Calculation of coupled secular oscillation frequencies and axial secular frequency in a nonlinear ion trap by a homotopy method

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In this paper the homotopy perturbation method is used for calculation of the frequencies of the coupled secular oscillations and axial secular frequencies of a nonlinear ion trap. 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. The homotopy perturbation method is used for solving the resulted system of coupled nonlinear differential equations and the resulted axial equation for obtaining the expressions for ion secular frequencies as a function of nonlinear field parameters and amplitudes of oscillations. The calculated axial secular frequencies are compared with the results of Lindstedt-Poincare method and the exact results.

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I. INTRODUCTION

The radio frequency (rf) quadrupole ion trap has three rotationally symmetrical hyperbolic electrodes. The ion trajectories in a trap with perfect rotational symmetry around the axial (z) direction and radial (r) direction can be derived analytically from the well-known Mathieu differential equation [1]. In an ideal ion trap the potential is pure quadrupole and the main properties of the movement of an ion which are obtained by the solution of Mathieu equation are as follows [2,3]:

(i) The movement in the axial (z) direction is completely decoupled from that in the perpendicular radial (r) direction due to the absence of "ross terms" of the form rz in the expression for the quadrupole potential.

(ii) The rf field amplitude varies in a linear manner with distance from the center in the r and z directions of the cylindrical coordinates and has only one parameter describing the periodicity.

(iii) The stability of ion trajectories of a given mass/charge ratio in an infinitely large quadrupole field does not depend on their initial starting conditions (position and velocity).

(iv) Only the two mass-related trapping parameters a and q of the dc and rf fields, respectively, determine whether the solution for the ion movement is stable or not?

(v) If the parameters a and q are kept inside the stability region of the stability diagram, in the absence of any auxiliary ac potentials applied the end-cap electrodes, the ions perform stable secular oscillations in the r and z directions with frequencies lower than half that of the driving voltage applied to the ion trap.

(vi) The frequency of the secular oscillation of an ion is independent of its displacement from the center.

In a practical ion trap the electric field distribution, deviates from linearity which is the characteristic of a pure quadrupolar trap geometry. This deviation is caused by misalignments, nonhyperbolic shapes, truncated electrodes, perforation in the electrodes, space charge potential of a large ion cloud [4], additional dipolar excitation potential [4,5] and collisions with the trap. These nonlinear agents superimpose weak multipole fields (e.g., hexapole, octapole, and higher-order fields) and the resulting nonlinear field ion traps exhibit some effects which differ considerably from those of the linear field traps [2,3]:

(i) The components of the rf field amplitude arising from the higher-order multipoles are nonlinear in the r and z directions of the cylindrical coordinates.

(ii) For multipoles higher than or equal to hexapoles, the secular frequencies of oscillation are no longer constant for constant field parameters, they now become amplitude dependent.

(iii) The ion trajectories in the r and z directions become amplitude dependent and are now coupled because of the existence of cross terms of the form rz in the expressions for the higher-order multipole potentials.

(iv) Several types of nonlinear resonance conditions exist for each type of multipole superposition, forming resonance lines within the stability region of the stability diagram. These are the nonlinear resonances that were first detected by Von Busch and Paul [6].

(v) Contrary to many experimental observations, the trajectories of ions with nonlinear resonances do not always exhibit instability. They take up energy from the rf drive field and thus increase their secular oscillation amplitude. Because of the amplitude dependence of the secular frequency, this frequency now drifts out of resonance, resulting in a kind of beat motion.

The equations governing the motion of the ion in the nonlinear ion trap are the nonlinear Mathieu type equations which cannot be solved analytically. Many simulation studies [7–10] and experimental studies [11,12] have been done on the effects of nonlinear terms in the nonlinear equation of motion. The superposition of weak higher multipole fields, not only slightly change the ion motion compared to their motion in pure quadrupole ion traps, it is the nonlinear resonances and other nonlinear effects which dramatically and

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qualitatively change the oscillation of ions in nonlinear traps.

Simulation studies have shown that the higher-order terms in the electric field make the ion secular frequency to shift with respect to the value $\omega_u=\beta_u\Omega/2(u=r\ or\ z)$. ω_u is the ion secular frequency in the radial and axial directions, Ω is the rf drive frequency applied to the central ring electrode and β_u is a function of Mathieu parameters a_u and q_u which can be calculated using continuous fraction relationship between these values [2,13]. For q_u values less than 0.4, β_u can be computed from Dehmelt approximation [2,13].

