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Optimization of ion trap geometries and of the signal-to-noise ratio for high resolution spectroscopy

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Physicists have always focused on designing and implementing methods which would eventually allow them to confine and levitate a particle in a well defined region in space, under conditions of minimal perturbations, in an almost interaction free environment. This led to the development of radically new techniques for trapping atomic particles. One major advantage of such a system lies in the fact that the apparatus used to prepare and manipulate atomic quantum states is already in place. It has been refined and developed for high precision spectroscopy, quantum logic and high accuracy frequency standards. This paper deals with optimization of ion trap geometries which are widely used in modern physics.

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1. Introduction

One of the most versatile tools used by modern day physics resulted from the goal of levitating an atomic particle within a region of small dimensions in space, in a well controlled manner. New and elaborate techniques have emerged, while conceptually new experiments have been performed in the last decades using trapped and laser cooled ions or atoms. Thus, single atoms are observed live and can be continuosly manipulated. Localization of ions results in unique characteristics: very narrow atomic lines, under weak perturbation by neighbouring particles [1, 2], as a consequence of accurate control of quantum states. An almost collision-free and interaction free environment is provided, which led to the most accurate measurements on fundamental constants in physics as well as stringent tests on quantum mechanics and quantum electrodynamics concepts. Applications range from high-precision measurement of *g* factors for electrons and protons and leptonic magnetic moments (quantum metrology), mass ratios, high *Z*-ion Spectra (Physica Scripta, Vol. T59 (1995)), quantum state engineering [3], quantum logic [4], study of non-neutral plasmas [5], development of new atomic clocks operating in the optical range [1, 6], to the study of ion chemical reactions. Quantum information processing (QIP) with trapped ions uses quantum entanglement in order to increase the signal-to-noise ratio in spectroscopy. Ion traps have also gained particular importance in the field of nuclear physics where they are used for the precise determination of nuclear binding energies, decay studies, and radioactive ion beam manipulation.

This paper deals with the study and design of new ion geometries intended for microparticle trapping, which would increase the signal-to-noise ratio and minimize the disturbing effects in high-resolution spectroscopy, with direct consequences on the long term stability of the confined particles. It is considered that these results might prove important for the design of new microtrap geometries operating in ultrahigh vacuum, in order to achieve quantum logic and develop new time-frequency standards based on trapped atomic ions, with enhanced properties compared to present day ones. Section 2 is a review of some considerations on quadrupolar ion traps and their specific characteristics. Section 3 presents the effect of trap nonlinearitities and anharmonicities, as a consequence of the presence of high order terms in the series expansion of the trap potential. Section 4 presents the microparticle trapping setup which was designed and realized, based on a hexapolar trap geometry. Section 5 is dedicated to discussions and conclusions.

2. Ion traps. General Considerations.

Since trapping field is strongly inhomo-geneous, the average force acting on a particle is not necessarily zero. Through adequate choice of the field amplitude and frequency Ω, a time averaged restoring force for all three directions can result, directed towards the trap centre. A harmonic binding force is chosen for simplicity reasons and hence, a quadrupolar field results. Its parabolic potential can be expressed as:

$$\Phi = \frac{\Phi_0}{2r_0^2}\left(\alpha x^2 + \beta y^2 + \gamma z^2\right), \qquad (1)$$

where $\Phi_0 = U_0 + V_0 \cos \Omega t$ stands for the oscillating electric potential, U_0 and V_0 are the continuous and the RF trap voltages, respectively, while α, β and γ are constants depending of the field to be generated and Ω represents the rapidly oscillating field frequency. The constants are chosen to satisfy the Laplace equation $\Delta\Phi = 0$ which, besides the trivial case $\alpha + \beta + \gamma = 0$, leads to the solution $\alpha = \beta = 1$ and $\gamma = -2$. This is the case for rotational symmetry around the *z*-axis, which gives the following quadratic potential:

$$\Phi = \Phi_0 \frac{\left(r^2 - 2z^2\right)}{r_0^2 + 2z_0^2}, \qquad (2)$$

where r_0 and z_0 are the trap radial and axial dimensions, as seen in Fig. 1 [2]. The trap electrodes are shaped as hyperboloids of revolution. In order to achieve three-dimensional trapping of electrically charged particles, ion traps have been designed, such as the Penning and Paul traps. A sketch of the electrode configuration for these traps is shown in Fig. 1. The Penning trap was used in order to confine electrons or protons, by means of a homogeneous magnetic field and a static electric quadrupole field. The static electric field is responsible for axial confinement while the magnetic field forces the particles to describe radial orbits around the trap axis. H. Dehmelt invented ingenious methods of cooling, perturbing, storing (one single electron was trapped for more than 10 months [7]), and communicating with the trapped particles, thus forcing them to reveal their properties. In the combined electric and magnetic fields in the Penning trap, charged particles describe a complicated motion.

