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ON THE MULTIPOLAR ELECTROMAGNETIC TRAPS

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Confinement of ion clouds in multipole traps is studied, with an accent on ion stability which is shown to be phase and position dependent. Ion dynamic is studied by means of the numerical integration of the equations of motion. The trajectories envelope and the phase-dependence of ion location in the quadrupole and sextupole rf traps are studied.

1. INTRODUCTION

In many spectroscopic applications [1–11] it is desired to use radiofrequency (RF) traps which can trap large numbers of particles with decreasing energies. Higher order electromagnetic traps enable storing an increased number of low energy particles, compared to the Paul trap. This paper deals with the dynamics of particle trapped in a RF quadrupole and sextupole rf traps.

A comparative study between the dynamics of a charged particle in a quadrupole Paul trap and in a sextupole trap respectively, is presented. The frontiers of the domains covered by the trajectories are described using a fourth order Runge-Kutta method. Within the frame of the pseudopotential approximation, the system has been described both classically and semiclassically.

The paper is organized as follows: Section 2 deals with the equations of motion describing the ion motion in electromagnetic traps. The next section focuses on electrodes' shape calculation for rf traps. Numerical integration of the equations of motion allowed us to represent ion trajectories in Section 4. Finally, some concluding remarks are drawn.

2. MULTIPOLE ELECTROMAGNETIC TRAPS

The classical Hamiltonian of an ion of electric charge Q and mass M, trapped by an electromagnetic field of electric potential Φ and constant magnetic induction $\vec{B}$, can be expressed as

$$H = \frac{1}{2M}\left[\vec{p} - \frac{1}{2}Q\vec{B}\times\vec{r}\right]^2 + Q\Phi(\vec{r},t), \tag{1}$$

where $\vec{r} = (x, y, z)$ and $\vec{p} = (p_x, p_y, p_z)$ stand for the particle position and impulse vectors respectively. If $\vec{B} = 0$, then for the ion stability it is required that the electric potential $\vec{B} = 0$ to be time dependent. In the case of RF traps we choose $\Phi(\vec{r},t) = A(t)f(\vec{r})$, where A is a function of $T = 2\pi/\Omega$ period. Customarily, the temporal term is chosen $A(t) = U_0 + V_0\cos\Omega t$, with U_0 and V_0 representing the dc and ac trapping voltage amplitudes, respectively, applied on the trap electrodes. The equations of motion for the particle are described by

$$M\ddot{\vec{r}} = Q\left(\vec{E} + \vec{r}\times\vec{B}\right), \tag{2}$$

where $\vec{E} = -\nabla\Phi$ stand for the electric field within the trap. Generally, these equations describe a nonlinear and non-autonomous system of differential equations. Analytic solution of this system exists only in a few particular cases. The numerical integration of this system reveals that the single-particle motion may exhibit chaotic dynamics in multipole RF traps, but not in the Paul trap. Hence, the multipole traps and their electromagnetic fields are studied concerning the stability regions for the particle motion as well as their phase portraits.

In case of axial symmetry, the Laplace equation solution may be expressed as

$$f(\vec{r}) = \sum_{n=0}^{\infty} C_n r^n P_n(\cos\theta), \tag{3}$$

where $r = |\vec{r}|$ and $\theta = \arccos(z/r)$, while P_n are the Legendre polynomials. The term corresponding to $n = 2$ in eq. (3) describes some ideal quadrupole traps: the Paul trap $(\vec{B} = 0)$, where the confined particle behaves as a parametric harmonic oscillator and the Penning trap ($V_0 = 0$), case when the particle is described by an autonomous harmonic oscillator Hamiltonian. If $V_0 \neq 0$ and $C_n \neq 0$ for indexes $n > 2$, the ion motion is described by a nonlinear and non-autonomous dynamic system. Using the pseudopotential method we may introduce the effective potential

$$\Phi_{\text{ef}}(\vec{r}) = U_0 f(\vec{r}) + \frac{QV_0^2}{4M\Omega^2}\left[\nabla f(\vec{r})\right]^2. \tag{4}$$

