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An approximate image solution method for the electrostatic quadrupole lens

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While no simple image method exists that yields an exact solution for the potential around the parallel conducting cylinders of a quadrupole electrostatic lens, we have found that using two line image charges in each cylinder makes an excellent approximation. Graphs are presented of the equipotentials and contours of electric field squared for different rod spacing.

I. INTRODUCTION

The standard repertory of techniques found in college texts for solving electrostatic boundary-value problems includes separation of variables, image methods, and complex variable methods, as well as the numerical procedure known as the relaxation method.^{1–6} Each of these works very well for certain geometries of conducting boundaries, but there is one commonly used device for which none of these is manageable. This is the quadrupole electrostatic lens which was developed for the original ammonia maser and continues as an essential component of molecular-beam spectrometers. It consists of four parallel cylinders placed with their axes at the corners of a square with two at a positive potential and two negative. The same geometry occurs in the quadrupole mass spectrometer except with an applied rf potential instead of dc. The purpose of this article is to describe a technique which can deal with this configuration.

It is perhaps surprising that neither a conformal mapping nor an image method, both of which work easily for a set of two parallel cylinders,⁷ can handle this four-cylinder geometry. Two parallel, oppositely charged line charges generate equipotentials, all of which have circular cross section, but the equipotentials of four line charges are not circular. The same problem prevents the use of any simple conformal mapping technique: No simple analytic function maps into a set of four circles of the appropriate form. The numerical relaxation method would be possible, but a very fine mesh would be needed to match the cylinder surfaces, and it also requires a large number of mesh points extending out into the unbounded region outside the cylinders.

Of all the standard techniques, the image method seems

to come closest to working. It does have the proper behavior both in the region near the center and at large distances outside the rods. The only problem is that its equipotentials are not quite circular. We decided to try using more than one line charge in each cylinder to see if this could change the equipotentials into a more nearly circular cross section. As a criterion for quality of fit to the given circular equipotential, we used the mean-square difference between the given potential and the potential produced by the line charges. The positions and charges of the line charges were varied to minimize this mean-square difference. The result was the discovery that a total of only eight line charges, one pair per cylinder, gives an excellent match to the circular cross section for all except the closest settings of the rods. We will now discuss the fitting procedure and show some of the results of the technique for different spacings of the four rods and also for sets of six parallel cylinders.

II. PROCEDURE

If we have m line charges arrayed perpendicular to the $x - y$ plane with their intersections through the plane at the coordinates (x_i, y_i) ; then the potential at a point (u, v) in SI units, will be

$$V(u, v) = \sum_{i=0}^{m-1} \frac{-\lambda_i}{4\pi\epsilon_0} \ln[(u - x_i)^2 + (v - y_i)^2]. \quad (1)$$

We want to match this to the surface of the cylindrical rods by adjusting the charges λ_i and their locations (x_i, y_i) so as to minimize the mean-square difference between it and the given potential at the surface of the rods. This process is greatly simplified by taking into account the symmetry of a configuration such as that of the quadrupole electrostatic lens. Let us consider an even number n of

cylinders with their axes located at the points whose polar coordinates in the x - y plane are given by $r_k = r, \theta_k = 2\pi k/n$ for $k = 0, \dots, n-1$. The potentials of the cylinders will be $+V_0$ for k even and $-V_0$ for k odd. For each line charge located at coordinates (x, y) in the $k = 0$ cylinder, symmetry requires another at $(x, -y)$ and a corresponding pair inside each of the other cylinders. Thus each choice of line charge automatically specifies an additional $2n-1$ line charges. With this taken into account, the sum over i in Eq. (1) can be replaced by a double sum over j (with two per cylinder) and p , the index for pairs of line charges within each cylinder:

$$V(u, v) = \frac{-1}{4\pi\epsilon_0} \sum_{p=0}^{q-1} \sum_{j=0}^{2n-1} \lambda_p s_n s_j \ln[(u - s_x x_p - s_y y_p)^2 + (v - t_x x_p - t_y y_p)^2]. \quad (2)$$