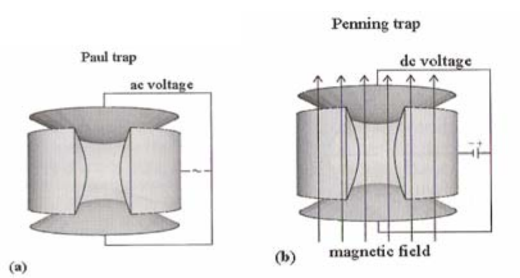

Fig. 1. Basic arrangement for Paul and Penning traps. The inner electrode surfaces are hyperboloids. (a) The dynamic stabilization in the Paul trap is given by the ac-voltage $V_0 cos\Omega t$; (b) The static stabilization in the Penning trap is given by the dc-voltage $U=U_0$ and the axial magnetic field B (Figure reproduced from [4]).

The electrodynamic trap currently used in trapped ion physics was invented in the 1950s by W. Paul. The idea is that since a charged particle can not be confined in three dimensional space using static electric fields, an inhomogeneous quadrupole electric field oscillating at radio-frequency (RF) is applied instead, forming a potential with the shape of a saddle spinning at the RF frequency, while a weak static potential is simultaneously applied in the z direction [2], [5]. This potential harmonically confines ions in the region where the field exhibits a minimum [8], in conditions of dynamical stability. Classical ion dynamics is described by homogeneous Hill (Mathieu) equations [2]. A stability diagram is associated to each Mathieu equation, while the the final stability diagram is the overlaping of the stability regions for the axial and radial directions.

3. Trap nonlinearities and anharmonicities. Theory and modelling

Lately, an ever increasing interest appeared towards the production of cold antihydrogen by recombination of positrons and antiprotons, as well as simultaneous trapping of different atomic species. With this aim, particles of opposite charge and different mass have to be confined simultaneously in the same region of space. There are two different kinds of ion traps which satisfy this requirement: nested Penning traps and the combined trap. A combined trap consists of a Penning and a super-imposed Paul trap. The resulting trap potential is identical with that given by Eq. (2). Such a potential would be usually produced by hyperbolic geometry electrodes, as already shown. In fact, real traps are quite different compared to ideal ones, due to holes drilled into the electrodes (with an aim to achieve optical pumping, fluorescence detection and laser cooling of the charged particles), imperfect electrode shape, misalignments and space charge. As a result, the electric potential which describes the trap presents radial and axial asymmetries. According to Pahl et al. [9], the potential in such a configuration is calculated using the method of successive overrelaxation. The electric potential can be expanded in a power-series:

$$\Phi(r,z) = \Phi_0\left(C_0 + \frac{C_2}{\rho^2} H_2(r,z) + \ldots + \frac{C_n}{\rho^n} H_n(r,z)\right), \qquad (3)$$

where $n = 0, 2, 4, \ldots$,

$$H_2(r,z) = 2z^2 - r^2, \quad H_4(r,z) = 8z^4 - 24z^2r^2 + 3r^4,$$
$$H_6(r,z) = 16z^6 - 120z^4r^2 + 90z^2r^4 - 5r^6, \qquad (4)$$

are the spherical harmonics and $\rho^2 = r_0^2 + 2z_0^2$. The term *n=2* stands for the quadrupole term, the *n=4* one is the octupole term, while *n=6* represents the dodecapolar part of the potential. For rotational symmetry, such as this is case, the odd coeficients vanish in Eq. (3). The terms of orders higher than the quadrupole one, C_2, may be considered as perturbing potentials. They induce parasitic effects such as motion resonances asymmetry, shift of motional eigenfrequencies with the increase of the excitation amplitude, space charge shifts and instabilities associated to particle dynamics for certain operating points in the stability diagram, for the Mathieu type equa-tion of motion. These shifts are very important in case of Penning traps, where high resolution mass spectroscopy is performed. Thus, we can regard the potential as consisting of a pure quadrupole (ideal) part, on one hand, and of the smaller high order terms which represent the perturbing part, on the other side.

