PHYSICAL ELECTRONICS

Original article
DOI: https://doi.org/10.18721/JPM.18206

THE INFLUENCE OF FIELD MISALIGNMENT AND ELECTRIC FIELD ASYMMETRY ON THE STABILITY ZONES OF A COMBINED ION TRAP

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Abstract. This study continues a series of articles devoted to the operating features of ion-optical devices with periodic electric power supply and constant homogenous magnetic field, used in mass spectrometers. It has been shown how the structure of combined ion trap stability diagram is changed when the trap configuration deviates from the ideal one. The influence of an angle between the electric field symmetry axis and a magnetic field direction as well as the influence of the electric field asymmetry on the pattern of stability zones were found. The results obtained are worthy of use both for estimating the impact of manufacturing defects and for designing new nonclassical ion traps.

Keywords: combined ion trap, stability zones, mass spectrometry, ion confinement

Funding: The research was funded in part within the framework of the FFZM-2022-0009 topic (State registration No. 122040600002-3) of the State Assignment No. 075-01157-23-00, dated 29.12.2022, of the Ministry of Science and Higher Education of the Russian Federation for Institute for Analytical Instrumentation of RAS (St. Petersburg).

Citation: Berdnikov A. S., Egorova A. V., Krasnova N. K., Masyukevich S. V., Solovyev K. V., The influence of field misalignment and electric field asymmetry on the stability zones of a combined ion trap, St. Petersburg State Polytechnical University Journal. Physics and Mathematics. 18 (2) (2025) 60–68. DOI: https://doi.org/10.18721/JPM.18206

Научная статья
УДК 621.384.8
DOI: https://doi.org/10.18721/JPM.18206

ВЛИЯНИЕ НЕСООСНОСТИ ПОЛЕЙ И АСИММЕТРИИ ЭЛЕКТРИЧЕСКОГО ПОЛЯ НА ЗОНЫ УСТОЙЧИВОСТИ КОМБИНИРОВАННОЙ ИОННОЙ ЛОВУШКИ

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Аннотация. Данное исследование продолжает цикл статей, посвященных особенностям функционирования ионно-оптических устройств с периодическим электрическим питанием и постоянным однородным магнитным полем, применяемых в масс-спектрометрии. В статье показано, как диаграмма устойчивости комбинированной ионной ловушки меняет свою структуру при отклонении конфигурации ловушки от идеальной. Определено влияние величины угла между осью симметрии электрического поля и направлением магнитной индукции, а также влияние нарушения осевой симметрии электрического поля на картину зон устойчивости. Полученные результаты целесообразно использовать как для оценки влияния дефектов изготовления либо юстировки на работу классической комбинированной ловушки, так и для проектирования новых неклассических ионных ловушек.

Ключевые слова: комбинированная ионная ловушка, зона устойчивости, масс-спектрометрия, удержание ионов

Финансирование: Работа частично профинансирована в рамках темы FFZM-2022-0009 (номер гос. регистрации 122040600002-3) Государственного задания Министерства науки и высшего образования Российской Федерации № 00-23-01157-075 от 29.12.2022 для Института аналитического приборостроения Российской академии наук (Санкт-Петербург).

Ссылка для цитирования: Бердников А. С., Егорова А. В., Краснова Н. К., Масюкевич С. В., Соловьев К. В. Влияние несоосности полей и асимметрии электрического поля на зоны устойчивости комбинированной ионной ловушки // Научно-технические ведомости СПбГПУ. Физико-математические науки. 2025. Т. 18. № 2. С. 60–68. DOI: https://doi.org/10.18721/JPM.18206

Introduction

A combined ion trap is commonly understood as a Penning trap with oscillating voltages supplied to its electrodes. This trap is actually a combination of Penning and Paul traps [1, 2]. The combined ion trap, although it has the disadvantages of each of its components, has a number of advantages, in particular, an increased stability zone.

It is convenient to construct the stability zones of ions in a combined trap in a rotating coordinate system, which makes it possible to separate the variables and obtain a pair of independent Hill equations [3] (in the particular case, the Mathieu equations). The stability zone of the system is constructed in this case as the intersection region of the stability zones of the obtained Hill equations.

However, this technique is effective only for systems with axial symmetry. A number of configurations of the combined trap are not intended for an axisymmetric system but preserve linearity of the equations of ion motion. The latter makes it possible to study the nature of ion motion using the analytical tools of Floquet theory [4, 5]. We already adopted an approach based on this theory in our previous studies [6–8]. It allows to directly establish the conditions for stability of ion motion, facilitating the study of the system and allowing to draw conclusions about its possible operating modes.