Here, we have summed j over all $2n$ line charges which arise from one chosen set of coordinates (x_p, y_p) . The $s_n, s_x, s_y, t_x,$ and t_y arrays are determined strictly from the symmetry

$$\begin{aligned} s_n &= (-1)^{\text{int}(j/2)}, \\ s_x &= \cos[2\pi \text{int}(j/2)/n], \\ s_y &= (-1)^j \sin[2\pi \text{int}(j/2)/n], \\ t_x &= \sin[2\pi \text{int}(j/2)/n], \\ t_y &= (-1)^{j+1} \cos[2\pi \text{int}(j/2)/n]. \end{aligned} \quad (3)$$

The mean-square difference between this line charge potential and the given potential can be determined for a sample of points (we used eight) on the surface of the cylinder which lies on the x axis. This is an analytical, albeit messy, function of the $\lambda_p, x_p,$ and y_p that we may call $S(\lambda_p, x_p, y_p)$, or simply $S(x_i)$ for short. We begin with an initial guess for the coordinates and charges x_i . The function $S(x_i)$ is expanded as a Taylor series to second order about this initial set of values of x_i . The minimum of the resulting paraboloid can be found by solving the $3q \times 3q$ linear system of equations:

$$\sum_j \left(\frac{\partial^2 S}{\partial x_i \partial x_j} \right) (x_j - x_{j0}) = \left(\frac{-\partial S}{\partial x_i} \right), \quad (4)$$

where the derivatives are evaluated analytically at the ini-

tial values. The solutions are used as a second approximation and the process repeated until the value of S stops decreasing. Convergence is reasonably fast when only one line charge pair per cylinder is used, provided that the initial guess is fairly close. If not, the process has a tendency to diverge rather than converge.

We used a microcomputer running the BASIC language to evaluate the derivatives from the analytical expressions and solve the equations.

III. RESULTS

The solutions that we obtained for sets of four cylinders using only one line charge pair per cylinder were surprisingly good, the rms deviation being on the order of 10^{-5} to 10^{-4} for rod spacings in the range corresponding to those used in electrostatic lenses. Contour maps of the potential produced by the line charge fit are shown in panels (a) of Figs. 1-7 for a range of spacings.

Since the second-order Stark energy of a diatomic molecule in a quadrupole lens is proportional to the square of the magnitude of the electric field, we have also plotted contour maps of this parameter in panels (b) of Figs. 1-7. It is interesting to see how the contours of E^2 deviate from circles as one moves away from the axis; for close rod spacings, they bulge into the gaps, while for large spacings, they bulge into the cylinders. The "optimal" spacing would strike a balance between these extremes, keeping circular contours out to as large a distance from the axis as possible.

We also used the image solutions to evaluate the coefficients in the cylindrical harmonic expansion of the potential

$$V(u, v) = \sum_q a_q \cos(q\theta) \left(\frac{r}{a-b} \right)^q, \quad (5)$$

where b is the rod radius, and a is the radius of the circle on which the rod axes lie. This was done by Simpson's rule integration around a circle of radius $a-b$. These coefficients, along with the optimum line charge densities and locations, are tabulated in Table I for a range of rod spacings. It is the second-order coefficient that determines the desired function of the quadrupole lens; higher-order terms

