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Application of a static magnetic field to the mass filter of a quadrupole mass spectrometer

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Abstract

We consider the case of a generalised quadrupole mass spectrometer in which a static magnetic field is applied to the body of the filter. We have solved numerically the extended Mathieu equation numerically constructing a theoretical transmission mass spectrum. The analysis shows for what values of the parameters an enhancement of the quadrupole resolution is achieved. Initial experimental results for argon confirm the predicted theoretical trends. © 1999 Elsevier Science Ltd. All rights reserved.

1. Introduction

The mass filter of a quadrupole mass spectrometer (QMS) has been simulated [1,2] using a numerical solution to the Mathieu equation for finite length lens with electric excitation of the electrodes. For certain values of the direct and rf fields only ions of a particular charge to mass ratio are passed successfully through the filter. In this article the application of a magnetic field to the mass filter will be considered in addition to the conventional electric fields. It will be assumed in the model that the QMS contains hyperbolic rods as electrodes and the magnetic field penetrates the full length of the mass filter assembly.

2. Theory

The force felt by the ion in the presence of electric and magnetic fields is the Lorentz force. If the electric field is given by the conventional hyperbolic potential for hyperbolic electrodes where U is the direct potential applied to the rods, V the amplitude of the rf, f the frequency of the sinusoidal field and r_0 the inscribed radius of the electrodes, for a general magnetic field $\mathbf{B} = (B_x, B_y, B_z)$ the coupled equations of motion are

$$\frac{d^2x}{d\xi^2} = -x(a - 2q\cos 2\xi) + \left(\frac{dy}{d\xi}b_3 - \frac{dz}{d\xi}b_2\right), \tag{1}$$

$$\frac{d^2y}{d\xi^2} = y(a - 2q\cos 2\xi) + \left(\frac{dz}{d\xi}b_1 - \frac{dx}{d\xi}b_3\right), \tag{2}$$

$$\frac{d^2z}{d\xi^2} = \left(\frac{dx}{d\xi}b_2 - \frac{dy}{d\xi}b_1\right). \tag{3}$$

The equations have been written in a dimensionless form where the only dimension that appears is that of length displacement. The time t has become $t = 2\xi/\omega$ where the angular frequency is related to the frequency of the alternating rf by $\omega = 2\pi f$. The direct potential U and the alternating potential amplitude V are related to a and q, respectively, as $a = 4eU/m\omega^2 r_0^2$ and $q = 2eV/m\omega^2 r_0^2$, where the mass of the ion is given by m. The components of the magnetic field $\mathbf{B}$ become $(b_1, b_2, b_3) = (2eB_x/m\omega, 2eB_y/m\omega, 2eB_z/m\omega)$. We notice that if the magnetic field is taken to be zero the coupled differential equations reduce to the familiar Mathieu equations. The geometry of the equations of motion is given in [1]. To solve the differential equations numerically for a finite mass filter it is necessary to rewrite the equations in terms of first-order differentials. The effective velocities become variables and instead of having three equations there are six coupled equations. The resulting set of equations can be solved numerically using a fourth-order Runge–Kutta

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technique. The magnetic field **B** is general. To solve numerically a particular **B** must be chosen. Solving numerically the coupled equations give the trajectories of the ions through the mass filter.

From the trajectories it is possible to determine the conditions which give successful ion transmission for a given charge to mass ratio. This depends on the values of the direct voltage U, the rf amplitude V, the rf voltage frequency f, the inscribed radius of the quadrupole rods r_0, the magnetic field **B**, the initial velocity and position of the ion and the initial phase. The first four parameters appear as the variables of a and q in the Mathieu equation, ($\mathbf{B} = 0$). For **B** non-zero we have further dependence (also in a and q), of ion charge, mass and frequency. For a real QMS the resolution may be defined as the width of the peak in the mass spectrum, (transmission peak), at 10% peak height for a particular ion. For simulation it is necessary to collate the information from successive ion trajectories into a peak. In previous work [2] this has been achieved for the $\mathbf{B} = 0$ case. In this article, we consider the effect of a constant magnetic field on the shape of the transmission peak for ion passage through the quadrupole mass filter.

