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Influence of a geometrical perturbation on the ion dynamics in a 3D Paul trap

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ABSTRACT

In ion traps, the purity of the Quadrupole potential is essential. Any perturbations in potential caused by geometrical imperfections or the presence of other ions alter the dynamics of trapped ions. In this paper the effect of a particular perturbation on dynamics of trapped ions in a 3-D quadrupole trap is analyzed and we have compared the experimental findings with simulations. To see the effect of geometrical perturbation, the position of a filament reaching into the trap (which acts as the perturbing element) is altered. The equi-frequency line on the $a-q$ Mathieu plot was scanned at different filament insertion heights. We studied the effect of filament current and the duration of loading. The distorted potential within this trap has been theoretically calculated and simulated using SIMION. An analytical expression for potential inside the trap is fitted to the potential values obtained from the simulation and the numerical solutions of the equation of motion of trapped ions is obtained. The motional frequencies are then calculated from the Fourier transformation of the simulated ion trajectories at any given trapping potential and compared with our experimental findings. The shift in the secular frequency with respect to the level of insertion of the filament within the trap is evaluated.

1. Introduction

Confinement of charged particles in an ion trap offers unique advantages allowing state of the art experiments to be performed enabling us to have profound insight in the fields of atomic, nuclear and quantum physics. Ion traps are extensively used in the different fields of scientific applications like mass spectrometry, several atomic and nuclear physics related experiments and more recently in the field of quantum computations [1–4]. Starting with Paul [5] and Dehmelt [6] several other researchers [7–9] have extensively worked in this field presenting innovative and improved models of ion traps. Improvement in design of ion traps and theoretical simulations to achieve the near ideal quadrupole field is an ongoing process in the field. In principle trapping of charged particles is not a difficult task but utilization of traps as devices for quantum engineering, precise mass measurements and high precision studies in atomic and molecular physics, requires a suitable design and precise machining and a thorough understanding of the fields that are generated within. In the past 30 years enormous work has been done in the field of ion traps in this direction.

For an ideal 3-D Paul trap the field inside varies linearly with distance from the trap center. The potential inside is given as

$$\phi = \frac{U_{dc}+V_{rf}\cos\Omega t}{2r_0^2}(2z^2-x^2-y^2) \tag{1}$$

where U_{dc} and V_{rf} are the amplitudes of the static and time varying trapping potentials (RF potentials) applied across the trap electrodes and Ω is the angular frequency of the RF potential. The size of the trap is defined in terms of the radius of the ring electrode (r_0) and the separation of end-caps ($2z_0$) and maintains r_0/z_0 equal to $\sqrt{2}$. The ion motion for an ideal trap can be described by Mathieu equations as discussed in [10,11]. In practice, it is difficult to make an ideal trap as described in theory. Manufacturing errors and several other modifications made in the trap for the convenience of specific experiments cause deviations in the potential as described in Eq. (1). Any deviation from this 'ideal' quadrupole potential is expressed either by a multipole expansion of the generalised potential [12] or suitable modifications in the Eq. (1) [13]. This deviation of the potential from the ideal quadrupole form alters the characteristics of the trapped ions, manifesting as nonlinear effects which are broadly classified into three ways.

The first one is where the trapped ions exhibit instabilities even though the trap is operated within its stability region. These instabilities were first seen by Busch and Paul [14] and were termed as black holes and canyons. Measurement of the number of

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trapped ions at different operating points provides an experimental verification [15–17] of the occurrence of these instabilities. These instabilities occur when a weak multipole higher order potential is superimposed on the pure quadrupole potential. Wang et al. [18] have given a theoretical explanation for such instabilities where they say that at certain operating points the superposition of the motional frequencies and their overtones are an integral multiple of the drive frequency, causing the transfer of energy from the drive field to the trapped ions. In addition it results in coupling of the ion motions in the r and z directions. This causes the excitation and ejection of trapped ions at frequencies other than the harmonic motional frequencies [19–21]. These nonlinear effects can be used in isotope separation of ions in a Paul trap [22].

The second effect is a non-linear effect manifesting as anharmonic oscillations of trapped ions leading to an asymmetry in the so-called frequency response curve [7]. The magnitude and distortion of these anharmonic oscillations depend upon the extent of nonlinearities in the trap. In addition to this the asymmetry in the resonance curves also depends upon the strength of the excitation field used to detect the ions and is important especially in mass spectrometry [11].

The third observed effect in ion traps is the shift in the secular frequencies due to nonlinearities in the trapping field. As ions move away from the center of a non-ideal trap, where the field within varies nonlinearly with the distance from the trap center, the secular frequencies exhibit a shift from those calculated for an ideal trap. The shift in the ion oscillation frequency depends upon the polarity, strength and order of that particular multipole present [23]. This geometrically driven nonlinear effect exhibits a shift in the stability region and is observed in hybrid [24] and stretched mode [25] of Paul traps. This shift in the stability region is explained either by numerical methods [26,27] or by including weak nonlinear potentials in the Mathieu equations that describe the motion of trapped ions [28].

