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Calculation of secular axial frequencies in a nonlinear ion trap with hexapole, octopole and decapole superpositions by a modified Lindstedt–Poincare method

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ABSTRACT

In this paper the modified Lindstedt–Poincare method is used for calculation of axial secular frequencies of a nonlinear ion trap with hexapole, octopole and decapole superpositions. The motion of the ion in a rapidly oscillating field is transformed to the motion in an effective potential. The equations of ion motion in the effective potential are in the form of a Duffing-like equation. With only octopole superposition the resulted nonlinear equations are symmetric, however, in the presence of hexapole and decapole superpositions, they are asymmetric. For asymmetric oscillators, it has been pointed out that the angular frequency for positive amplitudes is different from the angular frequency for negative amplitudes. Considering this problem, the modified Lindstedt–Poincare method is used for solving the resulted nonlinear equations. As a result, the ion secular frequencies as a function of nonlinear field parameters are obtained. The calculated secular frequencies are compared with the results of some other methods and the exact results. There is an excellent agreement between the results of this paper and the exact results.

1. Introduction

In an ideal ion trap the potential is pure quadrupole and the main properties of the movement of an ion are obtained by the solution of Mathieu equation [1]. In a practical ion trap, however, the electric field distribution deviates from linearity which is the characteristic of a pure quadrupolar trap geometry. This deviation is caused by many different agents such as the truncation of electrodes.

These nonlinear agents superimpose weak multipole fields (e.g., hexapole, octopole, decapole, and higher order fields) and the resulting nonlinear field ion traps exhibit some effects which differ considerably from those of the linear field traps.

The equation governing the motion of the ion in the nonlinear ion trap is the nonlinear Mathieu equation which cannot be solved analytically. The superposition of weak higher multipole fields changes the motions of ions compared to their motions in a pure quadrupole ion trap.

Knowing the secular frequencies of an ion motion in a practical ion trap is crucial for mass spectrometry in connection with, for example, the resonance ejection of the trapped ions from the trap. So, the main purpose of the present work is the calculation of the axial secular frequencies.

Simulation studies [2] have shown that hexapole superposition decreases the secular frequency, positive octopole superposition increases the ion secular frequency and the negative octopole superposition decreases the secular frequency. Experimentally, it has been shown that [3] the octopole and hexapole superposition resulted in a decrease in ion secular frequency.

In a series of papers, Sevugarajan and Menon [4–6] have studied the nonlinear Paul trap. They have applied the Lindstedt–Poincare technique, the modified Lindstedt–Poincare technique and the multiple scales perturbation technique for solving the nonlinear equation of ion motion in nonlinear ion trap. Also, in two previous studies [7,8] done on nonlinear ion traps by one of the present authors, the homotopy perturbation method [9–12] was used to study the secular frequencies in nonlinear ion traps. When the hexapole superposition is considered, the resulting nonlinear equation has a quadratic nonlinearity and we know that the angular frequency for positive amplitudes is different from the angular frequency for negative amplitudes in nonlinear oscillator with

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quadratic nonlinearity. In all the above studies [4–8] it has been assumed that the angular frequency for positive amplitudes is equal to the angular frequency for negative amplitudes.

In studying the quadratic nonlinear oscillator and mixed parity nonlinear oscillator by the method of harmonic balance, Hu [13,14] has used the sign function for incorporating the inequality of angular frequency for negative amplitudes and positive amplitudes. In this paper, we use this technique for studying the asymmetric nonlinear oscillators.

The exact solution for nonlinear equation of an anharmonic oscillator with quadratic nonlinearity and the exact expression for its period have been studied by some authors [15,16]. They have found the exact expression for the period of nonlinear oscillator in terms of complete elliptic integrals. We have used the results of these papers and have calculated the exact frequencies of an anharmonic oscillator with quadratic nonlinearity. The version 7 of mathematica software has been used for calculation of elliptic integrals.

