Harmonic linear Paul trap: Stability diagram and effective potentials

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We present the single-particle stability diagram for the radial motion in a linear Paul trap in a situation where the applied axial dc potential gives rise to a harmonic defocusing radial potential. Although most linear Paul trap experiments have been conducted in a regime where this approximation is reasonably valid, the effect of the axial confinement on the stability of the radial motion has not previously been analyzed. The defocusing effect in both radial directions leads to a stability diagram different from that of the two-dimensional quadrupole mass filter, and hence points toward new studies of few ion dynamics. Expressions for the effective or pseudopotentials for one and two charged particles are presented and discussed.

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Since the first realization of two- and three-dimensional radio frequency traps for charged particles in the 1950's [1] (generally referred to as Paul traps), many varieties of such traps have been suggested and constructed [1]. Even though the linear Paul trap in retrospect seems to be one of the most obvious configurations for obtaining three-dimensional confinement, it was first proposed and demonstrated by Prestage *et al.* [2] 10 years ago. In all Paul traps the charged particles have a spatially dependent micromotion at the driving frequency superposed on a typically slower harmonic motion. In contrast to the original three-dimensional hyperbolic Paul trap [1], the linear trap has a trap axis rather than just a single point in coordinate space where the micromotion vanishes. This fact has been the main reason for the popularity of the linear Paul trap in atomic physics, quantum optics, and metrology, since a string of ions rather than just a single ion can be studied without unwanted Doppler shifts induced by micromotion. Several proposals for realization of quantum computers have also been based on a string of ions in a linear Paul trap [3,4]. Furthermore, since in *any* point in space there is no micromotion along the trap axis direction, it is possible to laser cool large ion clouds along this axis without the heating effects connected with the micromotion-induced Doppler shifts [5]. This has enabled investigations of large ion Coulomb crystals [6,7].

Generically, a linear Paul trap is just a quadrupole mass filter [1] with dc voltage confinement along the center axis (z axis) as sketched in Fig. 1. The defocusing effect of the dc axial potential in the radial plane is obvious from the Laplace law, and it has also been accounted for in previous descriptions of the motion of ions in such traps [8]. The question of under which axial confinement conditions stable radial motions exist has, however, not been addressed previously.

In this Brief Report, we provide a stability diagram for the radial motions in the case of a harmonic dc potential along the z axis. Though this might seem to be a special case, at least at small distances from the trap center, it is generally a good approximation. Furthermore, we discuss some of the special features of such traps in contrast to the quadrupole mass filter and the original Paul trap, and point toward theoretical and experimental investigations. We finally present expressions for the effective or pseudopotential for this trap in the case of one and two charged particles.

When discussing the radial motion of charged particles, from now on referred to as ions, in linear Paul traps, the similar motion in the quadrupole mass filter is often the starting point. For the mass filter (Fig. 1 with $U_{\mathrm{end}}=0$), the motion of a single ion in the xy plane is described by the following equations:

$$\ddot{x}+(a-2q\cos 2\tau)x=0, \tag{1}$$

$$\ddot{y}-(a-2q\cos 2\tau)y=0, \tag{2}$$

where

$$a\equiv\frac{4QU_{\mathrm{dc}}}{M\Omega^2 r_0^2},\quad q\equiv\frac{2QU_{\mathrm{RF}}}{M\Omega^2 r_0^2},\quad \text{and } \tau\equiv\frac{1}{2}\Omega t. \tag{3}$$

Here U_{RF} and Ω are the amplitude and frequency of the applied RF field, respectively, M the mass and Q the charge of the ion, r_0 the minimum distance from the electrodes to the trap axis z, while U_{dc} refers to a dc voltage applied to diagonal electrodes. The derivatives are given with respect to the dimensionless time τ.

Stable radial motion for a single ion is achieved whenever the dimensionless parameters q and a are within the hatched areas denoted A and B in Fig. 2 [9]. The quadrupole mass filter description is, however, a reasonable approximation for the radial motion in linear Paul traps only when the defocusing effect of the axial confinement can be neglected, i.e., typically when the middle electrodes are much longer than the radial spacing of the electrodes. In the opposite case, where the middle electrodes are short, the defocusing effect can be strong and significant for the stability of the radial motion. In the specific case of $U_{\mathrm{dc}}=0$, the equations of radial motion can now be written:

$$\ddot{x}+(a-2q\cos 2\tau)x=0, \tag{4}$$

$$\ddot{y}+(a+2q\cos 2\tau)y=0 \tag{5}$$

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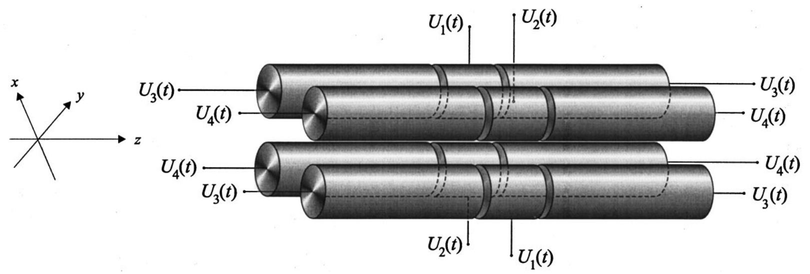

