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Minimized computational time method for the dynamics of ions trapped in an ideal quadrupole ion trap

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ABSTRACT

We present a method based on the series solution of the differential equations to solve numerically the equation of motion of a single ion trapped in an ideal quadrupole ion trap. Every time step, the solution is approximated by a polynomial whose degree and the time step have been optimized to get the minimum computational time with the best accuracy. The initial results were compared to those given by the analytical solution of the Mathieu equation, then the effects of a dipolar and quadrupolar excitation, and the cooling by a buffer gas, presented as a viscous drag, have been added without reference to any analytical solution. The results were compared to chosen examples from the ion trap literature.

1. Introduction

An ideal three-dimensional quadrupole ion trap is made of a ring closed by two end caps. The three electrodes have hyperbolic shape. When a voltage $U_{DC} + V_{RF}\cos(\Omega t)$ is applied to the ring, a time varying quadrupolar potential is created and ions are trapped. The motion of the trapped ions is governed by the Mathieu equation [1]

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

where $u = x, y$ or z, $\tau = (\Omega t)/2$ and a_u, q_u are the Mathieu parameters. Two couples of these parameters are defined; (q_z, a_z) for the direction of the trap's axis z and $(q_{x,y} = -(q_z/2), a_{x,y} = -(a_z/2))$ for the x, y directions. q_z and a_z are given by [1,2]

$$q_z = \frac{8QV_{RF}}{m(r_0^2 + 2z_0^2)\Omega^2}$$
$$a_z = \frac{16QU_{DC}}{m(r_0^2 + 2z_0^2)\Omega^2} \tag{2}$$

where Q is the ion's charge, m its mass, r_0 is the radius of the ring and $2z_0$ is the distance between the end caps.

For an ion to be trapped, its corresponding q_z and a_z must be chosen inside some regions in the q_z–a_z plane. Usually, the lowest domain centered around $a_z = 0$ is used (Fig. 1).

Stable solutions of the Mathieu equation are given by

$$u_a = A\sum_{n=-\infty}^{+\infty} C_{2n}\cos[(\beta_u + 2n)\tau] + B\sum_{n=-\infty}^{+\infty} C_{2n}\sin[(\beta_u + 2n)\tau] \tag{3}$$

β_u and C_{2n} are given by the recursion formula [1]

$$\beta_u^2 = a_u + f(\beta_u) + f(-\beta_u)$$
$$f(\beta_u) = \frac{q_u^2}{(\beta_u + 2)^2 - a_u - (q_u^2)/((\beta_u + 4)^2 - a_u - \cdots)} \tag{4}$$

$$\frac{C_{2n}}{C_{2n\mp 2}} = -\frac{q_u}{(\beta_u + 2n)^2 - a_u - (q_u^2)/((\beta_u + 2n \pm 2)^2 - a_u - \cdots)} \tag{5}$$

One can take $C_0 = 1$ and calculate A and B from the initial conditions.

$\beta_u(\Omega/2)$ is the fundamental frequency. Its maximum value corresponds to $\beta_u = 1$ which has an occurrence when $a_u = 0$ and $q_u \approx 0.908$.

To find the trajectory of a trapped ion, many algorithms have been implemented. One designated MA uses the analytical expression above to calculate the position of the ion at any time [3]. A Simulation Program for Quadrupolar Resonance (SPQR) calculates numerically the ion's positions using the Bulirsch–Stoer method [3]. It has been followed by a more general program called Field Interpolation Method (FIM) [3]. Another program called ITSIM, calculates the ion's trajectory using a Taylor series expansion [4]. A more recent version of ITSIM uses the Runge–Kutta method [5]. A generalized Molecular Dynamics (MD) algorithm has also been used [6] where the verlet algorithm has been adopted to solve the equations of motion. SIMION [7] software is also used for simulating the traps.

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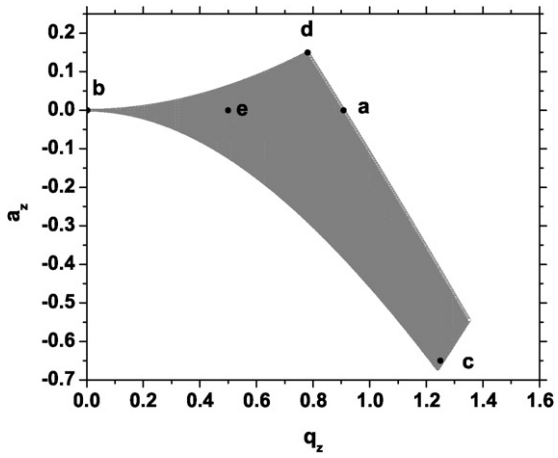

Fig. 1. Lowest stability domain of the three-dimensional quadrupole ion trap.

In the programs, SPQR, FIM and generalized MD, terms higher than the quadrupolar have been included in the trapping potential to simulate not only the ideal trap but also real traps. The other features of the trap such as dipolar or quadrupolar excitations are included in these programs and in ITSIM.

The collisions with the molecules of a buffer gas were included in ITSIM by considering a simple model of damping force. For FIM it is more complicated where the Langevin theory is used.

In this work, we want to calculate the position of a single ion in an ideal Paul trap. We considered a pure quadrupolar potential for the trapping field. Our main objective is to find the trajectory of a single ion for a relatively large time with minimum computational time and good accuracy. We choosed to solve numerically the equation of motion using power series.

2. Series solution of the Mathieu equation

When considering the variable $\xi = \Omega t$, Eq. (1) becomes

$$\frac{d^2u}{d\xi^2} + (a'_u - q'_u \cos\xi)u = 0 \tag{6}$$

with $a'_u = a_u/4$ and $q'_u = q_u/2$. ξ is the phase of the AC component of the trapping field.

