

# Numerical method for calculating of potential distribution in non-ideal multipole ion guides

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An accurate numerical method for calculating the potential distribution useful for 2D problems is proposed. Numerical results for quadrupole mass filter, hexapole, and octupole ion guide are presented and discussed.

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## 1. Introduction

Invention by W. Paul in 1953 [1] of the radiofrequency (rf) quadrupole mass filter (QMF) marks the beginning of a new era for the devices dedicated to the ion beam manipulation, and ion storage. The huge interest shown in our days for such devices is justified by their wide applicability. Fields as: high resolution atomic spectroscopy, atomic clocks based on stored ions in rf traps [2], radioactive ion beam manipulation in nuclear physics [3, 4], mass filters, mass spectrometry [5], quantum computing [6], and many other, from macro to nano scale could not be conceived without such devices.

We focus now on 2D rf confining devices. The well known is the QMF. An easy way to build a device that approximates an ideal QMF is to use parallel cylindrical electrodes (Fig. 1).

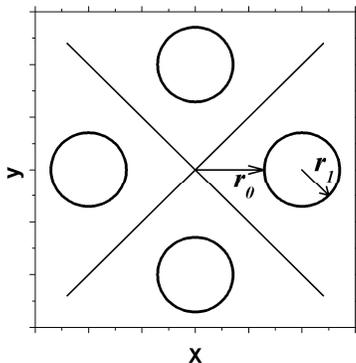


Fig. 1. Cross-sectional view of a four electrodes QMF; arbitrary units. The two crossing lines represent the region of vanishing potential.

However, such geometry does not ensure the ideal quadrupolar potential of a QMF. In the 2D model, the scalar potential of such a device can be expressed as

$$\phi(r, \theta, t) = \frac{U + V \cos(\Omega t)}{2} \sum_{k=0}^{\infty} C_k \left(\frac{r}{r_0}\right)^k \cos(k\theta) \quad (1)$$

Since this electrode setup preserves the four-fold symmetry, only terms with  $k = 2, 6, 10, \dots$  appear in the sum of equation (1). The first nonlinear component, i.e. the dodecapole  $C_6$  may be minimized if we chose a ratio  $r_1/r_0$  of about 1.14511 [7-9].

The section dedicated to numerical results will provide evidence that such an optimum ratio exists for hexapole and also for octupole ion guides.

## 2. The method

The method proposed here finds the multipole coefficients  $C_k$  in the case of a  $2n$ -fold symmetry where  $2n$  cylindrical rods are used to build a  $2n$ -pole ion guide.

Due to the above mentioned symmetry, in a Hexapole Ion Guide (6-pole IG) only the coefficients  $C_k$  with  $k = 3, 9, 15, \dots$  survive, while for the octupole configuration only the coefficients with  $k = 4, 12, 20, \dots$  are needed. Generally, for a  $2n$ -pole symmetry, only the coefficients with  $k = n, 3n, 5n, \dots$  appear.

**First step of the method.** Due to this particular symmetry, we used the *boundary element method* to calculate the potential inside a circular sector (Fig. 2). For a  $2n$ -pole ion guide, the central angle of this sector is set to  $\pi/n$ .

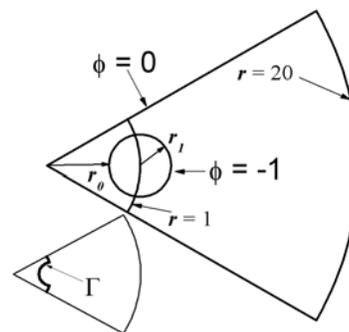


Fig. 2. The circular sector where the potential was calculated using the boundary element method. In a  $2n$ -pole ion guide, the central angle is  $\pi/n$ .

On the sector boundary the potential,  $\phi$ , vanishes, and on the inner circle of radius  $r_1$  is chosen as  $-1$ . The center of this circle lies on the boundary of a circular area of radius 1. The radius of the sector is chosen 20.

**The second step of the method.** The calculated values for the potential were then fitted to multipole expansion, and the coefficients  $C_k$  of the multipole moments have been evaluated by using the least square deviation method.

At this stage, only the points belonging to the  $\Gamma$  curve (see the inset in Fig.2) were used. More precisely, a linear system of 50 coefficients  $C_k$  was solved by minimizing the least square deviation of the potential obtained in step one.

The numerical calculus was performed using a homemade script written in Scilab [10].

### 3. Numerical results

**Maximum ratio  $r_1/r_0$  of 2n-pole IG.** For the geometry in Figure 2, there is a maximum value of the ratio  $r_1/r_0$  for which two adjacent rods contact each other in the IG. In other words, there is a ratio,  $r_1/r_0$ , for which the circle of radius  $r_1$  becomes tangent to the angular boundary of circular sector in Fig. 2. Since in the case of 2n-pole geometry the central angle is  $\pi/n$ , this maximum ratio is precisely given by  $(r_1/r_0)_{\max} = (1/\sin \frac{\pi}{2n} - 1)^{-1}$ . Therefore, for QMF this ratio satisfies  $r_1/r_0 < 2.4$ , for Hexapole Ion Guide  $r_1/r_0 < 1$ , and  $r_1/r_0 < 0.62$  in the case of an Octupole Ion Guide.

