lens. Throughout the treatment the angle of divergence, α, will be considered large enough so that its square and terms proportional to its square will be significant. Variations in other quantities will be considered small enough that their squares and also all cross products can be neglected. The first and most lengthy step will be to find an equation of motion in the lens, or field space, which is accurate to the second order. The procedure will be to express all quantities, including the field intensity, in terms of the mean ion beam and its parameters; and in particular all variables will be expressed as fractional deviations from the mean values so that any power of these variables can be expressed as a convergent power series.

* Present address: Minnesota Mining and Manufacturing Company, St. Paul, Minnesota.
[1] G. Herzog, Z. Physik 89, 447 (1934).
[2] W. Henneberg, Ann. Physik 19, 335 (1934).
[3] E. Bruche and O. Scherzer, *Geometrische Electronenoptik* (Julius Springer, Berlin, 1934).
[4] R. G. E. Hutter, Phys. Rev. 67, 248 (1945).

Consider a sector shaped field area of total angle Φ and coordinates r, ϕ for the particle and with object space and image space to the left and right, respectively, as in Fig. 1. There will be a homogeneous magnetic field of intensity B, perpendicular to the r, ϕ plane, and a cylindrical electric field of intensity $E=E_0r_0/r$, in the opposite direction to the radius vector. The values of B and E_0 must be such that the mean ion beam, consisting of ions of charge e, mass m_0, velocity v_0 and entering perpendicular to the field area at r_0, will describe a circle of radius r_0 and exit again perpendicular to the field boundary and along the optic axis.

If we consider f to be that fraction of the centripetal force produced by the electric field we have

$$f(m_0v_0^2/r_0)=eE_0, \tag{1a}$$

$$(1-f)(m_0v_0^2/r_0)=eBv_0, \tag{1b}$$

and we can express E_0 and B in terms of the mean ion beam parameters and the dimensionless field characteristic f. Thus $f=0$ for a pure magnetic field and $f=1$ for a pure electric field.

Now consider the motion of any given particle with charge e, mass m, and velocity v. Forces on the particle will have components along the unit radius vector $\mathbf{R}_1$, and the unit vector perpendicular to it, $\boldsymbol{\phi}_1$. There will be no forces perpendicular to the r, ϕ plane. The differential equation of motion is:

$$\begin{aligned} m[d^2r/dt^2-r(d\phi/dt)^2]\mathbf{R}_1 &\\ +(1/r)(d/dt)[mr^2d\phi/dt]\boldsymbol{\phi}_1 &\\ =-(eE_0r_0/r)\mathbf{R}_1-e\mathbf{v}\times\mathbf{B} &\\ =-e[Brd\phi/dt+E_0r_0/r]\mathbf{R}_1 &\\ +eB(dr/dt)\boldsymbol{\phi}_1. & \end{aligned} \tag{2}$$

Equation (2) immediately gives two differential equations involving the time rate variation of r and ϕ. Since the equation involving ϕ can easily be integrated to

$$d\phi/dt=eB/2m+C/r^2, \tag{3}$$

where C is a constant of integration; and since

$$dr^2/dt^2=(d\phi/dt)^2(d^2r/d\phi^2) + (d\phi/dt)(dr/d\phi)^2(d/dr)(d\phi/dt), \tag{4}$$

it is possible to eliminate the time variable and obtain the differential equation of r as a function of ϕ. Before doing so let

$$r=r_0(1+\rho), \tag{5a}$$

where ρ will be a numeric representing the fractional deviation of r from the mean value r_0. If we also let:

$$m=m_0(1+\gamma), \tag{5b}$$

$$v=v_0(1+\beta), \tag{5c}$$

γ and β are also numerics representing the fractional

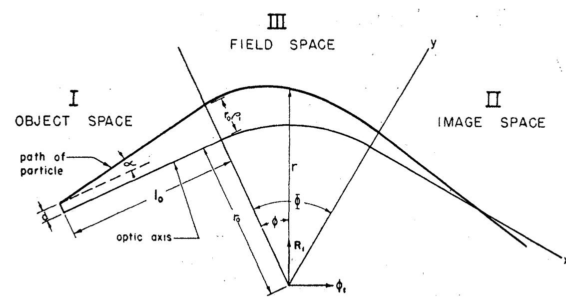

FIG. 1. Diagram showing path of a charged particle through a sector shaped electromagnetic lens. Particle is shown leaving object plane at a distance d from optic axis and at a diverging angle α.

deviations from the mean mass and mean velocity. The dependent variable ρ will be a function of its value at entry into the field area, of γ and β, and of the diverging angle α. If all these are zero ρ will also be zero and the particle will follow the optic axis. Since, in this derivation, α is to be an order of magnitude larger than the other independent variables, ρ and $d\rho/d\phi$ will both be considered roughly proportional to α so that only the cube and higher order terms in ρ and $d\rho/d\phi$ will be neglected. The squares and cross products of γ and β will be neglected.