In this paper we use the parameter expanding or modified Lindstedt–Poincare method proposed by He [17–19]. In this technique, a constant, rather than the nonlinear frequency, is expanded in powers of the expanding parameter to avoid the occurrence of secular terms in the perturbation series solution. We consider the first four multipoles of potential distribution inside the ion trap, i.e. quadrapole, hexapole, octopole and decapole terms. The resulting nonlinear equation has quadratic and cubic as well as quartic nonlinearity. Due to the inequality of angular frequency for negative amplitudes and positive amplitudes, we use the sign function for constructing the two auxiliary nonlinear equations. Then, the modified Lindstedt–Poincare method is used for solving the two auxiliary nonlinear differential equations and the ion secular frequencies are calculated. We compare the results of this paper with those obtained by using homotopy perturbation method [7,8] and with the exact results.

The outline of the paper is as follows: In Section 2 the axial equation of ion motion in a nonlinear ion trap is derived. In Section 3 the modified Lindstedt–Poincare method is applied to solve the equation of ion motion in nonlinear ion trap and the results are also given in this section. Finally, the concluding remarks are given in Section 4.

2. The axial equation of ion motion in a nonlinear ion trap

The axial equation of ion motion in the presence of hexapole and octopole superposition has been derived [7,8] before. However, we want to include the decapole superposition here, so we derive once again the equation of ion motion.

A solution of Laplace's equation in spherical polar coordinates $(\rho, \vartheta, \varphi)$ for a system with axial symmetry can be written in the following general form [20]:

$$\phi(\rho, \vartheta, \varphi) = \phi_0 \sum_{n=0}^{\infty} A_n \frac{\rho^n}{r_0^n} P_n(\cos\vartheta) \tag{1}$$

where $\phi_0 = U + V\cos\Omega t$ is the potential applied to the trap (U is a direct current voltage and V is the zero to peak amplitude of the sinusoidal RF voltage), A_n 's are arbitrary dimensionless coefficients, $P_n(\cos\vartheta)$ denotes a Legendre polynomial of order n, and r_0 is a scaling factor (i.e., the internal radius of the ring electrode).

When $\rho^n P_n(\cos\vartheta)$ is expressed in cylindrical polar coordinates (r, z) and the three higher order multipoles, i.e. hexapole, octopole and decapole corresponding to $n = 3$, 4 and 5 along with the quadrupole component corresponding to $n = 2$ are taken into account, the time dependent potential distribution inside the trap takes the form:

$$\phi(r, z, t) = \frac{A_2}{r_0^2} V \cos\Omega t \left[\frac{2z^2 - r^2}{2} + \frac{f_1}{r_0}\left(\frac{2z^3 - 3r^2 z}{2}\right) + \frac{f_2}{r_0^2}\left(\frac{8z^4 - 24z^2r^2 + 3r^4}{8}\right) + \frac{f_3}{r_0^3}\left(\frac{8z^5 - 40z^3r^2 + 15zr^4}{8}\right)\right] \tag{2}$$

where $f_1 = A_3/A_2$, $f_2 = A_4/A_2$ and $f_3 = A_5/A_2$. Here we have assumed the operation of the trap along the $a_u = 0$ axis in the Mathieu stability plot, that is, the DC component of ϕ_0 is equal to zero. The coefficients A_2, A_3, A_4 and A_5 refer to the weight of the quadrupole, hexapole, octopole and decapole superpositions, respectively.

According to classical mechanics [21], the motion of an ion in a rapidly oscillating field such as $\phi(r, z, t)$ (due to the largeness of Ω) can be averaged and transformed to the motion in an effective potential, $U_{eff}(r, z)$, related to $\phi(r, z, t)$ through the following relation:

$$U_{eff}(r, z) = \frac{e}{2m}\left\langle \left| \int \vec{\nabla}\phi(r, z, t)dt \right|^2 \right\rangle \tag{3}$$

Insertion of Eq. (2) for $\phi(r, z, t)$ in Eq. (3) and averaging with respect to time gives the following relation for $U_{eff}(r, z)$,

$$U_{eff}(r, z) = \frac{1}{\lambda}\omega_{0u}^2\left(\frac{m}{e}\right)\left[r^2 + 4z^2 + \frac{f_1^2}{r_0^2}\left(9z^4 + \frac{9}{4}r^4\right) + \frac{12f_1}{r_0}z^3 + \frac{f_2}{r_0^2}(16z^4 - 3r^4 - 12r^2z^2) + \frac{f_3}{r_0^3}\left(20z^5 - 40r^2z^3 - \frac{15}{2}r^4 z\right)\right] \tag{4}$$

where $\lambda = 2$ for $u = r$ (radial direction) and $\lambda = 8$ for $u = z$ (axial direction).

