

A Simple Reservoir Computing Approach to Determining Microparticle Mass-to-Charge Ratio

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Abstract

In this theoretical study, we implement a reservoir computing system to simulate mass-to-charge ratio determination for a single trapped microparticle. To achieve this, we numerically obtained trajectory images of a single silica microparticle in a quadrupole ion trap in air at room temperature. We demonstrated the capacity of the RC system to distinguish both between different types of trajectories and within identical trajectory classes. The system quantified the mass-to-charge ratio of the particles with corresponding determination errors of approximately 7% and 10%.

Keywords: Paul traps; Microparticle identification; Reservoir computing systems; Numerical simulation

1. INTRODUCTION

Trapping of charged objects is a versatile method for studying particles, necessary for various physical applications. For example, the widely known method of mass spectrometry was developed for charged objects. In the last decades there has been an active implementation of mass spectrometry methods and localization of micro- and nanoobjects in various fields of science: frequency standards [1–3], quantum computers [4,5], gravimetry [6–8], as well as trapping of viruses [9–11], proteins [12–14] and other biological objects [15,16] for non-destructive research and control. Electrodynamical traps are a fundamental tool in mass spectrometry [17–27] and chromatograph mass spectrometry [15,27] devices and are extremely important in these areas. Moreover, since weighing a particle using mechanical scales becomes impossible starting from a certain size, Paul traps are promising for mass evaluation of nano- and microparticles [28,29]. Additionally, electrodynamic traps allow one to study the interactions (such as chemical reactions) of various types of objects, ranging

from microparticles to molecular and atomic ions [30,31]. However, characterization of microparticles is challenging since every particle has a unique shape and mass even for the same material. Vinitsky et al. [32] showed that trapping a microparticle in viscous medium leads to the appearance of the new finite trajectories called “extended orbits”. The extended orbits can be divided in three distinguishable groups by their appearance: “butterfly” or “bowtie”, “diamond” and “cloverleaf” [32]. Different types can be observed depending on mass-to-charge ratio of the trapped particle or the trapping conditions.

Reservoir computing (RC) systems have been successfully used for classification and detection tasks: classification of spoken digits [33–36], detection of handwritten digits [37,38], drawings [39–41], or human motion [42]. Since the extended orbits depend on the mass-to-charge (m/Q) ratio and each type corresponds to certain m/Q values, usage of RC systems for extended orbits classification is promising for microparticles identification tasks.

In this work, we propose a method to determine mass-to-charge ratio of a trapped particle using RC system. First,

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we numerically solve equations of motion for a single microparticle in non-linear damping conditions, namely, at room temperature and atmospheric pressure with air as a surrounding media. Then we use the solutions to obtain the trajectories of particle motion. After that, we processed the obtained images for RC system training, and tested the system ability to determine mass-to-charge ratio based on the shape of particle trajectory.

2. MICROPARTICLE TRAPPING IN DAMPED MEDIUM

In this work, we consider particle trapping in a linear quadrupole trap shown in Fig. 1. Linear cylindrical electrodes provide confinement in xy plane via AC application, and end-cap electrode limits the particle's motion along z axis with DC.

Contrary to ion trapping, experiments with microparticles are frequently performed in viscous media at atmospheric pressure [43]. The presence of friction between a particle and surrounding medium allows to successfully confine the particle within the trap [32]. Moreover, trapping charged particles in a viscous medium results in so-called “extended orbits” [32].

The dynamics of a trapped particle is described by a system of three equations of motion (along the x , y , and z axes, respectively). In the transverse xy -plane of the trap, the particle exhibits extended orbital trajectories driven by the interaction between the particle and the AC field generated by four cylindrical electrodes. Axial motion along the z -axis is governed by three primary factors: the electrostatic repulsion exerted by the DC field of the end-cap electrode, which provides an upward axial force, interaction with the surrounding medium and gravitational acceleration. The latter can be effectively counterbalanced by tuning the end-cap DC voltage.