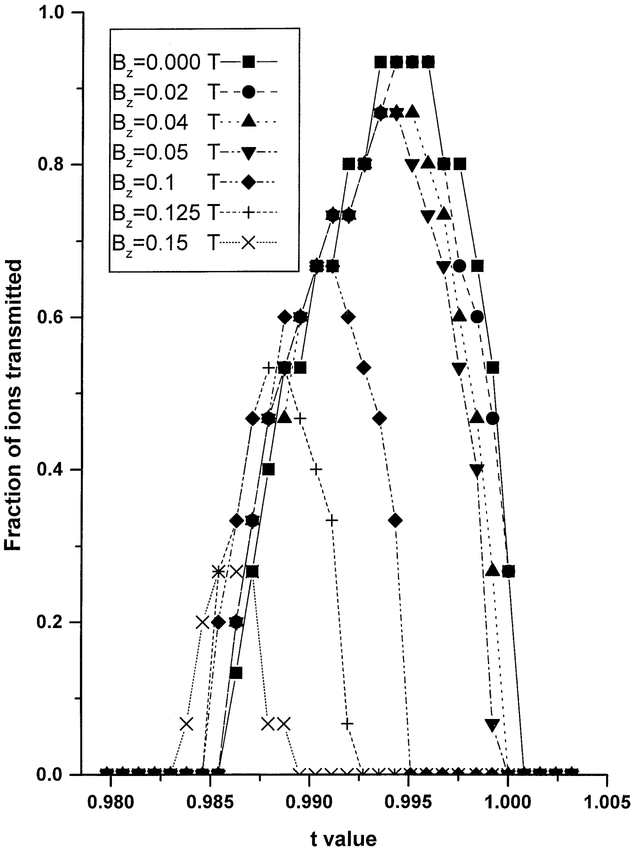

Fig. 1. The simulated mass spectrum (transmission peak) for varying magnetic field (B) applied in the z-direction. The vertical scale shows the fraction of ions transmitted through the QMS filter.

3. Simulation results

For various parameters, i.e. rf phase angle, a and q, a transmission peak can be simulated as one moves up the scan line through the tip of the stability diagram [1,2]. To achieve this, singularly charged nitrogen molecules were considered (28 AMU), with 100 cycles of rf applied to the quadrupole rods. The initial velocity of the ions was taken in the axial direction (z-axis), of the mass filter, and set equal to 1000 m/s. The initial value of the coordinates in the x and y directions (defined in the plane perpendicular to the axis of the quadrupole, connecting opposite rods of the mass filter), were 0.3 and 0.3 mm, respectively. The inscribed radius of the quadrupole mass filter was taken to be 2.75 mm. The position of the ion in the axial z-direction was taken to be zero, the entrance to the mass filter. The frequency of the rf voltage used in the simulation was 2 MHz. The parameters a and q were varied in a constant ratio by introducing a variable t. a_t and q_t are defined as $a_t = ta$ and $q_t = tq$, respectively. On the plots of the transmission peaks the fraction of ions transmitted are plotted against the value of t. For each value of t, 15 ions of various rf phases were considered in the simulation. The fraction of the ions transmitted is thus an average over rf phase angle values. A contribution to the average is made for each successful ion transmission.

Fig. 1 showed the effect of a constant magnetic field applied axially in the z-direction. The transmission peak remains mostly unchanged for the magnetic field applied upto the 0.05 T level. For the field value of 0.1 T and greater the peak is reduced in size becoming narrower moving to the left, (lower t).

Fig. 2 showed the behaviour of the resolution, measured at 10% peak height, as a function of magnetic field. For the magnetic field in the x-direction the resolution increases as B_x varied between 0 and 0.05 T. The resolution will not increase indefinitely since as B_x increases the peak height decreases (sensitivity). For variation of the magnetic field in the y direction resolution remains approximately constant (shown constant). Resolution again increased as B_z increased.

4. Experimental results

Argon gas was let into the vacuum system which housed the conventional QMS. The electronics of the spectrometer were tuned so a reasonable sized peak at 40 AMU was obtained on the pen-recorder. The transverse magnetic field was applied through the use of a bar magnet fixed in a steel yoke around the mass filter. Primarily we were interested whether the magnetic field