By ignoring the term proportional to f_1^2 compared with the term proportional to f_1 (because $f_1 = A_3/A_2$ is small in comparison to 1), the final form of $U_{eff}(r, z)$ reduces to the following form,

$$U_{eff}(r, z) = \frac{1}{\lambda}\omega_{0u}^2\left(\frac{m}{e}\right)\left[r^2 + 4z^2 + \frac{12f_1}{r_0}z^3 + \frac{f_2}{r_0^2}(16z^4 - 3r^4 - 12r^2z^2) + \frac{f_3}{r_0^3}\left(20z^5 - 40r^2z^3 - \frac{15}{2}r^4 z\right)\right] \tag{5}$$

The classical equation of ion motion in the effective potential $U_{eff}(r, z)$, and with no excitation potential applied to the endcap electrodes is given by:

$$\frac{d^2\vec{r}}{dt^2} + \frac{e}{m}\vec{\nabla}U_{eff}(r, z) = 0 \tag{6}$$

where $\vec{r}$ is the position vector of the ion. Combining equations (5) and (6), we get the equation of motion in the axial (z) direction as:

$$\frac{d^2z}{dt^2} + \omega_{0z}^2 z + \alpha_2' z^2 + \alpha_3' z^3 + \alpha_4' z^4 + \alpha_5' r^2 z + \alpha_6' r^2 z^2 + \alpha_7' r^4 = 0 \tag{7}$$

This is the equation in z direction which is coupled to equation in r direction. Since we are interested in axial secular frequencies, we put $r = 0$ in Eq. (7) and get an equation in axial direction which depends only on z variable:

$$\frac{d^2z}{dt^2} + \omega_{0z}^2 z + \alpha_2' z^2 + \alpha_3' z^3 + \alpha_4' z^4 = 0 \tag{8}$$

where

$$\omega_{0z} = \frac{q_z\Omega}{2\sqrt{2}} \tag{9}$$

$$q_z = \frac{4eV}{mr_0^2\Omega^2} \tag{10}$$

$$\alpha_2' = \frac{9f_1\omega_{0z}^2}{2r_0} \quad (11)$$

$$\alpha_3' = \frac{8f_2\omega_{0z}^2}{r_0^2} \quad (12)$$

$$\alpha_4' = \frac{25f_3\omega_{0z}^2}{2r_0^3} \quad (13)$$

In Eq. (8), by introducing the dimensionless variable x through the relation $x = z/r_0$, and omission of index z from ω_{0z} (for simplicity) we get the equation,

$$\ddot{x} + \omega_0^2 x + \alpha_2 x^2 + \alpha_3 x^3 + \alpha_4 x^4 = 0, \quad x(0) = A, \quad \dot{x}(0) = 0 \quad (14)$$

where $\alpha_2 = (9/2)f_1\omega_0^2$, $\alpha_3 = 8f_2\omega_0^2$ and $\alpha_4 = (25/2)f_3\omega_0^2$.

There are several methods [22–25] that can be used for solution of the nonlinear Eq. (14). In the next section of this article we have used the modified Lindstedt–Poincare method for solving this equation.

3. Application of modified Lindstedt–Poincare method for solution of the axial equation of motion and the results

The nonlinear differential equation $\ddot{x} + \omega_0^2 x + \alpha_2 x^2 + \alpha_3 x^3 + \alpha_4 x^4 = 0$ is the equation of a mixed parity nonlinear oscillator and the amplitudes of oscillations for this oscillator are not the same when $x \geq 0$ and $x \leq 0$. We assume that the positive amplitude is A and the negative amplitude is $-B$ (B is positive). Now we construct the two auxiliary equations by using sign function.

$$\ddot{x} + \omega_0^2 x + \alpha_2 x^2 sgn(x) + \alpha_3 x^3 + \alpha_4 x^4 sgn(x) = 0, \quad x \geq 0, \quad x(0) = A, \quad \dot{x}(0) = 0 \quad (15)$$

$$\ddot{x} + \omega_0^2 x - \alpha_2 x^2 sgn(x) + \alpha_3 x^3 - \alpha_4 x^4 sgn(x) = 0, \quad x \leq 0, \quad x(0) = B \quad \dot{x}(0) = 0 \quad (16)$$

