A New Class of Ordered Structures in a Paul Trap: Classically Stable Clusters of Positively and Negatively Charged Particles

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Abstract

We show that in the pseudo-potential approximation stable clusters of ions of both signs of charge can exist in a Paul trap.

A Paul trap (1) is an electrodynamical device for the stable confinement of charged particles. It consists of a ring electrode and two polar end caps. An ac voltage applied between ring electrode and the electrically connected end caps generates an oscillating electric quadrupole-field which focuses free electric charges towards the center of the trap. The focusing action of a Paul trap is very similar to the method of strong focusing employed in modern particle accelerators. Here, large quadrupole magnets of alternating polarity are positioned along the circumference of the accelerator generating an oscillating quadrupole field in the rest frame of the revolving particles. It can be shown that the time averaged net force resulting from such an oscillating potential is a harmonic force focusing the particles towards the beam axis of the accelerator. The two dimensional focusing action corresponding to the toroidal topology of an accelerator is turned into 3D focusing, i.e., confinement, in the case of the spheroidal topology of the Paul trap.

The time-averaged trapping potential generated by a Paul trap, the so-called "pseudo-potential" is of the form of an axisymmetric harmonic oscillator and explicitly given by (1-5)

$$V(x,y,z) = \frac{1}{2} m\left(\omega_x x^2 + \omega_y y^2 + \omega_z z^2\right) \qquad (1)$$

The pseudo-oscillator's frequencies ω_x, ω_y and ω_z are related to the oscillation frequency Ω of the ac voltage applied to the trap by (1-5)

$$\omega_x = \omega_y = \left(a + \frac{1}{2}q^2\right)^{1/2}\frac{\Omega}{2}; \quad \omega_z = \left[2\left(q^2 - a\right)\right]^{1/2}\frac{\Omega}{2} \qquad (2)$$

Here, a and q are dimensionless parameters which are related to the various physical parameters of the trap by (1-5):

$$a = \frac{8\,ZeU_0}{m\Omega^2\left(r_0^2 + 2z_0^2\right)}; \quad q = \frac{4ZeV_0}{m\Omega^2\left(r_0^2 + 2z_0^2\right)} \qquad (3)$$

U_0 and V_0 are the dc and ac components of the applied voltage, respectively, m is the mass of the particle, Z its charge, and r_0 and z_0 are the radius of the ring electrode and half the end cap separation, respectively. With the help of a Paul trap, single atomic ions can be fixed motionless in space and even photographed when illuminated with a cooling laser (2-5). This in itself already constitutes a considerable achievement, in view of the fact that not even 40 years ago Schrödinger was of the opinion that "...we never experiment with just one electron or atom or (small) molecule. In thought experiments we sometimes assume we do; this invariably entails ridiculous consequences" (6). Many

experimental groups have by now produced undisputable evidence that, contrary to Schrödinger's conviction, experiments with single electrons, atoms and ions are indeed possible (2-5,7). In a Paul trap the confined charged atomic (or sub-atomic) particle will be located close to the minimum of the secular oscillator potential (1). Additionally applied (laser) cooling (8) can push it even further towards the minimum. This is obviously an ideal situation for spectroscopy: Close to the minimum all the electric fields vanish and the atomic (ionic) energy levels can be observed with little external perturbation. Indeed the levels can be so precisely defined that an ion trap might well be the core of a future atomic clock which uses transitions in a single trapped ion as a frequency reference (9). Storing more than one charged particle in a Paul trap is not just more of the same. (10) A qualitatively new phenomenon arises, first described by Wuerker, Shelton and Langmuir in 1959 (11): The particles can arrange in regular shapes in a quasi "crystalline" structure. This situation is bistable. An external perturbation can disrupt the geometric pattern and knock the crystal into a cloud state, in which the particles swirl around in the trap like the contituents of a gas. The geometric patterns in the crystalline state can be understood as the minimal energy configurations of charged particles in the pseudo-potential (1). While Wuerker, Shelton and Langmuir worked with macroscopic charged aluminum particles, crystallization of ions was shown only very recently. (2-5) So far only geometric patterns formed by ions of one and the same charge polarity were obtained and investigated experimentally. The purpose of this note is to show that it is possible that a new class of geometric structures consisting of ions of both signs of charge exist. To this end, let us first investigate the potential landscape of a negatively charged ion in the field of a two-ion cluster. (2-5) In the following, we will neglect the jitter-motion of the ions (the "micro-motion") due to the time-varying applied ac field and work in the pseudo-potential approximation. We call the ions of the two-ion cluster B and C. In equilibrium, ion B is located at position ($x = -\xi_0$, 0,0) and ion C at ($x = \xi_0$, 0,0). Because of the fact that in a Paul trap the pseudo potential is steeper in z-direction than in x-y direction, the ions will not explore the z-direction in the crystalline minimal energy state. Because the pseudo potential is rotationally symmetric in the x-y-plane (see (1) and (2)), we could choose ions B and C as being located on the x-axis of the trap with no loss of generality. The situation is

depicted in Fig. 1.