For a single ion confined in an ideal trap, the motional frequencies depend solely upon the mass, charge, operating parameters and trap dimensions. The motional frequencies get modified due to the presence of other ions and aberrations in the trap geometry. Several researchers have seen that when ions of a single species are collectively excited the motional resonances do not depend on the number of ions trapped, i.e., no observable shift in the motional resonance frequencies is seen due to the space charge effect [22,29]. On the contrary the individual motional frequency and also in some cases the collective ion motion especially when two or more species are trapped simultaneously exhibit change in ion oscillation frequency with increasing number of ions [30]. It may be noted that for collective excitation the requirement of the excitation energy is higher than that required for an individual ion motion.

In the present study we keep the excitation level small enough to enable individual ion excitation, so that the space charge effect is visible. At the same time the perturbations in the trapping field due to geometrical aberrations are also discernible, which also causes the shift in motional frequencies. To understand the effects individually we reduce the geometrical perturbations to a minimum, a point where only space charge effect is expected. These perturbations are important and affect high precision studies which rely on the accurate measurements of motional frequencies.

In almost all earlier studies, the potential within a non-ideal trap is considered to be rotationally symmetric. In the current work we discuss the change in the trapped ion characteristics when they are subjected to a slightly asymmetric potential caused due to geometric modifications. In our experiment a filament, placed slightly above the lower end-cap, alters the potential within the trap and also causes the breakage of rotational symmetry. Cumulative effects of the breakage of rotational symmetry and alteration of the trapping potential lead to changes in the trapped ion motion. In this paper we discuss the shift in motional frequencies due to the geometry driven perturbations and also due to the presence of ions, through our experimental and theoretical studies. It is mainly the filament that is placed above the lower end-cap (modeling as an additional electrode) which alters the trapping potential and causes a change in ion motional behavior, compared to the presence of other trapped ions. We discuss the effect of geometrical imperfections by analyzing the perturbed potential theoretically. We simulate the potential using SIMION and fit it to an analytic expression. The ion oscillation frequencies are then calculated by taking Fourier transform of the simulated ion trajectory for this potential expression, using the same approach as adopted by Douglas and Konenkov [31].

2. Theory of trapping

In an ideal Paul trap, the time dependent potential given in Eq. (1) is responsible for confining the ions close to the trap center. The motion of trapped ion is described by Mathieu equations [32] and is expressed as

$$\frac{d^2u_i}{d\tau^2}+(a_i-2q_i\cos 2\tau)u_i=0 \tag{2}$$

where u_i represents the position coordinate in Cartesian coordinate system and the normalized time τ is $\Omega t/2$. The parameters, a_i and q_i, are the functions of trapping potentials and are defined as

$$a_z=\frac{8QU_{dc}}{mr_0^2\Omega^2},\quad a_x=a_y=\frac{-4QU_{dc}}{mr_0^2\Omega^2} \tag{3}$$

$$q_z=\frac{-4QV_{rf}}{mr_0^2\Omega^2},\quad q_x=q_y=\frac{2QV_{rf}}{mr_0^2\Omega^2} \tag{4}$$

where m and Q are the mass and charge of trapped ions respectively.

The solutions of Eq. (2) represent the motion of ion in the trap and are comprised of the secular motion modulated at the drive frequency (Ω). The secular motional frequency ($\omega_i, i=z,r$) depends on the mass, charge of trapped ions and operating parameters of the trap. In the pseudo potential well model [6], the secular frequency ω_i is expressed as a function of the parameter β_i, which is a function of a_i and q_i defined in Eqs. (3) and (4). For small values of a_i and q_i (<0.4) the parameter β_i can be well approximated by $\sqrt{a_i+q_i^2/2}$. In other cases β_i can be written as a solution of a continuous function in a_i and q_i [10,11]. These expressions are applicable only for an ideal Paul trap and any imperfection calls for modification in the expressions.

3. Experiment

The experimental set-up used in current studies is similar to that reported in our earlier paper [33]. The ion trap consists of a set of three hyperbolically shaped electrodes (Fig. 1a). The ring electrode radius (r_0) is 20 mm. The ring electrode has four symmetrically positioned holes each measuring 8 mm in diameter to facilitate steering of a laser beam [34]. The lower end-cap has two symmetric rectangular slots to place the filaments and the slots are positioned at 5 mm away from the center of the lower end-cap (Fig. 1b). In our experiments a filament of dimensions 22 mm × 4 mm is inserted within the trapping region through one of these slots while the other one is kept empty. To observe the effects, the height of the filament is changed for each set of experiments. For trapping, an RF potential at a fixed drive frequency ($\Omega/2\pi=500$ kHz) along with a DC potential was