Appl. Phys. B 61, 159–163 (1995)

Applied Physics B Lasers and Optics

Dynamics of a single particle in a Paul trap in the presence of the damping force

T. Hasegawa, K. Uehara

Department of Physics, Faculty of Science and Technology, Keio University, 3-14-1 Hiyoshi, Kohoku-ku, Yokohama 223, Japan
(Fax: + 81-45/563-1761)

Received: 22 July 1994/Accepted: 17 November 1994

Abstract. The motion of a single charged particle in a Paul trap in the presence of the damping force is investigated theoretically and the modified stability diagrams in the parameter space are calculated. The results show that the stable regions in the a–q parameter plane are not only enlarged but also shifted. Consequently, the damping force causes instability in some cases, contrary to intuition. As a by-product of the calculation, we derive new theoretical approximate expressions for the secular-oscillation frequency. In the limiting case of no damping, these formulas are in good agreement with early measurements done by Wuerker et al.

PACS: 07.60. – j

The motion of charged particles confined in a Paul trap is composed of a superposition of two parts, a fast oscillation called the micromotion synchronized with the driving field and a slow oscillation called the secular motion. In the standard configuration of the Paul trap, the stability and the normalized secular-oscillation frequency of a single particle are determined by two dimensionless constants denoted by a and q. In early experiments, Wuerker et al. made a visual observation of the motion of aluminum microparticles (a few microns in diameter) in a Paul trap [1]. They measured the secular-oscillation frequency of a single confined particle when $a = 0$ (zero-applied dc voltage) as a function of q, which is proportional to the amplitude of the ac voltage. The observed frequencies were compared with a theoretical approximate formula which was calculated from the harmonic pseudopotential neglecting the micromotion. Agreement was good only when the parameter q was small. On the other hand, when a few or more particles were stored, they observed that the particles were arrayed as a crystal (ordered state) or moved around in a random fashion like a cloud (disordered state), depending on the parameters a, q, or the background pressure. This experiment and recent observations of similar order–disorder transitions of trapped ions [2–4] suggest that the damping force corresponding to collisional cooling or laser cooling plays an important role in the dynamics of the particles in a Paul trap.

In the present paper, we deal theoretically, in connection with these experiments, with two fundamental problems concerning the dynamics of a single particle in a Paul trap, i.e., the effects of the damping force and approximate formulas for the secular-oscillation frequency. First, we investigate the influence of the damping force on the stability of motion of a single particle, although it is not understood yet how this problem is related to the dynamics (other than the motion of the center of mass) of multiparticle systems. We treat a simple case in which the damping force is proportional to the velocity of the particle. Statistical fluctuations are neglected. This situation is appropriate particularly for collisional cooling of a microparticle by a background gas [1]. The equations of motion are then a set of Mathieu's equations with a damping term. Although this type of equation is a standard mathematical problem as shown in some textbooks [5–7], there has been no detailed discussion, so far as we know, about the stability of three-dimensional motion of a particle in the presence of the damping force. For example, it has not been illustrated explicitly how the stability diagram in the a–q parameter plane is modified by the damping force. Our analysis shows that the stable parameter regions (stable regions, for short) are not only enlarged, as we can expect intuitively, but also shifted. As a consequence, it happens in some cases that a set of the values of a and q giving the stable confinement in the absence of the damping force, falls in the unstable region in the presence of damping. In the stable regions (except on the boundaries) in the presence of damping, the particle exhibits a damping oscillation converging to the center of the trap. Second, as a by-product of the analysis, we derive new approximate formulas for the secular-oscillation frequency. It is then shown that, in the limiting case of no damping, these formulas are in good agreement with the experimental data of Wuerker et al. [1].

1 Condition for stable confinement

We consider a particle of mass M and electric charge Q in a Paul trap with a ring diameter $2r_0$ and an end-cap separation $2z_0$. We assume that the damping force F is given by $F = -Dv$, where v is the velocity of the particle and D is a constant. Then, when the ac voltage of peak amplitude V_0 and angular frequency Ω in series with the dc voltage U_0 is applied between the ring and the end caps, the equations of particle motion are given by

$$\frac{d^2u}{d\tau^2} + 2\kappa\frac{du}{d\tau} + (a_u - 2q_u\cos 2\tau)u = 0, \qquad (1)$$

where u stands for x, y, or z (the z-axis is the symmetry axis). The dimensionless variables and constants τ, κ, a_u and q_u are defined by