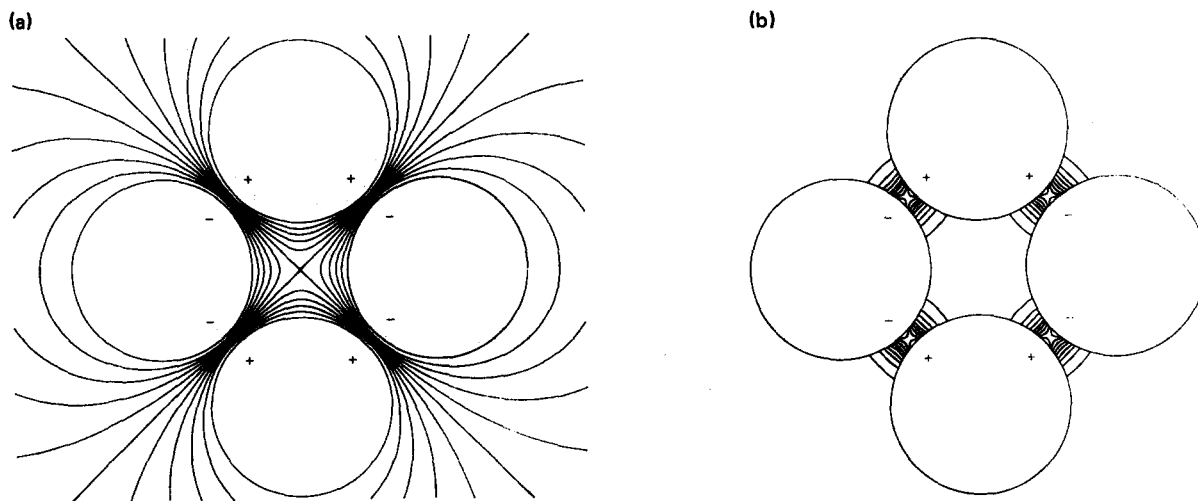


Fig. 1. Image solution for four conducting cylinders of radius 0.02 m with their axes on a circle of radius 0.03 m. (a) Equipotentials; (b) level contours of E^2 .

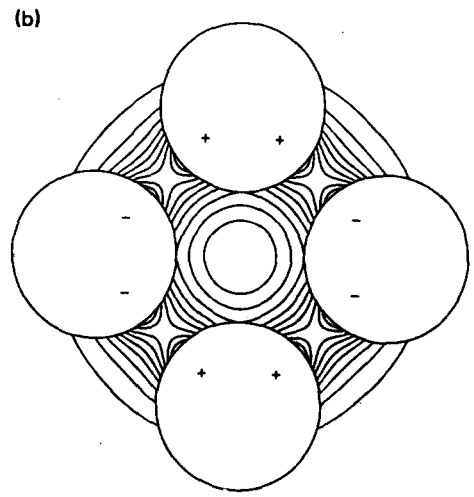
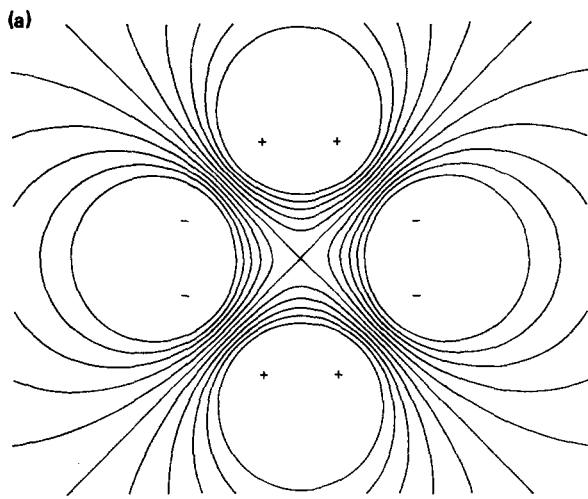


Fig. 2. Image solution for cylinders on a circle of radius 0.035 m. (a) Equipotentials; (b) level contours of E^2 .

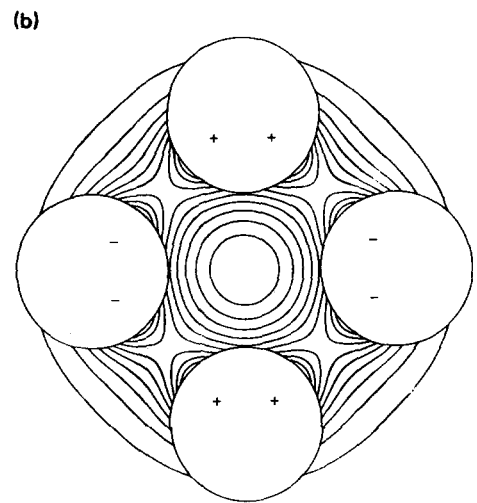
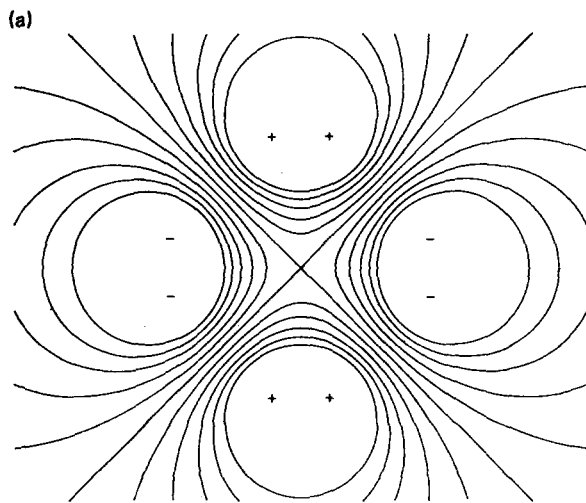


