Simple electrodes for quadrupole ion traps

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Quadrupole traps for charged particles often involve electrodes with portions carefully machined to the shape of hyperboloids. It is shown here that the more important features of such traps can be achieved using electrode shapes which are much easier to fabricate. Detailed numerical calculations are reported on some sample electrodes. The numerical method can be easily extended to other shapes which accommodate specialized laboratory situations.

I. INTRODUCTION

Quadrupole ion traps are used in a wide variety of research applications. It is well known that it is not possible to construct static electric fields which will trap ions in all three dimensions. However, it is possible to build an effective trap by either adding a magnetic field[1] (Penning trap) or by making the electric field time dependent[2] (Paul trap). For many applications it is desirable to achieve a special electric-potential function which is referred to below as the "ideal." It is generally desirable for the electric-potential function to have both cylindrical and reflection symmetry. With these symmetry restrictions, a general potential can be expressed in the form,

$$V(r,z) = C_0 + C_2 H_2(r,z) + C_4 H_4(r,z)$$
$$+ C_6 H_6(r,z) + C_8 H_8(r,z) + \dots , \qquad (1)$$

where

$$H_2(r,z) = (2z^2 - r^2)/s^2 ,$$
$$H_4(r,z) = (8z^4 - 24z^2 r^2 + 3r^4)/s^4 ,$$
$$H_6(r,z) = (16z^6 - 120z^4 r^2 + 90z^2 r^4 - 5r^6)/s^6 ,$$
$$H_8(r,z) = (128z^8 - 1792z^6 r^2 + 3360z^4 r^4$$
$$- 1120z^2 r^6 + 35r^8)/s^8 .$$

The H_j functions (spherical harmonics) are homogeneous polynomials in z/s, r/s with the numerical coefficients chosen so that each satisfies the Laplace equation. The C_j are constants (independent of position) with the units of potential, and s is a distance to be chosen to suit the circumstances of the problem. The ideal potential referred to above corresponds to the first two terms of this expansion. A special quality of the ideal potential is that the equations of motion of trapped particles are particularly simple. For instance, for the Paul trap, the r and z components have separate equations of motion, making it relatively easy to specify stability criteria. Also, in a Penning trap, the ideal potential yields axial, cyclotron, and magnetron frequencies which are independent of the amplitude of excitation (neglecting relativistic effects). Thus a trap with the ideal potential is sometimes described as "harmonic." Some relatively recent reviews cover both the operations and the applications.[3,4]

II. THE PROBLEM

To achieve the ideal potential represented by the first two terms of Eq. (1), three electrodes are needed, each a hyperboloid (and therefore infinite in extent). The electrodes which produce the ideal potential are referred to below as ideal electrodes. The three electrodes, each conforming to an equipotential surface of the ideal potential function, consist of a central "ring" electrode and "endcaps" on either side. Some errors are caused by making finite electrodes; however, these can be minimized by careful treatment of the truncation boundaries.[5] The hyperbolic electrodes are difficult to fabricate and for many purposes it is worth considering a much simpler shape. The purpose of this paper is to point out that it is possible to achieve a good approximation to the ideal with very simple electrodes.

The electrode structures examined below have the same general topology as the ideal electrodes. They have cylindrical and reflection symmetry, and involve a region of space substantially surrounded by a ring and two endcaps. To preserve the reflection symmetry, the two endcap electrodes must have the same potential (assuming they have the same shape). By appropriate choice of the potentials of the two free electrodes, it is possible to make C_0 and C_2 match any preset conditions. To make the other terms small with a three-electrode system, it is necessary to choose the shapes of the electrodes carefully. A more general version of Eq. (1) involves terms with odd powers of z and r, and also terms involving the angle coordinate. Such terms are not included here because it is easy to choose experimental conditions which, in principle, make them zero. If the electrodes and applied potentials have reflection symmetry, the odd-order terms will all be zero, and if the electrodes have cylindrical symmetry, the terms involving the angle coordinate all vanish. In practice, errors in fabrication or mounting (also nonuniform contact potentials) can cause these terms to be nonzero. The term of order one $[C_1 H_1(r,z)]$ caused by these laboratory errors can be made small by either choosing a different origin of coordinates for the expansion, or by making the endcap potentials unequal. If the machining and mounting are precise enough to make the third-order term small, then it is appropriate to look for electrode shapes which make the fourth-order term small.