We look for the solution $u(\xi)$ as a power series [8]

$$u = \sum_{n=0}^{\infty} a_n(\xi - \xi_0)^n \tag{7}$$

where ξ_0 is an arbitrary constant.

The second derivative is then

$$\frac{d^2u}{d\xi^2} = \sum_{n=0}^{\infty}(n+1)(n+2)a_{n+2}(\xi - \xi_0)^n \tag{8}$$

$\cos(\xi)$ is replaced by its Taylor expansion around ξ_0

$$\cos(\xi) = \sum_{n=0}^{\infty} c_n(\xi - \xi_0)^n \tag{9}$$

with

$$\begin{aligned} c_0 &= \cos(\xi_0) \\ c_1 &= -\sin(\xi_0) \\ c_n &= -\frac{c_{n-2}}{n(n-1)} \quad \text{for} \quad n \geq 2 \end{aligned} \tag{10}$$

Replacing (7)–(9) into Eq. (6), and after minor manipulations one obtains

$$\sum_{n=0}^{\infty}(n+1)(n+2)a_{n+2}(\xi - \xi_0)^n + \sum_{n=0}^{\infty}[a'_u a_n - q'_u \sum_{l=0}^{n} c_l a_{n-l}](\xi - \xi_0)^n = 0 \tag{11}$$

Equating the different powers of $\xi - \xi_0$ gives the recursion relation

$$a_{n+2} = \frac{q'_u \sum_{l=0}^{n} c_l a_{n-l} - a'_u a_n}{(n+1)(n+2)} \tag{12}$$

a_0 and a_1 are determined from the initial conditions

$$\begin{aligned} a_0 &= u(\xi_0) \\ a_1 &= \frac{du}{d\xi}|_{\xi=\xi_0} = \frac{v(t = \xi_0/\Omega)}{\Omega} \end{aligned} \tag{13}$$

where v is the velocity.

When using Eq. (7), one always stops the sum at a certain value n_{max} of n. In that case, u is determined with a good precision only if $\xi - \xi_0$ is not too large. If we want a good precision from $\xi = 0$ to a relatively large value ξ_{max}, the solution is either to use a large value of n_{max} or to divide the interval $[0, \xi_{max}]$ into small intervals of width $\Delta\xi$ and calculate the coefficients a_n for every one of them using the relation (12). a_0 and a_1 are determined from the initial conditions for the first interval and by imposing the continuity of u and its derivative when going from an interval to the next. In this case ξ_0 can be taken equal to $N\Delta\xi$ with N the interval number starting from 0 for the first one. Eq. (7) is then used as

$$u(\xi) = \sum_{n=0}^{n_{max}} a_n^N(\xi - N\Delta\xi)^n \quad \text{for} \quad N\Delta\xi \leq \xi < (N+1)\Delta\xi \tag{14}$$

The upper index N has been used to discriminate between the coefficients of (7) in the different intervals. The initial conditions (13) become

$$\begin{aligned} a_0^0 &= u_0 \\ a_1^0 &= \frac{v_0}{\Omega} \end{aligned} \tag{15}$$

for the first interval, with u_0 the initial position and v_0 the initial velocity. For the other intervals, one uses Eq. (14) and its derivative to get

$$\begin{aligned} a_0^N = \sum_{n=0}^{n_{max}} a_n^{N-1}\Delta\xi^n &= (\cdots(a_{n_{max}}^{N-1}\Delta\xi + a_{n_{max}-1}^{N-1})\Delta\xi + a_{n_{max}-2}^{N-1})\Delta\xi + \cdots + a_1^{N-1})\Delta\xi + a_0^{N-1} \\ a_1^N \sum_{n=1}^{n_{max}} n a_n^{N-1}\Delta\xi^{n-1} &= (\cdots(n_{max}a_{n_{max}}^{N-1}\Delta\xi + (n_{max}-1)a_{n_{max}-1}^{N-1})\Delta\xi + (n_{max}-2)a_{n_{max}-2}^{N-1})\Delta\xi + \cdots + 2a_2^{N-1})\Delta\xi + a_1^{N-1} \end{aligned} \tag{16}$$

For the minimization of the computational time, we start from the observation that the bigger is $\Delta\xi$, the smaller is the number of times we need to calculate the coefficients a_n to approximate the function $u(\xi)$ in the interval $[0, \xi_{max}]$. In fact the number of intervals is the integer closest to $\xi_{max}/\Delta\xi$. Then large values of

$\Delta\xi$ tend to reduce the computational time. But when $\Delta\xi$ is large, we expect that the degree of the polynomial approximating $u(\xi)$ must be high to give a good precision and this tends to increase the computational time. We then looked for a value of $\Delta\xi$ and its corresponding n_{max} giving the minimum computational time for a chosen precision.

2.1. Minimization procedure

We used a C program to optimize for a value of $\xi_{max} = 10^6 \times 2\pi$. This value corresponds to 10^6 periods of the AC trapping field. With the analytical expression (3), we calculated u_a from $t = 0$ to a maximum time $t_{max} = \xi_{max}/\Omega$ with a step $\Delta\xi_0 = (2\pi)/100$, means a time step $\Delta t_0 = 2\pi/(100\Omega)$. In Eq. (3), n was varied from −100 to 100. For many initial conditions we considered an n varying from −200 to 200. There was no difference with the case n from −100 to 100. We took $a_u = 0$ and $q_u = 0.908$. These values of the Mathieu parameters have been chosen because they give $\beta_u \approx 1$ then the position u is the most rapid oscillating function and the degree of the polynomial to use for the approximation must be the highest. The initial velocity of the ion has been taken as 0 to be between the positive and the negative values. The initial position was 0.01 m. For the $N_t = 10^8 + 1$ values of the position u_a, we calculated their corresponding positions u obtained from Eq. (14). To use this last, we divided the total interval $[0, \xi_{max}]$ into small intervals of width $N_i\Delta\xi_0$ with N_i varying from 1 to 50. Means that the analytical expression has been compared to 50 polynomials given by Eq. (14). For every polynomial, we varied n_{max} with a step of 1, starting from 2, until getting the value giving the minimum error. The error has been defined as the root mean square of $u_a - u$ divided by the maximum of u_a