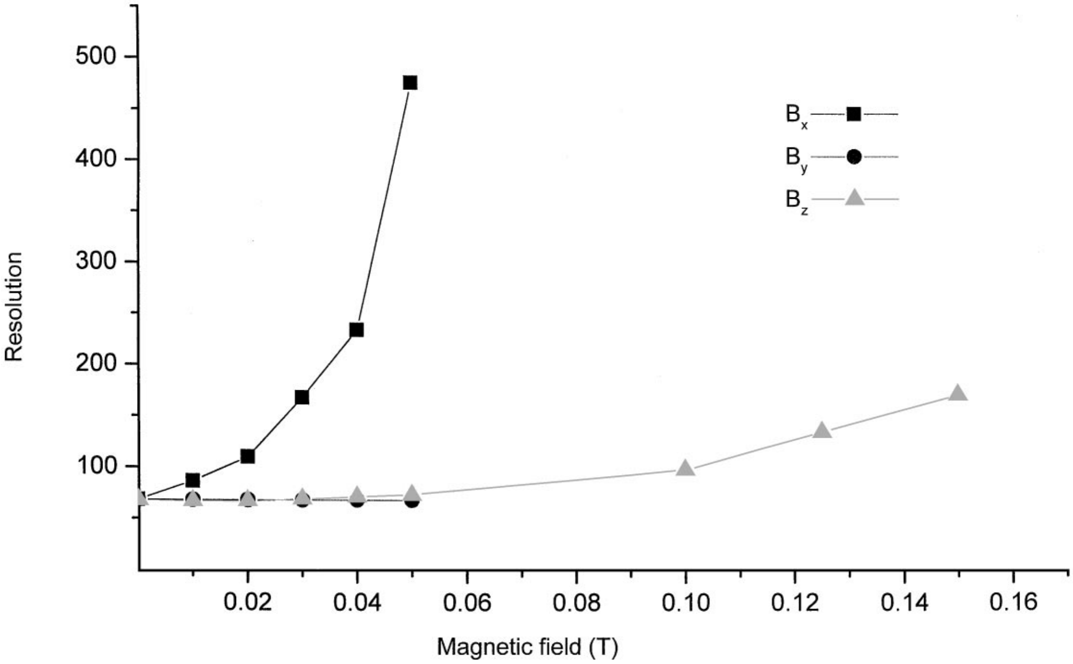

Fig. 2. The effect of magnetic field on resolution applied in the *x*-, *y*- and *z*-direction, respectively.

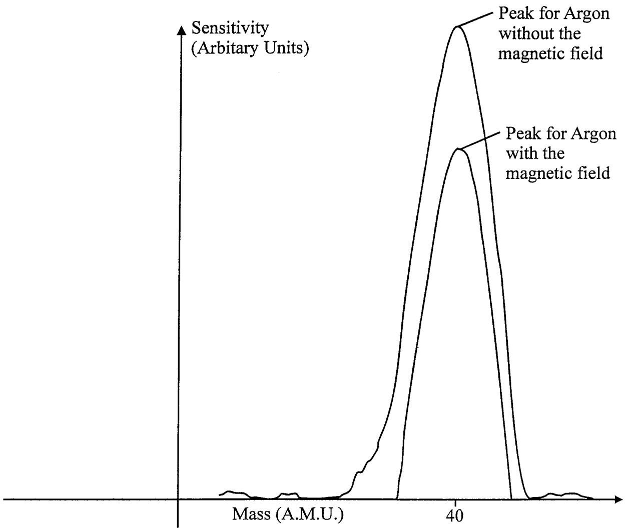

Fig. 3. Experimental mass spectrum for argon gas. The upper curve is the peak without magnetic field and the lower peak is the transmission peak with a constant transverse magnetic field.

would reproduce the effects on the transmission peak of the simulation. No accurate measure of the strength of the magnetic field was made. Unlike the simulation we were using argon gas was used with rf voltage at 4 MHz. Fig. 3 shows two argon mass spectra. The upper plot shows the argon peak without the magnetic field, whereas the lower peak shows the argon peak in the presence of the transverse magnetic field. It is clear that both low mass and high mass sides are sharper and that the resolution has improved. Sensitivity has been reduced and both effects agree with the simulation.

5. Discussion and conclusion

Clearly the application of a magnetic field shows some benefit for the operation of a QMS, giving improved resolution. An analytical solution for the constant magnetic field case would be useful in determining the condition for stable trajectories through the mass filter. Such a solution is underway. We have solved the system of linearised coupled differential equations derived from the equation of motion of the ion through the mass filter for $q = 0$ and the magnetic field taken to be a constant. A full solution with all the parameters taken into account is thus feasible.

References

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