Observation of a ring Coulomb crystal of Ca\(^+\) ions in a linear hexapole rf ion trap

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**Abstract**

Linear multipole rf ion traps generate very flat pseudopotentials in the radial direction that result in producing new types of Coulomb crystals by applying laser cooling to trapped ions. In essence, a large number of cold ions can be trapped in the larger trapping volume than that of a linear quadrupole trap of comparable size. The extensive almost field-free region is of advantage for studies of low temperature ion-molecule reactions and high-resolution spectroscopy. The ion Coulomb crystals in linear multipole traps have interesting features, and some of those do not occur in a linear quadrupole trap.

Our previous simulations show that crystallized ions form cylinder-like and ring structures in a linear octupole and multipole rf ion traps [1]. In the experiment, cylinder-like crystals of Ca$^+$ ions were successfully observed for large number of Ca$^+$ ions using the cryogenic linear octupole trap [2]. However, a ring Coulomb crystal with the small number of ions, which open up novel applications for quantum information processing and quantum computing, was not confirmed. Here we report experimental observation of planar ring Coulomb crystals consisting of a small number of ions in a cryogenic linear hexapole rf ion trap. Moreover the comparison of the observed images with the simulation images and a brief discussion about the problems in the simulation are also presented.
Simulated Ca\(^+\) Coulomb crystals in a linear octupole rf ion trap [1]

Demonstration experiment: cylinder-like Coulomb crystal of alumina charged particle in a linear octupole trap

**Linear Paul trap**

**Linear Octupole trap**

Trapping condition

\[ f = 133 \text{Hz} \]
\[ V_{ac} = 2.0 \sim 5.0 \text{kV} \]
\[ V_z < 2.0 \text{kV} \]

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**Linear hexapole rf ion trap**

![Diagram of the trap](image)

**Characteristics**
- Compact linear hexapole trap
  - Efficient laser-cooling of Ca\(^+\) ions and LN\(_2\)-cooling of trap electrodes (for UHV)
- Selectable observation direction (\(\theta = 0^\circ\) or \(90^\circ\) to the trap axis)
- Use of rod electrodes with a smaller diameter than that of standard hexapole rods (\(d = r_0\))
  - to increase the detection efficiency for the observation angle \(\theta = 90^\circ\)
- Adjustment of imaging optics (3x, 6x and x10) outside the vacuum chamber
- DC correction voltages (\(V_{dc1}\)~\(V_{dc6}\)) can be applied to all hexapole rods to manipulate a shape of a Coulomb crystal.

**Dimensions**
- Rod \(\phi\) 2.0 mm
- \(r'_0 = 3.5\) mm
- \(r_0 = 3.0\) mm
- \(z_0 = 9.5\) mm
- Cryogenic plate (~80K)

**Dimensions**
- Length: 50 mm
- Width: 19 mm
- Depth: 32 mm
Laser stabilization system

Energy level diagram of Ca$^+$

- $^2P_{3/2}$
- $^2P_{1/2}$
- $^2D_{3/2}$
- $^2D_{5/2}$
- $^2S_{1/2}$

Frequency stabilized He-Ne laser

Temperature stabilized transfer cavity
FSR 630 MHz
$R = 99.9\%$

Oscillator

Oscilloscope

High voltage amplifier

Peltier element

Peltier controller

Photodiode

Amplifier

DAQ

PC

Laser frequency controller

Amplifier

TOPTICA DL-100

Piezo transducer

Grating

Optical isolator

Wavemeter

Dichroic mirror

Frequency stabilized He-Ne laser

$\lambda = 633\text{nm}$

For laser cooling (~0.2mW, 397nm)

For stabilizing 866nm laser
**Observation direction**

**Standard observation (θ = 90°)**

**Observation along the trap axis (θ = 0°)**

**Typical experimental parameters**

RF and DC voltages: $f = 4.4$ MHz, $V_{ac} = 200V_{p-p}$, $V_z = 1$-5 V

Correction voltages (rod electrodes): $V_{dc1-dc6} < ±2$ V

Cooling lasers (power): 397nm (~0.2mW), 866nm (~2mW)

UHV chamber: < 10^{-7} Pa @ LN$_2$ cooled

To manipulate a shape of an ion Coulomb crystal, the DC correction voltages are applied to all hexapole rods (see left).
Experimental Results

◆ Standard observation \((\theta = 90^\circ)\)

1. cylindrical crystals

\[ \kappa = 0.11264 \]

\[ V_z = 1.21V \]

\[ V_z = 2.02V \]

\[ \sim 0.2\text{mm} \]
For large Coulomb crystals (> 1mm) cylindrical and hollow structures can be explained by the shape of the effective trapping potential (see the left graph), because the overall spatial distribution of the large number of ions is not much affected by local distortion of the potential. However, the smaller ion crystals are deformed by the local distortion such as the patch effect of electric charges, even if the hexapole fields provide stronger confinement force to trapped ions compared to the octupole field [2]. The information of the potential distortion is needed to explain the observed shapes of the small Coulomb crystals.
2. Small crystals with a hollow structure

- Experimental conditions: $f = 4.4$ MHz, $V_{ac} = 52.7$ V, $V_z = 1.2$ V, $V_{dc2} = V_{dc4} = V_{dc6} = 0.04$ V, $V_{dc1} = V_{dc3} = V_{dc5} = 0$ V.
1. Observation of ring Coulomb crystals