$$\tau = \Omega t/2, \qquad (2)$$

$$\kappa = D/M\Omega, \qquad (3)$$

$$a_x = a_y = -(1/2)a_z = -8QU_0/M\Omega^2(r_0^2 + 2z_0^2), \qquad (4)$$

and

$$q_x = q_y = -(1/2)q_z = 4QV_0/M\Omega^2(r_0^2 + 2z_0^2). \qquad (5)$$

If $\kappa = 0$, (1) is the Mathieu's equation. Even if $\kappa \neq 0$, however, by using a transformation

$$u = w\exp(-\kappa\tau), \qquad (6)$$

(1) can be reduced to the Mathieu's equation for w with the parameter a replaced by $a - \kappa^2$:

$$\frac{d^2w}{d\tau^2} + (a - \kappa^2 - 2q\cos 2\tau)w = 0, \qquad (7)$$

as shown in textbooks [5–7]. In (7), the subscripts of a and q are omitted for simplicity. Since the properties of the Mathieu functions have been studied in detail, the discussion of the stability of a particle in the case of $\kappa \neq 0$ appears straightforward. But it is not so because, owing to the damping factor $\exp(-\kappa\tau)$ in (6), u may be stable (bounded) even if w is unstable (unbounded). We neglect the effect of the finite size of the trap.

The complete solutions of (7) can be expressed by

$$w = A\exp(\mu\tau)\phi(\tau) + B\exp(-\mu\tau)\phi(-\tau), \qquad (8)$$

where A and B are arbitrary constants and μ is a function of $a - \kappa^2$ and q. We can assume that $\phi(\tau)$, which represents the micromotion, is a periodic function of τ with a period π and is written in the form

$$\phi(\tau) = \sum_{s=-\infty}^{\infty} C_s\exp(2s\tau i). \qquad (9)$$

From the condition that $\exp(\mu\tau)\phi(\tau)$ is a solution of (7), we obtain a recurrence relation for C_s

$$C_s + \xi_s(C_{s-1} + C_{s+1}) = 0, \qquad (10)$$

where

$$\xi_s = q[(2s - \mu i)^2 - a + \kappa^2]^{-1}. \qquad (11)$$

If (10) holds, $\exp(-\mu\tau)\phi(-\tau)$ is also a solution of (7).

Here, we define an infinite determinant $\Delta(\mu)$ by

$$\Delta(\mu) = \begin{vmatrix} \ddots & & & & & & \\ \xi_{-2} & 1 & \xi_{-2} & & & & \\ & \xi_{-1} & 1 & \xi_{-1} & & & \\ & & \xi_0 & 1 & \xi_0 & & \\ & & & \xi_1 & 1 & \xi_1 & \\ & & & & \xi_2 & 1 & \xi_2 \\ & & & & & & \ddots \end{vmatrix}, \qquad (12)$$

where all matrix elements outside of the three diagonals are zero. Then, the condition that the infinite set of equations (10) for all s have non-trivial solutions, C_s requires

$$\Delta(\mu) = 0. \qquad (13)$$

From (13) and a relationship between $\Delta(\mu)$ and $\Delta(0)$ [5]:

$$\Delta(\mu) = 2\left[\Delta(0)\sin^2\frac{\pi}{2}\sqrt{a-\kappa^2} - \sin^2\frac{\pi\mu i}{2}\right] \times (\cos\pi\mu i - \cos\pi\sqrt{a-\kappa^2})^{-1}, \qquad (14)$$

we obtain the final exact expression for μ as:

$$\mu = \pm\frac{2i}{\pi}\sin^{-1}\left[\Delta(0)\sin^2\frac{\pi}{2}\sqrt{a-\kappa^2}\right]^{1/2}, \qquad (15)$$

where $\Delta(0)$ is a function of $a - \kappa^2$ and q as given by (12).

As is seen from (15) or (12), μ has an arbitrariness of $+2ni$ (n is an arbitrary integer) and can be written as

$$\mu = \pm(\alpha + \beta i) + 2ni, \ (\alpha \geq 0, 0 \leq \beta \leq 1). \qquad (16)$$

Then, $\alpha + \beta i$ is a complex, imaginary or real number corresponding to the following three cases. β represents the dimensionless secular-oscillation frequency normalized by $\Omega/2$.