Therefore, to simulate the motion, we can describe the particle dynamics only in xy plane. In this case, we consider interaction of a particle with the electrodynamic potential and the interaction between the particle and the surrounding medium.

Following Vinitsky [32] approach, we can write equations of motion of a single particle in nonlinear friction environment. Introducing dimensionless terms, we obtain dimensionless equations of motion

$$\ddot{X}(t') + [a + 2q \cos 2t'] X(t') + b \left(1 + c \sqrt{\dot{X}(t')^2 + \dot{Y}(t')^2} \right) \dot{X}(t') = 0, \quad (1)$$

$$\ddot{Y}(t') + [a - 2q \cos 2t'] Y(t') + b \left(1 + c \sqrt{\dot{X}(t')^2 + \dot{Y}(t')^2} \right) \dot{Y}(t') = 0, \quad (2)$$

where $a = 4QU / m\omega^2 r_0^2$, $q = 2QV / m\omega^2 r_0^2$ are Mathieu coefficients, $b = 2\gamma_{ST} / \omega$ is proportional to the linear fric-

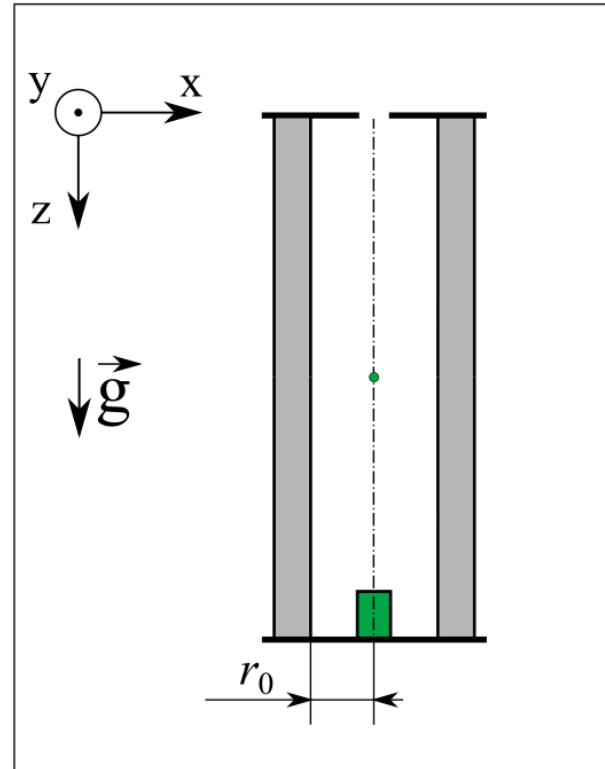


Fig. 1. Schematic diagram of a linear quadrupole trap with four cylindrical electrodes (gray rectangles) a single end-cap electrode (green rectangle): r_0 is a trap radius, the dash line represents the trap main axis. The free fall acceleration vector $\mathbf{g}$ is aligned with the axis z .

tion term, and $c = \alpha\omega / 2$ is proportional to non-linear friction term, $t' = \omega t / 2$ is dimensionless time; m and Q are mass and charge of a trapped particle, r_0 is a trap radius, V and ω are the AC amplitude and frequency, $\alpha = 3\rho D_r / 16\mu$, $\mu = 1.82 \cdot 10^{-5}$ Pa·s is dynamic viscosity of air at 20 °C, D_r is hydrodynamic radius of a particle, ρ is the surrounding medium density, γ_{ST} is Stokes friction coefficient. Note that the equations do not account for gravity since it is possible to compensate with end-cap electrodes (illustrated in green in Fig. 1).

Since the dynamics of a particle motion is directly related to its physical characteristics, it is possible to use RC systems to recognize the orbits of single trapped particles and, consequently, to determine their size, mass, and charge.