Substitution of expressions (1a), (1b), (4), (5a), (5b), and (5c) into the coefficient of $\mathbf{R}_1$ in Eq. (2) will result in:

$$\begin{aligned} d^2\rho/d\phi^2-(2C/r_0^2)(d\rho/d\phi)^2(d\phi/dt)^{-1}(1+\rho)^{-3}-(1+\rho) &\\ =-(1+\gamma)^{-1}[(1-f)(v_0/r_0)(1+\rho)(d\phi/dt)^{-1} &\\ +f(v_0^2/r_0^2)(1+\rho)^{-1}(d\phi/dt)^{-2}]. & \end{aligned} \tag{6}$$

From Eq. (3) the constant C and therefore $d\phi/dt$ in general can be evaluated in terms of the angular velocity possessed by the particle at the time of entry into the field area. Using the subscript 1 to denote values at $\phi=0$,

$$(d\phi/dt)_1=(v_1\cos\alpha)/r_1=v_1(1-\tfrac{1}{2}\alpha^2)/[r_0(1+\rho_1)]. \tag{7}$$

A particle entering the field area at a point other than r_0 will undergo a change in energy because of the variation in potential in the cylindrical condenser. By equating energy terms we can solve for v_1 in terms of the initial velocity and the point of entry into the field area. We obtain:

$$C=[1+f-\rho_1^2-f^2\rho_1^2-\alpha^2+2\beta+\gamma-f\gamma]v_0r_0/2, \tag{8}$$

$$\begin{aligned} d\phi/dt=[1-\rho-f\rho+\tfrac{3}{2}\rho^2+\tfrac{3}{2}f\rho^2-\tfrac{1}{2}\rho_1^2 &\\ -\tfrac{1}{2}f^2\rho_1^2-\tfrac{1}{2}\alpha^2+\beta]v_0/r_0. & \end{aligned} \tag{9}$$

Substitution of (8) and (9) in (6) will finally result in an equation in which the mean values m_0, v_0, and r_0 will cancel out, and only the small fractional deviations ρ, ρ_1, α, β, and γ remain. These quantities can all be expanded in convergent power series, and by doing this and dropping all terms of higher than second order we get a differential equation as follows:

$$\begin{aligned} d^2\rho/d\phi^2+(1+f^2)\rho-\delta &= (1+f)(d\rho/d\phi)^2-\tfrac{1}{2}(1+f^2+4f^3)\rho^2 \\ &\quad -\tfrac{1}{2}(1+f+f^2+f^3)\rho_1{}^2-\tfrac{1}{2}(1+f)\alpha^2, \end{aligned} \quad (10)$$

where

$$\delta=\gamma+(1+f)\beta. \quad (10a)$$

The quantity δ represents variation in the particle other than those of position and direction in the ion optical system.

Exact solutions to this type of equation are not known; however, we are interested only in solutions that will satisfy it to a second-order approximation. To find these we can replace the second-order terms on the right by the square of the *first-order* solution and its derivative.

The only first-order terms are those on the left-hand side. When set equal to zero they constitute the differential equation used by Herzog.[1] The solution is straightforward and corresponds to the Gaussian dioptrics of the system. Calling the first-order solution ρ_g we have:

$$\rho_g(\phi)=a\sin((1+f^2)^{\frac{1}{2}}\phi)+b\cos((1+f^2)^{\frac{1}{2}}\phi)+\delta/(1+f^2). \quad (11)$$

a and b are the two constants of integration. The second-order approximation to Eq. (10) is then:

$$\begin{aligned} d^2\rho/d\phi^2+(1+f^2)\rho &= (1+f)(d\rho_g/d\phi)^2 \\ &\quad -\tfrac{1}{2}(1+f^2+4f^3)\rho_g{}^2-\tfrac{1}{2}(1+f+f^2+f^3)\rho_{g1}{}^2 \\ &\quad -\tfrac{1}{2}(1+f)\alpha^2+\delta, \end{aligned} \quad (12)$$

where the right-hand side is a function of ϕ alone.

General solutions to equations of type (12) are known, and it can be shown by the method of undetermined coefficients that a general solution to (12) is

$$\begin{aligned} \rho(\phi) &= a\sin(\kappa\phi)+b\cos(\kappa\phi)+\delta/\kappa^2-\tfrac{1}{4}K_1(a^2+b^2) \\ &\quad +\tfrac{1}{6}K_2ab\sin(2\kappa\phi)-(K_2/12)(a^2-b^2)\cos(2\kappa\phi), \end{aligned} \quad (13)$$

where a and b are the two arbitrary constants of integration and κ, K_1, and K_2 are functions of the field characteristic f defined as

$$\kappa=(1+f^2)^{\frac{1}{2}}, \quad (14a)$$

$$K_1=(1+f^2+4f^3)/\kappa^2, \quad (14b)$$

$$K_2=(3+2f+3f^2+6f^3)/\kappa^2. \quad (14c)$$

The constants of integration are determined by the boundary conditions in the object space (see Fig. 1):

$$\rho(0)=(d+\alpha l_0)/r_0, \quad (15)$$

where d is the object ordinate and l_0 is the object distance; and

$$\rho'(0)=\alpha[1+\rho(0)], \quad (16)$$

since α is equal to the ratio of velocity components at the field boundary. Here the prime signifies derivation with respect to ϕ.

