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Minimisation of the aberrations of electrostatic lens systems composed of quadrupole and octupole lenses

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Abstract

Aberrations are investigated and compared for two types of multiplets based on electrostatic quadrupole and octupole lenses: "mid-acceleration" systems where an accelerating potential is applied to the middle lenses of a set of quadrupole lenses and systems where some of the quadrupole lenses are replaced by combined quadrupole–octupole lenses. It is shown that for systems consisting of three lenses the mid-acceleration type has the smaller aberrations. For systems consisting of four or five lenses the third order aperture aberration can be eliminated in the quadrupole–octupole type. The mid-acceleration type has the advantages of lower levels of chromatic and fifth order aperture aberrations and also relative simplicity of construction and voltage adjustment. (Int J Mass Spectrom 189 (1999) 19–26) © 1999 Elsevier Science B.V.

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1. Introduction

The performance of a mass spectrometer is characterized by the resolving power and the sensitivity of the instrument. In the case of mass spectrometers of the double focusing type formed by magnetic and electric sectors, both characteristics can be improved by using quadrupole lenses.

The resolving power of a mass spectrometer is given by

$$R = D/(Ms_1 + s_2 + \Delta) \quad (1)$$

where D is the mass dispersion, s_1 and s_2 are the widths of the entrance and exit slits, respectively, M is the linear magnification of whole system, and Δ is the total aberration blurring in the image plane. It can be derived from Eq. (1) that both resolving power and sensitivity can be increased by reducing aberrations and by increasing the ratio D/M [1].

If the dispersion elements are specified then the ratio D/M can be varied by varying the excitation of the lens that precedes the sector magnet. The mass dispersion itself can be varied by varying the excitation of the lens that follows the sector magnet [2]. Both lenses must be diverging in order to make D/M and D larger than when there are no lenses at all. Therefore, quadrupole lenses that are diverging in one plane and converging in the perpendicular one should be employed here rather than round lenses. Quadrupoles would provide not only an increase in the value of D/M, and hence in the resolving power, but also

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focus the ion beam in the perpendicular plane, which would result in an increase in the sensitivity. These are benefits that result from the specific first order properties of quadrupole lenses.

The aberrations of quadrupole lenses, where the most important are the aperture and chromatic aberrations, are as a rule higher than those of round lenses. Since the resolving power of a mass spectrometer depends on the aberrations in a straightforward way [see Eq. (1)] the problem of aberration reduction is of great importance. The third order aperture aberration of a quadrupole lens system can be reduced by using octupoles. The quadrupole–octupole correctors have been studied in detail in connection with electron microscopy and probe forming systems. A comprehensive survey of the subject is given in [3]. The corrector that can meet the demands of electron microscopy has to be complicated. Because of the quadrupole lens astigmatism the system should consist of at least four quadrupole lenses to focus charged particles just as a round lens (regular quadruplet). Three octupoles have to be incorporated in the system to enable complete correction of the third order aperture aberration.

The situation is easier in mass spectrometry. Since sector fields focus ion beams in the plane of dispersion, fewer quadrupole lenses are needed to provide stigmatic focusing in the image plane, especially since the linear magnifications can be different in the two directions. Also, complete correction of the aperture aberration is not necessary in this case since the main requirement is the reduction of the aperture aberration in the plane of dispersion. Therefore using even only one octupole can improve the performance of the sector field mass spectrometer [1].

The first order chromatic aberration can be reduced using combined electrostatic and magnetic quadrupoles whose excitations are connected by the achromatic condition. This method involves magnetic elements and leads to a complicated construction of the focusing system.

In the present article an alternative method of aberration reduction is described. It consists of applying an accelerating potential to some lenses of a quadrupole system and leads to simultaneous reductions of both chromatic and aperture aberrations in a purely electrostatic device. The method is very simple and in many cases is preferable to octupole correction. A detailed comparison of the new method and the octupole correction is also made.