Fig. 3. Image solution for cylinders on a circle of radius 0.040 m. (a) Equipotentials; (b) level contours of E^2 .

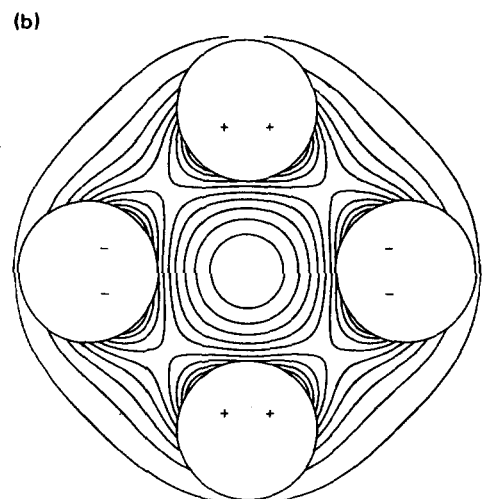
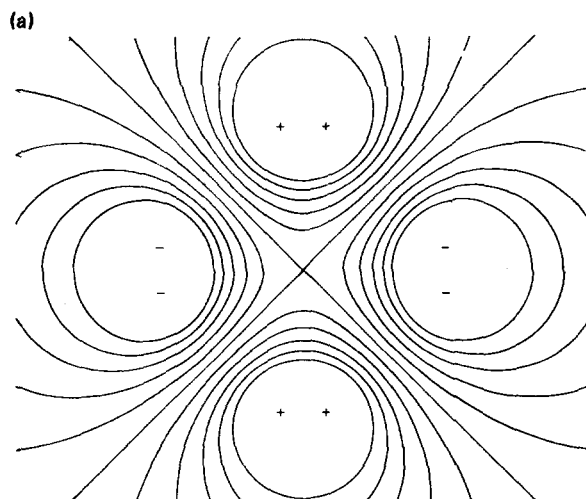


Fig. 4. Image solution for cylinders on a circle of radius 0.045 m. (a) Equipotentials; (b) level contours of E^2 .