When (15) and (16) are carried out, it can be seen that both a and b contain terms proportional to the first power of α plus terms proportional to α^2. In addition, b also contains terms proportional to δ and d/r_0. We will assume that d/r_0 is a numeric of order equal to or greater than α^2, so that its square and cross product with α can be neglected. This restriction is not detrimental, since in practice object ordinates are either zero or the result of a second-order aberration of a previous system. The constants of integration are then easily evaluated as follows:

$$a=\alpha/\kappa-\alpha^2 l_0(\tfrac{1}{3}K_2-1)/r_0\kappa, \quad (17a)$$

$$\begin{aligned} b &= d/r_0-\delta/\kappa^2+\alpha l_0/r_0+\alpha^2(\tfrac{1}{4}K_1)(1/\kappa^2+l_0{}^2/r_0{}^2) \\ &\quad +\alpha^2(K_2/12)(1/\kappa^2-l_0{}^2/r_0{}^2). \end{aligned} \quad (17b)$$

We can now write an equation of motion for the particle in the image space II (see Fig. 1) with coordinates y and x:

$$y=r_0\rho(\Phi)+x\rho'(\Phi)[1-\rho(\Phi)], \quad (18)$$

where the coefficient of x is the divergence angle as the particle leaves the field area.

Performing operations indicated in (18) and using the above values for the constants of integration we obtain an equation of motion in the image space which can be divided into four groups of terms:

$$\begin{aligned} y &= d\{\cos(\kappa\Phi)-(\kappa x/r_0)\sin(\kappa\Phi)\} \\ &\quad +(r_0\delta/\kappa^2)\{1-\cos(\kappa\Phi)+(\kappa x/r_0)\sin(\kappa\Phi)\} \\ &\quad +\alpha\{(r_0/\kappa-\kappa x l_0/r_0)\sin(\kappa\Phi)+(l_0+x)\cos(\kappa\Phi)\} \\ &\quad +\alpha^2\{[-(\tfrac{1}{3}K_2-1)l_0/\kappa-(3K_1+K_2)x/12\kappa \\ &\quad -(3K_1-K_2)\kappa x l_0{}^2/12r_0{}^2]\sin(\kappa\Phi) \\ &\quad +[(3K_1+K_2)r_0/12\kappa^2+(3K_1-K_2)l_0{}^2/12r_0 \\ &\quad -(\tfrac{1}{3}K_2-1)x l_0/r_0]\cos(\kappa\Phi) \\ &\quad +[K_2 l_0/6\kappa+(\tfrac{1}{6}K_2-\tfrac{1}{2})(1/\kappa^2-l_0{}^2/r_0{}^2)\kappa x] \\ &\quad \times\sin(2\kappa\Phi)+[(\tfrac{1}{3}K_2-1)x l_0/r_0-(1/\kappa^2 \\ &\quad -l_0{}^2/r_0{}^2)r_0K_2/12]\cos(2\kappa\Phi) \\ &\quad -[(1/\kappa^2+l_0{}^2/r_0{}^2)K_1r_0/4]\}. \end{aligned} \quad (19)$$

The largest contribution to this ordinate will, in general, be due to the terms containing the first power of α. Conditions under which the coefficient of α vanishes result in first-order focusing. We shall call all values of x for which this is true l_i, the image distance, and shall also define two new symbols for simplicity as follows: $n_0=l_0/r_0$, ratio of object distance to mean radius, and $n_i=l_i/r_0$, ratio of image distance to mean radius. We then have the well-known conditions for first-order focusing:

$$n_0n_i-1/\kappa^2=(1/\kappa)(n_0+n_i)\cot(\kappa\Phi). \quad (20)$$

Expression (19) without the terms containing α and with $x=l_i$ then becomes the image ordinate at a first-order focal point. The coefficient of d is the magnification M of the system, and the term containing δ is the dispersion D due to the mass and/or velocity difference:

$$M=\cos(\kappa\Phi)-\kappa n_i\sin(\kappa\Phi), \quad (21)$$

$$D=(r_0\delta/\kappa^2)[1-\cos(\kappa\Phi)+\kappa n_i\sin(\kappa\Phi)]. \quad (22)$$

These equations are the same as found previously by Herzog.

The last group of terms in (19) represents the widening of the image due to the square of the diverging angle α and is thus the second-order angular aberration. It is a complicated function of the geometry of the system and of the field characteristic f [see Eqs. (14)]. The geometry of the system is represented by the field angle Φ and the object and image distances. The expression can be simplified if we define a quantity independent of Φ which will express the degree of asymmetry of the system, i.e., the relation between the object and image distances. We define z as:

$$z=\cos(\tan^{-1}(\kappa n_i))/\cos(\tan^{-1}(\kappa n_0)).^{[5,6]} \quad (23)$$

For symmetry $n_0=n_i$ and $z=1$. When $n_i=\infty$, $z=0$; when $n_0=\infty$, $z=\infty$. Then, in terms of z and Φ,

$$\kappa n_i=[1/z+\cos(\kappa\Phi)]/\sin(\kappa\Phi) \quad (24)$$

$$\kappa n_0=[z+\cos(\kappa\Phi)]/\sin(\kappa\Phi). \quad (25)$$

Upon substituting (24) and (25) into the last group of terms in (19), we obtain an expression for the second-order angular aberration which can be reduced by trigonometric manipulation to:

$$L=-\{K_3[(z+1)\csc^2(\kappa\Phi/2)+(z^2-z-1+1/z)\csc^2(\kappa\Phi)]+K_4[z^2+1/z]\}\alpha^2 r_0. \quad (26)$$

Here L is used to denote the second-order angular aberration, and K_3 and K_4 are combinations of K_1 and K_2 such that $K_3=(f+5f^3)/[2(1+f^2)^2]$ and $K_4=(\frac{1}{2}-\frac{1}{3}f+\frac{1}{2}f^2-f^3)/(1+f^2)^2$. The magnification and dispersion are also simplified when expressed in terms of z.

$$M=-1/z, \quad (27)$$

$$D=r_0\delta(1+1/z)/\kappa^2. \quad (28)$$

Equations (26), (27), and (28) express the three most significant properties of sector shaped electromagnetic lenses of the type discussed here.