**Quadrupole mass filter.** The QMF case was numerically analyzed to optimize and to verify the accuracy of numerical method. In this case, the literature [7-9], provides accurate data. As can be seen from Table 1, our method found the optimal ratio  $r_1/r_0 = 1.14511$ , at which dodecapole coefficient,  $C_6$  vanishes.

Table 1. First five coefficients for QMF.

$r_1/r_0$	$C_2$	$C_6$	$C_{10}$	$C_{14}$	$C_{18}$
2.0	-1.0374	0.036963	4.6485E-4	5.5010E-6	2.1921E-6
1.9	-1.0348	0.033981	7.7856E-4	-5.0199E-7	1.1063E-6
1.8	-1.0319	0.030748	0.0010985	2.6404E-6	5.9722E-8
1.7	-1.0287	0.027247	0.0014277	1.8728E-5	-2.2810E-7
1.6	-1.0252	0.023406	0.0017399	4.5479E-5	3.9726E-7
1.5	-1.0213	0.019166	0.0020096	7.7451E-5	9.6689E-7
1.4	-1.0169	0.014486	0.0022399	1.2250E-4	3.4950E-6
1.3	-1.0119	0.0092884	0.0024035	1.7850E-4	8.2380E-6
1.2	-1.0062	0.0034833	0.0024693	2.4406E-4	1.5994E-5
1.14511	-1.0028	1.1012E-7	0.0024493	2.8319E-4	2.1926E-5
1.1	-0.99970	-0.0030387	0.0023951	3.1642E-4	2.7941E-5
1.0	-0.99214	-0.010415	0.0021193	3.8864E-4	4.5327E-5
0.9	-0.98326	-0.018819	0.0015510	4.4576E-4	6.8878E-5
0.8	-0.97265	-0.028474	5.5488E-4	4.5731E-4	9.7180E-5
0.7	-0.95977	-0.039672	-0.0010740	3.6348E-4	1.2205E-4
0.6	-0.94377	-0.052787	-0.0036575	4.5605E-5	1.1811E-4
0.5	-0.92335	-0.068271	-0.0077232	-7.3516E-4	1.2361E-5
0.4	-0.89622	-0.086757	-0.014119	-0.0024780	-3.9917E-4
0.3	-0.85817	-0.10894	-0.024314	-0.0062643	-0.0016982
0.2	-0.80022	-0.13482	-0.040821	-0.014580	-0.0056475
0.1	-0.70897	-0.16254	-0.060309	-0.029257	-0.013299

**Hexapole Ion Guide (6-pole IG).** Table 2 presents numerical results obtained considering the geometry shown in Fig. 3. In this case, it is also possible to find a ratio for which the coefficient  $C_9$  also vanishes. Indeed, for  $r_1/r_0 = 0.5628305$ , the coefficient  $C_9$  is  $-3.4364 \cdot 10^{-9}$ , close enough to zero to qualify this ratio as an optimal one.

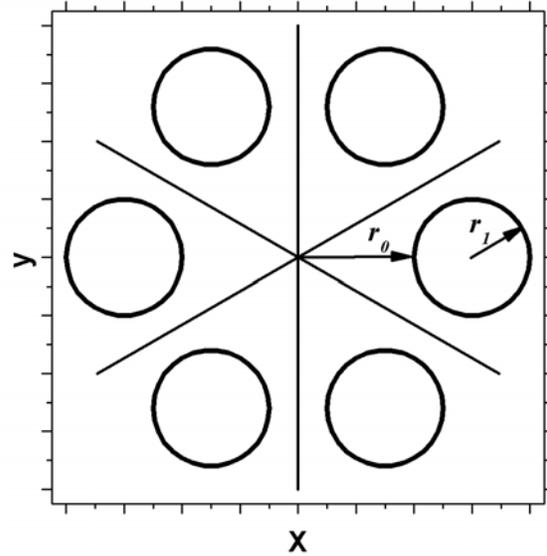


Fig.3. Cross-sectional view of the 6-pole IG; arbitrary units. The three crossing lines represent the 2D locus where the potential of this configuration is zero.

Table 2. The first five coefficients for the 6-pole IG.