Some example calculations are reported below to show that simple electrodes are capable of adequately producing the ideal potential over a substantial volume. The basic computational method as it applies here is described in some detail in Ref. 5. The general method has previously been used by Harting and Read[6] for electron lens calculations. Only a brief summary of the method is given here. In this
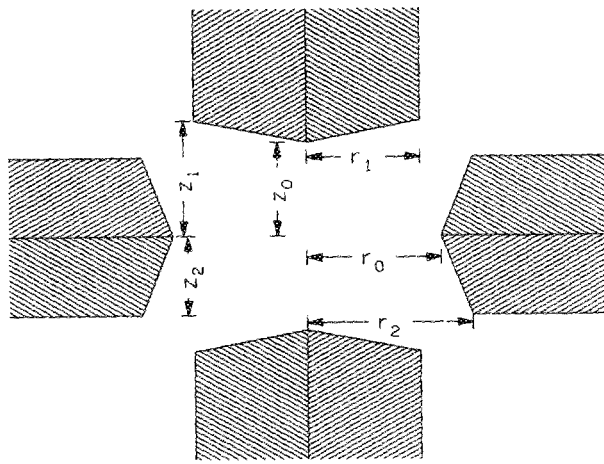
FIG. 1. A drawing of the trap geometry examined in this paper. The electrodes are cylindrically symmetric about the z axis.

FIG. 2. Sample plot of the potential function $V(r,z)$ vs z for three values of r.

procedure the surface-charge density on all the electrode surfaces is determined numerically, using the condition that the potential is known on all the electrode surfaces. Then either the C_j or the potential can be calculated by application of Coulomb's law. The numerical representation of the surface-charge density involves the arbitrary division of the electrode surfaces into N small areas each of which has approximately uniform surface charge density across it. The surface-charge distribution is represented by giving N numbers, each of which provides the assumed constant surface-charge density on one of the surface elements. One of the principal computational chores is the solution of N linear algebraic equations. The values of N used were of the order of 100. Much larger values of N require a large amount of computation time and tend to cause digital truncation error to be a significant problem. Much smaller values of N cause unacceptable errors in the results.

III. RESULTS

A diagram of the example electrode shape examined in this paper is displayed in Fig. 1. Detailed calculations of the surface-charge densities have been carried out for a variety of the variables defined in Fig. 1. By using a simple search procedure it is easy to find values of the dimensions which yield small values of C_4. It is even reasonable to search for conditions which make C_6 small also. In the following dis-
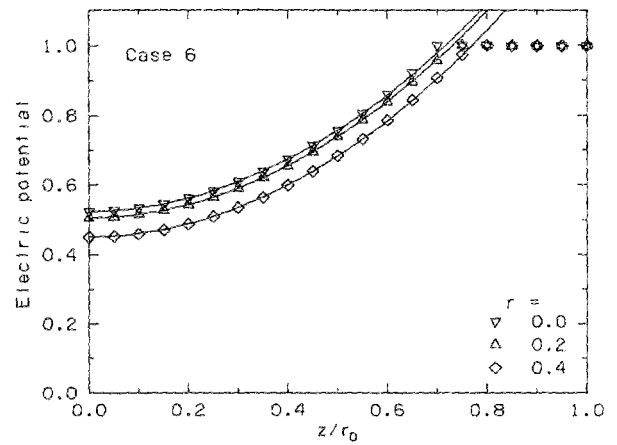
cussion, all dimensions are given relative to r_0 and the length variables are therefore treated as dimensionless.