SPECIAL CASES

The manner in which the second-order angular aberration behaves with changes in any of the independent variables will be examined by considering some special cases.

First consider the aberration when Φ is an integral multiple of π/κ. It will be seen that Eq. (26) fails to yield finite answers. However, correct expressions for these cases can be derived from the last group of terms in Eq. (19). With the help of Eqs. (20), (24), and (25) it can be shown that when Φ is equal to $k\pi/\kappa$, where k is any integer, then z must equal $(-1)^{k+1}$ and n_0 is equal to $-n_i$. Thus, when k is odd,

$$L=-[3K_1+K_2+\kappa^2 n_0^2(3K_1+3K_2-12)]\alpha^2 r_0/6\kappa^2. \quad (29)$$

When k is even, $L=0$. Inspection of Eq. (28) shows that the dispersion D is also zero when k is even. Thus, whenever the field angle is an even multiple of π/κ, the system behaves in the same manner as the well-known 360° pure magnetic case.

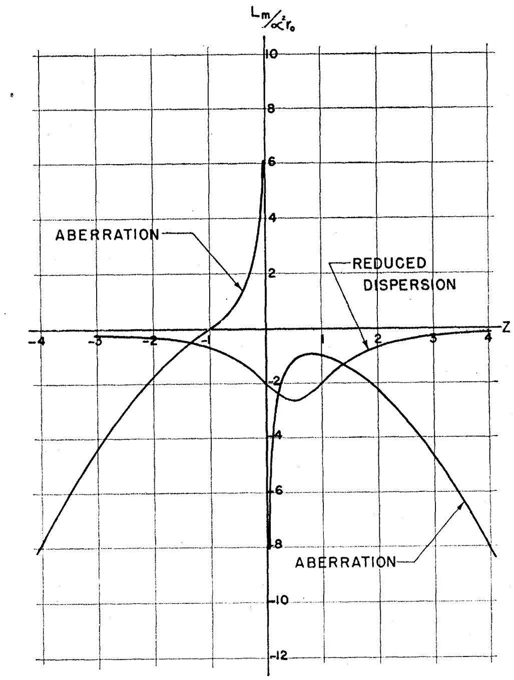

FIG. 2. Angular aberration L_m for pure magnetic sector lens as given by Eq. (30). The ordinate scale for reduced dispersion is the coefficient of δ/α^2 rather than the coefficient of $\alpha^2 r_0$ in Eq. (30).

Pure Magnetic Field

For a pure magnetic field f is equal to zero, $\kappa=1$, $K_3=0$, and $K_4=\frac{1}{2}$. Then (26) becomes

$$L_m=-[z^2+1/z]\alpha^2 r_0/2. \quad (30)$$

This is the same expression as given by Bruche and Scherzer.[3] Figure 2 shows the variation of L_m with z. The second-order angular aberration has its minimum value in an asymmetrical analyzer for which $z=(0.5)^{\frac{1}{3}}=0.794$.

In mass spectrometers employing a sector magnetic field for making mass separations a quantity which is a better "figure of merit" for the resolving power than the dispersion is the "reduced dispersion." It is defined as the ratio of the dispersion to the angular aberration and is obtained by dividing Eq. (28) by (30). Its dependence on z is also plotted in Fig. 2. The maximum absolute value occurs when $z=\frac{1}{2}$. Thus a slightly asym-

[5] With the help of the focusing relationship (20) it can be shown that $\tan^{-1}(\kappa n_i)+\tan^{-1}(\kappa n_0)+\kappa\Phi=\pi$, which reduces to Barber's (reference 6) theorem for the pure magnetic case where $\kappa=1$.

[6] N. F. Barber, Proc. Leeds Phil. Soc. 2, 427 (1933).

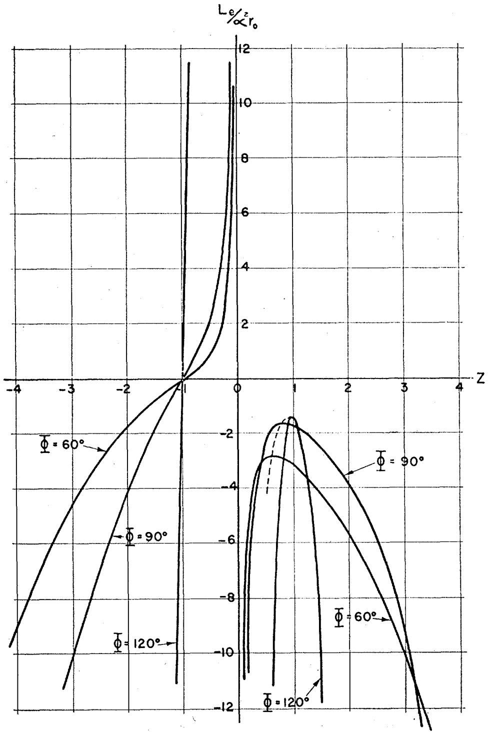

FIG. 3. Angular aberration L_e for pure electric sector lens as given by Eq. (31). Dotted curve shows loci of points of minimum aberration.

metrical analyzer, gives a reduced dispersion $\frac{1}{3}$ higher than the symmetrical analyzer used in most single focusing magnetic deflection mass spectrometers.