An important problem of trap geometry optimization consists in the determination of the electrode shape, so that the quadrupole term in the expressions of the electric potential Φ and of the Φ_{ef} to be dominant in an extended neighborhood of the trap center. In case of axial symmetry

$$\Phi(\bar{r},t)=A(t)\,g(\rho,z),\qquad g(\rho,z)=\sum_{n=0}^{\infty}D_nH_n(\rho,z),\tag{5}$$

$$\Phi_{\mathrm{ef}}(\bar{r})=U_0 g(\rho,z)+\frac{QV_0^2}{4M\Omega^2}\left[\left(\frac{\partial g}{\partial\rho}\right)^2+\left(\frac{\partial g}{\partial z}\right)^2\right],\tag{6}$$

where $\rho=\sqrt{x^2+y^2}$ and the spherical harmonics H_n is a polynomial in ρ and z which can be expressed using a homogeneous polynomial of order n satisfying the Laplace equation. The equations of motion can be expressed in cylindrical coordinates as

$$\ddot{\rho}=-\frac{Q}{M}\frac{\partial\Phi}{\partial\rho}+\frac{L_z^2}{M^2\rho^3}-\omega_c^2\rho,\qquad \ddot{z}=\frac{Q}{M}\frac{\partial\Phi}{\partial z},\tag{7}$$

$$\rho^2\ddot{\theta}=-2\rho\dot{\rho}\dot{\theta}-\omega_c\rho\dot{\rho}-\frac{Q}{M}\frac{\partial\Phi}{\partial\rho},\tag{8}$$

where L_z is the angular moment on the z axis given by

$$L_z=M\rho^2\dot{\theta}+\frac{1}{2}\omega_c M\rho^2,\qquad \omega_c=\frac{QB}{M}.\tag{9}$$

The equations of motion are concretely determined by fixing the D_n coefficients in the multipole expansion (5).

3. MULTIPOLE RF TRAPS AND ELECTRODE SHAPE

In spherical coordinates the ideal potential function of a $2n$-pole is given by

$$\Phi(r,\theta,\varphi)=Ar^nP_n(\cos\theta).\tag{10}$$

There are different ways to choose the constant A in (10). For reasons which will become obvious, A was chosen such as the potential function be zero in the trap centre, $\Phi(0,z_0)=\Phi_0/2$, and $\Phi(0,-z_0)=(-1)^n\Phi_0/2$. Thus, in cylindrical coordinates, a simple calculus gives the potential functions for the quadrupole trap as

$$\Phi(\rho,z)=\Phi_0\left(2z^2-\rho^2\right)/4z_0^2,\tag{11}$$

for the sextupole and octupole traps we infer

$$\Phi(\rho,z)=\Phi_0\left(2z^2-3\rho^2\right)z/4z_0^3,\tag{12}$$

and

$$\Phi(\rho,z)=\Phi_0\left(8z^4-24z^2\rho^2+3\rho^4\right)/16z_0^4,\tag{13}$$

where z_0 stands for the closest distance between endcap and the trap center on the z axis. As for a Paul trap, the electrode shape for a multipole trap results by solving the equations $\Phi(\rho, z) = \pm\Phi_0/2$. This choice in not unique [1, 12]. For the quadrupole and octupole traps, the electrodes profile can be inferred by solving the equations $\Phi(\rho, z) = \alpha\Phi_0$ and $\Phi(\rho, z) = -\beta\Phi_0$, with and $\alpha + \beta = 1$. In case of the sextupole trap, the condition for the electrode surface to be symmetrical in respect to the $z = 0$ plane has to be explicitly imposed which results in the unique option $\alpha = \beta = 1/2$.

Besides the electrodes which intersect the z axis in $z = \pm z_0$ (endcaps), a $2n$-pole trap has $(n-1)$ ring electrodes. For instance, the electrodes shape for octupole trap is given by $\pm 8z_0^4 = 8z^4 - 24z^2\rho^2 + 3\rho^4$. A simplified design of a trap approximating the octupole potential function (13) is represented in Fig. 1. The closest distance between the middle ring to the z axis is given by $\rho_0 = z_0\sqrt[4]{8/3}$, while for the two lateral rings the corresponding distance is $r_{in} = z_0\sqrt[4]{8/15}$. Since a dc voltage applied together with the driving voltage proved to deteriorate the trap stability in multipole traps, the usual choice of Φ_0 is $\Phi_0 = V_0\cos(\Omega t)$.

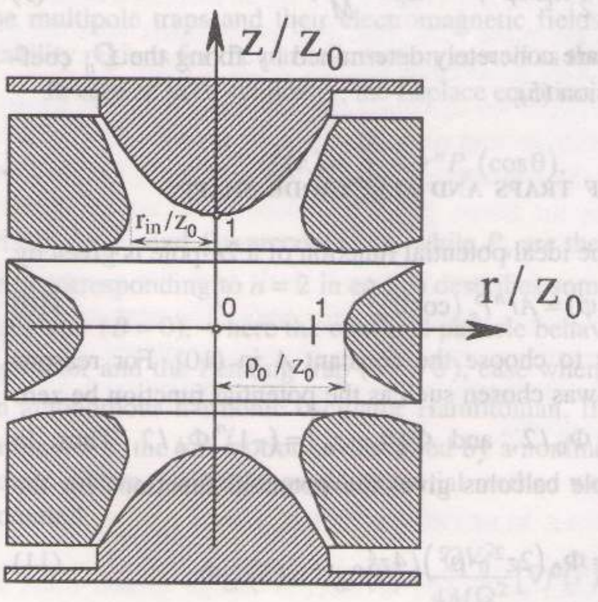

Fig. 1. – Electrode structure of the RF octupole trap.