Simulation studies [14] have shown that hexapole superposition decreases the axial secular frequency, positive octopole superposition increases the ion axial secular frequency and the negative octopole superposition decreases the axial secular frequency. Experimentally, it has been shown that [15] the octopole and hexapole superposition resulted in a decrease in ion secular frequency. Sevugarajan and his coworker [16] have found the equation of motion of the ion in axial (z) direction in the form of the Duffing equation and have applied the Lindstedt-Poincare technique for solving the resulting nonlinear equation and have obtained the secular frequency shift as a function of the strength of hexapole and octopole superposition. They have also studied coupled secular oscillations in nonlinear Paul trap using multiple scales method [17].

In this paper we use the homotopy perturbation method for studying nonlinear ion traps. We apply this method to solve the system of coupled nonlinear differential equations and also the Duffing-like equation of the axial direction and calculate the ion secular frequencies. We compare the results of this paper for the axial direction with those obtained by using Lindstedt-Poincare technique [16] and with the exact results.

The outline of the paper is as follows: in Sec. II the homotopy method is introduced. In Sec. III the equations of ion motion in a nonlinear ion trap are derived. In part A of Sec. IV the homotopy perturbation method is applied to solve the system of coupled nonlinear differential equations of ion motion in nonlinear ion trap. In part B of this section, the same method is used for solving the Duffing-like equation of the axial direction and the results are shown. Finally, the concluding remarks are given in Sec. V.

II. HOMOTOPY METHOD

The perturbation techniques which are usually considered in advanced courses of classical mechanics [18,19] are the Lindstedt-Poincare and the alternative Lindstedt-Poincare methods which are widely used for solution of nonlinear differential equations [20–23]. The standard Lindstedt-Poincare method is applicable to equations like $\frac{d^2x}{dt^2}+\omega_0^2x+\varepsilon f(x)=0$ which has a linear term (ω_0^2x) and a small perturbation parameter (ε). This method cannot be applied to a system with a nonlinear differential equation without linear term or without small parameter. In homotopy perturbation method [24–28] one does not need a linear term and small parameter. This method provides an approach to introducing an expanding parameter and a linear term. The homotopy perturbation method can solve various nonlinear equations.

For illustrating the basic idea of this method, we consider the following nonlinear differential equation,

$$A(u)-f(\vec{r})=0 \quad \vec{r}\in\Omega, \tag{1}$$

$$\text{with boundary conditions:} B\left(u,\frac{\partial u}{\partial n}\right)=0 \quad \vec{r}\in\Gamma, \tag{2}$$

where A is a general differential operator, B is a boundary operator, $f(\vec{r})$ is a known analytic function, and Γ is the boundary of the domain Ω. We suppose the operator A can be divided into two linear part (L) and nonlinear part (N). Then the Eq. (1) can be written as

$$L(u)+N(u)-f(\vec{r})=0. \tag{3}$$

By the homotopy technique, we construct a homotopy $v(\vec{r},p):\Omega\times[0,1]\rightarrow\Re$ which satisfies

$$\mathrm{H}(v,p)=(1-p)[L(u)-L(u_0)]+p[A(v)-f(\vec{r})]=0 \tag{4a}$$

or

$$\mathrm{H}(v,p)=L(v)-L(u_0)+pL(u_0)+p[N(v)-f(\vec{r})]=0 \tag{4b}$$

Where $p\in[0,1]$ is an embedding parameter, u_0 is an initial approximation of Eq. (1) which satisfies the boundary conditions.

From Eq. (4a) or (4b) we have

$$\mathrm{H}(v,0)=L(v)-L(u_0)=0 \tag{5}$$

and

$$\mathrm{H}(v,1)=A(v)-f(\vec{r})=0 \tag{6}$$

It is clear that when $p=0$, Eqs. (4a) or (4b) becomes a linear equation; and when $p=1$ it transforms to the original nonlinear equation. So the changing of p from zero to one is just that of $L(v)-L(u_0)=0$ to $A(v)-f(\vec{r})=0$.