Pure Electric Field

For a pure electric field, f is equal to 1, $\kappa=\sqrt{2}$, $K_3=\frac{3}{4}$, and $K_4=-1/12$, and Eq. (26) becomes

$$L_e=-[(3/4)((z+1)\csc^2(\Phi/\sqrt{2}) + (z^2-z-1+1/z)\csc^2(\sqrt{2}\Phi))-(z^2+1/z)/12]\alpha^2 r_0. \quad (31)$$

Unlike the pure magnetic case, the result depends upon the sector angle Φ of the cylindrical condenser, and the expression is more complicated algebraically. However, for any given value of Φ the same type of double branched curve as in the pure magnetic case can be expected. In Fig. 3 is plotted the angular aberration L_e as a function of z for three values of Φ.

As in the magnetic case, the lower right branch of the curve is the most interesting, as the other branch produces the trivial case at $z=-1$. In general the minimum absolute value of the aberration in the right-hand branch occurs for $z<1$. The dotted line traces the path of the minimum which can be seen to approach $-(4/3)\alpha^2 r_0$ as Φ approaches $\pi/2^{\frac{1}{2}}$. Because of the indeterminacy discussed previously, the plot for $\Phi=\pi/2^{\frac{1}{2}}$ would be a semi-infinite line extending down $z=1$ from a value of $-4/3$.

Simple Symmetric Systems With Superimposed Electrostatic and Magnetic Fields

As an example of how the field characteristic f affects the angular aberration consider the symmetric case, i.e., $z=1$. Then from (26):

$$L=-[2K_3\csc^2(\kappa\Phi/2)+2K_4]\alpha^2 r_0. \quad (32)$$

In Fig. 4 we have plotted the value of L for $f=1, \frac{1}{2}, 0, -\frac{1}{2}$, and -1. These five curves give us a general idea of the behavior of the aberration for symmetric cases as we vary the deflecting field from pure electric to pure magnetic, but with both tending to bend the ions in the same direction; and then on into the negative values of f, where the electric and magnetic fields oppose each other but the magnetic predominates.

We see that for the pure electric field the angular aberration has its minimum value of $-4\alpha^2 r_0/3$ for the familiar[7] case, $\Phi=\pi/\sqrt{2}$, when the object and image are located at the boundary of the field. Also, it is seen that for small negative values of f there exist cases where the second-order angular aberration is zero. These cases are of limited interest in our consideration. In general they will not give energy focusing. Also the construction of cylindrical electric condensers of sufficient size to give a uniform field over the region where an ion beam may travel requires a rather large air gap in the magnet with the result that the cost of the magnet and associated power source may be considerable.

SYSTEMS EMPLOYING ELECTRIC AND MAGNETIC FIELDS IN TANDEM

A number of successful double focusing instruments have been constructed employing sector electric and magnetic deflecting fields in tandem. In these systems the image point of the electric field serves as the object point of the magnetic field; and they are so constructed that any small chromatic aberrations occurring in the electric lens are canceled by an equal but opposite aberration in the magnetic lens. The compound system then possesses velocity focusing as well as first-order divergence focusing. Such a compound system is illustrated in Fig. 5. It is especially true in these systems that the second-order angular aberration is the limiting factor in either resolution or intensity. For example, the instrument of Bainbridge and Jordan[8] consists of a $\pi/2^{\frac{1}{2}}$ electrostatic analyzer followed by a 60° symmetric magnetic analyzer. The angular aberration in the electrostatic image plane is $-(4/3)\alpha^2 r_0$. Since the magnification of any symmetric magnetic system is -1, the $-(4/3)\alpha^2 r_0$ will be subtracted from the $-\alpha^2 r_0$ of the magnetic system leaving the net angular aberration as $+\frac{1}{3}\alpha^2 r_0$. The instruments of Dempster[9] and Mattauch[10] have similar residual angular aberrations.

[7] A. L. Hughes and V. Rojansky, Phys. Rev. **34**, 284 (1929).
[8] K. T. Bainbridge and E. B. Jordan, Phys. Rev. **50**, 282 (1936).
[9] A. J. Dempster, Phys. Rev. **51**, 67 (1937).
[10] J. Mattauch, Phys. Rev. **50**, 617 (1936).

With the help of the more general formula for angular aberrations, (26), it can be shown that it is possible to construct instruments which possess both velocity focusing and second-order divergence focusing.