This paper confirms that Floquet theory can be used to analyze ion traps based on non-axisymmetric hyperbolic electric fields with oscillating voltage immersed in a uniform magnetic field of arbitrary direction.

Stability of dimensionless trap model

For simplicity, we introduce dimensionless units of measurement [16], assuming that the dimensional coordinates $\mathbf{R} = (X, Y, Z)$ and time t are related as follows to the corresponding dimensionless coordinates $\mathbf{r} = (x, y, z)$ and time τ:

$$\mathbf{R} = \ell\mathbf{r},\ t = T\tau, \tag{1}$$

where ℓ, T are linear and time scales chosen from physical considerations.

The motion of a particle with charge e and mass m in a trap occurs in a constant uniform magnetic field with the strength B_0 and the direction set by the polar and azimuthal angles (θ, φ) relative to the coordinate system associated with the geometry of the electric quadrupole:

$$\mathbf{B} = B_0(\sin\theta\cdot\cos\varphi,\ \sin\theta\cdot\sin\varphi,\ \cos\theta) \tag{2}$$

and in an electric field (with oscillating voltage) quadratic with respect to the coordinates:

$$\begin{gathered} U = (U_0 - U_1 f(\omega t))\frac{\alpha X^2 + \beta Y^2 + \gamma Z^2}{\ell^2}, \\ f(\omega(t+\sigma)) = f(\omega t), \\ \alpha + \beta + \gamma = 0, \end{gathered} \tag{3}$$

where U_0, U_1 are the amplitudes of the DC and AC components of the supply voltage; ω is the angular frequency of the latter, σ is its period; α, β, γ are the parameters defining the geometry of the field.

The dimensionless equations of motion in these fields form a system

$$\begin{gathered} \ddot{x} = -2\alpha(a - 2q\cdot f(2\tau))x + \dot{y}b_z - \dot{z}b_y, \\ \ddot{y} = -2\beta(a - 2q\cdot f(2\tau))y + \dot{z}b_x - \dot{x}b_z, \\ \ddot{z} = -2\gamma(a - 2q\cdot f(2\tau))z + \dot{x}b_y - \dot{y}b_x, \end{gathered} \tag{4}$$

where the components of the dimensionless magnetic field are determined by the equality

$$\mathbf{b} = b(\sin\theta\cos\varphi, \sin\theta\sin\varphi, \cos\theta) = (b_x, b_y, b_z), \tag{5}$$

and the coefficients a, q, b for the given time scale $T = 2/\omega$ are determined by the relations

$$a = \frac{4eU_0}{\omega^2 m\ell^2},\ q = \frac{2eU_1}{\omega^2 m\ell^2},\ b = \frac{2eB_0}{\omega m}. \tag{6}$$

The dots above the variables in Eqs. (4) denote differentiation with respect to dimensionless time τ.

In the general case, system (4) has six independent parameters that affect stability:
traditional ones, a and q;
new ones, b, θ, φ, related to the strength and direction of the magnetic field;
two parameters of the geometry of the electric field, for example, α, β (taking into account the last equation in system (3)).

Evidently, the multidimensional region can only be visualized by sections whose dimensions do not exceed 3. Here we confine ourselves to traditional two-dimensional diagrams.

For a dimensionless magnetic field $\mathbf{b} = b\,(0, 0, 1)$ directed along the symmetry axis of the electric field, the form of equations (4) is simplified:

$$\begin{gathered}\ddot{x} = 2\alpha(a - 2q\cdot f(2\tau))x + b\dot{y},\\ \ddot{y} = 2\beta(a - 2q\cdot f(2\tau))y - b\dot{x},\\ \ddot{z} = -2\gamma(a - 2q\cdot f(2\tau))z = -(a_z - 2q_z\cdot f(2\tau))z,\end{gathered} \tag{7}$$

The electric field with axial symmetry corresponds to a set of parameters

$$(\alpha, \beta, \gamma) = (-1/4, -1/4, 1/2).$$

The diagrams for the stability zones below are given in the coordinates $(q, a) = (q_z, a_z)$.