FIG. 1. Sketch of a linear Paul trap. The trap consists essentially of four rod-electrodes in a quadrupole mass filter configuration. Each rod is sectioned into three, allowing a dc voltage $U_{\rm end}$ to be applied to the eight end-electrode pieces. The voltages $U_i(t)$ in the figure are given by $U_1(t) = -(U_{\rm RF}/2)\cos\Omega t$, $U_2(t)=(U_{\rm RF}/2)\cos\Omega t + U_{\rm dc}$, $U_3(t)=-(U_{\rm RF}/2)\cos\Omega t + U_{\rm end}$, and $U_4(t)=(U_{\rm RF}/2)\cos\Omega t + U_{\rm dc} + U_{\rm end}$.

with

$$a \equiv \frac{4QU_{\rm Eff}}{M\Omega^2 r_0^2}, \tag{6}$$

where $U_{\rm Eff}$ is a voltage proportional to the applied dc voltage $U_{\rm end}$ of the eight end-electrode pieces to accommodate axial trapping (see Fig. 1). The exact factor of proportionality depends on the specific trap geometry. Apparently, these equations of motion (4) and (5) are equivalent to those in Eqs. (1) and (2). There is, however, an important difference since the sign of the term containing the a parameter is now the same for the x and y motions. This means that the condition for stable motion is the same for the x and y directions, and the stability region for radial confinement is now given as the gray-shaded region in Fig. 2 [10]. It should be noted that, in order to obtain axial confinement, the a parameter must always be negative. In contrast to the mass filter or the original Paul trap, stable motion can in principle be obtained for any applied RF voltage, though the stability range for the a parameter rapidly gets narrow for large values of q. The stability region for the harmonic linear Paul trap presented in Fig. 2 contains the disjoint stability areas A (partly) and B for the mass filter. This feature is particularly interesting when comparing nonlinear dynamics of two or more ions in this type of trap with those of the mass filter as well as with those of the original Paul trap [5,11,12]. If an additional dc voltage is applied to diagonal electrodes, as often done with mass filters, the radial stability region becomes the intersection of two stability regions as the gray-shaded one in Fig. 2, displaced by $\pm a_{\rm dc}$ along the a axis, respectively. Here $a_{\rm dc}$ is the value of a associated by the applied diagonal dc voltage $U_{\rm dc}$.

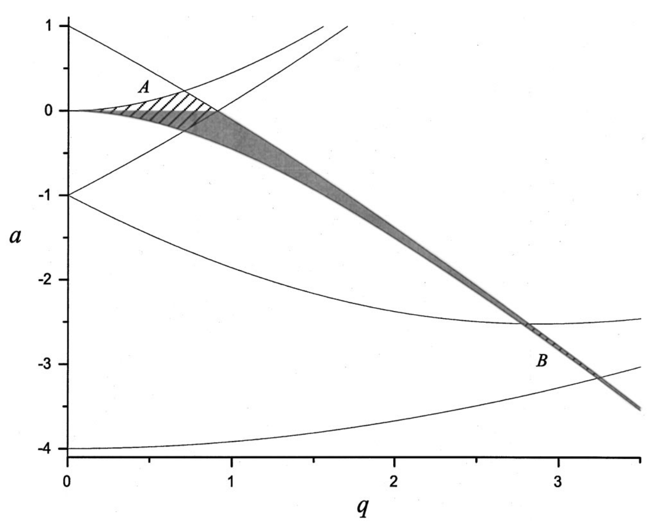

FIG. 2. Single-ion stability diagrams for the quadrupole mass filter (the hatched areas A and B) and for the harmonic linear Paul trap (gray-shaded area). The dimensionless parameters a and q are defined in the text.

If $a_{\rm dc}=0$ and $a, q^2 \ll 1$, the effective or pseudopotential for a single ion can be approximated by

$$U_{\rm Pseudo}(r,z) = \frac{1}{2}\omega_r^2 r^2 + \frac{1}{2}\omega_z^2 z^2, \tag{7}$$

with

$$\omega_r = \sqrt{a + \frac{1}{2}q^2}, \quad \omega_z = \sqrt{-2a} \quad \text{and} \quad r^2 = x^2 + y^2, \tag{8}$$

where a is defined as in Eq. (6) and ω_r and ω_z are the effective radial and the axial oscillation frequencies, respectively.