As noted in Fig. 5, the compound system contains eight geometrical parameters: Φ_e, r_e, l_{oe}, l_{ie}, Φ_m, r_m, l_{om}, and l_{im}. The subscript e refers to the electric system and m to the magnetic system. These are not all independent since the first-order focusing relationship (20) must be satisfied for both systems, and also any proportional change could be made on all the lengths involved without changing the characteristics of the system. Basically then, there are five independent variables. For mathematical work it is convenient to consider these as Φ_e, Φ_m, z_e, z_m and the ratio r_e/r_m. To obtain the desired results, two more conditions must be met by these parameters; the final first-order chromatic aberration must be zero and the final second-order angular aberration must also be zero. It is apparent that mathematical solutions will exist even though three of the five variables are arbitrarily specified.

For actual use solutions must be found which also satisfy a number of practical considerations. These are listed below:

1. All quantities must be real and all field angles must be positive.

2. The object and image distances for the electrostatic analyzer should be positive and greater than zero. Correction for the fringing field at entrance and exit can then be made using the calculations of Herzog.[11]

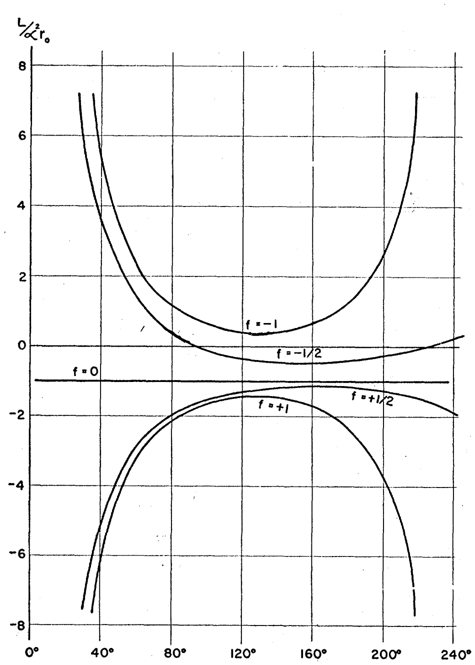

FIG. 4. Angular aberration of several cases of superimposed electric and magnetic symmetric analyzers as a function of the sector angle Φ.

[11] G. Herzog, Z. Physik 97, 596 (1935).

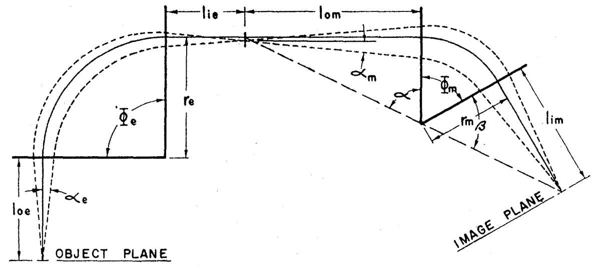

FIG. 5. Typical double focusing system employing electric and magnetic lenses in tandem.

3. The final image slit must be away from magnetic or electric fields so that it will be easy to use various kinds of detection systems for the ions, e.g., an electron multiplier of the Allen[12] type.

4. The ion source should be sufficiently removed from both the electric and magnetic analyzing fields that if an ion source magnet is used for collimating an electron beam in the source, its field will not affect the analyzers.

5. The magnetic field sector must be reasonably small, 90° or less, so that the cost of the magnet will not be unduly high.

6. The apparatus must not have unreasonable dimensional tolerances which would lead to exorbitant expense of construction.

To investigate cases where a combination of velocity focusing and second-order divergence focusing are possible, we will simply solve two simultaneous equations—the first being the velocity focusing condition, and the second the second-order divergence focusing condition.

These are:

$$M_m D_e + D_m = 0, \tag{33}$$

$$M_m L_e + L_m = 0. \tag{33a}$$

The dispersions symbolized by D_e and D_m are those suffered by an ion with the mean mass, m_0, but with a small velocity difference, β (see 5c). The equations can be solved by ordinary algebraic techniques and with the help of the following expressions from the preceding sections:

$$M_m = -1/z_m, \tag{27}$$

$$L_m = -(z_m^2 + 1/z_m)\alpha_m^2 r_m/2, \tag{30}$$

$$L_e = -\{9[(z_e+1)\csc^2(\Phi_e/\sqrt{2}) + (z_e^2 - z_e - 1 + 1/z_e)\csc^2(\sqrt{2}\Phi_e)] - [z_e^2 + 1/z_e]\}\alpha_e^2 r_e/12, \tag{31}$$

or

$$L_e \equiv -\alpha^2 r_e K_e \tag{34}$$

for simplicity. From (28), with $\delta = \beta$ and $\kappa = 1$,

$$D_m = r_m \beta(1 + 1/z_m). \tag{35}$$

[12] J. S. Allen, Phys. Rev. 55, 966 (1939); Rev. Sci. Instr. 18, 739 (1947).

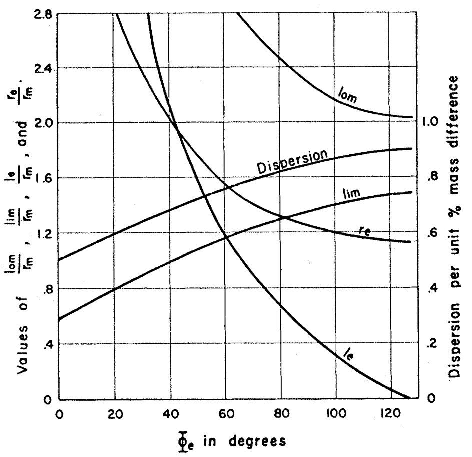

FIG. 6. Variation of ratios of l_{0m}, l_{im}, l_e and r_e to r_m as a function of Φ_e for instruments which employ electric and magnetic sector fields in tandem and for which there is first order velocity and second order angle focusing. Figure also shows corresponding dispersion per r_m per percent of mass difference.