The C_j are each linear functions of each of the electrode potentials. The zero of potential is arbitrary and here the potential is assumed to approach zero far from the electrodes. For the purposes of this paper it is not necessary to have a completely general solution. The values of C_j were calculated for a specific set of potentials on the electrodes. These special values of C_j are called A_j. The reference set of potentials are 0 for the ring and 1 for the endcaps (as defined here the A_j have the same units as the endcap potential). Scaling the results to other values of the endcap potential is straightforward. These results cannot be generally scaled to other ring potentials; however, in most circumstances it is only the potential difference between the endcaps and the ring which is important (for a more complete discussion see Ref. 5). A general solution would involve generating a second set of C_j with other values for the electrode potentials, including a nonzero value for the ring potential. The distance s in Eq. (1) is assigned the value r_0. With these normalizations the set of A_j are functions of the shape of the electrodes and are independent of the size or the potentials which are applied to the electrodes in use.

Table I contains results for eight cases which have been found to yield $A_4 = A_6 = 0$. Figure 2 displays the potential for case six as a function of axial position. The data points in the graphs are the calculated values and the solid lines are the ideal potentials as represented by the first two terms of

TABLE I. Data for eight sets of values for the variables defined in Fig. 1. The dimensions were selected to yield $A_4 = A_6 = 0$. The dimensions specified have been scaled to the condition $r_0 = 1$. The A_j are the spherical harmonic expansion coefficients with normalized potentials on the electrodes.

|	z_0	r_1	z_1	r_2	z_2	A_0	A_2	A_8
1	0.6122	0.8812	0.7952	1.1020	0.5913	0.545486	0.568051	0.002312
2	0.7000	0.6856	0.8182	1.0462	0.2678	0.497635	0.489588	0.000142
3	0.7000	0.6950	0.8197	1.1147	0.2949	0.508734	0.478829	0.000103
4	0.7000	0.7095	0.8224	1.3654	0.4438	0.524285	0.463748	0.000053
5	0.7000	0.7799	0.8518	1.1000	0.4000	0.492112	0.488948	0.000623
6	0.7071	0.8435	0.8728	1.2340	0.5956	0.493999	0.476988	0.000569
7	0.8000	0.7884	0.9356	1.2030	0.4569	0.441861	0.416657	0.000025
8	0.8000	0.8841	0.9683	1.2224	0.5573	0.435476	0.417169	0.000177

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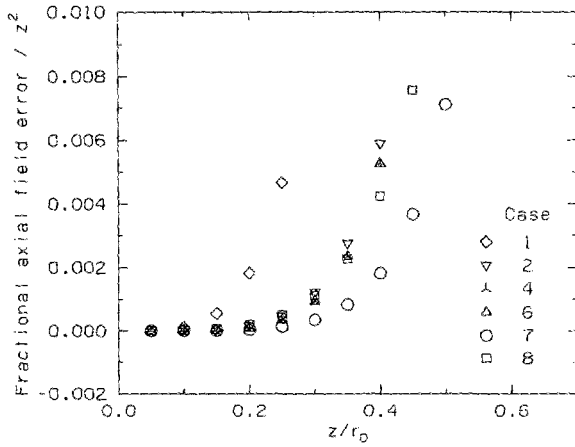
FIG. 3. Plot of E_f/z^2 vs displacement from the center of the trap. E_f is the fractional error in the electric field on the axis.

Eq. (1). Data are shown for $r = 0$, 0.2, and 0.4. Equation (1) with values of C_j derived from Table I can be used to calculate the potential near the center of the trap. Near the walls Eq. (1) is generally useless because too many terms contribute significantly to the sum. The data of Fig. 2 were calculated directly from the charge distributions without involving Eq. (1). The potential is reasonably close to the ideal all the way to the endcap.

The electric field on the z axis can be relatively easily calculated from the surface-charge distributions (the derivative of the potential can be done analytically). The electric field on the z axis corresponding to the ideal potential is $2A_2z$. The fractional error in the electric field is given by

$$E_f = \left(\frac{\partial V}{\partial z} - 2A_2z\right)\bigg/2A_2z$$

$$= 16\frac{A_4}{A_2}z^2 + 48\frac{A_6}{A_2}z^4 + 512\frac{A_8}{A_2}z^6 + \dots .$$

Figure 3 is a plot of E_f/z^2 vs z for several of the cases of Table I. The limit of these curves as z goes to zero is $16A_4/A_2$, a quantity which is small by design. The field errors displayed in Fig. 3 are all positive because the electrode shape chosen here has a sharp point on the z axis. This point contributes particularly large fields in a small volume near the point. Away from the polar axis the electric field is not necessarily in the same direction as the ideal, making a comparison more difficult. While the departures from the ideal are more difficult to display in other regions, the data of Fig. 3 are reasonably representative. Two of the cases are not included in the plot because case 3 is similar to case 2, and case 5 is similar to case 6.