$$\varepsilon_{rel} = \frac{(u_a - u)_{rms}}{\max(u_a)} = \frac{\sqrt{(\sum_{n=0}^{N_t}(u_a(n\Delta t_0) - u(n\Delta\xi_0))^2)/(N_t)}}{\max(u_a(0), u_a(\Delta t_0), \ldots, u_a(N_t\Delta t_0))} \quad (17)$$

Here we notice that when the mean value of $u_a - u$ is 0, $(u_a - u)_{rms}$ is the standard deviation $\sigma(u_a - u)$ of the difference $u_a - u$.

For every value of $\Delta\xi$ (every value of N_i), we looked for the smallest value of n_{max} giving $\varepsilon_{rel} < 5\,\%$ for the conditions described above. We finally get 50 values of N_i and their corresponding n_{max}. They are given in Fig. 2(a).

To estimate the computational time, we see that in the beginning of every interval, we need to calculate $n_{max} - 2$ coefficients a_n using Eq. (12), and a_0 and a_1 from Eq. (16). We neglect the computational time for the first interval where the relation (15) needs to be used for a_0 and a_1. This is true for large values of $\xi_{max}/\Delta\xi$. In Eq. (12) there is $n + 3$ multiplications, $n + 2$ additions, 1 substraction and 1 division. Neglecting the CPU time for the single substraction and the single division and neglecting the computational time for the additions (CPU time for the multiplication is much longer than the one for the addition), we find that calculating the a_n coefficients for n varying from 2 to n_{max}, takes a time proportional to $(n_{max}^2/2) + (3/2)n_{max} - 2$. For the calculation of a_0 we need n_{max} multiplications and n_{max} additions while the calculation of a_1 needs $2n_{max} - 2$ multiplications and $n_{max} - 1$ additions. Here also we neglect the computational time for the additions. The total number of multiplications is then $(n_{max}^2)/2 + (9/2)n_{max} - 4$ to which the computational time is proportional, with our assumptions.

We did not consider the calculation time for the coefficient c_l of the Taylor expansion of the cosine given by Eq. (10). In fact one can always find an integer value N_{cos} such that $N_{cos}\Delta\xi$ is a multiple of 2π. Thus the c_l coefficients will repeat themselves every N_{cos} intervals. They can then be calculated only one time for the first N_{cos} intervals and used in the proper places. The multiplication by q_u' can also be realized when calculating the c_l. The process of placing the c_l in the right places is also time consuming but we did not take this into account.

From the observation we made that the number of times the coefficients need to be calculated is inversely proportional to $\Delta\xi$ we took equal to $N_i\Delta\xi_0$, we arrive to the conclusion that the computational time for the calculation of the coefficients a_n is proportional to

$$T(N_i, n_{max}) = \frac{1}{N_i}\left(\frac{n_{max}^2}{2} + \frac{9}{2}n_{max} - 4\right) \quad (18)$$

This function is shown in Fig. 2(b) for the N_i and their corresponding n_{max} we found. It has a minimum for $Ni = 16$ for which $n_{max} = 11$.

One also needs to calculate the positions using Eq. (14), but if it is found that the optimum $\Delta\xi$ is small enough this is not necessary since the positions are already calculated at the beginning of every interval. That's what we supposed for the following.

We applied the procedure for an upper limit of the error of 10%. For every N_i, n_{max} was either equal or smaller than for the case of 5% maximum error. The minimum for the computational time remains at the same position.

To study the effect of the initial conditions and the Mathieu parameters on the results, we start from the observation that for every N_i we get the same n_{max} as in Fig. 2(a) by considering $\xi_{max} = 10^5 \times 2\pi$ and a maximum error of 0.5%. We used these new conditions to study the effect of a large number of parameters in a reasonable time.

For the initial conditions, we took 2 non zero speeds and 1 equal to zero. For these speeds we considered the positive and the negative directions. That makes 5 velocities. For every nonzero velocity we considered an initial position of 0, 1 mm and 1 cm. For the zero velocity we only considered the 1 mm and 1 cm initial positions.

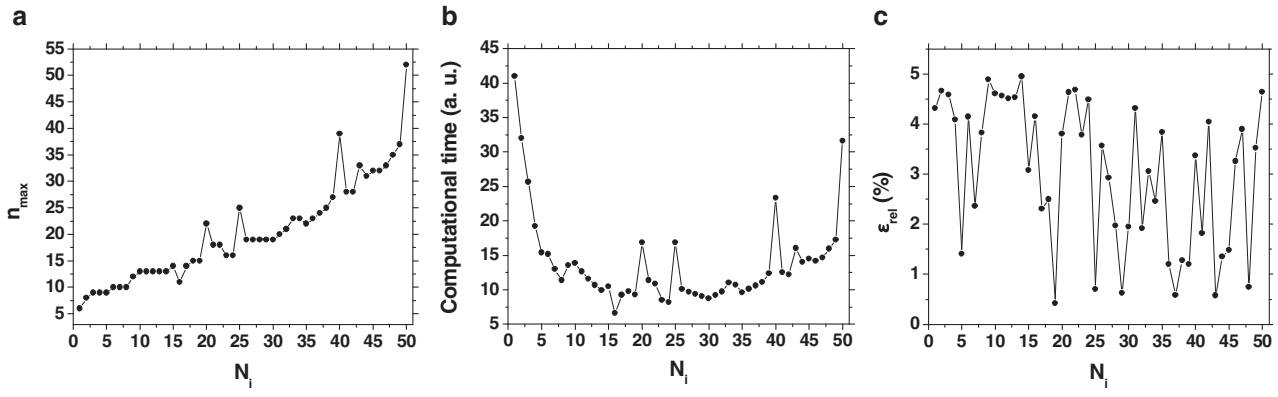

Fig. 2. (a) Minimum value of n_{max} giving an error smaller than 5% as function of N_i. (b) Computational time. (c) Error.