From (28), with $\delta=2\beta$ and $\kappa=\sqrt{2}$,

$$D_e=r_e\beta(1+1/z_e). \quad (36)$$

The square of the divergence angle of the mean beam as it enters the magnetic field, α_m^2, is of course the square of the diverging angle as it leaves the electric field—that is [see (16) and (18)],

$$\alpha_m^2=[\rho'(\Phi_e)]^2=z_e^2\alpha_e^2. \quad (37)$$

Thus in terms of the geometric parameters, Φ_e, Φ_m, z_e, z_m, and r_e/r_m, both (33) and (33a) can be satisfied if

$$z_m=\tfrac{1}{2}\pm[2K_e/(z_e^2+z_e)-\tfrac{3}{4}]^{\frac{1}{2}} \quad (38)$$

and

$$r_e/r_m=(1+z_m)/(1+1/z_e). \quad (39)$$

(39) is the velocity focusing condition which is the same as that derived by first-order theory. The quantity, $2K_e/(z_e^2+z_e)$, which we shall call A for convenience, is a function of Φ_e and z_e. Thus, whenever Φ_e and z_e are such that A is greater than $\frac{3}{4}$, there will be two real values of z_m, at least one of them positive, for which the second order angular aberration is zero. Φ_m, the magnetic field angle, does not enter into the mathematical conditions since, as noted earlier, the actual size of the angle does not influence the magnification, dispersion, or aberrations in a pure magnetic system. It does enter into the practical consideration, however. We shall now investigate the range of values possible in A with two objectives: (1) to find when $A>\frac{3}{4}$ and (2) to find the corresponding values of z_m. This second objective is of interest because of the manner in which the dispersive power of the instrument for a given percentage mass difference, γ, depends on z_m. From (28) with $\delta=\gamma$ and $\kappa=1$:

$$D=r_m\gamma(1+1/z_m). \quad (40)$$

Thus, the smallest possible value of z_m will produce a system with the largest dispersion. In terms of Φ_e and z_e,

$$A=3/2[(1/z_e)\csc^2\sqrt{2}\Phi_e/2+(1-1/z_e)^2\csc^2\sqrt{2}\Phi_e]-(1/6)(1-1/z_e+1/z_e^2). \quad (41)$$

It is evident that, at least for $z_e>0$, A can be easily made as large as desired by reducing the size of Φ_e, so that real values of z_m are assured.

Very small values of z_m could be had if the quantity A were near the value $\frac{3}{4}$. By holding Φ_e fixed and minimizing (41) with respect to z_e, we can find the minimum possible value of A, and the corresponding z_m as well as z_e for any given value of Φ_e. Table I shows minimum values of A and the corresponding values of z_e and z_m for values of Φ_e between 0 and $\pi/\sqrt{2}$ radians. This covers the entire range of possible values for $A_{\min}$ because of the manner in which Φ_e enters into (41). It can be seen that A is always greater than one, and that, therefore, second-order focusing can be achieved with some real and positive values of z_m for any values of Φ_e and z_e. Conversely, however, second-order focusing cannot be achieved in systems in which z_m is between 0 and 1. It can be seen that $A_{\min}$ is quite insensitive to changes in Φ_e. It approaches the value 1 as Φ_e approaches zero, which means very small negative values of z_m; however, when Φ_e is less than about 65°, values of z_e necessary for the minimum values of A are negative. Inspection of (25) will show that this would mean a negative value of the electric field object distance which violates our practical consideration No. 2.

TABLE I. Maximum dispersion mathematically obtainable for various values of Φ_e.

Φ_e	$A_{\min}$	z_e	z_m	Dispersion/$r_m\delta$
0°	1.000	−1.00		
20°	1.050	−1.092	−0.047, 1.047	−10.3, 0.978
40°	1.176	−1.568	−0.153, 1.153	− 2.77, 0.933
60°	1.311	−5.975	−0.249, 1.249	− 1.50, 0.900
80°	1.372	+2.643	−0.289, 1.289	− 1.23, 0.888
100°	1.362	+1.256	−0.282, 1.282	− 1.27, 0.890
120°	1.337	+1.014	−0.266, 1.266	− 1.38, 0.895
127°17′	1.333	+1.00	−0.264, 1.264	− 1.39, 0.896

Practical systems, in which the electric field angle Φ_e is less than 65° can, of course, be constructed. However, z_e must be positive and therefore the values of A will be greater than the minimums listed in Table I. Figure 6 illustrates how, for a given positive value of z_e, the geometric parameters of velocity focusing, second-order divergence focusing mass spectrometers vary with Φ_e. The value of z_e used is +1. Φ_m, the magnetic field angle, has been set at 60° for purposes of calculating values of l_{om} and l_{im}. Values of r_e/r_m and of the dispersion per unit percentage mass difference are independent of Φ_m. The value of r_m has been taken as unity. The value of the dispersion per unit percent mass difference is plotted as a "figure of merit" for the systems. It can be seen to vary from 0.5 to nearly 0.9 as Φ_e approaches $180/\sqrt{2}$ degrees. The dispersion in a typical first-order divergence focusing, velocity focusing instrument such as that of Bainbridge and Jordan[8] is 1.0. It can also be seen that for Φ_e less than 60°, values of r_e, l_{oe}, l_{ie}, and l_{im} become prohibitively large. The best dispersion occurs for $\Phi_e=180/\sqrt{2}$ degrees. However, in this case l_{oe} is 0, so that practical location of ion source (or collector) is not possible. The range between $\Phi_e=60°$ and 120° seems the most practical.

