Abstract  The effect of the presence of a finite number of ions on their parametric resonances inside a Paul trap has been investigated both experimentally and theoretically. The Coulomb coupling among the charged particles results in two distinct phenomena: one is the frequency shift of the trapped ion oscillators and second is the collective oscillation of the trapped ion cloud. We observe both in a linear trap configuration. It is found that the strength and the secular frequency of individual ion-oscillation decrease while the strength of the collective oscillation increases with increasing number of trapped ions. The observation has been modeled by considering the space charge potential as an effective dc potential inside the trap. It describes the observations well within the experimental uncertainties.

1 Introduction

Linear Paul trap [12,13] is a versatile tool for performing experiments of fundamental physics interests and commercial applications where from a single ion to a large number of ions, typically $10^4$, are required to trap depending on the aim of the experiment. The device is widely used in the field of quantum computation [14], atomic clock designing [6], precision spectroscopy [7,8], mass spectrometry [10] etc. In an ideal trap with a few ions, the ions exhibit in-phase harmonic oscillations with characteristic secular frequency. However considering the presence of Coulomb repulsion between the trapped ions, even the presence of a second ion inside the trap volume alters the trap potential. This has been studied by Paul [11] and Fischer [12] mostly empirically. Considering neighbouring interactions within mean field approach, we here show that the secular frequency shifts with the change in the number of trapped ions, as is consistent with the literature [13,14]. This approach is used to verify our experimental results and it agrees well with previous observations in a hyperbolic ion trap [16]. We report on the observation of collective oscillation of an ion cloud under certain experimental conditions in a linear Paul trap indicating strong coupling between the trapped ions.

A linear Paul trap uses a radio frequency (rf) potential ($V_0 \cos \Omega t$) in addition to a dc potential ($U$) for providing dynamical trapping of charged particles in the radial plane and a dc potential for providing axial confinement. As required for dynamical trapping the potential in the radial plane is quadrupolar in nature,

$$\Phi(x, y, t) = (U - V_0 \cos \Omega t) \left(\frac{x^2 - y^2}{2r_0^2}\right),$$

where $2r_0$ is the separation between the inner surfaces of the diagonally opposite middle electrodes. The equation of motion of a trapped ion in presence of this potential can be expressed by Mathieu’s differential equation,

$$\frac{d^2 u}{d\zeta^2} + \left(a_u - 2q_u \cos 2\zeta\right) u = 0,$$

with $u = x, y$, where

$$a_x = -a_y = \frac{4eU}{mr_0^2 \Omega^2},$$

$$q_x = -q_y = \frac{2eV_0}{mr_0^2 \Omega^2},$$

and $\zeta = \Omega t/2$. Solution of eqn. 2 shows that the ion oscillates with two different frequencies [17]; one equal to the frequency of the applied rf and is called micromotion while the other with a frequency $\omega_{\text{sec}} = \beta_u \Omega/2$ and is called secular motion. Here $\beta_u \approx \sqrt{a_u + q_u^2}/2$ for small $a_u$ and $q_u$.

Although the potential in ideal case is quadrupolar, in practice it appears with higher order terms that results in instability of the ion-motion in the trap [18].
The ion motion is parametrically excited when the frequency of oscillation at a given operating parameter \((a_u, q_u)\) satisfies a resonance condition with the frequency of the rf trapping potential \([15][21]\) as given by

\[
n_x \omega_{lx} + n_y \omega_{ly} = \Omega,
\]

where \(n_x, n_y = 0, 1, 2, 3... \) and \(n_x + n_y = k\) is the order of the multipole \([22]\), present in the trapping potential and higher than the quadrupole one \((k > 2)\). If one of the trap parameters is varied, a parametric resonance appears at a definite value subjected to the condition defined by eqn. \([4]\) and it gives rise to instabilities called “black canyons” within the stability diagram \([22]\). The position of such resonance on a trap operating parameter space (say, \(q\)) depends on various factors, such as the coupling between the axial and radial potentials \([23]\), space charge due to the trapped ions \([16]\) etc. Here we discuss the effect of space charge on a parametric resonance of an ion cloud in a linear Paul trap. It is observed that the position of a parametric resonance shifts to higher values of \(q\) as more ions are loaded into the trap. Earlier work with a hyperbolic trap reported a similar observation \([16]\) where the strength of the resonance has been shown unchanged with the increase in the trapped ion number. On the contrary, here we observe that the strength of the resonance decreases with the increase in the number of trapped ions. The observation of the shift has been explained with the help of a model that is consistent with earlier observation \([16]\) as well. It is shown that a collective oscillation of the trapped ions sets in with increasing space charge for which the strength of the parametric resonances becomes weaker in our experiment.