The embedding parameter p monotonically increases from 0 to 1 as the trivial problem $L(v)-L(u_0)=0$ is continuously deformed to the problem $A(v)-f(\vec{r})=0$ The basic idea of the homotopy method is that continuously deform a simple problem easy to solve into the difficult problem to be solved. The basic assumption is that the solution of Eqs. (4a) or (4b) can be written as a power series in p,

$$v=v_0+pv_1+p^2v_2+\cdots \tag{7}$$

Setting $p=1$ results in the approximate solution of Eq. (1),

$$u=\lim_{p\rightarrow 1} v=v_0+v_1+v_2+\cdots \tag{8}$$

This method, although, has eliminated limitations of the traditional perturbation methods, it can take full advantages of the traditional perturbation techniques and can be used for solving various strongly nonlinear equations.

III. EQUATIONS OF ION MOTION IN A NONLINEAR ION TRAP

A solution of Laplace's equation in spherical polar coordinates (ρ,ϑ,φ) for a system with axial symmetry can be written in the following general form [29]:

$$\phi(\rho,\vartheta,\varphi) = \phi_0 \sum_{n=0}^{\infty} A_n \frac{\rho^n}{r_0^n} P_n(\cos\vartheta), \tag{9}$$

where $\phi_0 = U + V\cos\Omega t$ is the sinusoidal rf field applied to the trap, 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 two higher-order multipoles, hexapole, and octopole corresponding to $n=3$ and $n=4$, along with the quadrupole component corresponding to $n=2$ are taken into account, the time dependent potential distribution inside the trap takes the form

$$\phi(r,z,t) = \frac{A_2}{r_0^2} V\cos\Omega t\left[\frac{2z^2 - r^2}{2} + \frac{f_1}{r_0}\left(\frac{2z^3 - 3r^2 z}{2}\right) + \frac{f_2}{r_0^2}\left(\frac{8z^4 - 24z^2r^2 + 3r^4}{8}\right)\right] \tag{10}$$

Where $f_1 = \frac{A_3}{A_2}$ and $f_2 = \frac{A_4}{A_2}$. 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, and A_4 refer to the weight of the quadrupole, hexapole and octopole superposition, respectively.

According to classical mechanics [30] the motion of an ion in a rapidly oscillating field like $\phi(r,z,t)$ (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:

$$U_{eff}(r,z) = \frac{e}{2m}\left\langle \left| \int \vec{\nabla}\phi(r,z,t)dt \right|^2 \right\rangle. \tag{11}$$

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

$$\frac{d^2\vec{r}}{dt^2} + \frac{e}{m}\vec{\nabla}U_{eff}(r,z) = 0, \tag{12}$$

where $\vec{r}$ is the position vector of the ion. From the above equations we get the equation of motion in the axial (z) direction as

$$\ddot{z} + \omega_{0z}^2 z + \alpha_2 z^2 + \alpha_3 z^3 - \alpha_4 z r^2 = 0. \tag{13}$$

And in the radial (r) direction as

$$\ddot{r} + \omega_{0r}^2 r - \alpha_5 r^3 - \alpha_6 r z^2 = 0, \tag{14}$$

where

$$\omega_{0u} = \frac{q_u \Omega}{2\sqrt{2}}, \tag{15}$$

$$q_z = -2q_r = \frac{4eV}{m r_0^2 \Omega^2}, \tag{16}$$

$$\alpha_2 = \frac{9 f_1 \omega_{0z}^2}{2 r_0}, \tag{17}$$

$$\alpha_3 = \left(8 f_2 + \frac{9 f_1^2}{2}\right)\frac{\omega_{0z}^2}{r_0^2}, \tag{18}$$

$$\alpha_4 = 3 f_2 \frac{\omega_{0z}^2}{r_0^2}, \tag{19}$$

$$\alpha_5 = \left(6 f_2 - \frac{9 f_1^2}{2}\right)\frac{\omega_{0r}^2}{r_0^2}, \tag{20}$$

$$\alpha_6 = 12 f_2 \frac{\omega_{0r}^2}{r_0^2}. \tag{21}$$

The nonlinear system of equations governed by Eqs. (13) and (14) represents the coupled ion dynamics in z and r directions. This system has the form of a homogeneous coupled Duffing oscillator with quadratic and qubic nonlinearities. It is similar to the nonlinear mechanical and physical systems with two degrees of freedom. It has been discussed in literature in connection with different problems extensively [31–34].