That means that we considered 14 different initial conditions. In our calculations, we represented the initial speeds by temperatures. The initial speed $|v_0|$ is taken

$$|v_0| = \sqrt{\frac{k_B T}{m}} \tag{19}$$

where k_B is the Boltzmann constant and T is the temperature. We see from Eq. (15) that the largest values of a_1^0 are obtained for the highest temperatures, the lowest masses and the lowest frequencies of the AC field. We then took, for the initial speeds, the case T = 10,000 K, m = 1 amu and $f = \Omega/(2\pi)$ = 100 kHz. The second velocity we considered corresponds to T = 0 which gives the speed 0, but may also approximate cases where the ion is very cold, has a big mass or a very high frequency of the trapping field. The third speed corresponds to an intermediate case with T = 300 K, m = 40 amu and f = 1 MHz.

The result is that for every N_i, n_{max} is independent of the initial conditions except for N_i = 31, 33 and 45 where there is a fluctuation of 1 unit.

We again took the initial conditions 0.01 m for the position and 0 for the velocity. We considered 3 other working points (q_u, a_u) = (0.002, 0), (0.5, 0) and (0.7809, 0.1499). This last gives β_u close to 1. For every one of them, we repeated the procedure. We find that, for every N_i the smallest value of n_{max} is obtained for (q_u, a_u) = (0.002, 0), then comes the value for (q_u, a_u) = (0.5, 0). One can then realize a good accuracy for these Mathieu parameters in a relatively small time. The curves of the computational time for (q_u, a_u) = (0.7809, 0.1499) and (0.908, 0) were more overlapping specially for the times close to the minimum. N_i = 16 and its corresponding n_{max} = 11 were giving an error larger than the maximum error. for (q_u, a_u) = (0.7809, 0.1499), N_i = 16 needed a minimum n_{max} of 14. That gives a longer computational time. We then excluded N_i = 16. Fig. 2(b) shows that the remaining minimum corresponds to N_i = 24. Its corresponding error is 4.49%.

We find N_i = 19 more interesting. It gives the minimum error which is more than 10 times smaller than for N_i = 24 and a computational time less than 14% higher. In the following we considered N_i = 19 as the optimum. It corresponds to $\Delta\xi = 0.38\pi$. The corresponding value of n_{max} is 15. N_i = 29, is also interesting. It gives a calculation time smaller than N_i = 19, but has an error 50% larger.

2.2. Test of the method

To test the method, we considered 5 working points (q_z, a_z). 4 of them were at the corners or near the limits of the first stability domain ((q_z, a_z) = (0.908, 0), (0.002, 0), (1.25, −0.65), (0.7809, 0.1499)) and one in the middle ((q_z, a_z) = (0.5, 0)). They are noted a, b, c, d and e in Fig. 1. For each one of them, we took the 14 initial conditions used in the previous paragraph. These cases are not related to any special experimental system. They have been taken to compare between the polynomial solution and the analytical one. With a C program we calculated the positions up to $\xi_{max} = 10^6 \times 2\pi$ with the step $\Delta\xi$ found previously. Both z_a given by the analytical expression (3) and z given by the polynomial (14) were calculated. For all the treated cases, the mean value of the difference $z_a - z$ was very close to 0, then the root mean square of $z_a - z$ was taken equal to the standard deviation of this difference. Eq. (17) was replaced by

$$\varepsilon_{rel} = \frac{\sigma(z_a - z)}{\max(z_a)} \tag{20}$$

For every working point the error was independent of the initial conditions. It was about 0.42% for (q_z, a_z) = (0.908, 0), about 0.043% for (q_z, a_z) = (0.002, 0), about 0.86% for (q_z, a_z) = (1.25, −0.65), about 1.1% for (q_z, a_z) = (0.7809, 0.1499) and about 0.022% for (q_z, a_z) = (0.5, 0). For every working point (q_z, a_z) we chosed one set of initial conditions and calculated z_a and z up to $\xi_{max} = 10^6 \times 2\pi$. The results for ξ close to 0 and to $10^6 \times 2\pi$ are shown in Fig. 3 (a)–(e). These figures show the mean value of $z_a - z$. We observe that in the scales shown, there is no significant difference between z_a and z for the small values of ξ and for the worst cases ((a), (c), (d)) small differences are seen for the large values of ξ.

For the five curves, the evolution of the error as a function of ξ_{max} has been calculated and is given in Fig. 3(f).

To get each one of the 5 curves, a Dell laptop with a processor x86 Family 6 Model 15 Stepping 13 GenuineIntel 1995 MHz, has been used. For the calculation of z, the computational time is about 75 s when the values of ξ and z are saved in the hard disk. It is less than 16 s without saving.

