COLOPHON

The attached paper has no connection with my current research in Computer Science and Digital Documents. It is another in my series of experiments to see how long it takes for me to re-build electronic versions of my published early papers as properly re-typeset 'PDF Normal' rather than just as a bitmap scan.

This particular paper appeared in the Journal of Physics section D in 1970. To my surprise this paper has been scanned in by the Institute of Physics and has been converted to PDF in 'Image plus Searchable Text' format. It is available via `http://www.iop.org/EJ/` to journal subscribers.

The fact that the 'underlying text' lay behind the above scanned image meant that I did not need to repeat the OCR process. I extracted the text using Acrobat's text extraction tool and then reformatted the paper using UNIX *troff* to set up the correct typeface (Times) and to get the line and page breaks as accurate as possible.

The five diagrams were extracted from the bitmap PDF version of the paper. They were then cleaned up in Adobe Photoshop and vectorized using Adobe Streamline. The lettering was re-set in Adobe Illustrator, using Helvetica and Helvetica-Oblique, before exporting each diagram to version 3.2 of Illustrator's Encapsulated PostScript (but with no TIFF preview). This Encapsulated PostScript was then incorporated into the paper using *psfig* .

This time taken to rebuild this paper was about 8 hours.

Electric field strengths and ion trajectories in sharp-edge field ionization sources

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Abstract. On the presumption that a sharp edge may be represented by a hyperbola, a conformal transformation method is used to derive electric field equations for a sharp edge suspended above a flat plate. A further transformation is then introduced to give electric field components for a sharp edge suspended above a thin slit. Expressions are deduced for the field strength at the vertex of the edge in both arrangements. The calculated electric field components are used to compute ion trajectories in the simple edge/flat-plate case. The results are considered in relation to future study of ion focusing and unimolecular decomposition of ions in field ionization mass spectrometers.

1. Introduction

Sharp edges such as razor blades and etched metal foils, are being increasingly used in field ionization mass spectrometers. The ion source in these instruments consists solely of a sharp edge suspended parallel to, and a small distance above, a slotted cathode (Robertson and Viney 1966). When a large potential difference is maintained between the edge and cathode, spontaneous ionization of molecules takes place in the vicinity of the edge. A quantitative knowledge of the electric field strength at any point in the ion source is of great importance in the study of ion focusing, unimolecular decay of ionized molecules and threshold field strengths for the ionization process. Equations have already been given for two simple ion source geometries by Brailsford and Robertson (1968) on the presumption that a sharp edge could be represented by a hyperbola of small radius of curvature. One of these arrangements, an edge suspended above a flat plate, is used in this paper as a basis for developing further equations applicable to the edge/slotted-plate case. The use of the calculated electric field components in a simple computation of ion trajectories is illustrated in §5.

2. Edge suspended above a flat plate

Although equations for this arrangement have already been given (Brailsford and Robertson 1968) a rather more satisfactory derivation will be presented briefly here, as many of the results are required for use in the edge/slotted-plate equations of §3.

Let $z = x + \mathrm{i}y$ and $w = u + \mathrm{i}v$. The transformation

$$w = \mathrm{i}k \cosh z \tag{1}$$

where k is a constant, transforms a series of lines parallel to the x axis in the z plane to a series of confocal hyperbolae, symmetric about the v axis, in the w plane (figure 1). The transform of the lines $y = O$ and $y = \frac{1}{2}\pi$ in the w plane resembles two perpendicular plates separated by a gap d. The line $\mathrm{Re}(w) = 0$, $\mathrm{Im}(w) \geq d$ corresponds to the line $y = 0$, and the line $\mathrm{Im}(w) = O$ corresponds to $y = \frac{1}{2}\pi$. A razor blade, or other sharp edge, can be approximated as a hyperbola of small radius of curvature. This hyperbola arises from a line $y = y_0$ (where $y_0 \simeq 0$) in the z plane.

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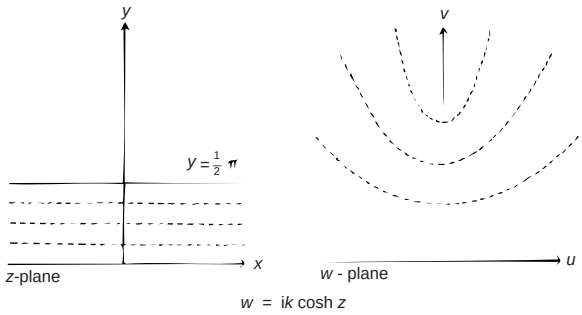

Figure 1. Conformal transformation for edge/flat-plate arrangement. The uniform potential distribution parallel to the *x* axis in the *z* plane is transformed to a series of confocal hyperbolae in the w plane.