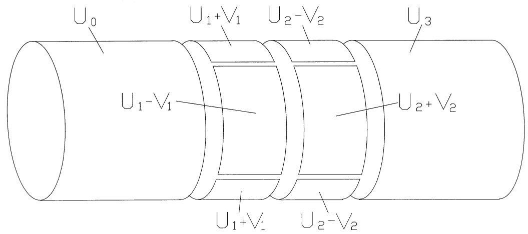

Fig. 1. A quadrupole lens doublet. The two central cyclinders are each cut into four quadrants. The quadrupole voltages $\pm V_1$ and $\pm V_2$ are superimposed on the mean voltages U_1 and U_2 of the inner cylinders.

The properties of the lenses have been computed using the CPO program [4], which uses the accurate surface charge method (also known as the boundary element method) for solving Laplace's equation.

2. Systems of two lenses

2.1. Geometry

Methods of simultaneous reduction of the first order chromatic and third order aperture aberrations by applying an accelerating potential to the second lens of a doublet have been studied in [5,6]. Systems consisting of two quadrupole [5] or two crossed aperture lenses [6] have been considered. Here we will briefly describe the main results that are of interest for mass spectrometer designers. For simplicity we restrict ourselves to the quadrupole lens doublets formed by cylindrical electrodes, which are easy to simulate using the computer program.

The doublet consists of two aligned cylinders cut by longitudinal slots into four equal parts each (Fig. 1). There are two additional long cylinders of the same radius at both sides of the doublet, terminated by disks at their ends. We have taken the diameter of the cylinders to be the unit of length. The length of each quadrupole lens measured between the centers of the

Table 1
Some ion-optical parameters of the quadrupole lens doublet operating in astigmatic modes and characterized by a zero first order chromatic aberration ($C_{cx} = 0$) and a negative or zero third order aperture aberration ($C_{30} \leq 0$) in the *xz* (DC) plane for a parallel input beam

Mode	U_0	U_1	U_2	U_3	V_1	V_2	f_{ix}	f_{iy}	$z(F_{ix})$	$z(F_{iy})$
1	1.0	0.4	5.0	4.0	1.068	1.40	10.65	1.82	14.88	0.60
2	1.0	0.5	4.0	4.0	0.933	1.20	12.31	2.10	16.74	0.74
3	1.0	1.0	4.0	4.0	0.971	1.20	16.25	2.56	20.95	0.94

gaps is then 0.5 and the gap width is 0.02. If the zero of the *z* axis is put at the center of the doublet then the terminating discs are at $z = \pm 6.0$.

The applied potentials are also indicated in Fig. 1. The source of charged particles is assumed to be at zero potential. Each of the four cylinders can be at a separate potential, the four potentials being denoted as U_0, U_1, U_2 and U_3, respectively. As shown, the quadrupole voltages $\pm V_1$ and $\pm V_2$ are superimposed on the quadrants of the two cut cylinders.

2.2. Aberration correction

Computations have shown that in such a system operating in an astigmatic mode, the first order chromatic and third order aperture aberrations can change sign or vanish in one direction. Correction has been achieved in the direction where the first quadrupole lens is diverging and the second one is converging. The main condition of the correction is that the absolute value of the potential U_2 applied to the second lens is higher than the absolute value of U_1 applied to the first one so that charged particles are accelerated between two lenses.

As in an example in Table 1 some characteristics of the corrected quadrupole lens doublet are given for three sets of operating voltages. The input ion beam is assumed to be parallel to the *z* axis. For all of the three modes the axial chromatic aberration coefficient in the *xz* plane C_{cx} is equal to zero and the aperture aberration coefficient in the same plane C_{30} is zero for the third mode and negative and very small for the first and second modes.

One can see that all three modes are strongly astigmatic and that the focal lengths and positions of the foci are very different in the *xz* and *yz* planes. This situation is favorable for using the doublet in sector mass spectrometers. The *xz* plane where the aberration correction takes place and the doublet shows weaker focusing should coincide with the dispersion plane of the spectrometer where the sector field focuses the ion beam itself and the aberration reduction is needed.

The stigmatic modes of the quadrupole lens doublet, which provide a point image of a point object, have been also studied. In this case the aberrations cannot be reduced to zero. Nevertheless reductions of both chromatic and aperture aberrations by an order of magnitude or more have been achieved in one transverse direction.