3. PROCESSING TRAJECTORY IMAGES WITH A RESERVOIR COMPUTING SYSTEM

In this work, we use the RC system with a state-dependent time delay to determine the mass-to-charge ratio m/Q of trapped particles. The incorporation of a state-dependent delay introduces highly complex, non-linear interactions, thereby significantly enhancing the linear separability and classification accuracy of high-dimensional datasets. A de-

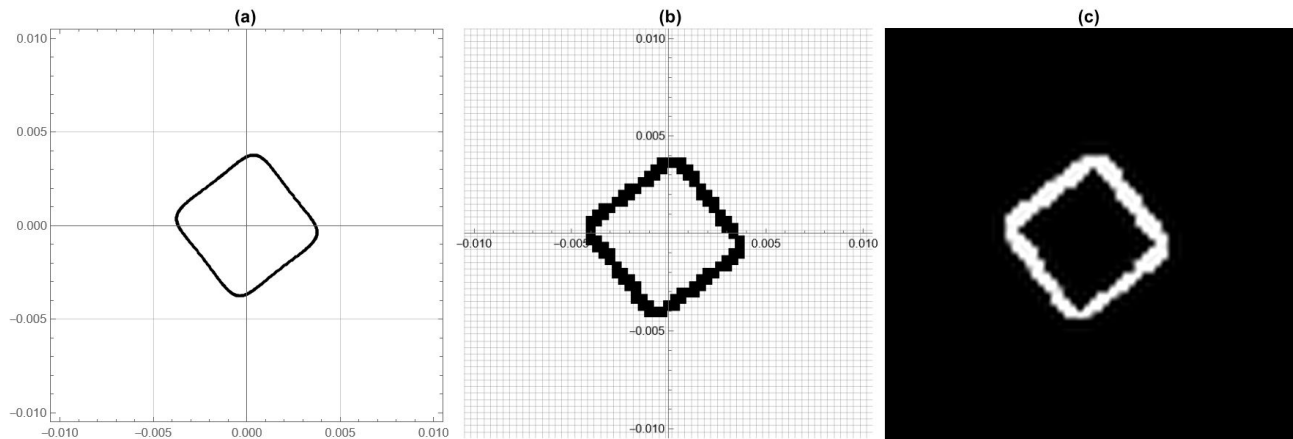


Fig. 2. The stages of the sampling process for $m/Q = 66.741 \text{ kg}/10^5 e$: (a) the trajectory obtained as a result of numerical simulation; (b) discretization of the trajectory; (c) binarized trajectory image.

tailed description of the RC system is provided in Ref. [44]. The following operational parameters have been used: modulation amplitude $\alpha = 0.7$, input cycle $T_{cc} = 1.2\tau$, constant delay time $\tau = 0.1N$, feedback strength $k = 0.6$.

Since particle orbits change significantly for different values of the mass-to-charge ratio m/Q , the RC system can be used to recognize different orbit types (e.g. “butterfly” or “diamond”) and to distinguish between the trajectories of particles with different m/Q ratios within a single type. The particle trajectory is approximated by a discrete set of points, which can be represented as pixels in a 64×64 grid or matrix, where each pixel has a value in the range $[0, 1]$, i.e., a black and white image is used.

The training database was created as follows:

- 1) Solving the equations of motion (1,2) of a charged microparticle and obtaining one period of the closed trajectory. To ensure a one-to-one correspondence between the trajectory type and the mass-to-charge ratio m/Q , the following localization parameters remain constant: the frequency ω and amplitude V of the alternating voltage on the trap electrodes, the radius r_0 and the trap length l , the density ρ and the dynamic viscosity μ of the surrounding medium. Only the mass-to-charge ratio m/Q changes.

- 2) Discretization of particle trajectories by applying a grid to the trajectory image.

- 3) Checking the grid elements: if there are particle trajectory points within a pixel, the pixel is assigned a value of 1.

Discretization of trajectories with a 64×64 grid is sufficient to display the required dependencies and trajectory patterns.