When describing the motion of two identical ions simultaneously present in the trap, the Coulomb interaction between them has to be taken into account. In this case it is practical to separate the motion of the ions into a relative and a center-of-mass motion. The latter is identical to the one presented in Eq. (7) for the motion of a single ion. Denoting the relative coordinates x, y, and z, the following equations are obtained for the relative motion:

$$\ddot{x} = \frac{x}{\rho^3} - (a - 2q\cos 2\tau)x, \tag{9}$$

$$\ddot{y} = \frac{y}{\rho^3} - (a + 2q\cos 2\tau)y, \tag{10}$$

$$\ddot{z} = \frac{z}{\rho^3} + 2az, \tag{11}$$

where $\rho = \sqrt{x^2+y^2+z^2}$ is the distance between the ions. Here all lengths are measured in units of $\sqrt[3]{2Q^2/\pi\varepsilon_0 M\Omega^2}$, which is of the order of a micron when Ω is in the MHz range. In the case where the center of mass motion is ceased by some cooling mechanism, Eqs. (9)–(11) describe completely the motion of the ions. Applying the same method as that used in Ref. [13] for determining the pseudopotential for two ions in the original Paul trap, the following pseudopotential is found:

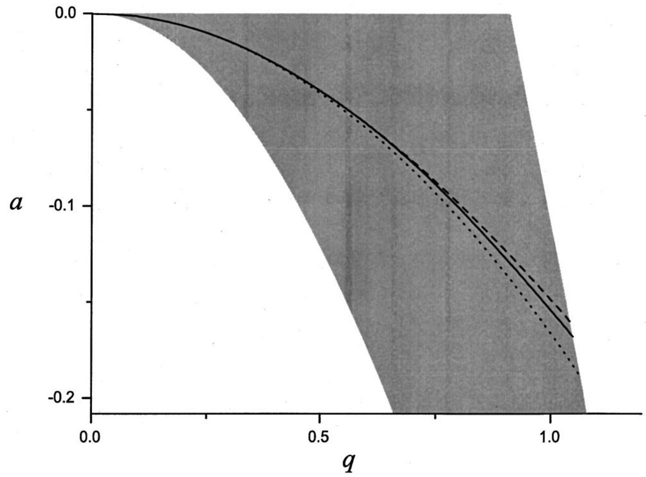

FIG. 3. Section of the stability diagram for the harmonic linear Paul trap (gray-shaded area). The curves represent the borderline for two-ion crystals being oriented along the z axis for the simplified pseudopotential given by Eq. (7) plus a $1/\rho$ Coulomb term (dotted line), for the pseudopotential given by Eq. (12) (dashed line), and from molecular dynamics simulations (solid line). Above the lines, the two-ion crystal is supposed to be oriented along the z axis.

$$U_{\mathrm{Pseudo}}(x,y,z)=\frac{1}{\rho}+\frac{1}{2}ar^2-az^2+\frac{q^2}{\Delta}\left((4-a)r^2+\frac{r^2}{\rho^3}-\frac{12x^2y^2}{\rho^5}\right), \tag{12}$$

where, again, $r^2=x^2+y^2$, $\rho^2=r^2+z^2$ and

$$\Delta=\left(4-a+\frac{1}{\rho^3}\right)\left(4-a+\frac{1}{\rho^3}-\frac{3r^2}{\rho^3}\right). \tag{13}$$

This expression is rather complicated, but for the limit where $a,q^2 \ll 1$ and $\rho \gg 1$, the potential reduces to the single-ion potential given by Eq. (7) with an additional Coulomb term $1/\rho$. When the two ions are close to their equilibrium distance at zero temperature, $\rho \gg 1$ is fulfilled if $a,q^2 \ll 1$. When such a simplified equation is used to determine the orientation of a two-ion crystal (defined as the equilibrium configuration at zero temperature) in the trap, one finds that the ion crystal will lie in the xy plane with no preferred orientation if $\omega_z > \omega_r$, while for $\omega_z < \omega_r$ its orientation will be along the z axis. The equilibrium distance would be $\omega^{-2/3}$ (in the scaled units used), where ω is the smallest of the secular frequencies. The borderline between these two types of orientation is defined by $\omega_r = \omega_z$, leading to $a=-\frac{1}{6}q^2$. The corresponding curve within the single-ion stability region is presented (dotted curve) in Fig. 3.