3. Systems of three lenses

3.1. Modes of operation

Having more variable parameters the quadrupole lens triplet presents a more flexible system than a doublet. In stigmatic modes the linear magnifications of a doublet are generally quite different in the *x* and *y* directions, which might be a limitation for some applications. The triplet allows the magnification ratio to be varied without changing the image position and it can be made equal to unity if necessary. The geometry of the system under study is similar to that shown in Fig. 1, with a third lens identical to the existing two being added. The zero of the *z* axis is again put at the center of the system. We take the *xz* plane to be the diverging–converging–diverging (DCD) plane and the *yz* plane to be the CDC plane. The triplet tends to be stronger in the CDC plane and so two modes of stigmatic focusing are possible. In both modes the trajectory shape in the DCD plane is similar although in the CDC plane trajectories do not cross the axis inside the triplet in the first mode of stigmatic operation but do cross it in the second mode, thus forming an intermediate line image.

We have restricted the present study to the symmetric triplet which has the same excitations for the first and third lenses. The first order properties are maintained the same throughout the study: the object plane is located at $z_0 = -4.3$ and the image plane at $z_i = 4.3$. Thus the linear magnification is always equal to unity.

3.2 Aberration reduction in mid-acceleration triplets

The first order chromatic and third order aperture aberrations of the triplet in both modes of operation can be significantly reduced merely by applying an accelerating potential to the middle lens as a whole [7]. The quadrupole voltages are re-adjusted to maintain the image at the same position ($z_i = 4.3$ in the present case). We refer to this as the "mid-acceleration" triplet. Note that unlike the doublet this system does not change the final energy of the beam. It is important that the reduction takes place in the diverging–converging–diverging plane where initially the aberrations are much greater. In the CDC plane they remain almost the same as in the conventional triplet.

Figs. 2 and 3 illustrate the aperture aberration of the conventional quadrupole triplet in the first mode of operation (in which trajectories do not cross the axis inside the lens). Trajectories having the initial slopes $x'_0 = y'_0 = \pm 0.004,\ 0.008, \ldots,\ 0.02$ are shown. The division of the cylindrical surface into rectangular segments created by the CPO program is also shown so that the positions of the three quadrupole lenses can be seen. We can see that the quadrupole triplet performance is mainly restricted by the large aberration in the DCD plane. Fig. 4 shows the aperture aberration in the DCD plane of the mid-acceleration triplet which results from applying an accelerating voltage of 4.0 to the middle lens and re-adjusting the quadrupole excitations to focus the beam at the same image plane. In this particular case the aperture aberration coefficient C_{30} is reduced to zero, while the coefficient C_{03} in the CDC plane remains almost the same as in the conventional triplet. The first two lines of Table 2 present the quadrupole

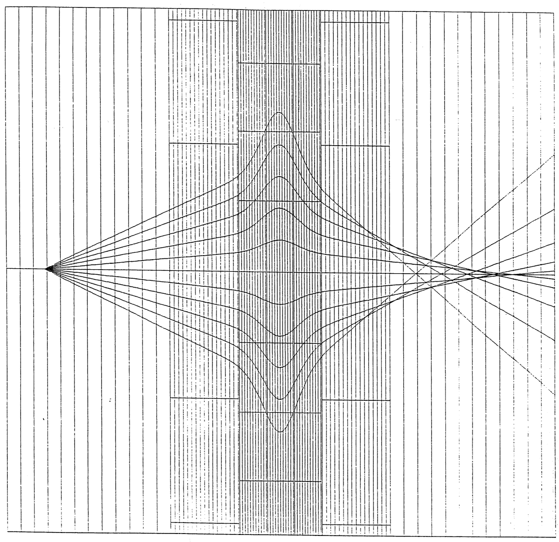

Fig. 2. Illustration of the aperture aberration in the *xz* plane of the conventional quadrupole triplet for the voltages given in the first line of Table 2. The initial trajectory slopes go from ± 0.004 to ± 0.020 in steps of ± 0.004. The field of view is $x = \pm 0.2$, $z = \pm 5.0$, and so the transverse direction is magnified by a factor of 25. The rectangles are the segments into which the cylindrical surfaces are subdivided by the CPO program.