$r_1/r_0$	$C_3$	$C_9$	$C_{15}$	$C_{21}$	$C_{27}$
0.95	-2.0466	0.37362	-0.027140	2.4349E-4	-4.8685E-4
0.90	-1.9863	0.31280	-0.0045022	-0.0021238	-1.9522E-4
0.85	-1.9257	0.25576	0.011756	-0.0024034	-1.8439E-6
0.80	-1.8647	0.20261	0.022894	-0.0015127	-2.9386E-4
0.75	-1.8032	0.15327	0.029810	3.5884E-4	-4.3637E-4
0.70	-1.7413	0.10759	0.033026	0.0026000	-3.5598E-4
0.65	-1.6787	0.065445	0.033079	0.0048382	4.9511E-5
0.60	-1.6155	0.026691	0.030404	0.0066869	6.8277E-4
.5628305	-1.5679	-3.4364E-9	0.026890	0.0076438	0.0012360
0.55	-1.5513	-0.0088045	0.025405	0.0078741	0.0014351
0.50	-1.4862	-0.041170	0.018431	0.0081842	0.0021500
0.45	-1.4196	-0.070567	0.0098204	0.0074451	0.0026754
0.40	-1.3514	-0.097084	-2.0543E-4	0.0055321	0.0028055
0.35	-1.2809	-0.12080	-0.011449	0.0023195	0.0023371
0.30	-1.2075	-0.14185	-0.023727	-0.0023348	0.0010191
0.25	-1.1299	-0.16025	-0.036947	-0.0086003	-0.0014697
0.20	-1.0460	-0.17582	-0.051079	-0.016746	-0.0055742
0.15	-0.95236	-0.18802	-0.066070	-0.027157	-0.011971
0.10	-0.84142	-0.19470	-0.081444	-0.040248	-0.021699
0.05	-0.69455	-0.18800	-0.094008	-0.054978	-0.035740

**Octupole Ion Guide (8-pole IG).** The diagram in Fig. 4 shows the geometry of an 8-pole IG, while Table 2 includes the data computed in this case. As in the previous cases, there is an optimal ratio  $r_1/r_0$  of about 0.372159, for which  $C_{12}$  is very close to zero.

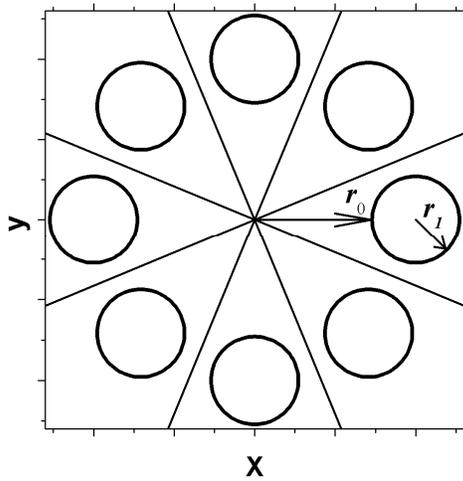


Fig. 4. Cross-sectional view of the 8-pole IG; arbitrary units.

Table 3. The first five coefficients for the 8-pole IG.

$r_1/r_0$	$C_4$	$C_{12}$	$C_{20}$	$C_{28}$	$C_{36}$
0.60	-2.6951	0.90820	-0.14127	0.042232	0.022758
0.55	-2.5099	0.61855	0.012037	-0.018961	4.2574E-5
0.50	-2.3297	0.38693	0.084580	-	-
0.45	-2.1541	0.20430	0.10216	0.0089739	0.0049172
0.40	-1.9829	0.063131	0.087709	0.011666	-
0.372159	-1.8892	-8.9177E-7	0.071811	0.026288	0.0038747
0.35	-1.8155	-0.043260	0.056938	0.029704	0.0025727
0.30	-1.6514	-0.12071	0.020175	0.029884	0.0091564
0.25	-1.4894	-0.17424	-0.016190	0.023238	0.011886
0.20	-1.3276	-0.20816	-0.048483	0.0093491	0.0092223
0.15	-1.1624	-0.22588	-0.074973	-	0.0015470
0.10	-0.98611	-0.22897	-0.095010	0.0084918	-
0.05	-0.77768	-0.21248	-0.10608	-0.027604	0.0099895
				-0.046268	-0.024288
				-0.062356	-0.040334

#### 4. Conclusions

Simulations of ion confining in 2D devices like Hexapole or Octupole Ion Guide need accurate estimation of the potential function in (1). Therefore, the method described here provided very useful numerical examples.

The results above demonstrate that optimal ratios  $r_1/r_0$  exist for Hexapole and Octupole Ion guides. The precision of the method compares well to other previously reported methods in the literature [7-9]. The method can easily be extended to any two-dimensional configuration of electrodes. The accuracy of the method greatly improves when, in the second step, the points used are close enough to the circle of radius 1.

The accuracy also increases when increasing the number of terms included in the series (1). In practice, the numerical errors in the second step also increase with the number of terms. Therefore, the number of terms will be chosen in such a manner to guarantee a minimal interpolation error.

The symmetry of the problem is a key factor for the accuracy of our method. As a result, regions like the circular sector in Fig. 2, must be carefully chosen when the symmetry is to be taken into account.

The lower the symmetry of the problem, the greater the number of terms in series (1).

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