The stability of ion motion in the axisymmetric hyperbolic electric field and the longitudinal magnetic field is studied in a coordinate system rotating around the z axis. Recall that if we introduce a complex variable $\xi = x + iy$ for $\alpha = \beta = -1/4$, then we obtain the following equation from the first two equations in system (7):

$$\ddot{\xi} = \frac{1}{2}(a - 2q\cdot f(2\tau))\xi - ib\dot{\xi}. \tag{8}$$

Next, moving on to the rotating coordinate system $\eta = x^* + iy^*$, using the transformation

$$\xi = \eta\cdot\exp(-ib\tau/2),$$

Eq. (6) is converted to the following form:

$$\ddot{\eta} - \frac{1}{2}\left(a - \frac{b^2}{2} - 2q\cdot f(2\tau)\right)\eta = 0. \tag{9}$$

Thus, we obtain the Hill equation shifted with respect to the parameter a. Then the stability of the system including the third equation of system (7) and Eqs. (8), (9) can be easily analyzed by the traditional method of superposition of stability zones of the Hill equation [1, 2].

Case I. Consider the case where the electric field is axisymmetric, namely, $(\alpha, \beta, \gamma) = (-1/4, -1/4, 1/2)$, and the magnetic field is directed at an angle θ to the z axis, i.e., there is misalignment between the magnetic field and the symmetry axis of the electric field. There is no dependence on the azimuthal angle, the strength of the dimensionless magnetic field is $\mathbf{b} = b\,(\sin\theta, 0, \cos\theta)$. Then system (4) takes the following form:

$$\begin{gathered}\ddot{x} = -2\alpha(a - 2q\cdot f(2\tau))x + b\dot{y}\cos\theta,\\ \ddot{y} = -2\beta(a - 2q\cdot f(2\tau))y + b(\dot{z}\sin\theta - \dot{x}\cos\theta),\\ \ddot{z} = -2\gamma(a - 2q\cdot f(2\tau))z - b\dot{y}\sin\theta.\end{gathered} \tag{10}$$

In turn, system (10) cannot be reduced to a set of Hill equations, but it remains linear with periodic coefficients and therefore is subject to analysis by the technique proposed in [6].

Let us rewrite Eq. (23) as follows:

$$\dot{\mathbf{x}} = \mathbf{A}(\tau)\mathbf{x},\ \mathbf{A}(\tau + A) = \mathbf{A}(\tau), \tag{11}$$

where

$$\mathbf{x} = (x_1\ x_2\ x_3\ x_4\ x_5\ x_6)^T = (x\ \dot{x}\ y\ \dot{y}\ z\ \dot{z})^T \tag{12}$$

(the superscript T denotes transposition);

$$\mathbf{A}(\tau) = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 0 \\ -2\alpha(a-2q\cdot f(2\tau)) & 0 & 0 & b_z & 0 & -b_y \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & -b_z & -2\beta(a-2q\cdot f(2\tau)) & 0 & 0 & b_x \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & b_y & 0 & -b_x & -2\gamma(a-2q\cdot f(2\tau)) & 0 \end{pmatrix}. \tag{13}$$

In accordance with Floquet theory [4, 5], the stability of solutions (13) is assessed through analysis of the monodromy matrix eigenvalues of system (11). The procedure for constructing stability diagrams of system (11)–(13) is described in sufficient detail in [6]; let us briefly recall its key points: the fundamental matrix of solutions $\mathbf{X}(\tau)$, $\mathbf{X}(0) = \mathbf{E}$ is constructed. Next, the spectrum of the monodromy matrix $\mathbf{X}(A)$ is analyzed. The spectral radius equal to unity corresponds to the values of the parameters representing stable motion.

Fig. 1 illustrates the evolution in the configuration of the first stability zone for $f(\tau) = \cos\tau$ at $b = 1$ with varying parameter θ.