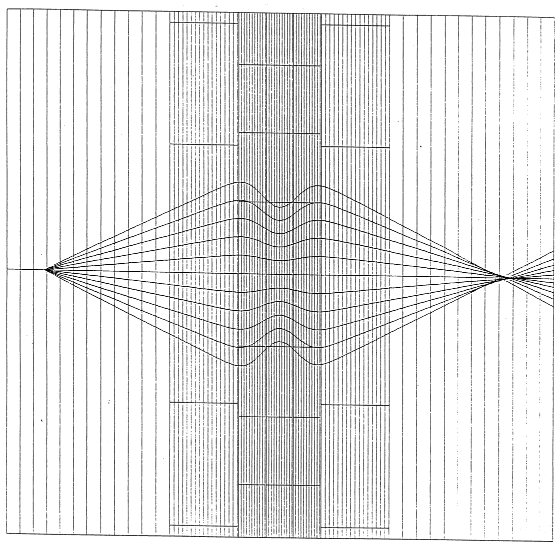

Fig. 3. Trajectories as specified in Fig. 2, for the *yz* plane of the conventional quadrupole triplet.

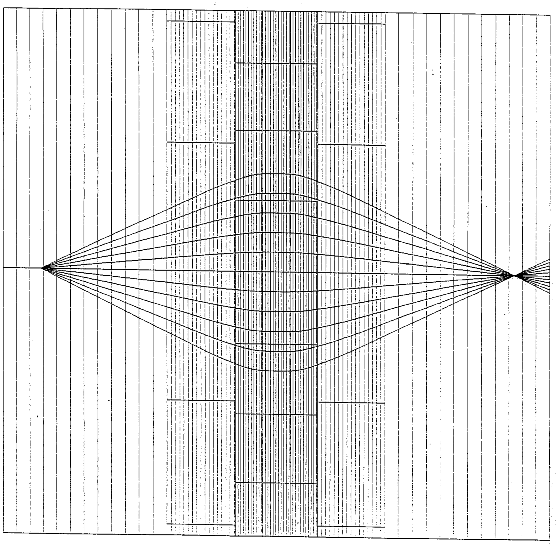

Fig. 4. Illustration of the zero aperture aberration in the *xz* plane of the mid-acceleration triplet (see the second line of the Table 2). The initial trajectory slopes go from ± 0.004 to ± 0.020 in steps of ± 0.004. The field of view is $x = \pm 0.2$, $z = \pm 5.0$.

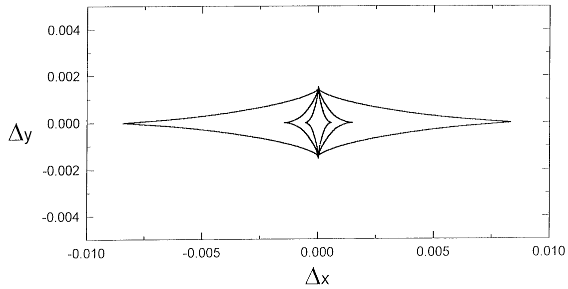

Fig. 5. Aberration figures in the image plane of the quadrupole triplet for the second mode in which trajectories in the CDC plane cross the axis inside the lens. Three stages in the progressive reduction of the aperture aberration are illustrated. The accelerating voltages applied to the middle quadrupole lens are 5 for the outer envelope and 8 for the middle and inner ones. The first and third quadrupoles have a voltage of 0.5 for the inner envelope. The initial trajectory slopes are given by $(x'^2_0 + y'^2_0)^{1/2} = 0.01$.

lens voltages and aberration coefficients for the same cases that are illustrated by Figs. 2, 3 and 4.

Three stages in the reduction of the aperture aberration in the second mode of operation where the triplet forms an intermediate line focus in the CDC plane are illustrated by Fig. 5. It shows the beam spot in the image plane for the case of a conical beam at the entrance of the triplet defined by the equation $(x'^2_0 + y'^2_0)^{1/2} = 0.01$. The outer and middle envelopes correspond to mid-acceleration voltages of 5 and 8, respectively. The inner envelope has been obtained by also applying a decelerating voltage of 0.5 to the first and third quadrupoles. For comparison, the size of the beam spot for the conventional triplet in the *x* direction is equal to 0.125, which is two orders of magnitude greater than the size of the inner envelope.