By putting $r=0$ in Eq. (13) one arrives at an equation in axial direction which depends only on z variable. In the resulted equation, by introducing the dimensionless variable x through the relation $x = \frac{z}{r_0}$, ignoring $\frac{9f_1^2}{2}$ in comparison with $8f_2$ in α_3 for simplicity and omission of index z from ω_{0z} we get the equation,

$$\ddot{x} + \omega_0^2 x + \alpha_2' x^2 + \alpha_3' x^3 = 0, \tag{22}$$

where $\alpha_2' = \frac{9}{2} f_1 \omega_0^2$ and $\alpha_3' = 8 f_2 \omega_0^2$.

In part A of the next section we try to apply the homotopy perturbation method to the system of coupled nonlinear Eqs. (13) and (14) for calculation of the secular frequencies. It will be shown that in first order approximation, the ratios of secular frequencies $\frac{\omega_z}{\omega_{0z}}$ and $\frac{\omega_r}{\omega_{0r}}$ can be calculated through analytic relations in terms of f_1 and f_2 (the nonlinear field parameters) and A_z and A_r (the amplitudes of oscillations). In second-order approximation the system of nonlinear equations is transformed to a pair of coupled nonlinear algebraic equations which cannot be solved analytically and needs numerical techniques.

The nonlinear differential Eq. (22) has the form of a Duffing oscillator without driving field. There are several methods that can be used for solution of the Duffing equation [19,20]. In part B of the next section we have used the homotopy perturbation method for solving this nonlinear differential equation of motion and have calculated the axial secular frequencies. We have compared the results with those obtained by some other models and with the exact results for Duffing equation without quadratic nonlinearity.

IV. APPLICATION OF HOMOTOPY METHOD FOR SOLUTION OF THE EQUATIONS OF MOTION

A. System of coupled equations

For solving the system of coupled nonlinear Eqs. (13) and (14) with initial conditions $z(0)=A_z$, $\dot{z}(0)=0$, $r(0)=A_r$ and $\dot{r}(0)=0$ we construct the following homotopies:

$$\ddot{z}+\omega_z^2 z+p[(\omega_{0z}^2-\omega_z^2)z+\alpha_2 z^2+\alpha_3 z^3-\alpha_4 z r^2]=0, \quad (23)$$

$$\ddot{r}+\omega_r^2 r+p[(\omega_{0r}^2-\omega_r^2)r-\alpha_5 r^3-\alpha_6 r z^2]=0, \quad (24)$$

where $p\in[0,1]$. When $p=0$, the equations become the linearized equations, $\ddot{z}+\omega_z^2 z=0$ and $\ddot{r}+\omega_r^2 r=0$ and when $p=1$, it turns out to be the original set of nonlinear equations. We assume that the periodic solutions to Eqs. (23) and (24) can be written as two power series in p,

$$z=z_0+pz_1+p^2 z_2+\cdots \quad (25)$$

$$r=r_0+pr_1+p^2 r_2+\cdots \quad (26)$$

Substitution of the series (25) into Eq. (23) and series (26) into Eq. (24), and collecting terms of the same power of p, gives the set of equations,

$$\begin{cases}\ddot{z}_0+\omega_z^2 z_0=0, \quad z_0(0)=A_z \quad \dot{z}_0(0)=0\\ \ddot{z}_1+\omega_z^2 z_1+(\omega_{0z}^2-\omega_z^2)z_0+\alpha_2 z_0^2+\alpha_3 z_0^3-\alpha_4 z_0 r_0^2=0, \quad z_1(0)=0, \quad \dot{z}_1(0)=0.\end{cases} \quad (27)$$

for z_0 and z_1, and the set of equations,

$$\begin{cases}\ddot{r}_0+\omega_r^2 r_0=0, \quad r_0(0)=A_r, \quad \dot{r}_0(0)=0\\ \ddot{r}_1+\omega_r^2 r_1+(\omega_{0r}^2-\omega_r^2)r_0-\alpha_5 r_0^3-\alpha_6 r_0 z_0^2=0, \quad r_1(0)=0, \quad \dot{r}_1(0)=0.\end{cases} \quad (28)$$

for r_0 and r_1.