2 Experiment

The experimental setup consisting of a linear Paul trap, an ionization setup, extraction and detection setup is shown schematically in figure 1. The linear trap is assembled from four three-segmented electrodes each placed at four corners of a square of side 12.73 mm. Each of twelve rods are of diameter 10 mm. The four middle rods are of length 25 mm while all others are 15 mm long. The separation between the surfaces of the diagonally opposite rods \((2r_0)\) is 8 mm. The middle electrode is separated from the end electrodes by a gap of 2 mm. The molecular nitrogen ions \((N^+_2)\) are created by electron impact ionization. The ions are dynamically trapped for few hundreds of milliseconds before they are extracted by lowering the axial potential in one direction. The extracted ions are detected by a channel electron multiplier. A time-of-flight technique has been employed for the detection of the number of trapped ions.

The trap is operated at a rf frequency of 1.415 MHz and the middle electrodes are kept at dc ground \((U = 0, a_u = 0)\). The end electrodes are kept at +20 V while trapping. At the time of extraction, the end electrodes at the ion-exit-side is switched fast from +20 V to −45 V. The number of trapped ions are varied by changing the creation time \((T_c)\) between 1 ms to 100 ms when the filament is kept on. The trap parameter \(q\) is varied by changing the rf amplitude while keeping the \(T_c\) same and the number of trapped ions is counted in each step. As expected, narrow nonlinear resonances appear within the stability diagram due to the presence of higher order multipoles of the trapping potential. The strongest observed resonance corresponds to the sixth order multipole \((k = 6)\) in our setup.

The \(q\) is varied in steps of 0.0004 about the sixth order parametric resonance while keeping all other parameters unchanged. Experimentally obtained ion numbers are normalized with respect to maximum ion number \((N_0)\) during a particular resonance experiment. The normalized ion count \((N_n)\) with the associated uncertainty has been plotted as a function \(q\) as shown in figure 2 which corresponds to a maximum detected ion number of 17. As observed in the stability diagram of the trap, the stability of trapping decreases as \(q\) is scanned to higher values around the sixth order nonlinear resonance. Therefore, a base line correction on the resonance line shape has been employed to obtain the figure 2. This resonance (figure 2) is then fitted with a Gumbel function as defined by

\[
n_n = N_0' + A \exp \left[ -\exp \left( -\frac{q - q'}{\sigma} \right) \right] - 1, \tag{5}\]

where \(\eta = (q - q')/\sigma\). Here \(q'\) is the parametric resonance center and \(\sigma\) is the full-width at half-maxima of the resonance and they can be determined from the fit. \(N_0'\) is an offset and \(A\) is a scaling factor. This Gumbel fit is justified due to the extreme nature of distribution of the ions which are excited and rejected by the parametric resonance. As can be seen from figure 2 the fitting curve (shown by solid line) lies within the experimental error bars with the adjacent \(R^2\)–square value of 0.98. The position of the resonance as obtained from this fit is \(q' = 0.4862(1)\) and the width of the resonance is \(\sigma = 0.0021(1)\).

3 Results and analysis

3.1 Shift in the resonance center

The number of trapped ions has been varied by increasing the ion creation time \(T_c\) and the same parametric resonance as described in Sect. 2 has been studied for each set. The parametric resonance corresponding to different number of trapped ions are obtained and three of them have been plotted in figure 3. The figure shows that the strength of the parametric resonance becomes weaker and the width gets broader as more ions are loaded into the trap. When the trap is loaded with its full capacity (corresponds to maximum detected count of 93 shown
in figure 3 and known from the loading capacity of the trap, the signature of the parametric resonance disappears. Each of the parametric resonances corresponding to different number of trapped ions has been fitted to the function described in eqn. 5 after necessary baseline correction, in order to determine the value of the resonance center ($q'$). The $q$ value at the resonance has been plotted as a function of the trapped ions ($N$) in figure 4. The detected ion number has been multiplied by a factor of 10 that approximately accounts for the efficiency of detection to estimate the number of ions confined in the trap and effectively contributes to the space charge.