The sign function is defined as:

$$\mathrm{sgn}(x) = \begin{cases} 1, & x > 0 \\ 0, & x = 0 \\ -1, & x < 0 \end{cases} \quad (17)$$

First, we consider the Eq. (15). It is convenient to introduce a small, dimensionless parameter ε which is the order of the amplitude of the motion and can be used as a crutch, or a book keeping device, in obtaining the approximate solution. In modified Lindstedt–Poincare method the solution x and the constant ω_0^2 are expanded in powers of the parameter ε (which is set equal to 1 at last step) as:

$$x = x_0 + \varepsilon x_1 + \varepsilon^2 x_2 + \cdots\cdots \quad (18)$$

$$\omega_0^2 = \omega_A^2 + \varepsilon\omega_{A1} + \varepsilon^2\omega_{A2} + \cdots\cdots \quad (19)$$

Substitution of these equations into Eq. (15), and collecting terms of the same power of ε, gives the following set of equations:

$$\ddot{x}_0 + \omega_A^2 x_0 = 0, \quad x_0(0) = A, \quad \dot{x}_0(0) = 0 \quad (20)$$

$$\ddot{x}_1 + \omega_A^2 x_1 + \omega_{A1} x_0 + \alpha_2 x_0^2 \mathrm{sgn}(x_0) + \alpha_3 x_0^3 + \alpha_4 x_0^4 \mathrm{sgn}(x_0) = 0, \quad x_1(0) = 0, \quad \dot{x}_1(0) = 0 \quad (21)$$

$$\ddot{x}_2 + \omega_A^2 x_2 + \omega_{A2} x_0 + \omega_{A1} x_1 + 2\alpha_2 x_0 x_1 \mathrm{sgn}(x_0) + 3\alpha_3 x_0^2 x_1 + 4\alpha_4 x_0^3 x_1 \mathrm{sgn}(x_0) = 0, \quad x_2(0) = 0, \quad \dot{x}_2(0) = 0 \quad (22)$$

In Eqs. (20)–(22) we have taken into account the following expression [26,27],

$$f(x) = f(x_0 + \varepsilon x_1 + \varepsilon^2 x_2 + \cdots) = f(x_0) + \varepsilon x_1 f'(x_0) + \varepsilon^2 \left[x_2 f'(x_0) + \frac{1}{2}x_1^2 f''(x_0)\right] + O(\varepsilon^3)$$

where $f'(x) = df(x)/dx$ and $d\mathrm{sgn}(x)/dx = d^2\mathrm{sgn}(x)/dx^2 = \cdots = 0$ for $x \neq 0$and $\mathrm{sgn}(x_0 + \varepsilon x_1 + \varepsilon^2 x_2 + \cdots) = \mathrm{sgn}(x_0)$

The first equation of this set can be solved easily, giving the solution $x_0(t) = A\cos\omega_A t$. We substitute $x_0(t)$ into Eq. (21) and expand the terms $x_0^2\mathrm{sgn}(x_0)$ and $x_0^4\mathrm{sgn}(x_0)$ in Fourier series and keep only the first four terms of the expansion of $\mathrm{sgn}(x_0)$. Having no secular term in solution $x_1(t)$, implies:

$$\omega_{A1} = -\frac{8A\alpha_2}{3\pi} - \frac{3A^2\alpha_3}{4} - \frac{32A^3\alpha_4}{15\pi} \quad (23)$$

Insertion of ω_{A1} in Eq. (19), neglecting the terms proportional to ε^2 and highers, and combining with $\varepsilon = 1$ at last step, the approximate amplitude dependent frequency, $\omega_A^{(1)}$, in first order is obtained as:

$$\omega_A = \omega_A^{(1)} = \sqrt{\omega_0^2 + \frac{8A\alpha_2}{3\pi} + \frac{3A^2\alpha_3}{4} + \frac{32A^3\alpha_4}{15\pi}} \quad (24)$$

