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Effect of magnetic field on the confinement of ions in a three-dimensional radio frequency quadrupole trap

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Abstract

The confining field of a three-dimensional radio frequency ion trap has been modified by the addition of a static uniform one-dimensional magnetic field. The physical properties of the confined ions under this combined field are not identical in z and r directions. Numerical calculations show that for a weak magnetic field the changes in the ion secular frequency are negligible for certain applications. (Int J Mass Spectrom 213 (2002) 177–181) © 2002 Elsevier Science B.V.

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1. Introduction

Many recent studies of collision phenomena and ion spectroscopy have been focused on the injection of externally generated electrons, ions, neutrals, or photons into a radio frequency (rf) quadruple ion trap. The rf ion trap is capable of confining the gaseous ions for a long time with a minimum of kinetic energy, of the order of a fraction of an electron volt (depending on the trapping parameters a_z, I_z and the applied rf voltage).

The rf ion trap has been potential applied to experiments involving the formation of interstellar molecules through cascade reactive collisions [1] and is especially well adapted for the production and investigation of multicharged ions produced in fusion-type plasma. The latter study is concerned principally with charge exchange rates of populations of multiply charged carbon ions [2].

In an earlier work [3–5], a method of employing a rf impulsional voltage was investigated. This method offers the advantage of a periodic large zero-voltage temporal zone for the injection of particles of well-defined collimated initial energy into the rf ion trap. The form of the applied rf impulsional voltage was such that the injected ion initial energy remained unchanged, was known precisely, and could be adjusted.

In general, for the purpose of collisional studies, the rf ion trap is coupled with a mass filter [1]. The rf ion trap acts as a reaction chamber and the mass filter is operated in the mass-selective mode. For a pure rf ion trap [6] operated in the mass-selective axial instability mode, the $I_{z,\max}$ value which is the maximum value of I_z corresponds to the point on the stability diagram boundary at which the $\beta_z=$ boundary intersect the a_z axis. The high-resolution mass-selective mode of

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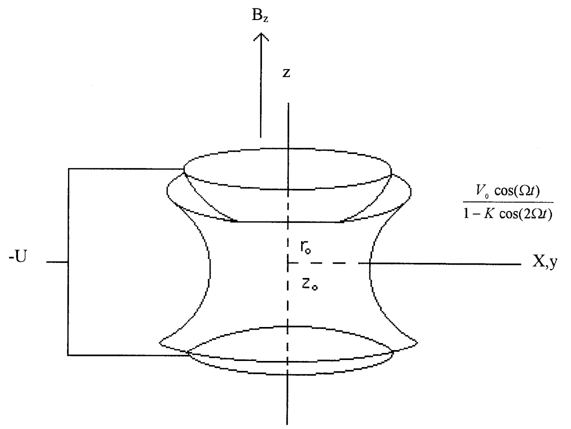

Fig. 1. Schematic representation of a rf ion trap.

the rf ion trap corresponds to the a_z and I_z values at the upper apex of the stability diagram.

In the present work, a system that employs a uniform one-dimensional magnetic field in the z direction, B_z, together with a rf impulsional voltage given by

$$V(t) = \frac{V_0 \cos \Omega t}{1 - k \cos 2\Omega t} \tag{1}$$

and a dc voltage has been studied. The motivation for this study was to determine the effect on ions confined in a rf trap of a weak magnetic field such as may be induced by some instruments in or near an ion pump or Tokamak experiment. With the application of a large magnetic field, this mode of rf ion trap operation may have application in the field of confining an uncharged magnetic dipole in three dimensions [7]. As will be seen, this investigation shows a new mode of ion trap operation that maybe useful for some applications.