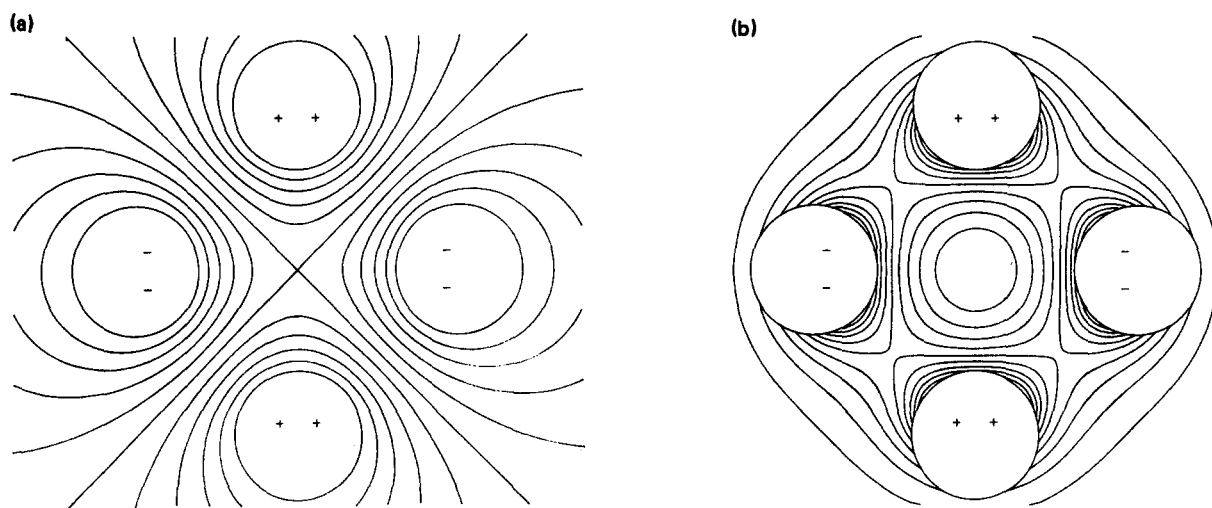


Fig. 5. Image solution for cylinders on a circle of radius 0.050 m. (a) Equipotentials; (b) level contours of E^2 .

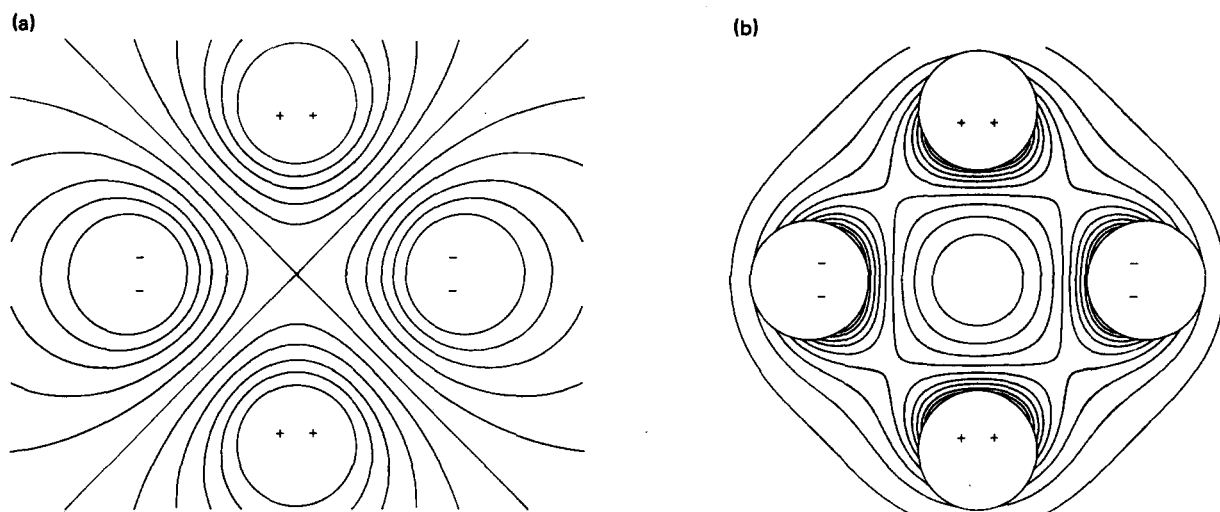


Fig. 6. Image solution for cylinders on a circle of radius 0.055 m. (a) Equipotentials; (b) level contours of E^2 .

