Double-well trap for charged microparticles

Olga Kokorina, Vadim Rybin, and Semyon Rudyi
ITMO University, St. Petersburg 197101, Russia
E-mail: kokorinaolga09@gmail.com

Abstract. We propose a double-well linear Paul trap for particle's spatial selection according to the charge-to-mass ratio. To perform spatial selection we implemented an experimental setup that permits to detect particles' positions in the double-well trap from three different view-points: top, front left, and front right. The setup gives an opportunity to monitor the particles' axial density distribution in real-time. We have shown a strong correlation between axial position of separated localization areas and the DC voltages applied to the rod and end-cap electrodes. We have experimentally determined the critical localization parameters where double-well mode acquires for all the trapped charged microparticles. According to the experimental data and a numerical simulation a upper value of charge-to-mass ratio of the trapped microparticles was estimated.

1. Introduction

For a series of theoretical works on traps for charged particles and experiments on ion localization W. Paul, N. Ramsay, and H. Delmelt were awarded the Nobel Prize in 1989 [1]. Today various trap configurations exist, such as Paul trap, surfaced trap, two-, and three-dimensional traps [2]. Electrodynamic traps can capture numbers of charged objects as elementary particles, ions, nano-, and microparticles, biomolecules [3]. Stable spatial particles’ localization permits the trapped particles laser cooling and particles’ selection according to the charge-to-mass ratio [4]. Nowadays, linear and surfaced traps are an element base of quantum computers [5, 6]. Antiprotons and other charged antiparticles at CERN store in electrodynamic traps. Thus, electrodynamic traps demand nuclear and atomic physics, mass spectrometry, plasma installations, and accelerator physics [7].

We consider a new direction in implementation the multipole linear electrodynamic traps: four-rod linear double-well Paul trap with several stable localization areas. Multipole electrodynamic trap’s configuration allows the charged particles selection in spatially separated local potential minima. Usually, linear multipole traps in the classical sense [8] have at least three localization areas in radial direction. We propose a new double-well multipole electrodynamic trap to implement the axial charge-to-mass separation method. To demonstrate the concept, we performed starch particles double-well trapping. As an experimental result, we show two Coulomb structures trapped in two separated areas. We determined power supply parameters, where all the trapped starch particles got separated into two potential wells. According to the obtained power supply parameters and numeric simulation results, we have estimated the upper value of charge-to-mass ratio of the trapped starch particles.
2. General concept
The quadrupole linear ion trap consists of four rod electrodes (mass filter) and two end-cap electrodes. Rod electrodes having different polarities form a quadrupole alternating electric field, which limits particle’s radial motion. End-cap electrodes restrict the axial dynamics of the particle. In the case of many-body localization in a linear quadrupole trap, the particles are arranged into a single Coulomb structure, replicating a single particle’s stable localization area. Note that the end-cap electrodes deform the mass filter’s quadrupole field. Thus, in a quadrupole trap with end-cap electrodes, the single localization area can split into two spatially separated areas [9]. Such factors as the geometry of the trap, the trapped particles’ charge-to-mass ratio, and the scheme and parameters of the trap’s power supply can affect the mentioned splitting phenomenon. Trap geometry involves the relative distance, size, and shape of the electrodes. The power circuit is a scheme of applying DC and AC voltages to the electrodes. The power supply parameters involve the AC voltage amplitude and frequency on rod electrodes and the DC voltages on rod and end-cap electrodes (Figure 1). In the work [10] was shown that a particle with a certain charge-to-mass ratio localizes in single-well or double-well mode depending on the trap’s power supply parameters. In case of single-well mode there is a single localization area in the geometrical origin of the trap. In turn, in double-well mode, there are two separate local minima. Thus, it is possible to design a trap with a power supply scheme, where both single-well and double-well modes for particles with a diverse charge-to-mass ratios will be implemented. The double-well trap’s design is bases on a quadrupole linear Paul trap construction, so it has the same geometry. The double-well trap’s principal difference is the power supply circuit, which is shown in Figure 1. The proposed power supply scheme can realize both single and double-well mode. The double-well trap power circuit is designed as follows: only AC voltage is applied to the rod electrodes 6 and 7, and only DC voltage is applied to the rod electrodes 4 and 9. DC voltage is applied to the end-cap electrodes 5 and 8. In this work, we determine DC voltage values on rod and end-caps where the trap’s mode changes from single-well to double-well. In the experiment, the amplitude of the AC voltage is fixed.