2. Theory

A schematic diagram of the electronic potentials and magnetic field to a rf ion trap [8] is shown in Fig.1. A negative dc voltage ($-U$) is applied to the two endcap electrodes and a rf voltage given by Eq. (1) is applied to the ring electrode where $\Omega/2\pi$ is the rf drive frequency, $V_0=(1-k)V_{max}$, $0\leq k<1$ is the modulation “index” parameter, V_{max} is the maximum value of V_{0-p}, and a uniform magnetic field B_z is applied in the z direction. This mode of the confining field is similar to the ion trapping properties of the Penning ion trap [9], i.e. the radial focusing of the ions by the dc voltage is overcome by a uniform axial magnetic field B_z except a periodic rf impulsional voltage is applied to the quadrupole ring electrode structure. For an ion of mass m and charge e placed in this field, the basic classical equation of ion movement can be described by Hill’s differential equation [10–12]. The resulting classical equation of ion motion in the z direction is not modified by the applied magnetic field

$$\frac{d^2 z(\xi)}{d\xi^2} + \left[a_z - 2I_z \frac{\cos(2\xi)}{1 - k \cos(4\xi)} \right] z(\xi) = 0 \tag{2}$$

in which $2\xi=\Omega t$ and the trapping parameters a_z and I_z are given as

$$a_z = \frac{-4eU}{mz_0^2\Omega^2} = -2a_r,$$

$$I_z = \frac{2eV_{max}(1-k)}{mz_0^2\Omega^2} = -2I_r \tag{3}$$

where z_0 is one-half the shortest separation of the endcap electrodes.

The effect of the magnetic field in the z direction causes the projection of ion motion in the plane perpendicular to z to turn if the field is sufficiently large. Therefore, the equations of the ion movement in the x and y directions are modified and can be written as

$$\frac{d^2 x(t)}{dt^2} + \frac{e}{mr_0^2}\left(U + \frac{v_0 \cos(\Omega t)}{1 - k \cos(2\Omega t)} \right) x(t) - \frac{eB_z}{m}\frac{dy(t)}{dt} = 0$$

$$\frac{d^2 y(t)}{dt^2} + \frac{e}{mr_0^2}\left(U + \frac{v_0 \cos(\Omega t)}{1 - k \cos(2\Omega t)} \right) y(t) + \frac{eB_z}{m}\frac{dx(t)}{dt} = 0 \tag{4}$$

where $r_0^2=2z_0^2$ is the square of the ring electrode diameter. One may recognize directly that $\omega_c=eB_z/m$ is the ion cyclotron frequency. The effect of B_z is to add one new term to each of equations of motion in the x and y direction, otherwise the equations of ion motion should be the same as before [5].

The solution of the equations of ion movement can be carried out independently for the z and r directions. There is a direct solution for the$z$ direction but, for the$r$ direction, let the equations of system (4) be coupled and assuming the following:

$$x_+(t) = x(t) + jy(t) \tag{5}$$

where $j=\surd(-1)$. The use of Eq. (5) in Eq. (4) will yield

$$\frac{d^2x_+(t)}{dt^2} + j\omega_c\frac{dx_+(t)}{dt} + \left[\frac{\mathrm{e}}{\mathrm{m}r_0^2}\left(\mathrm{U}+\frac{\mathrm{V}_0\cos(\Omega t)}{1-k\cos(2\Omega t)}\right)\right]x_+(t) = 0 \tag{6}$$

If we assume a solution of the form

$$x_+(t) = r(t)\exp\left(-j\frac{\omega_c}{2}t\right) \tag{7}$$

and substituting this solution [Eq. (7)] in Eq. (6), cast a new equation of ion motion which in the canonical form can be written as

$$\frac{d^2r(\xi)}{d\xi^2} + a'_r - 2I_r\frac{\cos(2\xi)}{1-k\cos(4\xi)}r(\xi) = 0 \tag{8}$$

where $2\xi=\Omega t$ and $a'_r=a_1+a_r$ in which $a_1=(\omega_c/\Omega)^2$.