Case 7 of Table I has the best value of A_8/A_2 suggesting that it might be a particularly favorable choice. Actually, any of these cases may be difficult to implement with enough precision to make the eighth-order term the dominant error in a laboratory situation. Case 1 has a small ring-endcap gap providing good shielding from external fields. Cases 2, 3, and 4 have a relatively large ring-endcap gap allowing easy access with light beams, etc. Case 6, also relatively open, has

already been used in an atomic spectroscopy application.[7] It may be helpful in visualizing the shapes to know that the diagram of Fig. 1 was drawn using the dimensions of case 6 from the table. For some purposes it would have been better to have a hole in the endcaps on the $r = 0$ axis (instead of a point), thereby reducing the electric-field anomaly and allowing a convenient access for ions, electron beams, etc. Such holes would not have greatly complicated the computations, and unless they were very large, they would not have interfered with making A_4 and A_6 small.

An investigation of the errors in the general method was reported in Ref. 5. Less extensive tests conducted in conjunction with the generation of the data of Table I confirm the general conclusion that the principal errors were due to representing the charge distribution on too coarse a grid. The grid used was kept relatively coarse to speed the calculation through the tedious search. Any small errors in the A_0 and A_2 can be easily compensated for by adjusting the potentials applied to the electrodes. Errors in the computation of A_4 and A_6 result in errors in the five length variables of Table I. The length data given in the table are estimated to have approximately four digit accuracy.

Might electrodes such as those of Fig. 1 be more sensitive to misalignments than hyperbolic electrodes? An easy and useful test is to make a small change in one of the dimensions and repeat the calculation to observe the change in the A_j. Tests made in conjunction with the work of Ref. 5 but not reported there yield the result that $\partial A_2/\partial z_0 = -0.72$ and $\partial A_4/\partial z_0 = 0.04$ for the case of ideal electrodes with $2z_0^2 = r_0^2$ (z_0 is the distance from the trap center to each of the endcaps). In changing z_0 both endcaps were displaced but their shape was not changed. Such tests were carried out both with truncated hyperbolas and with the design of Fig. 1. Some of the cases of Table I were found to have A_4 about twice as sensitive to this displacement as the ideal electrodes cited. Similar sensitivities were also found for truncated hyperbolas. A conclusion is that the electrodes examined here are not significantly more sensitive to laboratory errors than those with hyperbolic shapes.

In Fig. 1 the electrodes extend beyond the boundaries of the drawing. An assumption was made that in practice the portion off the drawing would involve wires and mounting brackets special to the particular installation. Thus, the impact of various ways of handling the remote portions was not systematically investigated. For the results of Table I electrodes were extended a short distance and simply terminated. In each case the straight boundaries parallel to the axes had a length of $1.5r_0$. To test the sensitivity to this dimension, some of the calculations were repeated with both ring and endcap extended by an additional $0.5r_0$. For cases 1, 4, and 7, the changes in A_4 were $(-1, -17, -10) \times 10^{-5}$, respectively. Generally, increasing the size of the endcap increases A_4, and expanding the ring decreases it. If the ring and endcap are close together, the region near the center of the trap is shielded from charges on the more remote parts of the electrodes. For cases where the intrinsic shielding is inadequate a reasonable step is to insert a relatively large extra electrode and empirically adjust its potential to produce optimum performance.

IV. DISCUSSION

Some general comments can be made about the use of the data of Table I in applications needing the ideal potential. In a common form of the problem the potential must approximate the ideal to some specified tolerance over a specified volume. This means that C_0 and C_2 have specified values, and limits are available for the other C_j. To meet these requirements with hyperbolic electrodes is straightforward with the condition that the minimum electrode size be large enough not to intrude on the specified volume. To meet these requirements with the electrodes of Fig. 1, it is necessary to have larger values of r_0 and z_0 (perhaps by a factor of 2 or 3) and therefore higher potentials.