We find that applying an accelerating voltage to the middle lens of the triplet not only compensates for the aperture aberration but also reduces the chromatic aberration. Fig. 6 shows the dependence of the chromatic aberration coefficients C_{cx} and C_{cy} in the *xz* (DCD) and *yz* (CDC) planes, respectively, on the magnitude of the accelerating potential applied to the middle lens. The quadrupole lens excitations are re-adjusted every time the accelerating potential is changed in order to maintain the image position in the same plane. The data refer to the second mode of operation. We see that the chromatic aberration coefficient in the *xz* plane can be reduced by nearly two orders of magnitude by increasing the acceleration although the coefficient in the *yz* plane does not change significantly.

Table 2
Chromatic and aperture aberration coefficients of the triplet systems; the first line refers to the conventional quadrupole triplet, the second to the mid-acceleration quadrupole triplet and the third to the quadrupole–octupole triplet with octupole excitations; in all cases the object is at $z_0 = -4.3$ (in units of the lens diameter) and the paraxial image is at $z_i = 4.3$ in both the *xz* (DCD) and *yz* (CDC) planes

	Quadrupole lens voltages		Aberration coefficients			
Triplet type	$U_1 = U_3$	U_2	C_{cx}	C_{cy}	C_{30}	C_{03}
Conventional Q	1.0 ± 0.617	1.0 ± 1.135	25.6	9.7	6.9×10^3	6.5×10^2
Mid-acceleration Q	1.0 ± 0.417	4.0 ± 1.128	5.6	10.0	0.0	6.0×10^2
QO	1.0 ± 0.867	1.0 ± 1.599	25.6	9.7	1.0×10^3	1.4×10^3

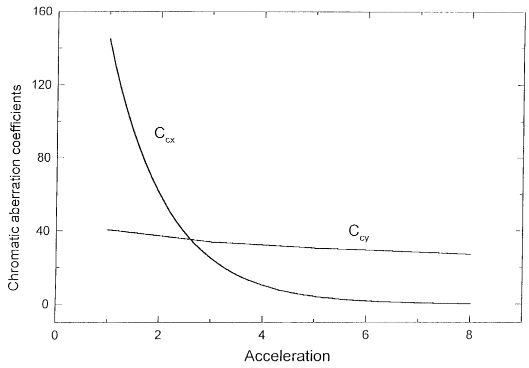

Fig. 6. Dependence of the chromatic aberration coefficients C_{cx} and C_{cy} on the magnitude of the accelerating potential applied to the middle lens of the quadrupole triplet in the mode of operation where the triplet forms an intermediate line focus in the CDC plane. The quadrupole lens excitations are re-adjusted to keep the first order properties unchanged.

4. Antisymmetric regular quadruplets

We have also briefly studied multiplets consisting of four quadrupole lenses. The system is formed by five identical cylinders. The central cylinder is not used as a lens and merely provides some spacing between the outer two doublets.

Practically, the quadruplet is the simplest quadrupole system that can be regular and therefore produce an undistorted sharp image for all positions of the object plane, just as a round lens. The regularity is most easily achieved in the antisymmetric quadruplet, which possesses a plane of geometrical symmetry and electrical antisymmetry due to the first and fourth lenses having equal excitations of opposite polarity, as have the second and third lenses. This quadruplet can be made regular by tuning only two voltages so that the focal planes in the x and y directions coincide.

The computations have shown that in a regular quadruplet the aberration coefficients are the same in the two principal planes and the aberration figures resulting from the axial chromatic and aperture aberrations are circular just as they are in a round lens, although the trajectory shapes are different in xz and yz planes.

Applying an accelerating voltage to the two middle lenses and re-adjusting the quadrupole voltages to keep the image position unchanged (mid-acceleration quadruplet) leads to a significant reduction of the aberrations both in the xz (DCDC) and yz (CDCD) planes. The first order chromatic aberration has been reduced by a factor of 2 to 3 and the third order aperture aberration by an order of magnitude, the aberration coefficients being the same in the xz and yz planes. An example of the results obtained for quadruplets is given in Table 3. The first two lines show the quadrupole lens excitations and aberration coefficients for the conventional and mid-acceleration quadruplets.