3.2 Theoretical model

A simple model has been employed to explain this observation reported in figure 4. The potential developed due to the presence of ions inside the trap increases with the space charge i.e. the number of trapped ions. Thus an ion inside the trap experiences an effective potential that depends not only on the applied trapping potential but also on the number of its neighbouring ions. The net force on a trapped ion is the resultant of the applied field and the interaction of the ion with all other ions inside the trap. In this model, it is assumed that the force on a trapped ion due to interaction with all other ions is proportional to the displacement from its equilibrium position. Again, the interaction increases with the space charge and hence the force scales proportional to the number of trapped ions ($N$). Thus the force of inter-
action in the radial plane and in the vicinity of a single ion due to all other ions can be represented by

\[ F_{1u} = (N - 1)V_I u \approx NV_I u, \quad (6) \]

where \( N \gg 1 \). Here \( V_I \) describes the mean field strength of the Coulomb interaction on an ion due to the charges inside the trap and contains the information about the effective volume of the trap, residual gas pressure etc. Incorporating the force of interaction in the trapping field defined by the potential in eqn. 1, the equation of motion in the radial plane can be written as

\[ \frac{d^2u}{d\zeta^2} + (a'_u - 2q_u \cos 2\zeta)u = 0, \quad (7) \]

where

\[ a'_u = a_u - \frac{4N\nu_I}{\Omega^2}. \quad (8) \]

The definition of the \( \beta \) parameter is modified by \( a'_u \) and can be redefined by

\[ \beta'_u = \sqrt{a'_u + \frac{q^2}{2}}. \quad (9) \]

Thus the secular frequency of the trapped ion decreases \([21]\) as \( \beta \) parameter is effectively decreased due to the space charge effect. Thus in order to match the secular frequency in presence of the space charge, the \( q \) value has to be increased. This implies that the position of the parametric resonance shifts to higher value of \( q \). If the parametric resonance shifts to a new position \( q' \) in presence of the space charge, it is given by

\[ q' = \sqrt{2(a - a') + q_0^2}, \quad (10) \]

where \( q' = q_0 \) is the parametric resonance center in absence of the space charge effect. From eqns. 8 and 10

\[ q' = \sqrt{\frac{8N\nu_I}{\Omega^2} + q_0^2}. \quad (11) \]

Eqn. 11 can alternatively be represented as

\[ q' = \sqrt{bN + c}, \quad (12) \]

with constants \( b \) and \( c \) defined as \( b = 8\nu_I/\Omega^2 \) and \( c = q^2 \).

The variation of the parametric resonance center with trapped ion number as presented in figure 1 has been fitted with the model function described in eqn. 12. However, due to the small trap volume and low detection efficiency the values of \( N \) are not widely spread and hence the fit resembles a straight line. The adjacent \( R^2 \)–square value of the fit is 0.92 and it yields \( b = 4.294 \times 10^{-6} \) and \( c = 0.2357 \). From the fitting, \( \nu_I = 4.2 \times 10^7 \) kg/s² and the unperturbed value of \( q \) has been obtained as \( q_0 = 0.4855 \).

![Fig. 4](image_url) Shift in the parametric resonance center (q') with trapped ion number (N). N is obtained after multiplying the detected ion count by a factor of 10. Solid line is a fit to the data points with the model function as described in the text.

![Fig. 5](image_url) Normalized ion number as a function of the frequency of the electric dipole excitation field for different number of trapped ions (mentioned inset). The resonance profile corresponding to a detected ion count of 27 appears to be noisy due to low number of ions. The second dip at 180.5 kHz in the resonance profiles for detected ion counts of 40 and 47 corresponds to collective oscillation of trapped ions.