The accuracy of the mass-to-charge ratio (m/Q) determination is evaluated as error γ :

$$\gamma = \frac{|m/Q_0 - m/Q_p|}{m/Q_0}, \quad (3)$$

where m/Q_0 is the true value, m/Q_p is the value determined by RC system.

Based on the results of numerical simulations for various particle mass-to-charge ratios m/Q , a database was created for training the RC system. To train the RC, the images obtained from the numerical simulations were binarized (Fig. 2).

Before applying to the reservoir computing system, each image is transformed into an input sequence compatible with the reservoir architecture.

Figure 3 illustrates the preprocessing procedure for a reservoir computing system configured with $N = 90$ nodes, a value selected to ensure visual clarity in the graphical representations. The initial trajectory is represented by a 64×64 matrix X , where elements correspond to the pixels of the binarized trajectory image. To transform the two-dimensional image into a RC system suitable representation, we apply two consecutive mask transformations. The first mask transforms the pixel matrix into a one-dimensional sequence to introduce spatial correlations, whereas the second mask partitions this serialized signal into time intervals, creating virtual nodes for processing via RC.

First, the input matrix X (Fig. 3, step 2) is multiplied from the left by the first mask M_1 (Fig. 3, step 1), according to the rule $H_1 = M_1 X$ (Fig. 3, step 3). The dimensions of M_1 are $N \times 64$, where $N = 90$ is the number of nodes in the reservoir computing system. Therefore, multiplication of the 90×64 mask M_1 by the 64×64 input matrix X produces the intermediate matrix H_1 with dimensions 90×64 . Through this transformation, the spatial data embedded within the initial trajectory image is projected onto the reservoir network.

The resulting matrix H_1 is then multiplied from the right by the second mask M_2 , according to the rule $H_2 = H_1 M_2$. The dimensions of M_2 are $64 \times Tin$ (Fig. 3, step 4), where Tin is the number of consecutive input clock cycles during which one trajectory image is introduced into the reservoir. As a result, the matrix H_2 has dimensions 90×15 (Fig. 3, step 5). Thus, each row of H_2 corresponds to one of the $N = 90$ reservoir nodes and