As one can see, the trapping parameter I_r is unchanged by the magnetic field B_z, but a new quantity a_1 is added to the trapping parameter a_r. The numerical solutions of Eqs. (2) and (8) are obtained using the matrix method [13,14]

$$\begin{bmatrix} u(\xi_0+\xi) \\ \dot{u}(\xi_0+\xi) \end{bmatrix} = \begin{bmatrix} m_{11} & m_{12} \\ m_{21} & m_{22} \end{bmatrix}\begin{bmatrix} u(\xi_0) \\ \dot{u}(\xi_0) \end{bmatrix} \tag{9}$$

Here u is one of the directions z or r, $\xi_0= 0$ is the initial phase of the rf drive voltage, and $\xi=\pi$ is the fundamental period. From the ion motion stability, i.e. $|m_{11}+m_{22}|\leq 2$, the value of the state transition matrix provides the parameters β_u which control the ion oscillation movements. In the fundamental form they have the following relations with the ion secular frequency for each of the$z$and$r$directions

$$\omega_z = \beta_z\frac{\Omega}{2}, \qquad \omega_r = \left[\left(\frac{\omega_c^2}{2\Omega}\right) + \beta_r\frac{\Omega}{2}\right] \tag{10}$$

It can be seen that the ion motion fundamental secular frequency ω_r is increased by a factor of $\omega_c^2/2\Omega$ which causes the iso-β_r lines to be drown closer. This change does not affect the ranged β_r from 0 to 1 over the interval $0<I_r\leq I_{r\max}$. Therefore, the dominant frequency in the ion motion never exceeds half the rf drive frequency voltage for the$z$direction whereas that for the$r$direction is increased by a factor of $\omega_c^2/2\Omega$ with respect to that without B_z. With respect to the first stability diagram, the trapping parameter a_r is shifted to α'_r within the limits of the trapping parameter a_z. In other words, any increment on the stability parameter a_r must lie within the a_z, I_z stability region.

3. Results and discussion

For the purposes of illustrating the effect of the a_1 on the first stability region, consider the first stability diagram in the plane (a_z, I_z) for $k=0.8$ without the use of magnetic field. Suppose a point A with the coordinate $a_z=-2a_r=0.15$ and $I_z=-2I_r=0.306$ which is situated at the tip of the stability region with the scan slope line of $a_z/I_z=-2U/[V_{\max}(1-k)]$ as shown in Fig. 2.

Suppose a value of $a_1=0.02$ is added to a_z of the point A as (a_1-2a_r) keeping the value of I_z constant. The new operating point B($a_z=0.17$, $I_z=0.306$) is obtained which is situated outside of the stability diagram and corresponds to unstable ion motion. To retrieve a working point corresponding to operation stable, one must reduce I_z to the value that lies on the $\beta_z=1$ stability boundary, e.g. this point is C($a_z=0.17$, $I_z=0.3$).

In Fig. 3, we have shown the relationship between stable operating points (a_z, I_z) on the $\beta_z=1$ stability boundary as a_1 is increased from zero and the corre-

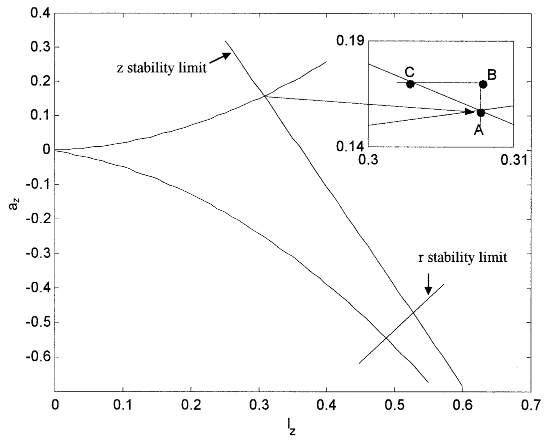

Fig. 2. The first stability diagram for k=0.8: point A(a_z=0.15, I_z=0.306) is the tip of the upper apex of the stability region, B(a_z=0.17, I_z=0.306), lies outside the stability diagram when B_z is applied, and C(a_z=0.17, I_z=0.3) is the working point obtained by reducing I_z to the value that lies on the β_z=1 stability boundary.

spondingly shifted value of I_z for a_z=0.15. For the negative part of stability diagram, ($-a_z$, I_z) the effect of increasing the parameter a_1 is almost the same as for the positive region except that the stability region is shifted in the direction of the I_z axis.