Separating real and imaginary parts from equation (1) we have

$$u = -k \sinh x \, \sin y \tag{2}$$

$$v = k \, \cosh x \, \cos y. \tag{3}$$

The inclusion of *i* in the transformation sets up the edge/flat-plate system with symmetry in a vertical plane (as opposed to a horizontal plane in Brailsford and Robertson 1968).

The equations of the hyperbolae in the *w* plane are obtained by eliminating *x* from equations (2)and (3) to give

$$\frac{v^2}{k^2 \cos^2 y} - \frac{u^2}{k^2 \sin^2 y} = 1. \tag{4}$$

The height *l* of the hyperbola representing the edge is obtained by putting $u = 0$, $y = y_0$ in equation (4) to give

$$l = k \cos y_{0.} \tag{5}$$

Since the hyperbolae are symmetric about an axis their vertex radius of curvature r_v can be found from Newton's formula (Starr 1957), which yields

$$r_\mathrm{v} = l \tan^2 y_{0.} \tag{6}$$

Let the potential difference between the two perpendicular plates in the *w* plane be *V*. This is also the potential difference in the 'parallel plate capacitor' formed by the plates $y = ½\pi$ and $y = 0$ in the *z* plane. If we now denote the horizontal and vertical electric field components in the *w* plane as F_u and F_v respectively it is easy to show that

$$F_u = \frac{-V}{(½\pi - y_0)} \, \frac{u \sin y \cos^3 y}{u^2 \cos^4 y + v^2 \sin^4 y} \tag{7}$$

$$F_V = \frac{V}{(½\pi - y_0)} \, \frac{v \cos y \sin^3 y}{u^2 \cos^4 y + v^2 \sin^4 y} \tag{8}$$

At the vertex of the hyperbola representing the edge we have

$$u = 0, \quad y = y_O \simeq 0$$

and thus, from equation (6) we have the further condition $r_\mathrm{v} \ll l$.

Under these conditions, and using equation (6), we find that (7)and (8) simplify to

$$F_u = 0 \tag{9}$$

$$F_{\text{vertex}} = F_v \simeq \frac{2V}{\pi (r_\mathrm{v} \, l)^{½}} \tag{10}$$

3. Sharp edge above a slotted plate

The introduction of a slot into an infinitely thin flat plate is effected by means of the following transformation

$$c = w + \frac{q^2}{4w} \tag{11}$$

where

$$c = a + \mathrm{i}b \quad w = u + \mathrm{i}v$$

and q is a constant. The effect of the transformation is shown in figure 2. Separating real and imaginary parts we obtain

$$a = u + \frac{q^2 u}{4(u^2 + v^{2)}} \tag{12}$$

$$b = v - \frac{q^2 v}{4(u^2 + v^{2)}} \tag{13}$$

where

$$u = -k \sinh x \sin y \tag{14}$$

$$v = k \cosh x \cos y \tag{15}$$

as in §2.

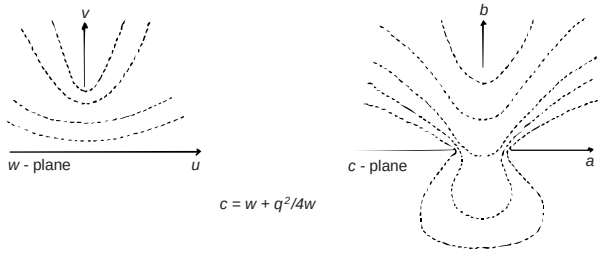

Figure 2. A further conformal transformation to convert from an edge/flat-plate to an edge/slotted-plate arrangement. Equipotentials are shown as broken lines.

The magnitude of the slot width can be found by setting $v = O$ in equation (12) and requiring that $(\partial a/\partial u)_{v=0}$=0. This condition shows that the slot width is $2q$. Transformations of the type shown in equation (11) are very common in the study of systems employing slotted electrodes (Allard and Russell 1963, Kober 1957, Naidu and Westphal 1966). More recently Gilliland and Viney (1968), using this transformation, obtain an expression for vertex field strength in the edge/slotted-plate system. However, for future use in studies on ion trajectories and flight times, as described in §5, we need a more general formulation of the field components at any point in the edge/slot system and this is developed here.

Equations (12) and (13) can be combined to give the equation of curves in the c plane

$$\frac{a}{u} + \frac{b}{v} = 2. \tag{16}$$

Hence

$$u = \frac{av}{2v - b} \tag{17}$$

$$v = \frac{bu}{2u - a}\,. \tag{18}$$

The height h of the curve representing the edge above the slotted plate, is obtained by putting $u = O$ in equation (13) to give

$$h = v - \frac{q^2}{4v}\,. \tag{19}$$

This curve corresponds to the undistorted hyperbola in the *w* plane where $v = l$ (see equation (5)).