Case I:

$$\Delta(0)\sin^2\frac{\pi}{2}\sqrt{a-\kappa^2} > 1$$

In this case,

$$\alpha = \frac{2}{\pi}\cosh^{-1}\left[\Delta(0)\sin^2\frac{\pi}{2}\sqrt{a-\kappa^2}\right]^{1/2} \qquad (17)$$

and $\beta = 1$. Since $\alpha \neq 0$, one of the two terms of (8) diverges as $\tau \to \infty$ and therefore, w is unstable. However, since u is composed of two terms with exponential factors $\exp[-(\kappa - \alpha)\tau]$ and $\exp[-(\kappa + \alpha)\tau]$, respectively, u is stable if $\alpha \leq \kappa$ and unstable if $\alpha > \kappa$. When $\alpha = \kappa$, one of the two terms represents a non-damping oscillation.

Case II:

$$0 \leq \Delta(0)\sin^2\frac{\pi}{2}\sqrt{a-\kappa^2} \leq 1$$

In this case, $\alpha = 0$ and

$$\beta = \frac{2}{\pi}\sin^{-1}\left[\Delta(0)\sin^2\frac{\pi}{2}\sqrt{a-\kappa^2}\right]^{1/2}, \qquad (18)$$

which takes a value between 0 and 1. Since $\alpha = 0$, w is stable and u represents a damping oscillation with a damping factor $\exp(-\kappa\tau)$. Therefore, the motion is stable.

Case III:

$$\Delta(0)\sin^2\frac{\pi}{2}\sqrt{a-\kappa^2} < 0$$

In this case,

$$\alpha = \frac{2}{\pi}\sinh^{-1}\left[-\Delta(0)\sin^2\frac{\pi}{2}\sqrt{a-\kappa^2}\right]^{1/2} \qquad (19)$$

and $\beta = 0$. As in Case I, u is stable if $\alpha \le \kappa$ and unstable if $\alpha > \kappa$. If $\alpha = \kappa$, the non-damping term gives a constant displacement from zero, superposed with the micromotion.

In summary, the boundary of stability is given by $\alpha = \kappa$. In the stable regions, except on the boundaries, the solution represents a damping oscillation which converges to zero. The normalized secular-oscillation frequency is 1, 0 and in-between, corresponding to Case I, Case III and Case II, respectively.

All the calculations so far are exact, but the formulas containing $\Delta(0)$ are not closed in the sense that $\Delta(0)$ consists of an infinite number of terms. For evaluation of these formulas, we must either use some closed approximate expressions, as derived in the next section, or repeat numerical calculations by replacing $\Delta(0)$ with a finite determinant of successively higher orders until they converge sufficiently.

In order for a particle to be stable three-dimensionally, the above requirement must be satisfied for two sets of parameters (a_z, q_z) and $(-\frac{1}{2}a_z, -\frac{1}{2}q_z)$ simultaneously from (4) and (5). The areas A and B in Fig. 1 show two calculated main stable regions in the a_z–q_z plane when $\kappa = 1.0$. The values of κ of order 1 used here are typical for a submicron particle in a background gas of a pressure higher than ≈ 0.01 Torr. The corresponding stable regions A′ and B′ for $\kappa = 0$ are also shown for comparison. It is seen, as one can expect, that the stable regions are enlarged when $\kappa \neq 0$. At the same time, however, the stable regions are shifted. As a consequence, a stable region or a portion of it in the absence of damping lies outside of the stable regions in the presence of damping. In other words, the damping force causes instability in some cases, contrary to intuition. In the regions of stable confinement for $\kappa \neq 0$, except on the boundaries, the particle exhibits a damping oscillation converging to the center of the trap.

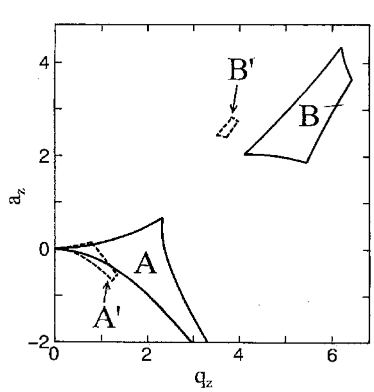

Fig. 1. Stability diagram in the a_z–q_z plane. Two main stable regions A and B for $\kappa = 1.0$ and the corresponding regions A′ and B′ for $\kappa = 0$ are shown