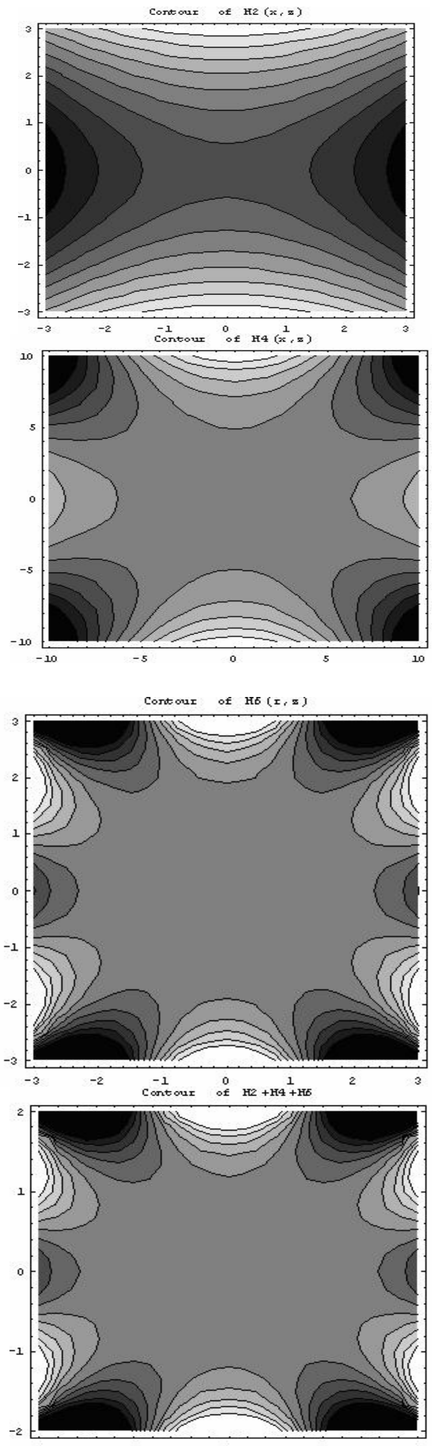

Fig. 2. Surface contours for the quadrupole, octopole and dodecapole terms of the potential and for a linear combination of them.

4. Results

We report a simple setup based on a linear hexapolar Paul trap consisting of six brass electrodes equally spaced on a 1.5 cm radius and two end cap electrodes, located at the trap ends. A sketch of the trap geometry we designed is presented in Fig. 4.

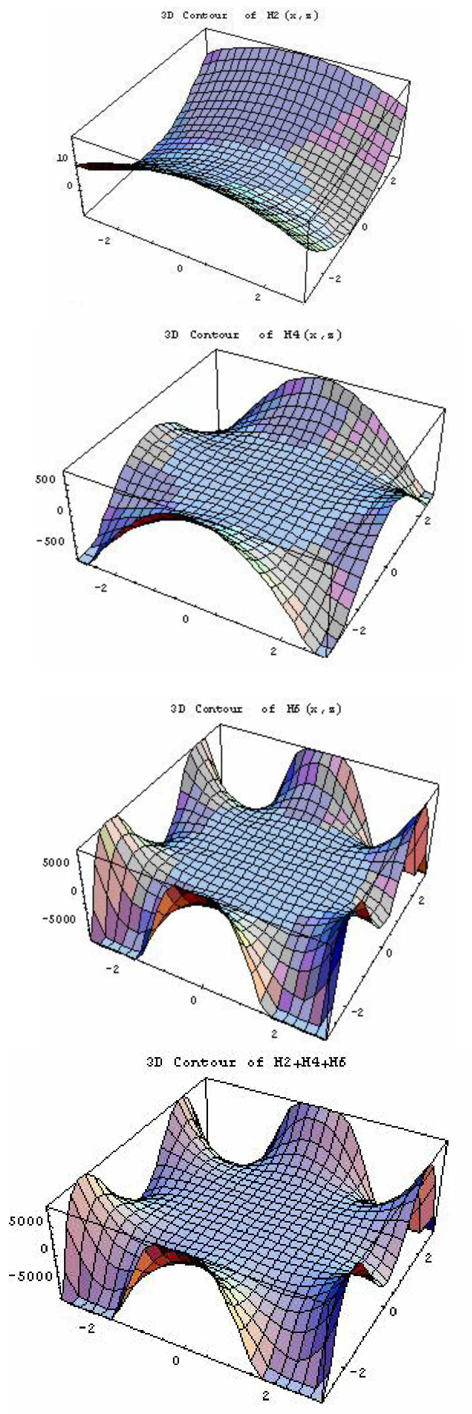

Fig. 3. Space (3D) contours for the quadrupole, octopole and dodecapole terms of the potential and linear combinatins of them.