When the full pseudopotential Eq. (12) is used, one finds that the two-ion crystal will be oriented either along the z axis or in the xy plane, as predicted by the above simple approximation. Due to the last term in Eq. (12), there are, however, only two possible orientations within the xy plane. The ions orient either along the line defined by $x=y$ or along the line defined by $x=-y$. This is in contrast to the hyperbolic Paul trap, where ''peculiar'' crystal orientations can be present [13,14]. Simulations performed using Eqs. (9)–(11) confirm this. Curves representing the borderlines for crystals oriented along the z axis derived from the full pseudopotential in Eq. (12) or obtained from molecular dynamics simulations based on Eqs. (9)–(11) are represented in Fig. 3 by the dashed and solid curves, respectively. While the simplified pseudopotential given by Eq. (7) plus the $1/\rho$ Coulomb term are appropriate for determining the two-ion crystal orientation for small values of q, it is clear from Fig. 3 that the more general potential given by Eq. (12) yields nearly the correct crystal orientation for all values of q.

Currently, we plan to investigate experimentally the validity of the pseudopotential approximation by studying the shape of ion Coulomb crystals as a function of trapping parameters, and we have initiated theoretical studies of the ion crystal stability within the single ion stability diagram shown in Fig. 3.

In the same way as a dc voltage applied to diagonal electrodes can be used to obtain mass selection in a quadrupole mass filter, the voltage on the end-electrode pieces U_{end} can be used to obtain mass selection in a harmonic linear Paul trap. Recently, we have been able to eject $^{25,26}Mg^+$ ions selectively, while keeping $^{24}Mg^+$ ions trapped in a linear Paul trap using this technique. This mass selection process has also been applied to show that $N_2{}^+$ molecular ions have been trapped and cooled translatorically by laser-cooled $^{24}Mg^+$ ions. The motion of the ions becomes unstable due to a vanishing effective potential in practically the entire xy plane simultaneously with an increasing U_{end}, in contrast to the mass filter for which the increase in U_{dc} leads only to instability along one specific axis. This difference may lead to a reduced heating and loss of the remaining ions when the axial voltage is used as the mass selector. Furthermore, in a linear Paul trap that meets the harmonic assumptions above, it is possible experimentally to investigate larger ion Coulomb crystals in RF traps under various effective harmonical confinement conditions. In such experiments, possible deviations of these crystals' outer shapes and inner structures from those predicted by the theory of Coulomb crystals in static harmonical potentials [15] can be studied.

In conclusion, we have presented a stability diagram for the linear Paul trap that in many situations is more appropriate than the stability diagram for the two-dimensional quadrupole mass filter. Expressions for the effective pseudopotentials for the one- and two-ion cases have been derived, and, we have pointed toward various new theoretical and experimental work involving harmonic linear Paul traps.

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[1] See, e.g., P. K. Ghosh, *Ion Traps* (Clarendon Press, Oxford, 1995), and references therein.
[2] J. D. Prestage, G. J. Dick, and L. Maleki, J. Appl. Phys. **66**, 1013 (1989).
[3] J. I. Cirac and P. Zoller, Phys. Rev. Lett. **74**, 4091 (1995).
[4] A. Sørensen and K. Mølmer, Phys. Rev. Lett. **82**, 1971 (1999).
[5] R. Blümel, C. Kappler, W. Quint, and H. Walther, Phys. Rev. A **40**, 808 (1989).
[6] G. Birkl, S. Kassner, and H. Walther, Nature (London) **357**, 310 (1992).
[7] M. Drewsen, C. Brodersen, L. Hornekær, J. S. Hangst, and J. P. Schiffer, Phys. Rev. Lett. **81**, 2878 (1998).
[8] M. G. Raizen, J. M. Gilligan, J. C. Bergquist, W. M. Itano, and D. J. Wineland, Phys. Rev. A **45**, 6493 (1992).
[9] There exists at least in principle an infinite number of regions of stable motion for the mass filter. The areas of the regions not presented in Fig. 2 are, however, very small, and will not be considered in the present paper.
[10] There exists also an infinite number of regions of stable motion for the harmonic linear Paul trap, but only the region depicted in Fig. 2 will be considered in the present paper.
[11] J. Hoffnagle, R. G. DeVoe, L. Reyna, and R. G. Brewer, Phys. Rev. Lett. **61**, 255 (1988).
[12] R. G. Brewer, J. Hoffnagle, R. G. DeVoe, L. Reyna, and W. Henshaw, Nature (London) **344**, 305 (1990).
[13] M. G. Moore and R. Blümel, Phys. Rev. A **50**, R4453 (1994).
[14] J. A. Hoffnagle and R. G. Brewer, Appl. Phys. B: Lasers Opt. **60**, 113 (1995).
[15] D. H. E. Dubin, Phys. Rev. Lett. **71**, 2753 (1993).