The theory developed here has been used to design a mass spectrometer for precision mass determinations;[13] numerous measurements[14,15] have been made. For this instrument $\Phi_e=90°$ and $\Phi_m=60°$, r_e and r_m are 18.87 and 15.24 cm, respectively. l_{oe}, l_{ie}, l_{om}, and l_{im} are 6.61, 6.61, 34.77, and 20.73 cm, respectively.

[13] A. O. Nier and T. R. Roberts, Phys. Rev. **81**, 507 (1951).
[14] Collins, Nier, and Johnson, Phys. Rev. **84**, 717 (1951); **86**, 408 (1952).
[15] R. E. Halsted, Phys. Rev. **88**, 666 (1952).

PHYSICAL REVIEW VOLUME 91, NUMBER 1 JULY 1, 1953

The Specific Heat Discontinuity in Antiferromagnets and Ferrites*

LOUIS N. HOWARD† AND J. SAMUEL SMART
United States Naval Ordnance Laboratory, White Oak, Maryland
(Received March 24, 1953)

It is shown that, in a molecular field approximation, the internal energy and specific heat of a ferromagnet and antiferromagnet have the same form, regardless of the number of sets of neighbors whose interactions are considered and of the signs of the interactions. The Néel theory is used to derive an expression for the discontinuity in specific heat in ferrites at the Curie temperature. This discontinuity ΔC is in general smaller than it would be for a ferromagnet or antiferromagnet with the same number of atoms. Numerical calculations indicate that for most ferrites ΔC should decrease monotonically as nonmagnetic atoms are substituted for magnetic atoms on the A sites. On the other hand, if the nonmagnetic atoms go on the B sites, ΔC should pass through a maximum.

THE usual approximation of exchange interactions by a molecular field gives an expression

$$E=-\tfrac{1}{2}(NkT_c)3S_0(S_0+1)^{-1}\sigma^2 \qquad (1)$$

for the internal energy of a ferromagnet. Here N is the total number of magnetic atoms, S_0 the spin quantum number of each atom, T_c the Curie temperature, and σ the reduced magnetization. The magnetic contribution to the specific heat of the material is then obtained by differentiating Eq. (1) with respect to T. It is found that at the Curie temperature the specific heat should have a discontinuity given by[1]

$$(\Delta C)_0=5NkS_0(S_0+1)[(S_0+1)^2+S_0^2]^{-1}, \qquad (2)$$

a result which depends only on S_0 and not on the molecular field or the Curie temperature.

It is easy to show that, for the same approximation, the same results obtain, regardless of the number of sets of neighbors whose interactions are considered and of the signs of these interactions if the magnetic atoms all occupy equivalent positions in the lattice. Thus Eqs. (1) and (2) hold for antiferromagnets as well as ferromagnets. Suppose we consider interactions of all sets of neighbors up to and including the ith. Then subdivide the original magnetic lattice into sublattices so that (a) all sublattices are equivalent under the group of translations of the original lattice, (b) each atom has only one kind of neighbors on any other sublattice, and (c) each atom has neither ith nor nearer neighbors on its own sublattice. Let the number of sublattices required be n. Then

$$E=-\tfrac{1}{2}(Ng\mu_B/n)\sum_{j=1}^{n}\mathbf{S}_j\cdot\mathbf{H}_j, \qquad (3)$$

where $\mathbf{S}_j$ is the average net spin on the jth sublattice and $\mathbf{H}_j$ is the molecular field acting on atoms on the jth sublattice. We may write

$$\mathbf{H}_j=\sum_{k=1}^{n}\gamma_{jk}\mathbf{S}_k, \qquad (4)$$

where $\gamma_{jk}\mathbf{S}_k$ is the internal field acting on an atom on the jth sublattice caused by its neighbors on the kth [$\gamma_{kk}=0$, from condition (c)]. Then Eq. (3) may be written in the form

$$E=-\tfrac{1}{2}(Ng\mu_B/n)\mathbf{S}'\gamma\mathbf{S}, \qquad (5)$$

where $\mathbf{S}$ is the column matrix with elements $\mathbf{S}_1, \cdots, \mathbf{S}_n$, $\mathbf{S}'$ is its transpose, and γ is the $n\times n$ matrix with elements γ_{jk}. Now if we use the result that the eigenvalues of γ are given by

$$\gamma\mathbf{S}=3kT_c[g\mu_BS_0(S_0+1)]^{-1}\mathbf{S}, \qquad (6)$$

* This work was supported in part by the U. S. Office of Naval Research.
† Now a National Science Foundation Fellow at Princeton University, Princeton, New Jersey.
[1] See, for instance, J. H. Van Vleck, *The Theory of Electric and Magnetic Susceptibilities* (Oxford University Press, London, 1932), p. 345.