With the same laptop, we used SIMION 7 and simulate a quadrupole ion trap having $r_0^2 = 2z_0^2 = (7\,\text{mm})^2$. We measured the time needed to calculate the evolution of the position of an ion of mass 40 amu starting from the center of the trap. The initial kinetic energy was 1 eV with the motion in the z direction. We considered a trapping field frequency of 1 MHz and a working point (q_z, a_z) = (0.5, 0). We saved the time and the axial position from 0 to 100 ms with a step of 19 μs. Without any plot in the screen, SIMION 7 takes more than 17 min to do the calculation. With our method we had the results in less than 8 s. Knowing that SIMION calculates the 3 components x, y and z of the position, the execution time of our method must be multiplied by 3 to get the comparison. We find that our method is about 60 time faster for the treated case.

3. Resonant excitation

When a small additional alternating voltage (tickle) is applied to the trap, the ions interact with it and the amplitude of their motion and their energy increases if the frequency of the tickle satisfies certain resonance conditions. This excitation can be either dipolar when it is applied between the trap's end caps or quadrupolar when applied between the end caps and the ring. In both cases we considered the additional voltage as

$$V_t = V_{0t} \cos(\omega t) \tag{21}$$

The Taylor expansion of the cosine in terms of $\xi - \xi_0$ is written

$$\cos(\omega t) = \sum_{n=0}^{\infty} ce_n (\xi - \xi_0)^n \tag{22}$$

with

$$\begin{aligned} ce_0 &= \cos(\xi_0) \\ ce_1 &= -\frac{\omega}{\Omega} \sin(\xi_0) \\ ce_n &= -\left(\frac{\omega}{\Omega}\right)^2 \frac{c_{n-2}}{n(n-1)} \quad \text{for} \quad n \geq 2 \end{aligned} \tag{23}$$

3.1. Dipolar excitation

When the tickle is applied between the end caps, the equation of motion (6) for the z direction becomes

$$\frac{d^2 z}{d\xi^2} + (a'_z - q'_z \cos\xi) z - f_t \cos\left(\frac{\omega}{\Omega}\xi\right) = 0 \tag{24}$$