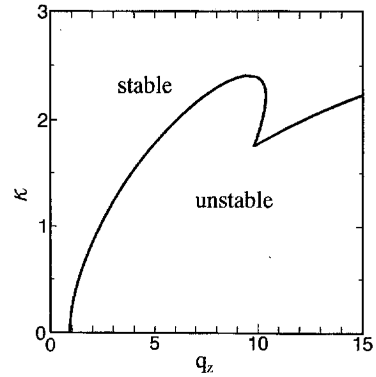

Fig. 2. Stability diagram in the κ–q_z plane when $a_z = 0$

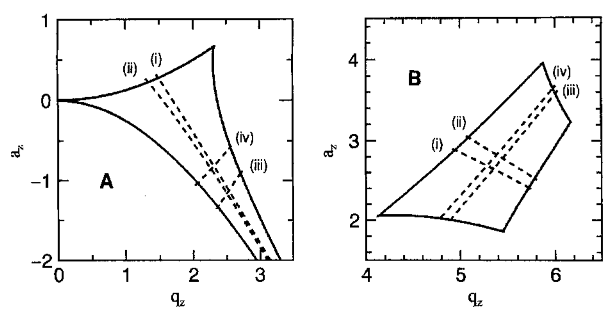

Fig. 3. 3 × 3 subsections of the stable regions A (*left*) and B (*right*) in Fig. 1. *Dashed line* (*i*) is the boundary between Case I ($\beta = 1$) and Case II ($0 \le \beta \le 1$) with respect to the motion in z-direction, and *line* (*ii*) represents that between Case II and Case III ($\beta = 0$) of the same motion. *Lines* (*iii*) and (*iv*) are the corresponding boundaries with respect to the motions in x- and y-directions

On the $a_z = 0$ line in Fig. 1, which means zero-applied dc voltage, the stable range of q_z is extended from $0 < q_z \le 0.91$ for $\kappa = 0$ to $0 < q_z \le 2.4$ for $\kappa = 1.0$. Figure 2 shows the boundary of stability in the $\kappa - q_z$ plane when $a_z = 0$. Note that two stable ranges of q_z appear when κ exceeds 1.75 and they merge into each other when κ exceeds 2.4. This means the linkage of A and B for large values of κ.

The stable regions A and B in Fig. 1 can be divided further into 3 × 3 subsections, as shown in Fig. 3, corresponding to the above-mentioned three cases of $\beta = 1$, $0 \le \beta \le 1$ and $\beta = 0$ for each motion in two orthogonal directions.

2 Approximate formulas of the secular-oscillation frequency and comparison with experiments

As a next step, we derive closed approximate formulas of the secular-oscillation frequency from (18) and compare them with experimental data. Since there is no systematic measurement done in the presence of the damping force, we are concerned with the theoretical formulas in the limiting case of $\kappa = 0$ and compare them with the experiments of Wuerker et al. [1]. However, all the formulas in the following are applicable to the general case if a is replaced by $a - \kappa^2$.

When $\kappa = 0$, the normalized secular-oscillation frequency β in the stable regions is given by

$$\beta = \frac{2}{\pi} \sin^{-1} \left[\Delta(0) \sin^2 \frac{\pi}{2} \sqrt{a} \right]^{1/2}. \tag{20}$$

If the infinite-order matrix in (12) is approximated by the central 3×3 matrix to calculate $\Delta(0)$, we can obtain a formula in which $\sin^2(\pi\beta/2)$ is exact to the first order of a and q^2 as

$$\beta = \frac{2}{\pi} \sin^{-1} \left(\frac{\pi}{2} \sqrt{a + \frac{q^2}{2}} \right). \tag{21}$$

Expansion of the right-hand side of (21) to the lowest-order term leads to the well-known approximate formula

$$\beta = \sqrt{a + \frac{q^2}{2}}, \tag{22}$$

which can be obtained also from the harmonic pseudopotential calculated by averaging the driving force over one cycle of the ac field [1].

By using a recurrence relation for the determinants of the central $(2n+1) \times (2n+1)$ and $(2n+3) \times (2n+3)$ matrices in (12) and putting $n \to \infty$, we obtain a formula in which $\sin^2(\pi\beta/2)$ is exact to the second order of a and q^2 as

$$\beta = \frac{2}{\pi} \sin^{-1} \left[\frac{\pi}{2} \sqrt{a + \frac{q^2}{2} - \frac{\pi^2}{12} a^2 + \left(\frac{25}{128} - \frac{\pi^2}{48} \right) q^4 + \left(\frac{1}{2} - \frac{\pi^2}{12} \right) a q^2} \right]. \tag{23}$$