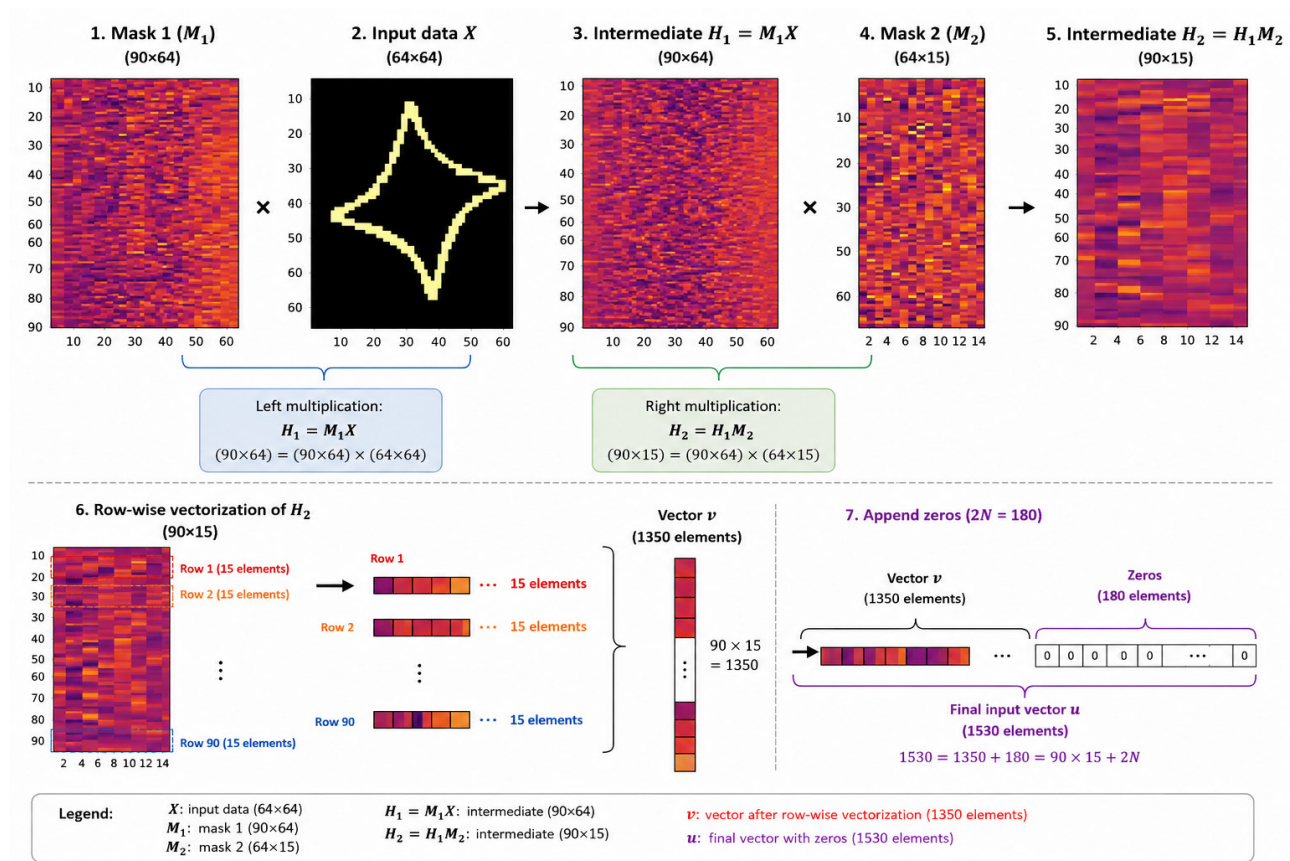


Fig. 3. Schematic representation of the trajectory image preprocessing procedure for the reservoir computing system at $N = 90$, where N is the number of nodes in the reservoir computing system. The original 64×64 image is transformed using two masking operations, vectorized, and supplemented with a zero-valued separation interval before being applied to the reservoir.

contains 15 values associated with the introduction of a single image. Equivalently, each column represents one of the 15 consecutive input steps and contains one input value for each reservoir node. In this way, the information contained in the original 64×64 trajectory image is distributed over the reservoir nodes and introduced into the system during 15 consecutive input steps.

For subsequent processing, the matrix H_2 is vectorized row by row. Since H_2 contains 90×15 elements, this operation produces a one-dimensional vector containing 1350 elements (Fig. 3, step 6).

Finally, $2N = 180$ zero-valued elements are appended (Fig. 3, step 7). The zero elements serve as a separation interval between two consecutive trajectory images. Since the reservoir possesses memory, some information associated with the preceding input might retain. If the next image is introduced immediately, the residual state might affect the reservoir response and, consequently, the processing of the new image. The zero-valued separation interval allows the influence of the previous image to decay before the next trajectory image is introduced.

After appending the zero-valued interval, the final input vector contains 1530 elements, corresponding to $90 \times 15 + 2 \times 90$. In this way, each 64×64 trajectory image is transformed into an input sequence distributed over

$N = 90$ reservoir nodes and introduced during 17 consecutive inputs.

4. RESULTS AND DISCUSSION

To evaluate the ability of the reservoir computing system to determine the mass-to-charge ratio of trapped microparticles, we consider two determination tasks with different levels of complexity. To ensure the best RC system performance, we varied the number of nodes N through the tasks and monitored the changes in determination error. The determination error γ (Eq. 3) for both tasks is shown on Fig. 4.