where

$$f_t = \frac{Q V_{0t}}{2 z_0 m \Omega^2} \tag{25}$$

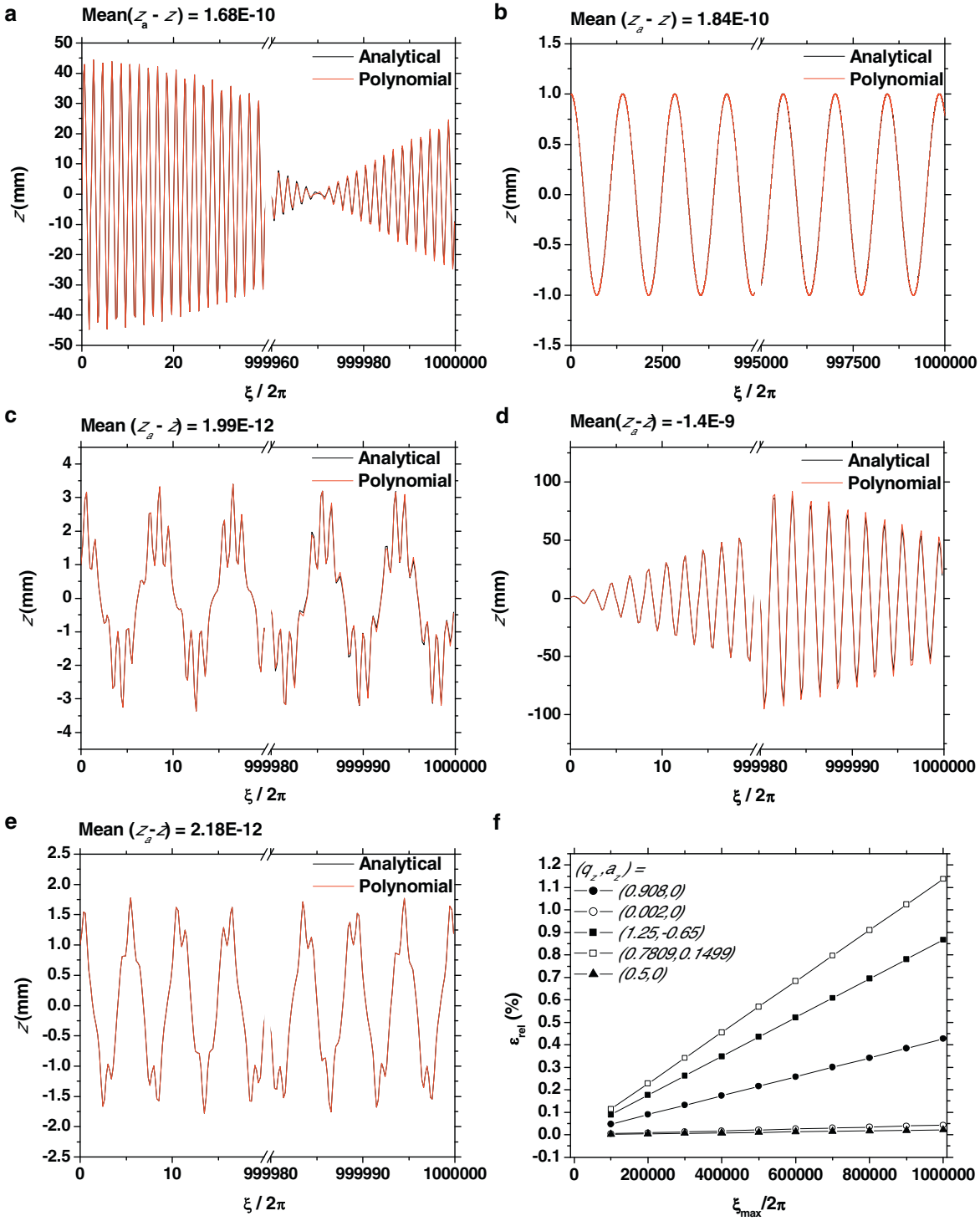

Fig. 3. (a) $(q_z,\ a_z) = (0.908,\ 0)$, $T = 10{,}000$ K, $m = 1$ amu, $f = 100$ kHz. (b) $(q_z, a_z) = (0.002, 0)$, $T = 0$. (c) $(q_z, a_z) = (1.25,\ -0.65)$, $T = 300$ K, $m = 40$ amu, $f = 1$ MHz. (d) $(q_z, a_z) = (0.7809, 0.1499)$, $T = 300$ K, $m = 40$ amu, $f = 1$ MHz. (e) $(q_z, a_z) = (0.5, 0)$, $T = 300$ K, $m = 40$ amu, $f = 1$ MHz. (f) Evolution of the error as function of ξ_{max}.

By taking z in the form given by Eq. (7) and after replacing into Eq. (24), the recursion relation (12) becomes

$$a_{n+2} = \frac{q'_z \sum_{l=0}^{n} c_l a_{n-l} - a'_z a_n + f_t c e_n}{(n+1)(n+2)} \tag{26}$$

This relation together with the continuity Eqs. (16) and (15) is used to find the axial position z as function of ξ.

As an example we considered a singly charged ion of mass 40 amu in a Paul trap with $z_0 = 1$ cm. The trapping field had a frequency of 1 MHz and the Mathieu parameters were $q_z = 0.5$ and $a_z = 0$. The tickle's amplitude was $V_{0t} = 10$ mV and the excitation lasts for 10 ms. The ion started from rest at $z = 1$ mm. The result is shown in Fig. 4.

We then considered excitations with frequencies starting from 0 and ending at 2 MHz with a step of 100 Hz and the same amplitude as before. The trap we considered had the same z_0 than in the previous case and the trapping field the same frequency. For every excitation we considered the ion starting from rest at $z = 0$. The

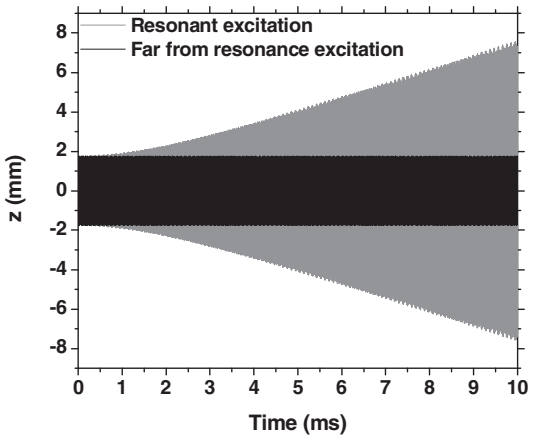

Fig. 4. Resonant and non resonant excitation for the conditions given in the text.

duration of this excitation is 10 ms also. For each tickle frequency, we looked for the maximum value of z the excitation gives to the ion. The calculations were done for two sets of Mathieu parameters; ($q_z = 0.5$, $a_z = 0$) and ($q_z = 0.8$, $a_z = 0.1$). The results are shown in Fig. 5. One can clearly see the fundamental frequencies $\beta_z(\Omega/2)$ and the harmonics $\Omega - \beta_z(\Omega/2)$, $\Omega + \beta_z(\Omega/2)$ and $2\Omega - \beta_z(\Omega/2)$ as given in Eq. (3).

Fig. 5(b) and (d) shows the fundamental frequencies with a 1 Hz step scan. By considering the position of the maximum, one deduces a value of β_z equal to 0.373738 for ($q_z = 0.5$, $a_z = 0$) and $\beta_z = 0.867044$ for ($q_z = 0.8$, $a_z = 0.1$). The theoretical values obtained from Eq. (4) are 0.373744 and 0.867043, respectively.

3.2. Quadrupolar excitation

When the excitation is quadrupolar, the resonance occurs for the ratios of the tickle's frequency to the RF frequency equal to $|n + \beta_u|$ with $-\infty < n < \infty$ [9]. The additional term in the ion's equation of motion is similar to the one due to the RF field provided the replacement of the RF amplitude by V_{0t} and Ω by ω. When using the parameter $\alpha = V_{0t}/V_{RF}$, Eq. (6) becomes

$$\frac{d^2u}{d\xi^2} + \left(a'_u - q'_u \cos\xi - \alpha q'_u \cos\left(\frac{\omega}{\Omega}\xi\right)\right) u = 0 \tag{27}$$

The recursion relation for the coefficients of the solution is then

$$a_{n+2} = \frac{q'_u \sum_{l=0}^{n} (c_l + \alpha c e_l) a_{n-l} - a'_u a_n}{(n+1)(n+2)} \tag{28}$$

We used this relation and similarly to the dipole excitation, we realized a scan of the tickle's frequency with 100 Hz step from 0 to 2 MHz. We looked for the maximum amplitude of z. We took the same conditions for the trap and ion as in the case of the dipole excitation, except for the ion's initial temperature which was taken as 300 K. We considered $\alpha = 10^{-4}$. The results we obtained for 2 sets of the Mathieu parameters are shown in Fig. 6. One can see the resonances at $\beta_z\Omega$, $(1 - \beta_z)\Omega$, $(1 + \beta_z)\Omega$ and $(2 - \beta_z)\Omega$.