4. ION DYNAMICS IN QUADRUPOLE AND SEXTUPOLE TRAPS

In an electromagnetic trap with rotational symmetry, the first anharmonic term of the electric potential multipole expansion is expressed by means of a third rank polynomial in coordinates. The equations of motion for an electrically charged particle in a third order electromagnetic trap are nonlinear, opposed to the ideal quadrupole Paul trap for which the Mathieu equations of motion are linear.

In the following, a comparative study between the dynamics of a charged particle in a quadrupole Paul trap and a third order electromagnetic trap respectively, is presented, together with the description of the frontier of the domain covered by the trajectories. The nonlinear differential equations with time periodical coefficients which describe the particle dynamics within the trap volume are integrated using the fourth order Runge-Kutta method.

The electric potential for the third order trap can be expressed in cylindrical coordinates as

$$\Phi(\rho, z) = \frac{\Phi_0}{4z_0^3}\left(2z^3 - 3\rho^2 z\right). \tag{14}$$

The four surfaces of the electrodes of a third order trap (two rings in this case, and two endcaps) are described by $\Phi(\rho, z) = \pm\Phi_0/2$. The inner distance between endcaps $2z_0$ and the inner radius of the two rings r_0 specifies the trap dimensions. These lengths are related by $r_0 = \sqrt[6]{2} z_0 \cong 1.12 z_0$.

For the third order trap, the following nonlinear differential equation system is obtained:

$$\ddot{\rho} = 2k\rho z + \left(\frac{L_z}{M}\right)^2 \frac{1}{\rho^3}, \quad \ddot{z} = k\left[\rho^2 - 2z^2\right],$$

$$\dot{\theta} = \left(\frac{L_z}{M}\right)\frac{1}{\rho^2}, \quad k = \frac{3Q\Phi_0}{4Mz_0^3}.$$

In order to compare the dynamics of an electrically charged particle in the third order trap and in the quadrupole Paul trap, we chose $L_z = 0$, $\Phi_0 = U_0 + V_0 \cos\Omega t$, $V_0 = 750$ V, $U_0 = 0$, $\Omega/2\pi = 500$ kHz. The charged particle is the simple ionized $^{137}Ba^+$ ion. The trap parameters in our example are $r_0 = 17.5$ mm and $z_0 = 12.4$ mm. For the ideal Paul trap, these conditions correspond to $a_z = 0$, and $q_z = 0.699$, namely parameter values within the stability diagram of the Mathieu equations. The initial conditions have been chosen so as the kinetic energy vanishes and $x = 3$ mm, $z = 1$ mm. The equations of motion have been integrated on a time interval equal with $128T$, with a constant step $T/128$, where T is the radiofrequency field period. The electric field phase has been defined as $2\tau = 2\pi t/T$. For the sextupole trap, the ac. voltage was $V_0 = 1500$ V.

Using a simple sort procedure, the ion trajectories envelope was inferred from a collection of ion positions. The ion positions for the kinetic energy extreme

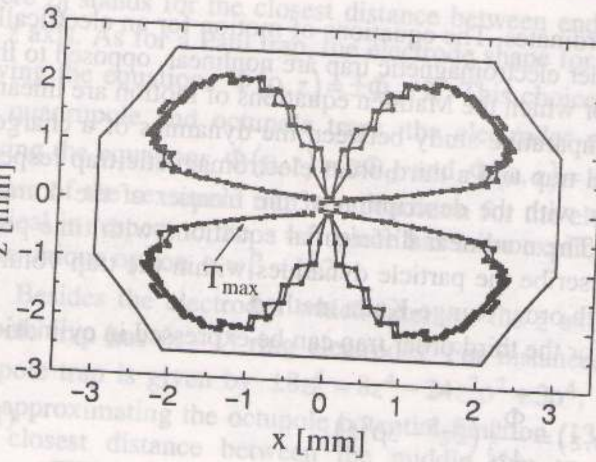

Fig. 2. – The ion positions at maximum kinetic energy T_{max} and the trajectories envelope for the quadrupole RF trap.