Finally, insertion of $\alpha_2 = 9/2f_1\omega_0^2$, $\alpha_3 = 8f_2\omega_0^2$ and $\alpha_4 = 25/2f_3\omega_0^2$ in this equation gives the result,

$$\frac{\omega_A}{\omega_0} = \frac{\omega_A^{(1)}}{\omega_0} = \sqrt{1 + \frac{12f_1A}{\pi} + 6f_2A^2 + \frac{80f_3A^3}{3\pi}} \quad (25)$$

In a similar way, for oscillation of ion in negative direction, from Eq. (16) we get the following result for ω_B,

$$\frac{\omega_B}{\omega_0} = \frac{\omega_B^{(1)}}{\omega_0} = \sqrt{1 - \frac{12f_1B}{\pi} + 6f_2B^2 - \frac{80f_3B^3}{3\pi}} \quad (26)$$

Now, we go to second order approximation. ω_{A1}, $x_0(t)$ and the first two terms of the Fourier expansion of $x_0^2\mathrm{sgn}(x_0)$ and $x_0^4\mathrm{sgn}(x_0)$ are inserted in Eq. (21) and it is solved for $x_1(t)$. The final result for $x_1(t)$ is,

$$x_1(t) = A' \cos\omega_A t + B' \cos 3\omega_A t \quad (27)$$

with $A' = -\frac{A^2\alpha_2}{15\pi\omega_A^2} - \frac{A^3\alpha_3}{32\omega_A^2} - \frac{4A^4\alpha_4}{35\pi\omega_A^2}$ and $B' = \frac{A^2\alpha_2}{15\pi\omega_A^2} + \frac{A^3\alpha_3}{32\omega_A^2} + \frac{4A^4\alpha_4}{35\pi\omega_A^2}$

Insertion of ω_{A1} and the solutions for $x_0(t)$ and $x_1(t)$ in Eq. (22), and implication for having no secular term in $x_2(t)$, gives the value of ω_{A2} as:

$$\omega_{A2} = \frac{8A^2\alpha_2^2}{75\pi^2\omega_A^2} + \frac{3A^4\alpha_3^2}{128\omega_A^2} + \frac{384A^6\alpha_4^2}{1225\pi^2\omega_A^2} + \frac{A^3\alpha_2\alpha_3}{10\pi\omega_A^2} + \frac{64A^4\alpha_2\alpha_4}{175\pi^2\omega_A^2} + \frac{6A^5\alpha_3\alpha_4}{35\pi\omega_A^2} \quad (28)$$

Insertion of calculated expressions for ω_{A1} and ω_{A2} in Eq. (19) along with $\varepsilon = 1$ and using the values of $\alpha_2 = 9/2f_1\omega_0^2$, $\alpha_3 = 8f_2\omega_0^2$ and $\alpha_4 = 25/2f_3\omega_0^2$ gives the final result for $\omega_A^{(2)}$, the second order approximate frequency and T_{A2}, the second order approximate period, in positive direction:

$$\frac{\omega_A}{\omega_0} = \frac{\omega_A^{(2)}}{\omega_0} = \frac{1}{\sqrt{210\pi}}\sqrt{L_A + \sqrt{S_A}}, \qquad T_{A2} = \frac{2\pi}{\omega_A^{(2)}} \quad (29)$$

where

$$L_A = 105\pi + 70A(18f_1 + A(40Af_3 + 9\pi f_2)) \quad (30)$$

and

$$S_A = 8A^2(186543f_1^2 + 768600A^2 f_1 f_3 + 710000A^4 f_3^2) + A(63f_1(5+27f_2A^2) + 100A^2(7+33f_2A^2)f_3)\pi + 11025(1+6f_2A^2(2+5f_2A^2))\pi^2 \quad (31)$$

In a similar way, for oscillation of ion in negative direction from Eq. (22) we get:

$$\frac{\omega_B}{\omega_0} = \frac{\omega_B^{(2)}}{\omega_0} = \frac{1}{\sqrt{210\pi}}\sqrt{L_B + \sqrt{S_B}}, \qquad T_{B2} = \frac{2\pi}{\omega_B^{(2)}} \quad (32)$$

where,

$$L_B = 105\pi - 70B(18f_1 + B(40Bf_3 - 9\pi f_2)) \quad (33)$$

and

$$S_B = 8B^2(186543f_1^2 + 768600B^2 f_1 f_3 + 710000B^4 f_3^2) - 840B(63f_1(5+27f_2B^2) + 100B^2(7+33f_2B^2)f_3)\pi + 11025(1+6f_2B^2(2+5f_2B^2))\pi^2 \quad (34)$$