5. Comparison of aberration reduction in multiplets of the quadrupole–octupole and mid-acceleration types

5.1. Geometry of the quadrupole–octupole lens

It is of interest to compare the proposed method of aberration reduction with the well known octupole correction. For this purpose we have also considered multiplets in which each lens is cut into eight identical parts instead of four. Depending on the applied voltages such a unit can operate either as a pure quadrupole (with the top and bottom parts at $U_0 + V$, the left and right parts at $U_0 - V$ and the diagonal parts at U_0) or as a pure octupole (with the top, bottom, left and right parts at $U_0 + W$ and the diagonal parts at $U_0 - W$) or as a combined quadrupole-octupole lens (with superimposed quadrupole and octupole voltages).

5.2. Comparison of quadrupole–octupole and mid-acceleration triplets

Some electron-optical characteristics of the triplets examined in the present study are listed in Table 2. The first line refers to the conventional quadrupole triplet, using cylinders split into four parts. When the cylinders are split into eight parts the excitations of the quadrupole type remain, and then the same first order properties are achieved under different quadrupole excitations because the sizes of the lens electrodes are different, but the axial chromatic and third order aperture aberrations remain the same.

The second line of Table 2 refers to the mid-acceleration triplet. The accelerating potential applied

Table 3
Chromatic and aperture aberration coefficients of systems of four and five lenses; the five split cylinders can be activated as quadrupoles (Q), octupoles (O), combined quadrupole–octupole (QO), or can be left neutral (N); the first line refers to the conventional quadruplet, the second to the mid-acceleration quadruplet and the third to the quintuplet with octupole excitations

	Quadrupole voltages		Aberration coefficients	
Type	$U_1 = U_4$	$U_2 = U_3$	$C_{cx} = C_{cy}$	$C_{30} = C_{03}$
Q, Q, N, Q, Q	1.0 ± 0.401	1.0 ± 0.708	15.5	1.8×10^3
Q, Q, N, Q, Q, mid-acc	1.0 ± 0.253	4.0 ± 0.719	6.0	2.2×10^2
Q, QO, O, QO, Q	1.0 ± 0.563	1.0 ± 0.996	15.5	0.0

to the middle lens as a whole is equal to 4.0 and the quadrupole voltages are re-adjusted to maintain the image at the same plane. It can be seen that in the DCD plane the chromatic aberration is reduced by a factor of 5 and the third order aperture aberration is eliminated while in the CDC plane both aberrations remain almost unchanged.

The third line of Table 2 shows the best results that have been achieved for the quadrupole–octupole triplets when the octupoles are excited. The chromatic aberration is not affected by exciting the octupoles and remains the same. The aperture aberration is reduced but not completely eliminated. The reason for this is that in the symmetric triplet three octupoles combined with quadrupole lenses cannot provide complete correction of the aperture aberration. The minimum spot size has been reached by gradually increasing all three octupole voltages in such a way that the beam spot in the image plane is reduced in all directions. At some stage of the procedure a further increase of the octupole excitations leads to an increase in the spot size. Thus one can easily determine the octupole voltages that provide the minimum aberration blurring. In the present case the octupole voltages that produce an optimal aberration reduction are $W_1 = \pm 0.5$, $W_2 = \pm 0.64$, $W_3 = \pm 0.2$.

Comparison of the last two lines of Table 2 shows that the mid-acceleration triplet provides much lower chromatic and aperture aberrations than the quadrupole–octupole triplet. The chromatic aberration is the same in the yz (CDC) plane for both systems but in the xz (DCD) plane it is smaller by a factor of 5 for the mid-acceleration triplet. The aperture aberration coefficient C_{30} in the DCD plane is zero for the mid-acceleration triplet and for the quadrupole–octupole one it is only reduced by a factor of 6.9 and remains finite. The aperture aberration coefficient C_{03} in the perpendicular CDC plane is smaller by a factor of 2.5 for the mid-acceleration triplet.

We can therefore conclude that the mid-acceleration type of triplet has the smaller aberrations.