- **Observation along the trap axis**

(a) Observation showing ion loss

(b) Laser beam direction

- Intensity (arb. units) vs. x (mm)
  - ~ 80 µm
  - ~ 50 µm
The ring structure was confirmed by direct observation from the axial direction in the linear trap as shown in Fig. (b). The cooling lasers were irradiated in the radial direction. The diameter of the ring crystal is about 50 µm. The crystal might be composed of less than 10 ions from the single ion image of Fig. (c). On the other hand, the structure of Fig. (a) is novel but we can not explain it using MD simulation so far.
2. Decay of the ring Coulomb crystal

The decay process of the ring Coulomb crystal was sequentially. Since the ring crystal was deformed by the distortion of the trapping potential and the radiation pressure force, the correction DC voltages ($V_{dc1}$-$V_{dc6}$) were applied to the hexapole rods to maintain the ring structure. As the number of ions decreases, the ring shape was deformed and finally disappeared. We assumed that the last image was composed of one or two ions.

*Note: This ion decay started after the liquid nitrogen vessel emptied, because an increase of the background pressure in the chamber triggered the ion loss.*
The equations of motion of the $i$-th ion are given by [1]

\[
\frac{d^2 x_i}{dt^2} = -\frac{3q x_i^2 \left(1 - y_i^2 / x_i^2 \right)}{m_i r_0^3} \left(V_{dc} - V_{ac} \cos \Omega t\right) + \frac{q \kappa V_{z_0}}{z_0^2} x + F_{Lx} + F_{Cx},
\]

\[
\frac{d^2 y_i}{dt^2} = \frac{6q x_i y_i}{m_i r_0^3} \left(1 - y_i^2 / x_i^2 \right) \left(V_{dc} - V_{ac} \cos \Omega t\right) + \frac{q \kappa V_{z_0}}{z_0^2} y + F_{Ly} + F_{Cy},
\]

\[
\frac{d^2 z_i}{dt^2} = -\frac{2q \kappa V_{z_0}}{m_i z_0^2} z + F_{Lz} + F_{Cz}.
\]

$F_c$: Coulomb interaction between ions
$F_L$: radiation pressure force by laser

The equations are numerically solved by 4th-order Runge-Kutta method.

In order to reproduce the observed images of ion Coulomb crystals by the MD simulations, the pseudopotential approximation was introduced[3]. In this case, the time-dependent trapping fields are replaced by the following fields:

\[
E_x = -\frac{9q V_{ac}^2}{mr_0^8 \Omega^2} x \left(x^2 + y^2 \right), \quad E_y = -\frac{9q V_{ac}^2}{mr_0^8 \Omega^2} y \left(x^2 + y^2 \right).
\]

In addition, the effect of elastic collisions by virtual very light atoms are included [3]. To simulate CCD images, probability density of ion trajectories is plotted. The parameters are set to $f = 4.4\text{MHz}$, $V_{ac} = 50\text{~}200\text{V}$, $r_0 = 2.0, 3.0 \text{ mm}$, $z_0 = 9.5\text{mm}$, and the geometric factor $\kappa = 0.11$, which is estimated from the numerically calculated potential using SIMION 3D code.
We carried out MD simulations of the trapped ions to obtain the structures and the average kinetic energies of Coulomb crystals and to reproduce the observed images. In the present simulation taking all forces into account, we obtain trajectories and velocities of all the trapped ions by solving Newton's equations of motion using 4th-order Runge-Kutta method[1]. Then we can evaluate average kinetic energies of ion crystals.

On the other hand, simulation images (as shown in the left Figs) are obtained by considering time-independent trapping forces by the radial pseudopotential and a axial harmonic potential in addition to Coulomb forces between trapped ions. Instead of a radiation pressure force, cold elastic collisions between trapped ions and virtual very light atoms are implemented [3].
Simulation Results

◆ Simulation of ring crystals for the ideal conditions

Simulation parameters: $f=4.4\, \text{MHz}$, $V_{ac}=58.8\, \text{V}$, $V_z=2.3\, \text{V}$ ($\kappa=0.11$). These values are the same as the apparent experimental conditions. The number of ions was assumed to be $N_{\text{ion}}=10$. 
Simulated ion temperature ($N_{\text{ion}}=10$)

In this simulation, the time-dependent rf fields were used to evaluate the average energy of Coulomb crystals. Then we translated the energies to the average kinetic temperatures ($T_{\text{ion}}$), which are plotted as a function of the secular temperature ($T_{\text{sec}}$).
Fitted result to the observed ring crystal

Up to now we can not reproduce the CCD image of the ring crystal by applying the apparent experimental parameters to the MD simulation. In actual ring crystals with a similar size are reproduced by applying the unexpected parameters (see below Figs.). This indicates that the local trapping potential was strongly modified. To exclude the local distortion effect as much as possible, much stronger trapping fields are needed, e. g. a smaller ion trap (possibly \( r_0 < 2 \text{mm} \)) with higher voltages should be used.

\( f = 4.4 \text{MHz}, V_{ac} = 200 \text{V}, r_0 = 2 \text{mm} \)

\( N_{\text{ion}} = 4, T_{\text{sec}} = 6 \text{mK} \)
Characterization of the ion Coulomb crystals in the hexapole trap is indispensable for experimental applications. In the next step, a realistic MD simulation method must be developed. Then we will apply such cold ions to study cold ion-polar molecule reactions by combining a Stark velocity filter (See below). In such experiments, sympathetically cooled molecular ions can also be used as cold ion targets [4, 5].
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References