By substituting into equation (19) and rearranging we obtain

$$l = \frac{h + (h^2 + q^2)^{1/2}}{2} . \tag{20}$$

The positive root of the quadratic equation for l has to be taken in order that $l \to$ as $q \to 0$.

The vertex radius of curvature s_v of curves in the *c* plane can be related to the corresponding value of r_v in the *w* plane. We find

$$r_v \simeq \frac{4l^2 s_v}{4l^2 + q^2} \tag{21}$$

provided that $8q^2 l r_v \ll 4l^2 + q^2$.

The electric field components $F_a F_b$ in the *c* plane are

$$F_a = F_u \left\{ \frac{2ub(a-u)}{16u^3 - 24au^2 + 2u(5a^2 + b^2 + q^{2)} - aq^2 - ab^2 - a^3} \right\} \tag{22}$$

$$F_b = F_v \left\{ \frac{16v^3 - 20v^2 b + 2v(3b^2 + a^2 + -q^{2)} + bq^2}{32v^3 - 48vu^2 b + 4v(5b^2 + a^2 - q^{2)} + 2bq^2 - 2a^2 b - 2b^3} \right\} . \tag{23}$$

At the edge vertex we know that

$$a = 0, \quad b = h, \quad u = 0, \quad v = l = \frac{h + (h^2 + q)^{1/2}}{2} .$$

These conditions, together with equation (21), will simplify equations (22) and (23) to give the form,

$$F_a = 0 \tag{24}$$

$$F_{\text{vertex}} = F_b \simeq \frac{2V}{\pi\{s_v (h^2 + q^2)^{1/2}\}^{1/2}} \tag{25}$$

provided that $y_0 \simeq 0$ which implies $s_v \ll (h^2 + q^2)^{1/2}$. These validity conditions ensure that the transformed profile in the *c* plane is very close to a hyperbolic shape, as was the case in the *w* plane, Equations (25) and (10) clearly become identical as $q \to 0$.

4. Plotting of equipotentials

In order to check that the transformations used in §§ 2 and 3 were having the desired effect, computations were carried out on the University of London ATLAS computer, to calculate the resulting equipotentials for various values of *x* and *y* substituted into equations (2) and (3) and also into equations (12–(15). Thus the equipotentials in the edge/flat-plate and edge/slot arrangements were obtained. As the ATLAS computer did not have graph plotting facilities, a graph plotting sub-routine was written into the computer program to plot out the transformed coordinates on the computer's line printer output. The results are shown in figures 3 and 4. The equipotentials in both cases are labelled with the value of *y* in the *z* plane which generates them. The values taken for slot width, height and radius of curvature were

$$q = 0.25 \text{ mm} \quad h = 0.25\text{mm} \quad s_v = 0.1\mu\text{m}.$$

These correspond closely to values encountered in practice (Brailsford 1969). The hyperbolic nature of the equipotentials is evident in figure 3 while figure 4 shows the nature of field penetration through the slot in the edge/slot system.

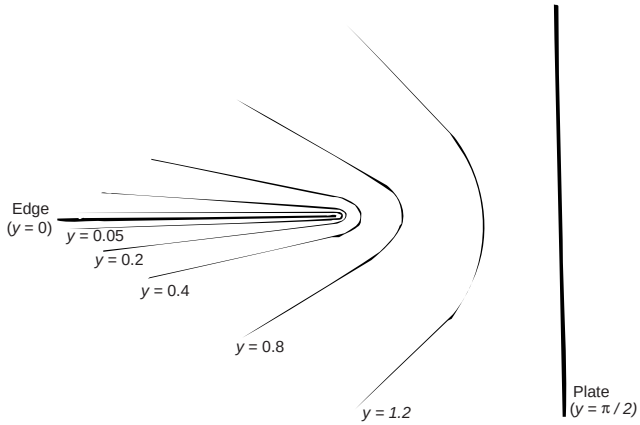

Figure 3. Computer calculated potential distribution in the edge/flat-plate system. Equipotentials are labelled with the value of y in the z plane which generates them.

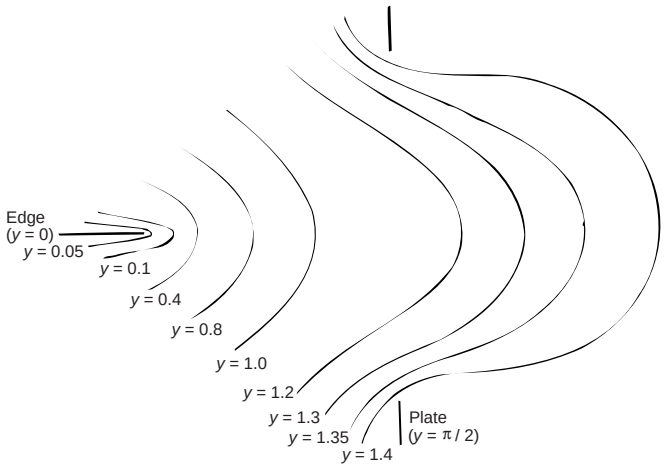

Figure 4. Computer calculated potential distribution in the edge/slotted-plate system. Equipotentials are again labelled with the value of y in the z plane which generates them.