3. The experiment
The experimental setup consists of a double-well trap, a power supply system, a registration system, a light-proof box, and a PC with Wolfram Mathematica 12.1. The setup is shown in the Figure 1. The double-well trap consists of four rod and two cylindrical end-cap electrodes mounted in a non-conductive plastic body. The length of the rod electrodes is 90 mm, the diameter of the rod and end-cap electrodes is 6 mm. The length between end-caps is 75 mm and the diameter of the trap is 25.5 mm (Figure 1). The power system consists of an autotransformer with a maximum voltage amplitude of 250 V and a frequency of 50 Hz, two DC voltage sources up to 300 V, and an AC-AC 27× transformer. The double-well trap and registration system are placed in a light-proof box. The registration system includes KLM-532/SNL-100 laser 1, optical beam expander 2, aperture 3, mirror 13, and three cameras 14-16. Laser radiation passes through the expander and the aperture, illuminates trapped particles, and permits the experiment’s visual registration. The presence of the collimated laser beam enhances the particles’ detection area. The cameras’ location make possible the registration of the particles’ position in the trap from three different view-points. We processed video stream from cameras 14-16 in the Wolfram Mathematica 12.1 software package. The measurement results were computed to estimate the particles axial distribution density.

The trapped particles replicates stable localization areas. We use charged starch microparticles with the charge-to-mass ratio of the order $10^{-4} - 10^{-3}$ C/kg as potential minima indicators. When the trap runs double-well mode, charged particles form two independent Coulomb
Figure 1. Schematic diagram of the experimental setup. The diagram uses the following designations: 1 is a laser KLM-532 / SNL-100, 2 is an optical beam expander, 3 is an aperture, 4 and 9 are cylindrical rod DC electrodes, 5 and 8 are end-cap DC electrodes, 6 and 7 are cylindrical rod AC electrodes, 10 and 12 are DC voltage sources, 11 is an AC voltage source, 13 is a mirror, 14-16 are side and front 30 fps@1280x960 cameras, 17 is a radius of the trap.

structures that can be registered visually, Figure 2b. The purpose of the experiment is to determine the power supply parameters – DC voltages on rod and end-cap electrodes, where the double-well mode appears. The experiment was performed the following way: firstly, we captured starch particles at 10 V DC on rod and end-cap electrodes. Secondly, we varied both DC voltages along the grid of values in the range of 30 – 290 V with 20 V step. During the experiment, cameras 14-16 take images of trapped Coulomb structures at each pair of rod’s and end-cap’s DC voltages. As a result of the experiment, we obtained the density peaks positions of the trapped particles for each pair of DC voltages. The Figure 2a displays the obtained density peaks positions for AC voltage fixed on 2700 V and end-cap DC voltage fixed on 10 V. Thus, by varying the DC values on rod electrodes and evaluating the particles’ distribution density, we have found the transition voltages’ values between single and double-well modes in the proposed trap for charged starch particles.

4. Results and discussion
According to the described experimental method we estimated density peaks for each DC voltage from the grid. For clarity in Figure 2a we show the coordinates of the trapped particles axial density peaks for 10 V on the end-caps, 2700 V on the AC rod electrodes, and variable DC voltage on the rod electrodes. The single-well mode realizes on the top of the Figure 2b for microparticles with charge-to-mass ratio of the order $0.5 \cdot 10^{-4}$ C/kg. There is a single localization area as in a classical Paul trap. The transition between single-well and double-well modes for all of starch microparticles is observed at $DC = 110$ V in Figure 2a. With a further increase of the DC voltage, the density peaks shift from the center of the trap at $L = 0$ to the end-cap electrodes at $L = -0.5$, and $L = 0.5$. In the bottom of the Figure 2b the double-well mode is demonstrated. Two independent peaks characterize two spatially separated Coulomb structures. In this case typical charge-to-mass ratio of captured particles is about $5 \cdot 10^{-4}$ C/kg. The top figure was taken at $DC = 30$ V, and the bottom one was taken at $DC = 270$ V.
Figure 2. a) Graph of the trapped particles density peaks dependent on the applied DC voltage at $AC = 2700$ V and $DC$ voltage on end-cap electrodes $EC = 10$ V. The parameter $Z_{[300 s]}$ is the coordinate of the peak density of particles on the main axis of the trap, normalized on the distance between end-cap electrodes 5 and 8. b) Images of trapped Coulomb structures in single-well and double-well modes.