The first equations of the two sets (27) and (28) can be solved easily, giving the solutions $z_0(t)=A_z\cos\omega_z t$ and $r_0(t)=A_r\cos\omega_r t$. Substitution of $z_0(t)$ into the second equation of set (27) and $r_0(t)$ into the second equation of set (28) and after doing some algebra, having no secular term for both $z_1(t)$ and $r_1(t)$, implies,

$$\omega_z^2=\omega_{0z}^2+\frac{3}{4}\alpha_3 A_z^2-\frac{1}{2}\alpha_4 A_r^2, \quad (29)$$

$$\omega_r^2=\omega_{0r}^2-\frac{3}{4}\alpha_5 A_r^2-\frac{1}{2}\alpha_6 A_z^2. \quad (30)$$

These relations can be written in the following forms in terms of f_1 and f_2 (the nonlinear field parameters) and A_z and A_r (the amplitudes of oscillations):

$$\frac{\omega_z^2}{\omega_{0z}^2}=1+\frac{3}{4}\left(8f_2+\frac{9}{2}f_1^2\right)\frac{A_z^2}{r_0^2}-\frac{3}{2}f_2\frac{A_r^2}{r_0^2}, \quad (31)$$

$$\frac{\omega_r^2}{\omega_{0r}^2}=1-\frac{3}{4}\left(6f_2-\frac{9}{2}f_1^2\right)\frac{A_r^2}{r_0^2}-6f_2\frac{A_z^2}{r_0^2}. \quad (32)$$

These are the approximate amplitude dependent secular frequencies of coupled secular oscillations in a nonlinear ion trap in first order of homotopy perturbation method. For going to higher-order approximation, the parameter-expanding method (the modified Lindstedt-Poincare method) [35] is applied. For this purpose, we construct the following homotopies,

$$\ddot{z}+\omega_{0z}^2 z+p(\alpha_2 z^2+\alpha_3 z^3-\alpha_4 z r^2)=0, \quad (33)$$

$$\ddot{r}+\omega_{0r}^2 r-p(\alpha_5 r^3+\alpha_6 r z^2)=0. \quad (34)$$

Now, we expand the coefficients of the linear terms (ω_{0z}^2 and ω_{0r}^2) into power series of p,

$$\omega_{0z}^2=\omega_z^2+p\omega_{1z}+p^2\omega_{2z}+\cdots \quad (35)$$

$$\omega_{0r}^2=\omega_r^2+p\omega_{1r}+p^2\omega_{2r}+\cdots\cdots \quad (36)$$

Substitution of the power series (25) and (35) into Eq. (33), and the power series (26) and (36) into Eq. (34) and collecting terms of the same power of p, results in the two sets of equations as follows:

$$\begin{cases}\ddot{z}_0+\omega_z^2 z_0=0\\ \ddot{z}_1+\omega_z^2 z_1+\omega_{1z}z_0+\alpha_2 z_0^2+\alpha_3 z_0^3-\alpha_4 z_0 r_0^2=0\\ \ddot{z}_2+\omega_z^2 z_2+\omega_{1z}z_1+\omega_{2z}z_0+2\alpha_2 z_0 z_1+3\alpha_3 z_0^2 z_1-\alpha_4 r_0(2z_0 r_1+z_1 r_0)=0\end{cases} \quad (37)$$

$$\begin{cases} \ddot{r}_0 + \omega_r^2 r_0 = 0 \\ \ddot{r}_1 + \omega_r^2 r_1 + \omega_{1r} r_0 - \alpha_5 r_0^3 - \alpha_6 z_0^2 r_0 = 0 \\ \ddot{r}_2 + \omega_r^2 r_2 + \omega_{1r} r_1 + \omega_{2r} r_0 - 3\alpha_5 r_0^2 r_1 - \alpha_6 z_0 (2 r_0 z_1 + z_0 r_1) = 0 \end{cases} \tag{38}$$

These two systems can be solved for six unknowns z_0, z_1, z_2 and r_0, r_1, r_2 subject to initial conditions,

$$z_0(0) = A_z, \quad \dot{z}_0(0) = 0, \quad z_1(0) = 0, \quad \dot{z}_1(0) = 0, \quad z_2(0) = 0, \quad \dot{z}_2(0) = 0, \tag{39}$$

$$r_0(0) = A_r, \quad \dot{r}_0(0) = 0, \quad r_1(0) = 0, \quad \dot{r}_1(0) = 0, \quad r_2(0) = 0, \quad \dot{r}_2(0) = 0. \tag{40}$$