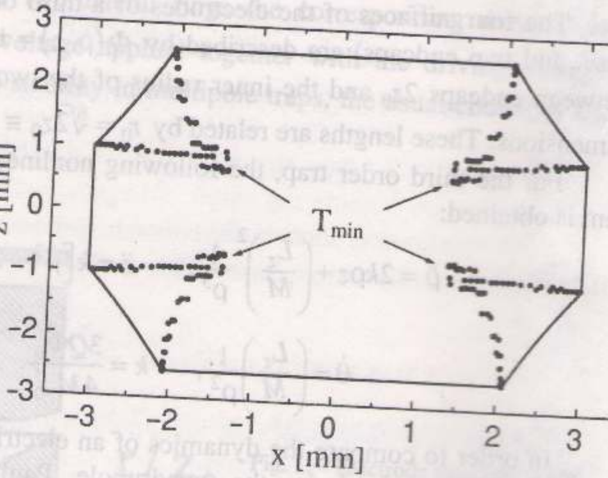

Fig. 3. – The ion positions at minimum kinetic energy T_{min} and the trajectories envelope for the quadrupole RF trap.

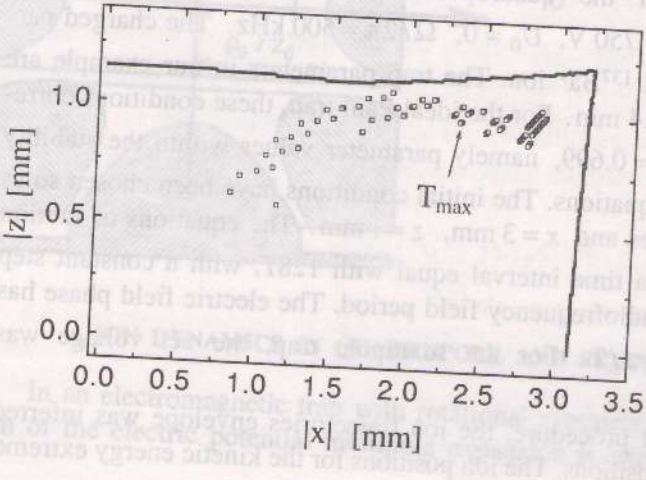

Fig. 4. – The ion positions at maximum kinetic energy T_{max} and the trajectories envelope for the sextupole RF trap.

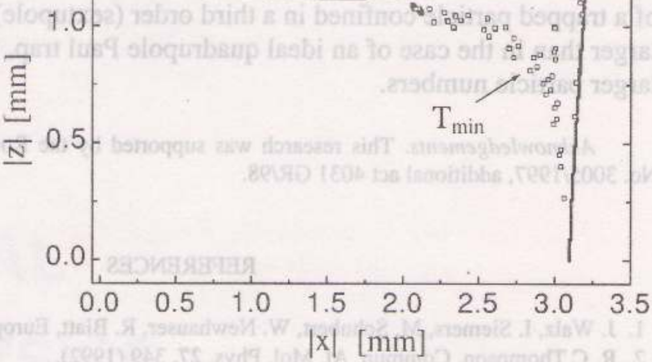

Fig. 5. – The ion positions at minimum kinetic T_{min} energy and the trajectories envelope for the sextupole RF trap.

values for a given phase 2τ were also collected. In case of the quadrupole trap, ion position at maximum and minimum kinetic energy is shown in Fig. 2 and Fig. 3, respectively. The rectangle without corners represents the trajectories envelope.

Fig. 4 and Fig. 5 show the corresponding graphs for the sextupole trap in the first quadrant of the $y = 0$ plane.

5. CONCLUSIONS

In order to optimize the multipole contributions to the stability domains of the electromagnetic traps, we introduced the classical Hamiltonian for an ion moving in the field of a multipole trap with periodical potential and we studied the nonlinear differential system of motion equations. The control parameters for the Hamiltonian of this dynamic system are function of the trap geometrical parameters and of the multipolar coupling constants. Within the frame of the geometrical control theory, the structural stability of the considered dynamic system has been investigated. The multipole expansion potentials have been considered as Morse functions, for which the harmonic approximation can be achieved, or as a function with degenerate critical points classified according to the catastrophe theory. The system we considered has also been characterized by means of an autonomous Hamiltonian, associated through the pseudopotential method, introducing an effective potential.

The frontiers of the stability domains and the periodical solutions of the sextupole trap have been analytically determined without using the pseudopotential approximation. We remark that a study over the stability of this nonlinear and non-autonomous dynamic system has not been performed yet in the literature. The kinetic energy decreases and the spatial extent of the ion clouds is larger compared to the corresponding quadrupole Paul trap. We have numerically integrated (based on the Runge-Kutta method) the nonlinear differential equations with the time periodical coefficients which characterize the dynamics of a trapped particle confined in a third order (sextupole) trap. These domains are larger than in the case of an ideal quadrupole Paul trap, which allows trapping of larger particle numbers.

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