Figure 3. The numerical simulation of the particle’s axial position module according to the charge-to-mass ratio and $DC$ voltage on the rod electrodes under the linear damping at $AC = 2700$ V and voltage on end-caps $EC = 10$ V, and the simulation time 300 s. The parameter $Z_{[300 s]}$ is the module of particle’s axial coordinate in millimeters where the trap’s geometric center is taken as the zero coordinate. In the area 1, localization is not feasible; in the area 2 the double-well mode realizes; the area 3 corresponds to the single-well mode implementation; in the area 4 particle’s localization is unstable on the 300 second of the simulation.

To analyze the dependence between starch particle’s charge-to-mass ratio and required $DC$ voltage for its stable localization in the single-well or the double-well mode we have performed the numerical simulation presented in the Figure 3. For plotting the diagram the FEM method had been applied. The charge-to-mass ratio sampling step is $10^{-5}$, $DC$ voltage sampling step is 10 V. Each colored pixel on the diagram corresponds to the particle’s certain position along the trap axis. All the simulating parameters such as the trap’s geometrical size and applied voltages match the experimental values. On the diagram’s legend, the particle’s axial position relative to the center of the trap is marked in millimeters. Using this diagram one can determine the particle’s charge-to-mass ratio if the $DC$ voltage and the particle’s axial coordinate is known.
To clarify this diagram let us consider a particular voltage $DC = 110 \text{ V}$ where the transition between single-well and double-well modes for all the starch microparticles was observed.

The area 4 corresponds to the unstable particle’s localization at the 300 s of the simulation. It means that the charge-to-mass ratio of those particles exceeds the threshold values on the red line for its stable motion at applied voltages. Throughout injecting these particles aspire to the geometrical center of the trap where the potential minimum is situated. This process is displayed in light blue and whitish colors corresponding to the localization at the distance up to ten millimeters from the center of the trap. However, according to the high charge-to-mass ratio, these particles leave the trap as a result the parametric excitation. Going along the horizontal line in the arrow direction we enter in area 3. At constant $DC = 110 \text{ V}$ for the particles with the charge-to-mass ratios from area 3, the single-well mode realizes. Such particles are trapped mostly in the trap’s center as in the top of Figure 2b. If we decrease the $DC$ voltage and continue being in area 3, a wide range of charge-to-mass ratios which can be localized in the single-well mode.

Continue moving along the horizontal arrow of constant $DC = 110 \text{ V}$ there is a point marked with star. It is the transition point between single-well and double-well modes. All the trapped particles turned to the double-well mode with since the upper charge-to-mass ratio value equals to $4.18 \cdot 10^{-4}$ at fixed $DC = 110 \text{ V}$. If the particle’s charge-to-mass ratio is less than that value and is still in the range of area 2, the double-well mode realizes. It means that particles with these charge-to-mass ratios localizes not around the center of the trap as in the bottom of Figure 2b, but closer to the end-cap electrodes as in the Figure 2b. Moreover, the particle’s trapping in the “left” or “right” well depends on the initial injection conditions. Moving to area 1 we see no pixels, it means that there is no localization there; particles which have charge-to-mass ratios from area 1 can not be trapped at $DC = 110 \text{ V}$.

It should be noted that if we look a little deeper at areas 2 and 3 there is an engaging fact: for each particle with certain charge-to-mass ratio has its own axial position at fixed $DC$ voltage. Let us go along the horizontal line in the arrow direction from area 3 to area 2. At this transition particles of a coarse-dispersed ensemble line up along the trap’s axis according to the charge-to-mass ratios. Particles with higher ratios localized around the trap’s center, and particles with lower ratios trapped closer to the end-cap electrodes. This effect makes it possible, in principle, a spatial particles’ selection with respect to the charge-to-mass ratio in a Paul trap with the asymmetrical power supply scheme. At fixed $DC$ voltage in the trap with asymmetrical power supply for particles with different ratios both single-well and double-well modes can be realized simultaneously. In this case three areas can be formed, for the particles with higher charge-to-mass ratios the single-well mode will be realized, and for the particles with lower ratios the double-well mode at the same $DC$ voltage. To perform particles selection from lower to higher charge-to-mass ratios the varying of the $DC$ voltage is required.