Wuerker et al. [1] measured the secular-oscillation frequency β in the z-direction (denoted by β_z in [1]) as a function of q_z when the dc voltage was zero, i.e., $a_z = 0$. When $a = 0$, (22), (21) and (23) are reduced to, respectively,

$$\beta^{(1)} = \frac{q}{\sqrt{2}}, \tag{24}$$

$$\beta^{(2)} = \frac{2}{\pi} \sin^{-1} \left(\frac{\pi q}{2\sqrt{2}} \right) \tag{25}$$

and

$$\beta^{(3)} = \frac{2}{\pi} \sin^{-1} \left[\frac{\pi}{2} \sqrt{\frac{q^2}{2} + \left(\frac{25}{128} - \frac{\pi^2}{48} \right) q^4} \right]. \tag{26}$$

The three functions $\beta^{(1)}$, $\beta^{(2)}$ and $\beta^{(3)}$ are plotted in Fig. 4 by the long-dashed, short-dashed and solid line, respectively. The experimental data of Wuerker et al. [1] are shown by circles in the same figure [8]. The known formula $\beta^{(1)}$ agrees with the experiment when q is small but deviates appreciably from it when $q \geq 0.4$, as was also pointed out in [1]. On the other hand, the new formulas $\beta^{(2)}$ and $\beta^{(3)}$ are in good agreement with the experimental data over the whole stable range $0 < q \leq 0.91$.

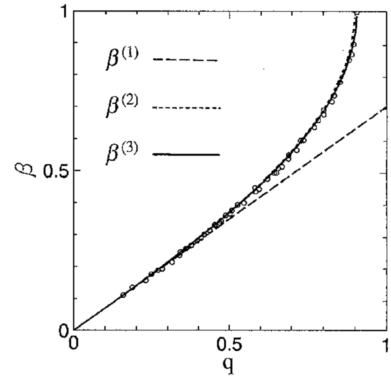

Fig. 4. Theoretical and experimental secular-oscillation frequency β as a function of q when $a = 0$. The theoretical approximate formulas $\beta^{(1)}$, $\beta^{(2)}$ and $\beta^{(3)}$ are given by (24), (25) and (26), respectively, in the text. The experimental data of Wuerker et al. are shown by *circles*

A still higher-order approximate formula than (23) is necessary to calculate β for the other stable region B′ in Fig. 1.

Practically exact numerical values of β can be calculated from (20) by using a determinant of a sufficiently high order in $\Delta(0)$. The difference between the "exact values" and $\beta^{(3)}$ in the range $0 < q \leq 0.91$ is only 0.001 at most.

Another well-known relation $\beta_z = 2\beta_x$ ($= 2\beta_y$) between the secular-oscillation frequencies in two orthogonal directions, when $a_z = 0$, is also an approximate formula. This fact is verified experimentally in Fig. 1 of [1] as a deviation of the $\beta_z = 2\beta_x$ line from the $a_z = 0$ line. We can obtain a more accurate approximate formula from (25) as

$$\sin\left(\frac{\pi \beta_z}{2} \right) = 2 \sin\left(\frac{\pi \beta_x}{2} \right). \tag{27}$$

3 Conclusion

We treated theoretically the dynamics of a single particle in a Paul trap in the presence of the damping force. It was shown that the regions in the a–q plane for stable confinement are not only enlarged but also shifted compared to those for no damping force. In addition, new approximate expressions for the secular-oscillation frequency were obtained and, in the limiting case of no damping, they are in good agreement with the experiments of Wuerker et al. Theoretical studies of the effects of the damping force on a system of two or more particles are in progress.

Acknowledgement. The authors wish to thank A. Hübler for helpful discussions.

References

1. R.F. Wuerker, H. Shelton, R.V. Langmuir: J. Appl. Phys. **30**, 342 (1959)
2. F. Diedrich, E. Peik, J.M. Chen, W. Quint, H. Walther: Phys. Rev. Lett. **59**, 2931 (1987)
3. J. Hoffnagle, R.G. DeVoe, L. Reyna, R.G. Brewer: Phys. Rev. Lett. **61**, 255 (1988)
4. R. Blümel, J.M. Chen, E. Peik, W. Quint, W. Schleich, Y.R. Shen, H. Walther: Nature **334**, 309 (1988)
5. N.W. McLachlan: *Theory and Application of Mathieu Functions* (Dover, New York 1964)
6. A.H. Nayfew, D.T. Mook: *Nonlinear Oscillations* (Wiley, New York 1979) p. 300
7. D.W. Jordan, P. Smith: *Nonlinear Ordinary Differential Equations* (Clarendon, Oxford 1987) p. 257
8. The curve in Fig. 6 of [1] is not a theoretical curve but a smooth line connecting the data points