On the basis of this characteristic behavior of an rf ion trap under the application of the magnetic field, we may achieve a new mode of scanning the stability regions. As the trapping parameter a_z is fixed for a given I_z, it is possible to vary the modulation index k from zero to one in order to sweep the tip of the stability diagram. This mode of operation will reduce the size of stability region, i.e. as the values of I_z decreases when k increases (see also [5]), therefore the iso-β_u lines which control the ion secular frequency become closer. The innate narrowness of the stability region and the expected rapid transition from stable to unstable ion trajectories as k is varied so that the quadrupole should give higher resolution in a short number of rf cycles.

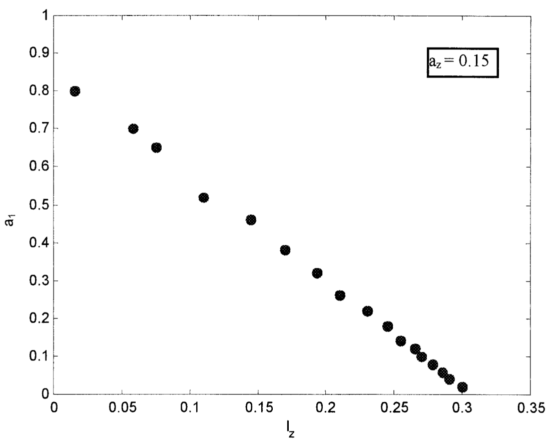

Fig. 3. Variation of a_1=(ω_c/Ω)2 against the trapping parameter I_z for a fixed value of a_z=0.15. The locus of these datum points corresponds to the β_z=1 boundary of he stability diagram.

Although the rf ion trap with the supplied magnetic field operate in the rf-only mode, consider the adiabatic operating region of the stability diagram, e.g. the linear part of I_z–β_z curve in which ions have harmonic oscillation, $a_z\sim 0$ and $I_z\leq 0.15$ when k=0.8, for the determination of the difference in ion secular frequency with or without applied magnetic field. For this purpose, the equivalent points have been defined as the operating points in two different stability diagrams, i.e. k=0 and k=0.8, which have the same value of β_z. Indeed, these points are associated with the same ion secular frequencies ω_z. in the case of k=0, the well known expression for adiabatic region is $\beta_z=(\sqrt{}2/2)\ q_z$, and from equivalent point, for k=0.8, we have found $\beta_z=1.8I_z$. This adiabatic stability region allows a simple relationship between β_z and the stability parameter I_z such as $\omega_z=(1.8I_z)\Omega/2$. We use this relationship to derive the ion secular frequency in the $r$direction

$$\omega_r=\left[\left(\frac{\omega_c}{\Omega}\right)^2+\frac{1.8}{2}I_z\right]\frac{\Omega}{2} \tag{11}$$

In order to provide a comprehensive minimum effect of the magnetic field on the trapped ion secular frequency let $B_z=10^{-4}$ T which is close to the earth magnetic field (47×10^{-6} T). For the assessment of numerical calculations we use the following parameters: I_z=0.1, $\Omega/2\pi$=1/11 MHz and Xe^+ ion. With the applied magnetic field, the fundamental ion secular frequency has been found to be $f_r=\omega_r/2\pi$= 4090.9053 Hz and in the absence of magnetic field, f_r=4090.9048. For a stronger magnetic field, i.e. the stray field near a Tokamak, the ion secular frequency for $B_z = 10^{-2}$ T, has been obtained as $f_r = 4098.3989$ Hz.

4. Conclusion

We have examined the effect of a uniform magnetic field on the confined ion in a rf ion trap. On the basis of stable ion motion characteristic behavior, different values of B_z has been used to calculate the ion secular frequencies. There was no significant change in the ion secular frequency, when a near earth magnetic field of $B_z = 10^{-4}$ T was used. Whereas, a high stray field near a Tokamak of $B_z = 10^{-2}$ T had a significant effect on the ion secular frequency.

However, from these calculation it can be concluded that the effect of a weak magnetic field on the ion secular frequency can be negligible for some application if $\omega_c/\Omega \ll 1$.

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