4.1. Mass-to-charge determination for two trajectory types

In the first task, the dataset contained two clearly distinguishable types of particle trajectories: “butterfly” and “diamond” trajectories. For butterfly trajectories, the mass-to-charge ratio varied from 9.68 to 9.76, whereas for diamond trajectories it varied from 66.2 to 68.9.

For each trajectory type, 130 samples were used. From each subset, 95 trajectories were randomly selected for training, 10 for validation, and 25 for testing. Thus, the

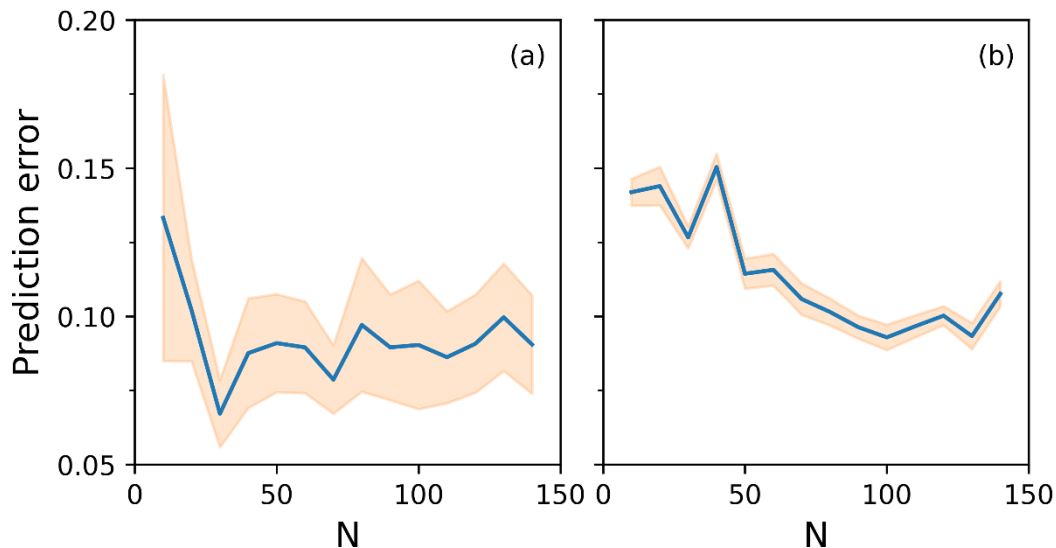


Fig. 4. Error of the mass-to-charge ratio determination as a function of the number of reservoir nodes for (a) mass-to-charge determination for two trajectory types (Task 1) and (b) mass-to-charge determination within a single trajectory type (Task 2). The solid line represents the mean determination error, and the shaded region represents the standard deviation.

complete dataset contained 170 training samples, 30 validation samples, and 60 test samples.

The goal of the reservoir computing system was to determine the mass-to-charge ratio directly from the particle trajectory. The best obtained determination accuracy corresponded to an error of approximately 7% (Fig. 4a).

Figure 4a shows the dependence of the mass-to-charge ratio determination error on the number of reservoir nodes N for Task 1. The solid line represents the mean determination error, while the shaded region indicates variations over repeated runs. The error decreases significantly as N increases from 10 to 30 and reaches its minimum value of approximately 7% at $N=30$. A further increase in the number of reservoir nodes does not lead to a systematic improvement, with the mean error remaining approximately within the 8–10% range. Thus, $N=30$ provides the best performance for this task among the considered reservoir sizes.

However, this task is relatively simple from the classification point of view. The two considered trajectory types have significantly different geometries and are also associated with well-separated ranges of mass-to-charge ratio. Therefore, the reservoir can use pronounced differences between butterfly and diamond trajectories when estimating the corresponding mass-to-charge ratio.

4.2. Mass-to-charge determination within a single trajectory type

In the second task, only diamond-shaped trajectories were considered. The dataset included particles of 12 different sizes, with each particle size corresponding to a different mass-to-charge ratio. Overall, the mass-to-charge ra-

tios covered a substantially broader range, from 4266 to 13065.