4. Buffer gas cooling

The collisions of the trapped ions with a light buffer gas induces the damping of their motion. This effect can be modeled by a viscous drag where the damping force is written $\vec{F} = -(Q/K)\vec{u}$, $\vec{v}$ the ion's

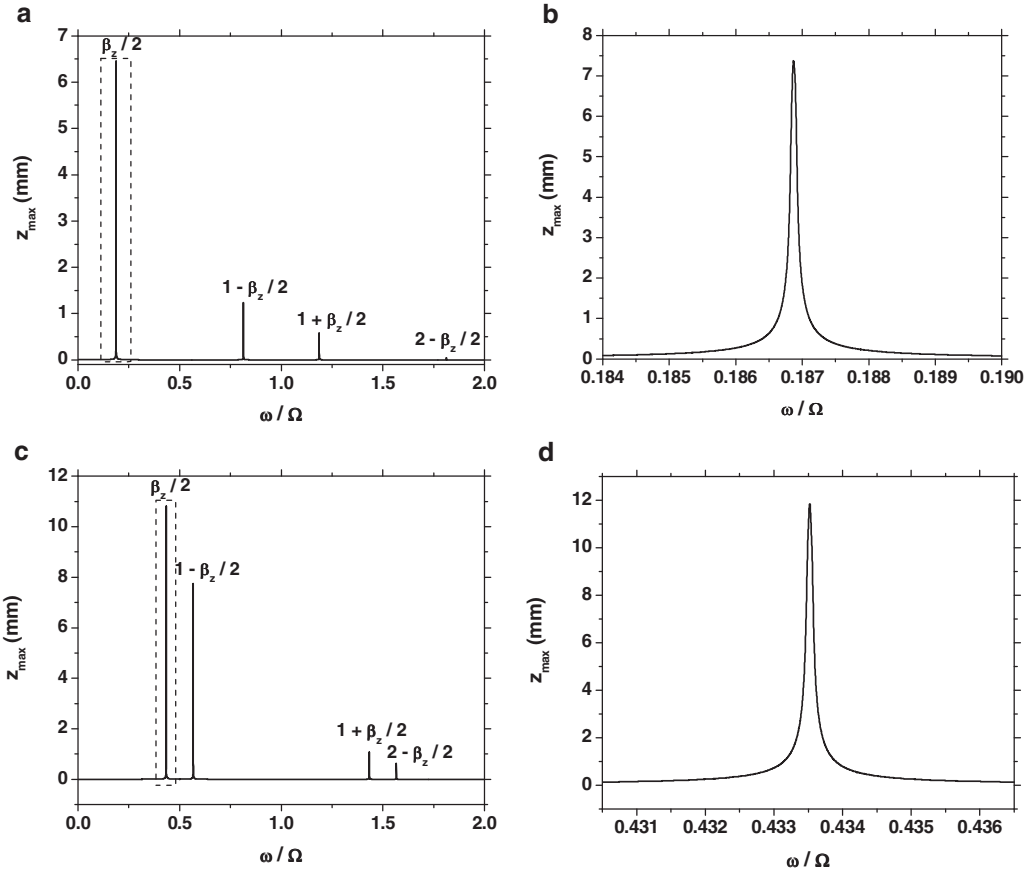

Fig. 5. Dipolar excitation scan (a) ($q_z = 0.5$, $a_z = 0$). (b) 1 Hz step scan around the fundamental frequency. (c) ($q_z = 0.8$, $a_z = 0.1$). (d) 1 Hz step scan around the fundamental frequency.

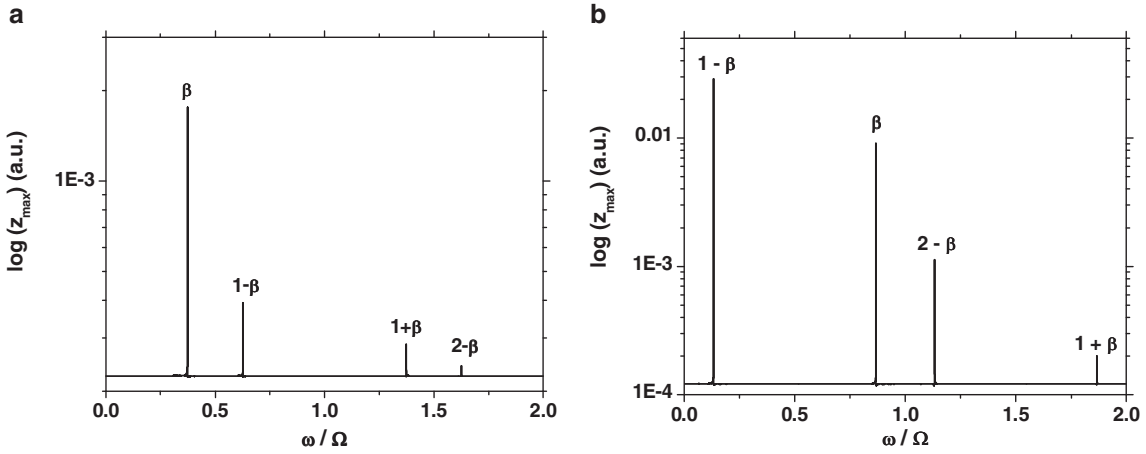

Fig. 6. Quadrupolar excitation scan (a) ($q_z = 0.5$, $a_z = 0$). (b) ($q_z = 0.8$, $a_z = 0.1$).

velocity and K its mobility [10]. This last is usually expressed as

$$K = \frac{760}{p}\frac{T}{273.15}K_0 \tag{29}$$

p being the buffer gas pressure in Torr, T its temperature in K and K_0 the reduced mobility one finds tabulated in the specialized literature.