In these relations A is the positive amplitude and is equal to maximum value for x and x_{max} can be obtained by using the relation $z_0/r_0 = 1/\sqrt{2}$ for ion trap and inserting z_0 for z in equation $x = z/r_0$ gives $A = 1/\sqrt{2}$. As mentioned earlier, the amplitude in negative direction, B, is different from A and can be calculated in terms of A. For calculation of B, the both side of Eq. (14) is multiplied by $\dot{x}$ and then integrated [14], giving the result,

$$\frac{1}{2}\dot{x}^2 + \frac{1}{2}\omega_0^2 x^2 + \frac{1}{3}\alpha_2 x^3 + \frac{1}{4}\alpha_3 x^4 + \frac{1}{5}\alpha_4 x^5 = C \quad (35)$$

where C is the constant of integration. Insertion of initial conditions in Eq. (35) gives the result,

$$\frac{1}{2}\omega_0^2 A^2 + \frac{1}{3}\alpha_2 A^3 + \frac{1}{4}\alpha_3 A^4 + \frac{1}{5}\alpha_4 A^5 = \frac{1}{2}\omega_0^2 B^2 - \frac{1}{3}\alpha_2 B^3 + \frac{1}{4}\alpha_3 B^4 - \frac{1}{5}\alpha_4 B^5 \quad (36)$$

Using version 7 of mathematica software, this equation can be solved analytically and B is calculated in terms of A.

It is clear that the second order approximate period is:

$$T_2 = \frac{T_{A2} + T_{B2}}{2} \quad (37)$$

So, the second order approximate secular frequency is:

$$\frac{\omega_2}{\omega_0} = \frac{2\pi}{T_2} = \frac{2}{\sqrt{210\pi}}\left(\frac{1}{\sqrt{L_A + \sqrt{S_A}}} + \frac{1}{\sqrt{L_B + \sqrt{S_B}}}\right)^{-1} \quad (38)$$

The perturbed secular frequencies can be calculated through the relation (38) as a function of field aberrations (parameters f_1, f_2 and f_3).

The values of ω/ω_0 for different values of f_1, f_2 and f_3 are given in Tables 1–4 and for comparison purposes the values of ω/ω_0 in homotopy perturbation approximation [7,8] are also given in the tables.

For a nonlinear oscillator with only a quadratic term as a nonlinearity ($\alpha_2 \neq 0$ and $\alpha_3 = \alpha_4 = 0$), the exact values of frequencies are available in the literature [15,16] and are given in terms of complete elliptic integrals (relation No. (46) of Ref. [16]). Mathematica software has been used for calculation of numerical values of elliptic integrals and finding the roots of cubic polynomial equations. For a nonlinear oscillator with mixed parity ($\alpha_2 \neq 0$, $\alpha_3 \neq 0$,

Table 1
Comparison of the calculated values of ω_2/ω_0 in this paper for only hexapole superposition with the values obtained by homotopy method [7,8] and the exact values.

f_1	B	ω_{2HPM}/ω_0	ω_2/ω_0	ω_{ex}/ω_0
0.01	0.722439	0.99958	0.999568	0.999569
0.05	0.792221	0.98916	0.987913	0.987926
0.10	0.913755	0.95235	0.939082	0.939193
0.11	0.947125	0.94052	0.921043	0.921214
0.12	0.986189	0.92654	0.897928	0.898204
0.13	1.03385	0.90979	0.867083	0.867561
0.14	1.09633	0.88933	0.822454	0.823418
0.15	1.19283	0.86329	0.742729	0.745686
0.155	1.28435	0.847030	0.644365	0.655595
0.1565	1.3404	0.841545	0.527906	0.582921

Table 2
Comparison of the calculated values of ω_2/ω_0 in this paper for only octopole superposition with the values obtained by homotopy method [7,8] and the exact values.