5. Conclusion

The present work demonstrates the way to perform the spatial selection of charged particles according to the charge-to-mass ratio in the Paul trap with the asymmetrical power supply scheme. Numerical calculations showed that single-well or double-well mode can be achieved at the proposed supply scheme. Those two modes corresponds to trapped charged particles with different charge-to-mass ratios. We showed that particles with wide range of charge-to-mass ratios may be trapped and spatially selected from lower to higher ratios. Then, it would be easier to manipulate particles which are localized in many spatially separated areas. Dealing with single ions, molecules and particles can be of service in applications working with monodisperse objects: mass-spectrometry, pharmaceuticals, virology, chemistry, in particular isotopes selection. To
realize the last application in the proposed trap extremely high accuracy of setting the voltages is required. To clarify the issue of spatial selection, it is necessary to study the following points. Firstly, to investigate a wider range of DC and AC voltages applied to the trap electrodes. Secondly, calculate the end-cap electrodes influence. Thirdly to consider other power supply schemes. Finally, traps with fields of higher multipole’s order could be studied.

References

[1] William D Phillips. Nobel lecture: Laser cooling and trapping of neutral atoms. Reviews of Modern Physics, 70(3):721, 1998.
[2] AJ Richard. The 3d quadrupole ion trap mass spectrometer as a complete chemical laboratory for fundamental gas-phase studies of metal mediated chemistry. Chemical communications, (14):1469–1481, 2006.
[3] Steve MM Sweet, Christopher M Bailey, Debbie L Cunningham, John K Heath, and Helen J Cooper. Large scale localization of protein phosphorylation by use of electron capture dissociation mass spectrometry. Molecular & Cellular Proteomics, 8(5):904–912, 2009.
[4] Roland Wester. Radiofrequency multipole traps: tools for spectroscopy and dynamics of cold molecular ions. Journal of Physics B: Atomic, Molecular and Optical Physics, 42(15):154001, 2009.
[5] Signe Seidelin, John Chiaverini, Rainer Reichle, John J Bollinger, Didi Leibfried, Joe Britton, JH Wesenberg, RB Blakestad, RJ Epstein, DB Hume, et al. Microfabricated surface-electrode ion trap for scalable quantum information processing. Physical review letters, 96(25):253003, 2006.
[6] Stephan Guilde, Mark Riebe, Gavin PT Lancaster, Christoph Becher, Jürgen Eschner, Hartmut Häffner, Ferdinand Schmidt-Kaler, Isaac L Chuang, and Rainer Blatt. Implementation of the deutsch–jozsa algorithm on an ion-trap quantum computer. Nature, 421(6918):48–50, 2003.
[7] Alexander Makarov, Eduard Denisov, Alexander Kholomeev, Wilko Balschun, Oliver Lange, Kerstin Strupat, and Stevan Horning. Performance evaluation of a hybrid linear ion trap/orbitrap mass spectrometer. Analytical chemistry, 78(7):2113–2120, 2006.
[8] Dieter Gerlich. Inhomogeneous rf fields: A versatile tool for the study of processes with slow ions. State-Selected and State-to-State Ion-Molecule Reaction Dynamics. Part 1: Experiment, 82, 1992.
[9] Olga Kokorina, Vadim Rybin, and Semyon Rudyi. Coulomb crystal splitting effect in a linear electrodynamic trap. Vibroengineering PROCEEDIA, 32:212–215, 2020.
[10] Olga O Kokorina, Vadim V Rybin, Semyon S Rudyi, and Yuri V Rozhdestvensky. Double-well effective potential in a linear paul trap with end-cap electrodes. In Quantum Nanophotonic Materials, Devices, and Systems 2021, volume 11806, page 118060U. International Society for Optics and Photonics, 2021.