5. Computation of ion trajectories and flight times

Many experimental and numerical methods exist for determining the trajectories of electrons and ions in a known potential distribution (Klemperer 1953). A particularly accurate numerical method, due to Goddard (1944), is based solely on the equations of motion of a charged particle in an electromagnetic field and involves no paraxial approximation. This method was used in a pilot calculation of ion trajectories in the calculated potential distribution of the edge/flat-plate arrangement. For a two dimensional problem, in a purely electrostatic field and a Cartesian coordinate system (x,y), the equations of motion, for particles of mass m and charge e, simplify to

$$m\frac{\mathrm{d}^2x}{\mathrm{d}t^2} = -e\frac{\partial V}{\partial x} \tag{26}$$

$$m\frac{\mathrm{d}^2y}{\mathrm{d}t^2} = -e\frac{\partial V}{\partial y} \tag{27}$$

The conformal transformations of §§ 2 and 3 give the electric field components $\partial V/\partial x$ and $\partial V/\partial y$ directly.

The Goddard method performs a stepwise integration of equations (26) and (27) to give position coordinates using a formula due to Milne (1933). A single-stage integration may also be performed, using Weddle's rule, to give x and y components of velocity at any point. Denoting these velocities as x' and y' respectively we can write

$$\tfrac{1}{2}m(x'^2+y'^2)=e\Delta V \tag{28}$$

where ΔV is the potential fallen through by the ions. Equation (28) is valid for charged particles initially at rest in the potential field, and by separately evaluating the two sides of this equation we have a means of checking the accuracy of the numerical integration.

The computer program using the above numerical integration procedure was written for the University of London ATLAS computer using EXCHLF autocode. In the early stages of the computation the time interval Δt used in the stepwise integration, was set at 10^{-14} seconds. The time interval was doubled after every 100 points computed to avoid excessive storage and time demands on the computer. A continuous check was maintained that both sides of equation (28) agreed to within 1%. If at any stage this was found not to be so, provision was made in the program for recalculating the relevant part of the trajectory with Δt set at a smaller value.

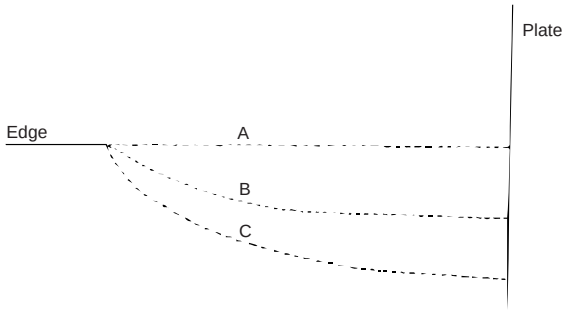

Figure 5. Typical trajectories in the edge/flat-plate system for ions of $m/e = 45$ and for three values of initial angle relative to the horizontal axis. Initial angles (relative to horizontal axis): A, 0°; B, 20°; C, 45°.

Three computed ion trajectories in the edge/flat-plate system are shown in figure 5 using the following parameters: $l = 0.25\text{mm}, r_v = 0.1\mu m, V = 8600v, m/e = 45$.

The ions were started off from rest at various positions on the edge hyperbola so that the initial trajectory angles, relative to the horizontal axis, were 0°, 20° and 45°. The total flight time from edge to plate of the 0° ions was 1.8 ns. The overall focusing effect of the accelerating field between edge and plate can clearly be seen.

6. Discussion

The transformations described in §§ 2 and 3 give useful formulae for the electric field at a sharp edge in the presence of two types of cathode. The electric field strengths obtained are cross section and take no account of end effects or surface roughness. Neglect of these factors seems justified at least for razor blades (Brailsford and Robertson 1968). Gilliland and Viney (1968) have shown that the geometrical form of the material lying behind the sharp edge has only a small effect on the vertex field strength.

The calculation of ion trajectories, using the general equations for electric field components given in §2, can be carried out relatively easily. Naidu and Westphal (1966) have studied ion focusing in an electron impact mass spectrometer by regarding the ion source and focusing system as being composed of several separate sub-units. They obtain field components in each sub-unit by the use of appropriate conformal transformations. The electric fields in an electron impact source are rather lower than in a field ion source, but in

principle there is no reason why similar calculations should not be carried out for a field ionization mass spectrometer.

The program described in §5 is presently being extended to deal with the edge/slotted-plate configuration. Flight times of ions obtained from these studies are being used to investigate the kinetics of unimolecular decomposition of molecular ions in high fields (P. J. Derrick and A. J. B. Robertson, to be published).

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