Now, similar to what we did in connection with the sets (27) and (28), we easily solve the first equations of the two sets (37) and (38) with the solutions $z_0(t) = A_z \cos \omega_z t$ and $r_0(t) = A_r \cos \omega_r t$. Substitution of $z_0(t)$ into the second equation of the set (37) and $r_0(t)$ into the second equation of the set (38), and having no secular term in both $z_1(t)$ and $r_1(t)$, implies,

$$\omega_{1z} = -\frac{3}{4}\alpha_3 A_z^2 + \frac{1}{2}\alpha_4 A_r^2, \tag{41}$$

$$\omega_{1r} = \frac{3}{4}\alpha_5 A_r^2 + \frac{1}{2}\alpha_6 A_z^2. \tag{42}$$

The results for the secular frequencies at this stage are equivalent to the results of first order calculation given in relations (29) and (30).

Now we can solve the second order differential equations for $z_1(t)$ and $r_1(t)$ subject to initial conditions given in Eqs. (39) and (40).

Substitution of the results for $z_1(t)$ and $r_1(t)$, along with the results for $z_0(t)$ and $r_0(t)$ in the third equations of the sets (37) and (38) gives the equations for $z_2(t)$ and $r_2(t)$ which to be solved. Having no secular term in $z_2(t)$ and $r_2(t)$ rises to a complicated coupled nonlinear algebraic equations for two unknowns ω_{2z} and ω_{2r} which cannot be solved analytically and needs numerical techniques.

B. Axial equation with no *r* dependency

For solving the nonlinear equation $\ddot{x} + \omega_0^2 x + \alpha_2' x^2 + \alpha_3' x^3 = 0$ with initial conditions $x(0) = A$, and $\dot{x}(0) = 0$, we apply the same procedure outlined in part A and construct the homotopy,

$$\ddot{x} + \omega^2 x + p[(\omega_0^2 - \omega^2)x + \alpha_2' x^2 + \alpha_3' x^3] = 0 \quad p \in [0,1]. \tag{43}$$

By writing the periodic solution to Eq. (43) as a power series in p,

$$x = x_0 + p x_1 + p^2 x^2 + \cdots \tag{44}$$

and substitution of this series into Eq. (43), gives the following set of equations:

$$\begin{cases} \ddot{x}_0 + \omega^2 x_0 = 0, \quad x_0(0) = A, \quad \dot{x}_0(0) = 0 \\ \ddot{x}_1 + \omega^2 x_1 + (\omega_0^2 - \omega^2) x_0 + \alpha_2 x_0^2 + \alpha_3 x_0^3 = 0, \quad x_1(0) = 0, \quad \dot{x}_0(0) = 0. \end{cases} \tag{45}$$

It is clear that $x_0(t) = A \cos \omega t$. Having no secular term in $x_1(t)$, implies

$$\omega = \sqrt{\omega_0^2 + \frac{3}{4}\alpha_3 A^2}. \tag{46}$$

This is the approximate amplitude dependent frequency in first order. Now we go to second order approximation by constructing the following homotopy,

$$\ddot{x} + \omega_0^2 x + p(\alpha_2 x^2 + \alpha_3 x^3) = 0 \tag{47}$$

We expand the coefficient of the linear term (ω_0^2) and the solution $[x(t)]$ into power series of p as

$$\omega_0^2 = \omega^2 + p\omega_1 + p^2 \omega_2 + \cdots, \tag{48}$$

$$x = x_0 + p x_1 + p^2 x_2 + \cdots. \tag{49}$$

Substitution of these series into Eq. (47), and collecting terms of the same power of p, results in the following set of equations:

$$\begin{cases} \ddot{x}_0 + \omega^2 x_0 = 0 \\ \ddot{x}_1 + \omega^2 x_1 + \omega_1 x_0 + \alpha_2 x_0^2 + \alpha_3 x_0^3 = 0 \\ \ddot{x}_2 + \omega^2 x_2 + \omega_1 x_1 + \omega_2 x_0 + 2\alpha_2 x_0 x_1 + 3\alpha_3 x_0^2 x_1 = 0. \end{cases} \tag{50}$$

The solution for the first equation is $x_0(t) = A \cos \omega t$. Insertion of this solution in the second equation and implication for no secular term in $x_1(t)$, gives the result,

TABLE I. The calculated values of $\frac{\omega}{\omega_0}$ for different values of f_1 and f_2 in Lindstedt-Poincare approximation and the homotopy method.