ω_{ex}/ω_0	ω_2/ω_0	ω_{2HPM}/ω_0	f_2
0.01	1.01491	1.01487	1.01487
0.05	1.0727	1.072	1.072
0.10	1.1414	1.1389	1.1389
0.15	1.2065	1.20173	1.2017
0.20	1.2682	1.2612	1.2612
0.25	1.3279	1.31776	1.3177
0.30	1.3849	1.37188	1.372
0.40	1.4923	1.4739	1.4739
0.50	1.5928	1.56905	1.569
−0.01	0.98490	0.984866	0.98487
−0.05	0.92255	0.921355	0.92136
−0.10	0.83983	0.833427	0.83343
−0.15	0.75162	0.730894	0.73099
−0.20	0.65918	0.598426	0.59968

Table 3
Comparison of the calculated values of ω_2/ω_0 in this paper for hexapole and octopole superpositions with the values obtained by homotopy method [7,8] and the exact values.

ω_{ex}/ω_0	ω_2/ω_0	ω_{2HPM}/ω_0	B	f_2	f_1
0.01	0.01	0.721825	1.0145	1.01478	1.01478
0.05	0.05	0.775049	1.06405	1.07113	1.07113
0.10	0.10	0.829421	1.11117	1.13924	1.13922
0.15	0.15	0.872078	1.1453	1.20693	1.20689
0.20	0.20	0.905442	1.16768	1.27422	1.27412
0.25	0.25	0.931747	1.17753	1.34054	1.3404
0.12	0.30	0.794033	1.36112	1.39889	1.39888
0.05	−0.05	0.824202	0.90861	0.883152	0.883223
0.07	−0.07	0.979204	0.858107	0.697807	0.700873
0.01	−0.10	0.733768	0.839123	0.824691	0.824691

Table 4
Comparison of the calculated values of ω_2/ω_0 in this paper for hexapole, octopole and decapole superpositions with the values obtained by homotopy method [7,8] and the exact values.

ω_{ex}/ω_0	ω_2/ω_0	ω_{2HPM}/ω_0	B	f_3	f_2	f_1
0.01	0.01	0.01	0.73513	1.01376	1.01302	1.01302
0.02	0.02	0.02	0.76452	1.02522	1.02192	1.02191
0.10	0.10	0.06	0.966336	1.0887	1.03603	1.03584
0.05	0.05	0.03	0.823497	1.05813	1.04941	1.0494
0.07	0.08	0.05	0.885144	1.08355	1.0603	1.06025
0.15	0.20	0.10	1.07527	1.16533	1.0811	1.08014
0.12	0.15	0.04	0.894785	1.16097	1.178	1.17802
0.14	0.30	0.12	0.949597	1.30046	1.31768	1.31774
0.13	0.40	0.16	0.92592	1.39876	1.43654	1.43667
0.03	−0.05	0.02	0.825353	0.908382	0.869339	0.869302
0.05	−0.01	0.04	0.935453	0.959367	0.844862	0.844401
0.01	−0.10	0.01	0.761675	0.837824	0.808704	0.808711
0.02	−0.08	0.03	0.89998	0.860218	0.702734	0.69135

$\alpha_4 \neq 0$), the exact values of frequencies can be calculated [28] by the integral,

$$\frac{\omega_{ex}}{\omega_0} = 2\pi\left(\int_0^A \frac{2dx}{\sqrt{A^2 - x^2 + 3f_1(A^3 - x^3) + 4f_2(A^4 - x^4) + 5f_3(A^5 - x^5)}} + \int_0^B \frac{2dx}{\sqrt{B^2 - x^2 - 3f_2(B^3 - x^3) + 4f_2(B^4 - x^4) - 5f_3(B^5 - x^5)}}\right)^{-1} \quad (39)$$

This integral is evaluated numerically by mathematica for ω_{ex}/ω_0, the exact values of frequencies.

In Table 1, it has been assumed that only the hexapole superposition exist and the other multipoles are absent. So, the exact values of secular frequencies (ω_{ex}/ω_0) for different values of f_1 ($f_2 = f_3 = 0$) are compared with the results of this paper (ω_2/ω_0) for second order approximation and the results of homotopy perturbation approximation obtained in references [7] and [8].

In Table 2, we have considered only the octopole superposition. In this table, the exact values of secular frequencies (ω_{ex}/ω_0) for different values of f_2 ($f_1 = f_3 = 0$) are compared with the results of this paper (ω_2/ω_0) for second order approximation and the results of homotopy perturbation approximation obtained in references [7] and [8].