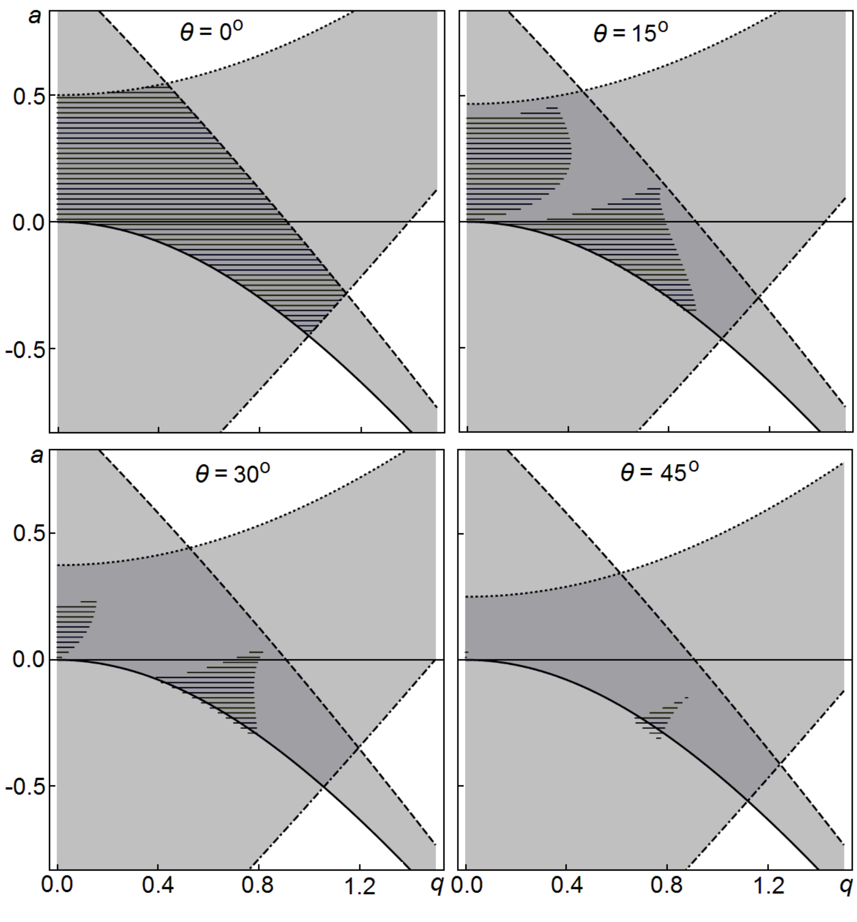

Fig. 1. Stability zones (hatched by horizontal lines) for different values of misalignment angle θ between the symmetry axis of the electric field and the direction of the magnetic field; $b = 1$; $f(\tau) = \cos\tau$ (Case I)

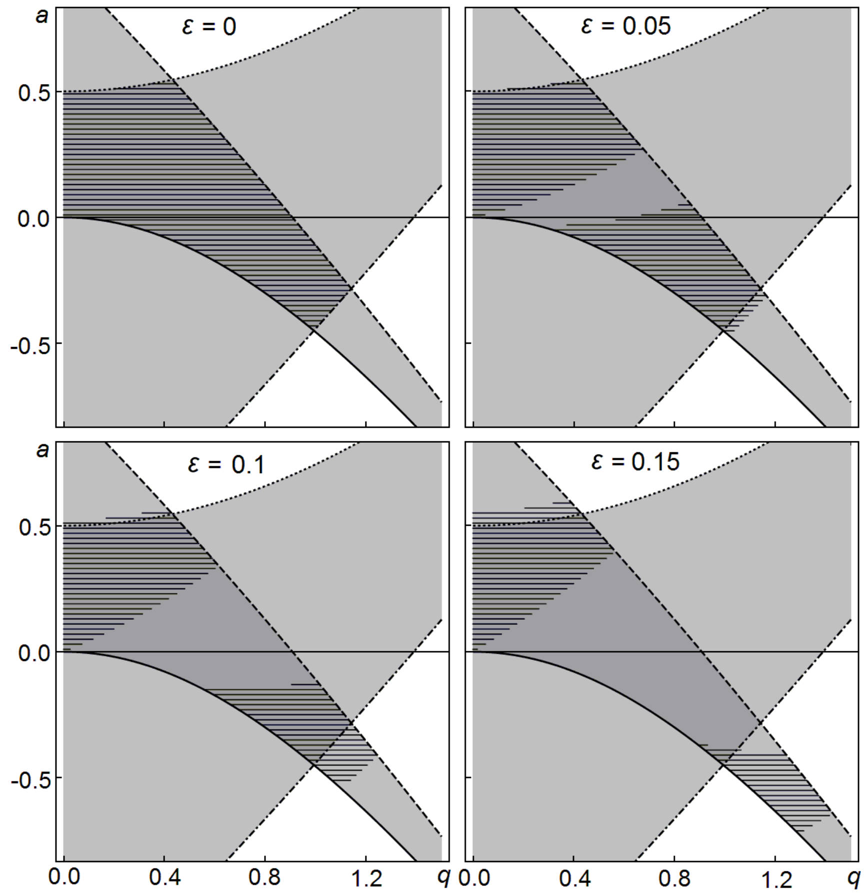

Fig. 2. Stability zones (hatched by horizontal lines) for different values of the electric field asymmetry parameter ε; $b = 1$, $f(\tau) = \cos\tau$ (Case II)