For each of the 12 particle sizes, 174 trajectories were available. From each dataset, 124 trajectories were used for training, 20 for validation, and 30 for testing. Consequently, the complete dataset consisted of 1488 training trajectories, 240 validation trajectories, and 360 test trajectories. In contrast to the first task, all trajectories in this dataset belong to the same diamond type. Therefore, the reservoir computing system cannot rely on pronounced differences between trajectory classes. Instead, the determination must be based on more subtle changes in the trajectory shape associated with variations in the particle parameters and the corresponding mass-to-charge ratio.

Despite the increased complexity of this problem, the reservoir computing system was able to estimate the mass-to-charge ratio over the entire range considered. The best determination result corresponded to a determination error of $\approx 9\%$ (Fig. 4b).

Figure 4b shows the dependence of the mass-to-charge ratio determination error on the number of reservoir nodes N for Task 2. The solid line represents the mean determination error, while the shaded region indicates its variation over repeated runs. In contrast to Task 1, the determination error generally decreases as the number of reservoir nodes increases. For small reservoirs, with $N \in [10, 40]$, the error remains relatively high, approximately 13–14%. Increasing N leads to a gradual improvement in the determination performance, and the minimum mean error of approximately 9% is obtained at $N=100$. A further increase in the number of nodes does not provide a consistent improvement, and the error remains close to 9–11%. These results indicate that a larger reservoir is re-

quired for the second, more complex task, in which the system must distinguish subtle differences between trajectories of the same type.

The moderate increase in error compared with the first task is consistent with the greater difficulty of distinguishing trajectories that belong to the same general orbit type and differ only in their detailed geometrical characteristics.

5. CONCLUSION

In this work, we used reservoir computing (RC) system to determine mass-to-charge ratio of a single silica microparticle trapped in a quadrupole ion trap with cylindrical electrodes. We numerically solved equations of motion of a trapped single particle in air at room temperature, and used the solutions to obtain trajectory images of single particles with size 20–30 μm . The obtained images were then preprocessed by binarizing and masking, and introduced to the reservoir computing system in 17 consecutive inputs. RC system was able to distinguish trajectories of two different types (“diamond” and “butterfly”) as well as trajectories of the same type (“diamond”).

Moreover, RC system determined mass-to-charge ratio with a determination accuracy $\approx 7\%$ when distinguishing trajectories of two different types and $\approx 10\%$ for a single trajectory type. Additionally, we showed that the determination accuracy depends on the number of input nodes N . We were able to achieve a low error value for a small reservoir ($N = 30$) when the system was trained to determine two different trajectory types. However, a larger reservoir ($N = 100$) was required to determine subtle differences between the trajectories of the same type.

Thus, combining electrodynamic trapping with the RC system allows fast and non-destructive characterization of the trapped charged microparticles based on their m/Q ratio with a high accuracy. The proposed method might be used to determine mass of a single particle with precision down to nanograms and charge with precision down to a dozen elementary charges, which currently cannot be achieved with other methods.

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УДК 537.291:531.751:004.85

Простой метод определения отношения массы-к-заряду микрочастиц с применением систем резервуарных вычислений

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Аннотация. В настоящей теоретической работе был реализован метод определения отношения массы к заряду для одиночной микрочастицы, локализованной в ловушке Пауля, с использованием системы резервуарных вычислений. Для выполнения этой задачи численно были получены изображения траектории одной микрочастицы диоксида кремния в квадрупольной ионной ловушке в воздухе при комнатной температуре. Была продемонстрирована способность системы резервуарных вычислений определять отношение массы-к-заряду как для частиц с различными типами траекторий, так и для частиц с идентичными траекториями. Система резервуарных вычислений количественно определила отношение массы к заряду частиц с соответствующими ошибками 7% и 10%.

Ключевые слова: ловушки Пауля; идентификация микрочастиц; системы резервуарных вычислений; численный расчет