3.3 Collective oscillation

One of the interesting results of our experiment is the suppression of parametric resonance (figure 3) when the trap is loaded almost to its full capacity (Sect. 3.1). This phenomenon can be qualitatively explained by the emergence of collective oscillation \([25, 26, 27]\) observed in our trap. As the coupling between the ions by inter-ionic Coulomb interaction becomes large due to large ion number, the cloud behaves as an effective single ion in the trap. Thus it requires more energy to excite a cloud as
4 Discussion

The effect of space charge on the parametric resonances of an ion cloud in a linear Paul trap has been reported in this article. Contrary to earlier report [16], vanishing parametric resonance as a function of space charge has been observed. The observation has been explained with the help of a model which is consistent with earlier report where the trapped ion number has been widely varied. In order to check the validity of the model, same average two-ion-interaction strength ($\bar{V}_I = 4.2 \times 10^7$ kg/s$^2$) and unperturbed parametric resonance center ($q_0 = 0.4855$) as obtained from the experiment using this model, have been considered and the number of trapped ions are taken over wide range as done in earlier work [16]. Figure 6 shows the same analytical behaviour of the model function (eqn. 12) that resembles the result reported by Alheit et al. [10]. However, this analytical work with same $V_I$ shows $q'$ to vary over a long range (0.486 to 0.602), on the contrary to the work performed with a fourth order parametric resonance in a hyperbolic trap [10]. This is likely to be coming from an overestimated value of the mean field in our experiment as compared to Alheit et al, where the trapped ion number is much larger within a large trap volume.

Our experiment is inconclusive about the observed reduction of the strength of parametric resonance. Therefore apart from the possibility of collective oscillation taking over the individual oscillations, the contradiction may stem from stronger higher-order-multipoles in the hyperbolic trap [10] as compared to that in our linear trap. The experiment has been performed with a fourth order parametric resonance in the hyperbolic trap while with the sixth order in this linear trap. It is also not mentioned whether the hyperbolic trap which has larger volume allowing more ions to be trapped, is loaded with its maximum capacity as done in our setup.

Though the actual spatial distribution of trapped ions is Gaussian [28, 29], the consideration of a simple uniform distribution [12] as is done here, is equally efficient to explain small variation of the parametric resonance line center. It shows that the space charge potential in the vicinity of a single ion within the trap can be considered as an effective dc potential. Such a model has been considered earlier to estimate the trapped ion number [30, 31]. From the model force defined in eqn. 6 the potential developed by the space charge can be calculated as

$$V_s = \frac{1}{2} NV_I u_0^2,$$

(13)

where $u_0$ is effective radial dimension where the mean field approximation can be considered to be fair. The maximum number of trapped ions ($N_{max}$) is limited by the depth of the pseudopotential $D_r$,

$$D_r = V_{smax} = \frac{1}{2}N_{max}V_I u_0^2.$$

(14)
By considering 1% of the radial trap dimension ($r_0 = 4$ mm) to be effective, efficiency of detection to be 10%, $V_I$ as obtained from the analysis and maximum detected ion number (93) in the experiment are consistent with each other for a pseudopotential depth $D_r = 15$ V. This study thus provides a significant value of the average strength of the Coulomb interaction which will help further the analytical investigation on the collective motion of a trapped ion cloud.

The signature of collective oscillation has not been observed via parametric resonance but it is quite prominent in the electric dipole excitation experiment. The following two reasons might be responsible for this non-observation. (1) The width of the parametric resonance is broader than the narrow collective oscillation resonance and hence the later remains hidden within the former. (2) The strength of higher order multipole (here, the sixth order) causing such parametric resonance is weak to excite a strong collective oscillation of a large ion cloud. Both of these possibilities need further investigation. In our trap setup the radial pseudopotential depth is kept around 15 V while the axial potential depth is 20 V. Thus the radial confinement is weaker as compared to the axial confinement. The first possibility should be studied with deeper radial pseudopotential and by varying $q$ in smaller steps so that sharper parametric resonance may be obtained with a signature of collective oscillation. The second possibility could be studied with a setup where the strength of the higher order multipole and hence the anharmonicity are controllable externally. For example, an additional rod may be introduced close to the trap-center and its potential can be adjusted externally and independent of the trap-supply-voltage.

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