5.3. Systems of four or five lenses

These multiplets consist of five cylinders, where all are cut into four (conventional and mid-acceleration systems) or eight (quadrupole–octupole systems) identical parts. In the first two cases the central split cylinder is not used as a lens, and merely provides some spacing between the outer two doublets. In the latter case each of the five lenses can operate as a pure quadrupole, a pure octupole or a combined quadrupole–octupole lens. We shall refer to this system as a quintuplet.

Table 3 is similar to Table 2 and presents lens voltages and aberration coefficients for systems of four quadrupole lenses and five quadrupole–octupole ones. The first line refers to the conventional regular quadruplet. The second one refers to the mid-acceleration quadruplet which is created by applying an accelerating voltage of 4.0 to the two middle lenses and re-adjusting the quadrupole voltages to maintain the first order properties unchanged. In this case the chromatic aberration coefficient is reduced by a factor of 2.5 in both the DCD and CDC planes. The aperture aberration coefficient is also reduced in both planes by an order of magnitude.

The third line of Table 3 refers to the quadrupole–octupole system. By activating three octupoles in the middle of the five cylinders split into eight parts each it becomes possible to eliminate the third order aperture aberration. We have considered the sequence Q, QO, O, QO, Q for the five lenses, where Q and O signify quadrupole and octupole, respectively. For the given object and image positions the third order aperture aberration becomes zero under the following octupole voltages: $W_1 = W_3 = \pm 0.91$ and $W_2 = \pm 1.47$. The paraxial trajectories remain the same as in the quadruplet because octupoles do not affect the first order properties (except for a very weak influence which can be corrected by small changes of the quadrupole voltages). It can be seen that the chromatic aberration is also unaffected by octupoles and remains the same in the conventional and quadrupole–octupole systems whether the octupoles are excited or not (see the first and third lines).

Thus the mid-acceleration quadruplet is characterized by the chromatic aberration which is 2.5 times smaller than that of the quadrupole–octupole system. However, for small beam angles the quintuplet provides smaller image blurring due to the aperture aberration than the mid-acceleration quadruplet. This statement is true for beam slopes which are less than 0.02. For larger slopes the fifth order aperture becomes dominant. In the mid-acceleration quadruplet the fifth order aperture aberration coefficients are $C_{50} = C_{05} = 1.1 \times 10^5$, which is nearly two order of magnitude smaller than for the quintuplet, where these coefficients are $C_{50} = C_{05} = 9.5 \times 10^6$. For instance if the beam slope is $x'_0 = 0.035$ then the spot size in the mid-acceleration quadruplet is smaller by a factor of 6 while for $x'_0 = 0.04$ it is smaller by an order of magnitude.

6. Discussion

An important advantage of the mid-acceleration quadrupole multiplets is their relative simplicity of construction and voltage adjustment. After applying an accelerating potential to the middle lenses of the multiplet the stigmaticity can be dealt with by adjusting only two quadrupole voltages both for the symmetric triplet and the antisymmetric quadruplet. In the quintuplet three octupole voltages have to be adjusted in addition to the quadrupole voltages. When tuning the octupole excitations the position of the paraxial image is displaced a little, therefore the procedure for voltage adjustment has to be iterative. Also the quadrupole–octupole system is very sensitive to any errors in octupole excitations, since even a small error can result in a significant image blurring.

The second advantage of the mid-acceleration system consists in the reduction of the chromatic aberration by a factor in the range from 2 to almost two orders of magnitude. The quadrupole–octupole system does not provide any reduction of the chromatic aberration.

The mid-acceleration systems also have advantages with respect to aperture aberrations. The third order aperture aberration of the mid-acceleration triplet is much smaller than that of the quadrupole–octupole one. On the other hand in the quadrupole–octupole quintuplet this aberration can be completely eliminated, while in the mid-acceleration quadruplet it is only reduced by approximately an order of magnitude. However at larger beam angles, when the fifth order aperture aberration becomes dominant, the mid-acceleration quadruplet produces smaller image blurring.

We can conclude that the performance of any instrument or experimental setup which makes use of quadrupole multiplets can be easily improved by applying mid-acceleration. The most obvious application of the suggested method is mass spectrometers with sector magnetic and electrostatic fields which normally employ quadrupole lenses for ion beam focusing.

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