When taking the damping force into account, the equation of motion (6) becomes

$$\frac{d^2u}{d\xi^2} + \gamma\frac{du}{d\xi} + (a'_u - q'_u\cos\xi)u = 0 \tag{30}$$

with $\gamma = Q/(m\Omega K)$. The recursion relation (12) becomes

$$a_{n+2} = \frac{q'_u\sum_{l=0}^{n} c_l a_{n-l} - a'_u a_n - (n+1)\gamma a_{n+1}}{(n+1)(n+2)} \tag{31}$$

We used this relation to study a case similar to the one given in Refs. [10,11] where the cooling of $133Cs^+$ ions by N_2 molecules was studied. The authors were using a two-dimensional quadrupole ion trap made of 4 parallel rods [1]. The distance between opposite rods was 13.8 mm. In the ideal case, the Mathieu Eq. (1) holds for x and y when z is the trap's axis. They considered the evolution of the position of an ion starting from 10^{-3} mm for 4 different buffer gas pressures and solved numerically the equation of motion.

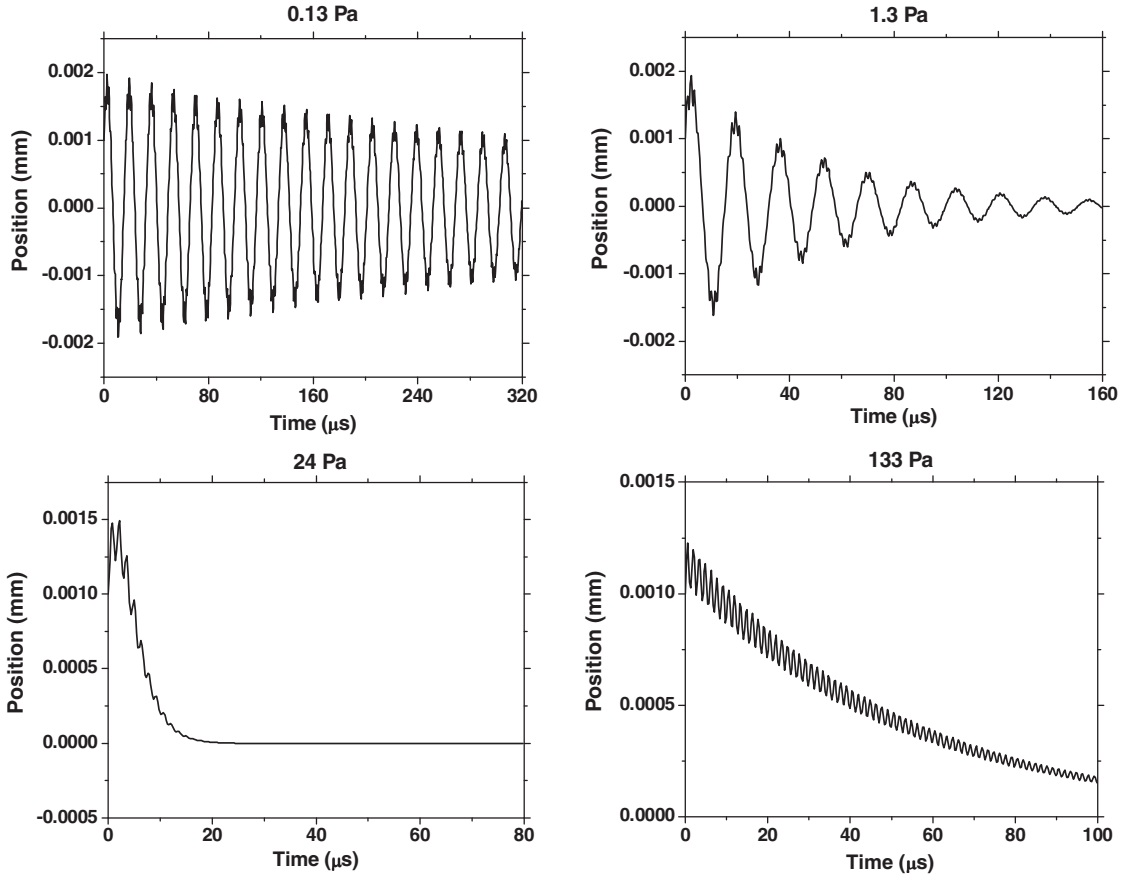

Fig. 7. Trajectories of Cesium ions in nitrogen buffer gas for different pressures.

The trapping field frequency was 700 kHz and the trap's Mathieu parameters were $q_x = 0.236$ and $a_x = 0$. We considered these conditions and an ion's temperature of 0.005 K. We took $K_0 = 2.21\ cm^2/V\,s$ for the reduced mobility from Ref. [12]. This is for a buffer gas temperature of 300 K. The results for the 4 pressures are given in Fig. 7. They look similar to the ones given in Refs. [10,11].

5. Conclusion

We have developed a numerical method for the study of the motion of individual ions trapped in an ideal quadrupole trap. We start from the equation of motion and replace the position by a power series of time. By replacing the analytical functions appearing in the equation of motion by their Taylor expansions we get a recursion relation for the coefficient of the position series. To use the method when the RF phase varies from zero to a maximum value, we divide the total phase interval into small intervals of width 0.38π and approximate the function giving the position by a polynomial of degree 15. These numbers have been chosen by comparing the polynomial solution to the analytical solution of the Mathieu equation and imposing upon the method to get the best accuracy with the minimum computational time. The application of this method to the cases of dipolar and quadrupolar excitation, and to the buffer gas cooling when considered as a damping mechanism inducing on the ion a force proportional to the velocity, gives good agreement with what one finds in the ion trap literature.

In a future development of the method, we can add higher order terms in the trapping potential to simulate real traps [13,14]. The equations of motion for x, y and z will not be independent as for the ideal trap but coupled [13]. They contain z and $r = \sqrt{x^2 + y^2}$ at powers higher than 1 [14]. Three power series of time are needed. One for each direction. One replaces them in the equations of motion, and looks for their recursion relations.

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