The multipole terms, such as the hexapole one and higher-order terms, are minimized by varying the shape of the electrodes. Present interest is focused on designing ion traps which could possibly increase the signal-to-noise ratio, under conditions of dynamical stability. An evergrowing interest was attracted by multipole traps, as it is considered that these traps can trap higher particle numbers, minimizing the second order Doppler effect. Recent experiments in quantum information physics have used either miniaturized Paul traps (for single ions) or linear radiofrequency traps (for strings of ions). Both situations enable strong confinement in the Lamb-Dicke regime [10]. Ion micromotion limits the cooling efficiency within the Paul trap. Traps designed to study ions and elementary particles are operated under ultrahigh vacuum conditions. Researches involving microparticles have been performed under standard temperature and pressure conditions, at atmospheric pressure. We report, for the first time to our knowledge, a hexapolar trap based miniaturized setup intended for microparticle storage, operating in air, under standard temperature and pressure reference (STP) conditions [11].

The trap length is around 85 mm. The trap electrodes are made of six brass bars, each one having a diameter of 10 mm. The setup is intended for studying the appearance of stable and ordered patterns for different electrically charged microparticle species, with an aim to increase the particle number and hence, the signal-to-noise ratio. Alumina was used in order to illustrate the trapping phenomenon, but other species are also considered. Specific charge measurements over the trapped microparticle species are expected to result, as the setup is currently under testing.

An electronic supply system was designed. It delivers an a.c. voltage V_0 with an amplitude of 0-4 kV and a variable frequency in the 40-800 Hz range, used in order to radially trap the charged particles. The V_0 voltage is obtained by means of a high voltage step-up transformer, driven by a low frequency (main) oscillator. The V_0 voltage can be amplitude modulated up to 100, using an auxiliary oscillator. The modulation frequency lies in the 10-30 Hz range. The electronic supply system also delivers a variable d.c voltage U_z, applied between the upper and lower multipolar trap electrodes, used to compensate the gravitational field and shift the particle position along the z-axis. Due to the electric field generated by U_z, the stored particles (microplasmas) can be positioned along the trap longitudinal axis x, where the trapping potential presents a minimum (vanishes for an ideal trap). Another d.c. variable voltage U_x is applied between the trap end cap electrodes thus preventing particle loss at the trap ends. The U_z and U_x voltages range lies between 0-700 V, while their polarity can be reversed.

5. Discussion and conclusions

We have studied the effect of trap nonlinearities and anharmonicites over the trapping phenomenon. Real traps differ from ideal traps, due to reasons caused by geometrical imper-fections, misalignments, holes drilled in the elec-trodes, etc. As it is known, these parasitic effects can degrade long term stability of trapped particle species and thus affect the resolution of the mea-surements. In such cases, the electric potential of the trap can be calculated through the method of over-relaxation and it is a series expansion in which we find the quadrupole (ideal) term and the parasitic terms, namely the high order terms. For an adequate choice of the trap geometry, in case of rotational symmetry, the odd terms vanish and we are left only with the even terms of the trap potential. Fig. 2 presents the surface contours associated to these terms. In order to minimize the parasitic effects, the contributions of the high order terms must be as small as possible. High resolution spectroscopy, quantum logic, nonlinear state engineering, quantum optics, quantum metrology and development of new, very accurate, frequency standards operating in the optical and microwave range, are all directions based on the progress made in the development of electromagnetic traps methods and technologies. Increasing the signal-to-noise ratio, while minimizing parasitic effects is a must for modern physics and key technology. With this aim in view, we have investigated linear Paul traps with multipolar geometries, operating in air, under standard temperature and pressure reference conditions. We focused on a hexapolar trap geo-metry intended for charged microparticle con-finement and for illustrating the appearance of planar and volumic structures for these micro-plasmas.

Fig. 4. Microparticle confinement setup based on a hexapolar trap geometry, operating in air, at standard temperature and pressure conditions.

In order to view the microplasmas a laser diode was used, mounted within one of the endcap electrodes. The microparticles are electrically charged and then introduced inside the trap. Microplasmas consisting of a few up to hundreds of microparticles have resulted. We have been able to see strings of microparticles, parallel strings, planar structures, volumic structures. Stable and ordered microplasma structures have been obtained. The microplasmas can be shifted both axially and vertically, using the two d.c. voltages U_x and U_z. A method of determining the space charge of the trapped microparticles is currently tested, which would have applications in environment monitoring. From the experimental data gathered, we can ascertain that the trap we designed enables trapping larger number of particles compared to quadrupolar geometries or even simple linear setups.

Microparticles are radially confined along the nodal line of the a.c. electric field at the center of the trap (*x*-axis), due to the trapping voltage. It is estimated that extending the research in this area might result in multipolar trap geometries which achieve larger signal-to-noise ratios, by trapping larger number of micro-particles, without an increase of the second order Doppler shift, of the micromotion or of the space charge parasitic effects. As a conclusion, multi-polar traps are expected to act as excellent can-didates for high-resolution spectroscopy, quantum computing, quantum metrology and high accuracy atomic frequency standards.

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