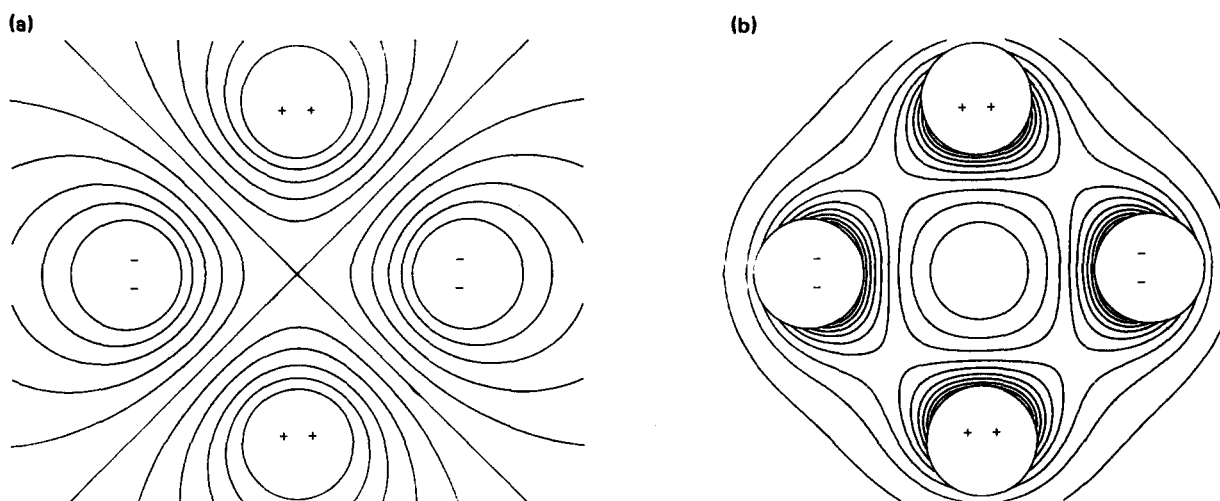


Fig. 7. Image solution for cylinders on a circle of radius 0.060 m. (a) Equipotentials; (b) level contours of E^2 .

Table I. Parameters determined for quadrupole lens with rods of radius 0.02 m, $V_0 = 1$ V, at various spacings.^a

a	x	y	λ	σ	a_2	a_6	a_{10}
0.030 m	0.01983 m	0.0109 71 m	135.03 pC/m	0.003 383 5 V	1.004 31 V	- 0.023 75 V	0.000 18 V
0.035	0.02751	0.0086 00	62.702	0.000 183 4	1.003 69	- 0.007 31	- 0.001 31
0.369 918	0.030 036	0.0080 484	54.1895	0.000 063 31	0.998 774	- 0.000 002	- 0.001 534
0.036 919	0.030 037	0.0080 482	54.1859	0.000 063 27	0.998 772	0.000 002	- 0.001 534
0.040	0.033 89	0.0073 26	45.397	0.000 013 7	0.988 95	0.011 59	- 0.001 41
0.045	0.039 81	0.0064 25	37.034	0.000 002 9	0.971 51	0.028 90	- 0.000 13
0.050	0.045 47	0.0057 39	31.982	0.000 001 4	0.954 39	0.043 98	0.002 06
0.055	0.050 97	0.0051 93	28.553	0.000 000 7	0.938 27	0.057 02	0.004 79
0.060	0.056 37	0.0047 47	26.049	0.000 000 4	0.923 24	0.068 33	0.007 81

^a The parameter a is the radius of the circle on which the rod axes lie, (x,y) are the coordinates of the first line charge, λ is its charge density, σ is the standard deviation of the fit to the given potential at the rod surface, and a_2 , a_6 , and a_{10} are the cylindrical harmonic coefficients.

give rise to aberrations. The symmetry of the four rods eliminates all orders except $2 \pmod 4$, so that after the second order, the next term would be the sixth order. One can see from the table that the sixth-order term passes through zero for a rod spacing with the rod axes on a circle whose radius is about 1.845 92 times the rod radius. This is a little closer than the factor of 2 that would be predicted by simply matching the curvature of the rod surface to the curvature of the hyperbolic equipotentials that would be given by a pure second-order cylindrical harmonic.

Although the fit of the image solution is quite good with only one line charge pair per rod, we were interested in seeing how much improvement would result from adding a second pair of line charges. The convergence was much slower, as one might expect, but eventually the rms difference between fit and given potentials was reduced by about two orders of magnitude. The improvement would not show up in a contour map, but would serve in cases where a more accurate representation is required.

It may be noted that the total surface charge per unit length on each cylinder has to equal the sum of the line charges/length on the image equivalent. Since there are four line charges in the two positive cylinders, the capacitance of the whole assembly is simply four times the table value of the fitted line charge divided by the 2-V potential difference.

We have also used the image technique to determine the

potential for a hexapole configuration. It seems to work just as well for this structure as for the quadrupole lens.

IV. CONCLUSION

We have presented a simple computer-based technique for solving for the potential in an electrostatic quadrupole lens. The results are interesting in their own right, but the technique should also be a useful addition to the standard lexicon of tricks for dealing with boundary value problems.

ACKNOWLEDGMENT

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