An application where simple electrodes might be useful is mass spectroscopy. In one kind of mass spectrometer, the electric potentials are made time dependent in such a way that ions with small masses have unstable orbits for one reason, and ions with large masses have unstable orbits for another reason.[8] With the ideal potential the stability conditions are well defined and it is possible to create a situation in which only ions in a narrow mass range have stable orbits. Particles with unstable orbits leave the trap rather quickly. Also some of the particles in stable orbits are removed because the orbits intersect one of the electrodes. Many such traps have been built and found to give good service. It is clearly possible to arrange the electrodes of Fig. 1 (or other simple shapes) such that near the trap center the orbits of the ions and the stability conditions are not materially changed. A failing of the simple electrodes is that near the electrode surfaces the orbits are much more complex, blurring the distinction between stable and unstable orbits. Ions near the center which fail to meet the stability conditions will move out where the fringing field may produce stability or at least a long lifetime. The impact of this problem on mass resolution can't be easily evaluated. Fulford *et al.* and Mather *et al.*[9] experimentally investigated the performance of some traps that had cylindrical rings and plane endcaps. They found the mass resolution to be significantly lower than they were accustomed to finding with hyperbolic electrodes. It is not clear what the specific failing of the cylindrical traps was. The design has the endcap and ring quite close together, resulting in high electric fields in a place easily available to the trapped particles. Also, as implemented, the endcaps had large holes such that A_4 may not have been small.

In some precise atomic physics measurements the potential function must be very close to the ideal. In many of these experiments the precise fields are achieved by having a way to compress the cloud of ions into a relatively small volume near the center of the trap.[4] While the electrodes used have typically been modified hyperbolas, in some cases extra "compensation" electrodes have been added so that C_4 can be electrically adjusted to zero.[10] In many of these experiments it is important to closely approximate the ideal field near the trap center while giving little concern to irregularities near the electrodes. For this situation the design of Fig. 1 is quite appropriate. It might be desirable to add electrodes to a design such as that in Fig. 1 to allow compensation for some mounting errors. There is a significant need for the extra electrodes to have both reflection and rotation symmetry, with the penalty that it would be possible to compensate only those errors with these symmetries.

Gabrielse and MacKintosh[11] have examined the electrostatic properties of cylindrical traps where it is possible to solve the Laplace equation using series methods. They show that A_4 can be made zero by appropriate choice of the ratio of height to radius. They also consider the option of dividing the cylindrical ring electrode into three parts such that the outer two can be used as compensation electrodes. This arrangement allows the user to empirically adjust A_4 to zero after assembly is complete. This analysis is based on very small interelectrode gaps. While a practical design may require larger gaps and other holes, the adjustment should have enough latitude to cover these problems. This is a good example of how extra electrodes can be used to compensate for incomplete design information. For the case of the Penning trap the potentials normally do not vary rapidly with time and the potentials for the extra electrodes can be derived from a simple resistive divider network. In Paul traps, high-frequency potentials are needed and the divider network is not so easy to adjust. Also, in many applications the test for small A_4 is very difficult.

V. CONCLUSIONS

Normally the most effective way to generate a close approximation to the ideal potential distribution is to use hyperbolic-shaped electrodes. This is especially true if the application demands that the close approximation extend all the way to the electrodes. The only intrinsic problem with hyperbolic electrodes is the truncation. The truncation errors can be made small either by careful design[5] or by inserting compensation electrodes.[10] Practical problems with hyperbolic electrodes are that they are difficult to fabricate and, in some applications, it is necessary to make holes which spoil the ideal fields. The simple electrodes discussed above can, in some applications, be adequate and much easier to fabricate. With electrodes requiring only simple lathe cuts it is possible to be rather free with making access holes and special mounting fixtures, while preserving some of the more important features of the potential distribution. In circumstances where the dominant errors in the potential function are caused by alignment or machining errors, the simple electrodes may have a positive advantage.

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