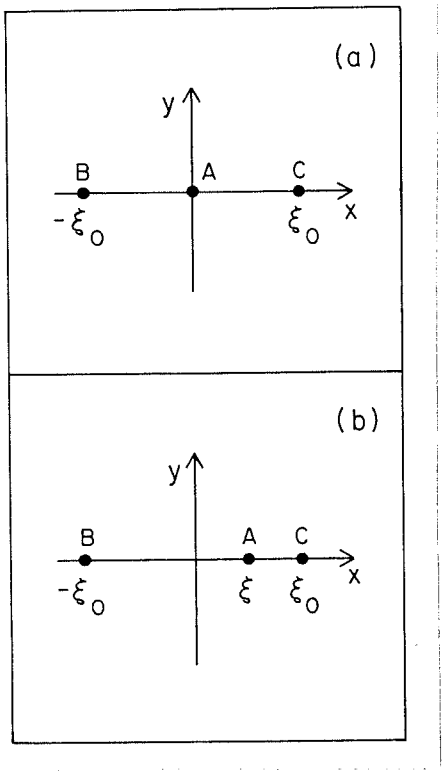

Fig. 1: Test charge A probing the field of the two ion cluster (B, C) in the x-y plane of a Paul trap. a) Equilibrium position. b) A probes the field along the "dangerous" x-axis for stability investigations.

The test charge A initially located at the origin (see Fig. 1(a) experiences two types of forces when displaced from the origin: (i) the harmonic pseudo-potential force which tries to focus the test charge back to the origin and (ii) an electro static force which tries to pull the test charge either toward ion B when A is displaced to the left, or toward C when A is displaced to the right. While the electrostatic force acts as a defocusing force in x-direction, it helps to focus the test charge when A is displaced in y or z direction. The "dangerous" direction, therefore, is the x-direction and the origin is locally stable for A only if the pseudo force locally wins out over the Coulomb force. For small displacements ξ of A in x-direction, the Coulomb force acting on A is given by

$$F_C(\xi) = \frac{QZe^2}{4\pi\,\varepsilon_o\,\xi_0^2}\cdot\frac{4\xi}{\xi_0} \qquad (4)$$

where Q is the charge of A, Z is the charge of B,C and ε_0 is the dielectric constant. The focusing pseudo fore is given by:

$$F_s(\xi) = -m\left(\omega_x^{(A)}\right)^2 \xi \qquad (5)$$

In order for the focusing force F_S to win out over the Coulomb force F_C , we must have $|F_S| > |F_C|$, or, substituting the experessions (2), (3) for ω_X,

$$0 < 16\frac{m}{M}\frac{\eta^2}{\eta - 4} < 1. \qquad (6)$$

We introduced the mass M of the ions B, C and the charge ratio $\eta = Z/Q$. The first thing to realize in (6) is that ηmust be larger than 4. This is indeed necessary since otherwise the test charge A would screen the charge B with respect to C (or vice versa) to an extend where the two-ion cluster would no longer be stable. In fact, for $\eta < 4$, the ions located initally, according to Fig. 1a)or 1b), would first collapse towards each other and then burst apart, forming an ion cloud in the trap.

For given mass ratio m/M, the left-hand side of (6) is a minimum for $\eta = 8$. Therefore, the maximal range of allowed mass ratios is given by

$$\frac{m}{M} < \frac{1}{256} \qquad (7)$$

If the test charge is an electron, this inequality can easily be fulfilled for any convenient choice of atomic ions for B, C. In case A is itself an ion, (7) can be fulfilled only with heavy molecules, substituting the ions B, C. According to the above derivations, it seems very plausible that stable multicharged clusters can exist in a Paul trap. But a number of open questions remain.

(a) The origin is only locally stable. The potential barrier separating A from B and C, respectively, must be high enough so that ion A is well below the barrier for temperatures currently reachable in ion traps.

(b) The barrier must be thick enough to avoid fast quantum tunneling. On the other hand, a thin barrier allows for the study of quantum tunneling effects. "Dissipative tunneling" can be studied if laser cooling is present. There is even the remote possibility of "watching" an ion tunneling through the barrier by means

of the spontaneous photons scattered off the ion if cooling (or accelerating) laser light is irradiating the ion while tunneling.

(c) The influence of the micro motion on the dynamics of ion A has to be studied. A preliminary study was presented in ref. 12, indicating that, despite the shaking action of the time varying quadrupole field, ion A is stable.

(d) The most burning question in this context is how to generate the multicharged cluster in the first place. This is indeed tricky. It may be possible by sequentially loading the ion trap. First ion A is loaded and placed close to the origin by the various cooling techniques nowadays available. Only then ions B and C are loaded.

In summary, we have shown that based on the pseudo potential approximation ions of both charge signs, simultaneously present in a Paul trap, can form ordered geometric structures in analogy to the known structures formed by ions of only one charge polarity. We suggest that multicharged clusters be used in quantum tunneling experiments to shed more light on the nowadays much discussed questions of (dissipative) tunneling in non-integrable potentials.

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