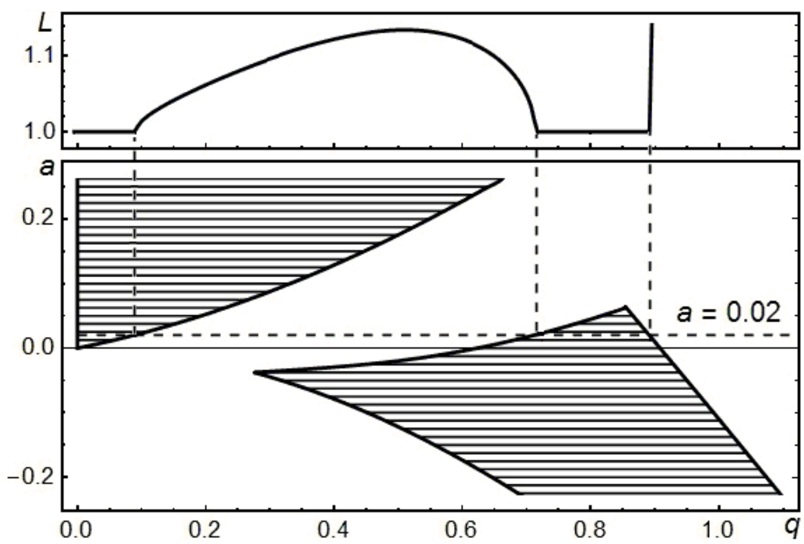

Fig. 3. Diagram (q, a) (lower part of figure) and dependence of $L(q)$ (upper part): the former shows the configuration of stability regions in coordinates (q, a), the second shows the change in the spectral radius of the monodromy matrix L from identity to non-identity and vice versa at the boundaries of stability regions with the parameter q varying along the line $a = 0.02$ (horizontal dashed line)

Case II. Consider a situation where the axial symmetry of the electric field is broken. We introduce the parameter ε, lying in the range $0 < \varepsilon < \min(\alpha,\beta)$, and analyze the case of an electric field with geometric parameters $(\alpha, \beta, \gamma) = (-1/4 - \varepsilon, -1/4 + \varepsilon, 1/2)$. The condition that the sum of the parameters be equal to zero is satisfied, we have a field with equipotentials that are hyperboloids of revolution for $\varepsilon = 0$, a harmonic non-axisymmetric field for $\varepsilon \neq 0$. The system of equations of motion is the same: (11)–(13). Although all components (5) of the magnetic field strength **b** are important in this case, for ease of visualization, we focus on the option $\mathbf{b} = b\,(0, 0, 1)$. The result presented below is obtained by performing the above sequence of steps. Fig. 2 shows a change in the configuration of the first stability zone of the combined trap for $f(\tau) = \cos\tau$ at $b = 1$ with varying ε.

Note that the diagrams (Figs. 1, 2) were obtained by a technique refining the boundary points as transition points to/from non-identity of the spectral radius of the monodromy matrix, previously used for a simpler system [7, 8]. This approach is illustrated in Fig. 3, where the upper part shows the dependence of the spectral radius of the monodromy matrix L on the parameter q of Eqs. (10) with the parameter $a = 0.02$ (option $b = 1$, $\varepsilon = 0.05$); the lower part of the figure shows the correspondence of q values for the variation in the spectral radius to the boundaries of the stability regions of system (10).

Conclusion

The misalignment of the electric and magnetic fields, as well as the non-axisymmetry of the electric field, significantly affect the structure of the stability diagram of a traditional (axisymmetric) combined ion trap and lead to a change in this diagram. The latter is divided into fragments, defining the behavior of the system in a new way depending on the values of the non-ideality factors.

The results and methodology obtained can be used both to assess the influence of manufacturing and alignment defects on the operation of a traditional ion trap and to design new traps without axial symmetry.

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Received 03.11.2024. Approved after reviewing 05.12.2024. Accepted 05.12.2024.
Статья поступила в редакцию 03.11.2024. Одобрена после рецензирования 05.12.2024. Принята 05.12.2024.