In Table 3, the hexapole and octopole superpositions are considered and the exact values of secular frequencies (ω_{ex}/ω_0) for different values of f_1 and f_2 ($f_3 = 0$) are compared with the results of this paper (ω_2/ω_0) for second order approximation and the results of homotopy perturbation approximation obtained in Refs. [7,8].

Finally, in Table 4, the hexapole, octopole, and decapole superpositions are considered and the exact values of secular frequencies (ω_{ex}/ω_0) for different values of f_1, f_2 and f_3 are compared with the results of this paper (ω_2/ω_0) for second order approximation and the results of homotopy perturbation approximation obtained in references Refs. [7,8].

As is seen in Tables 1–4, the results of this paper are in excellent agreement with the exact results.

4. Conclusion

In this paper we have derived the equation of ion motion in axial direction of a nonlinear ion trap. The nonlinear ion trap is generated by superposition of weak multipole fields on the pure quadrupole field. Hexapole, octopole, and decapole field superpositions are considered. The computed axial equation of ion motion is a nonlinear equation with quadratic, qubic and quartic nonlinearity. We have used the modified Lindstedt–Poincare method for solution of the resulted equation and calculation of the axial secular frequencies of the ions in the trap. The results of this paper are compared with the exact results and the results of the homotopy perturbation method. There is an excellent agreement between the results of this paper and the exact results.

References

[1] N.W. McLachlan, Ordinary Non-linear Differential Equations in Engineering and Physical Sciences, Oxford University Press, UK, 1958.
[2] J. Franzen, Int. J. Mass Spectrom. Ion Process 125 (1993) 165.
[3] M. Nappi, V. Frankevich, M. Soni, R.G. Cooks, Int. J. Mass Spectrom. Ion Process 177 (1998) 91.
[4] S. Sevugarajan, A.G. Menon, Int. J. Mass Spectrom. 189 (1999) 53.
[5] S. Sevugarajan, A.G. Menon, Int. J. Mass Spectrom. 197 (2000) 263.
[6] S. Sevugarajan, A.G. Menon, Int. J. Mass Spectrom. 209 (2001) 209.
[7] A. Doroudi, Phys. Rev. E 80 (2009) 056603–56611.
[8] A. Doroudi, Int. J. Mass Spectrom. 296 (2010) 43.
[9] J.H. He, Phys. Lett. A 350 (2006) 87.
[10] J.H. He, Phys. Lett. A 347 (2005) 228.
[11] J.H. He, Chaos Soliton Fractals 26 (2005) 695.
[12] J.H. He, Appl. Math. Comput. 156 (2004) 591.
[13] H. Hu, J. Sound Vib. 293 (2006) 462.
[14] H. Hu, J. Sound Vib. 299 (2007) 331.
[15] B.F. Apostol, J. Theor. Phys. 86 (2003) 1.
[16] P. Amore, F.M. Fernandez, Eur. J. Phys. 26 (2005) 589.
[17] J.H. He, Int. J. Nonlin. Mech. 37 (2002) 309.
[18] J.H. He, Int. J. Nonlin. Mech. 37 (2002) 315.
[19] J.H. He, Int. J. Mod. Phys. B 20 (2006) 1141.
[20] J.D. Jackson, Classical Electrodynamics, John Wiley & Sons Inc, 1999.
[21] L.D. Landau, E.M. Lifshitz, Mechanics, Reed Publishing Ltd, 1981.
[22] A.H. Nayfeh, Problems in Perturbations, Wiley, New York, 1985.
[23] A.H. Nayfeh, D.T. Mook, Non-linear Oscillations, John Wiley and Sons, Inc, New York, 1995.
[24] D.D. Ganji, H. Seyed, Hashemi Kachapi, Prog. Nonlin. Sci. 2 (2011) 1.
[25] D.D. Ganji, H. Seyed, Hashemi Kachapi, Prog. Nonlin. Sci. 3 (2011) 1.
[26] P. Amore, A. Aranda, J. Sound Vib. 283 (2005) 1115.
[27] A. Belendez, T. Belendez, A. Marquez, C. Neipp, Chaos. Solitons Fractals 37 (2008) 770.
[28] A.Y.T. Leung, Z. Guo, J. Sound Vib. 325 (2009) 287.