f_1	f_2	Lindstedt-Poincare	This paper (homotopy method)
0.05	0.05	1.06445	1.0640
0.10	0.10	1.0525	1.1112
0.15	0.15	1.1301	1.1453
0.20	0.20	1.1312	1.1677
0.25	0.25	1.1111	1.1775
0.05	−0.05	0.9144	0.9086
0.1	−0.10	0.8078	0.7447

$$\omega_1 = -\frac{3}{4}\alpha_3 A^2. \quad (51)$$

The second equation of the set is solved for this value of ω_1 and the final solution for $x_1(t)$, along with the solution for $x_0(t)$ are inserted in third equation of the set. No secular term for $x_2(t)$ implies that

$$\omega_2 = \frac{5}{6}\frac{\alpha_2^2 A^2}{\omega^2} - \frac{3}{128}\frac{\alpha_3^2 A^4}{\omega^2}. \quad (52)$$

Combining these results with $p=1$ gives rise to the result

TABLE II. Comparison of the calculated values of $\frac{\omega}{\omega_0}$ in this paper with the values of the Lindstedt-Poincare approximation and the exact values.

f_2	Lindstedt-Poincare	Homotopy method (this paper)	Exact results
0.01	1.015	1.0149	1.01487
0.05	1.075	1.0727	1.072
0.10	1.15	1.1414	1.1389
0.15	1.225	1.2065	1.2017
0.20	1.30	1.2682	1.2612
0.25	1.375	1.3279	1.3177
0.30	1.45	1.3849	1.372
0.40	1.60	1.4923	1.4739
0.50	1.75	1.5928	1.569
−0.01	0.9850	0.98490	0.98487
−0.05	0.9250	0.92255	0.92136
−0.10	0.850	0.83983	0.83343
−0.15	0.7750	0.75162	0.73099
−0.20	0.70	0.65918	0.59968

$$\omega_0^2 = \omega^2 + \omega_1 + \omega_2 = \omega^2 - \frac{3}{4}\alpha_3 A^2 + \frac{5}{6}\frac{\alpha_2^2 A^2}{\omega^2} - \frac{3}{128}\frac{\alpha_3^2 A^4}{\omega^2}. \quad (53)$$

This equation can be solved for ω and the final result is:

$$\omega = \sqrt{\frac{\omega_0^2 + \frac{3}{4}\alpha_3 A^2 + \sqrt{\omega_0^4 + \frac{3}{2}\alpha_3 A^2 \omega_0^2 + \frac{21}{32}\alpha_3^2 A^4 - \frac{10}{3}\alpha_2^2 A^2}}{2}}. \quad (54)$$

In this relation A is the maximum value for x and x_{max} can be obtained by inserting z_0 for z in equation $x=\frac{z}{r_0}$. Insertion of the expressions for A, α_2, and α_3 in Eq. (53) gives the final result,

$$\frac{\omega}{\omega_0} = \sqrt{\frac{1 + 3f_2 + \sqrt{1 + 6f_2 + \frac{21}{2}f_2^2 - \frac{135}{4}f_1^2}}{2}}. \quad (55)$$

The perturbed frequencies can be calculated through the relation (55) as a function of field aberrations (parameters f_1 and f_2). It is clear from the relation that ion secular frequency is dependent on the sign of the octopole superposition and independent of the sign of the hexapole superposition. According to the relation (55), hexapole superposition decreases the axial secular frequency, positive octopole superposition increases the ion axial secular frequency and the negative octopole superposition decreases the axial secular frequency.

The values of $\frac{\omega}{\omega_0}$ for different values of f_1 and f_2 are given in Table I and for comparison purposes the values of $\frac{\omega}{\omega_0}$ in Lindstedt-Poincare approximation [16,20] which can be calculated by the relation

$$\frac{\omega}{\omega_0} = 1 + \frac{144f_2 - 405f_1^2}{96} \quad (56)$$

are also given in the table.

For a Duffing oscillator with only cubic term as nonlinearity ($\alpha_2=0$), the exact values of frequencies are available in literature and can be calculated by the relation

$$\frac{\omega}{\omega_0} = \frac{\pi\sqrt{1+4f_2}}{2F\left(\frac{\pi}{2};\frac{2f_2}{1+4f_2}\right)} \tag{57}$$

Where $F(\frac{\pi}{2};k)=K(k)$ is the complete elliptic integral of the first kind.

In Table II, the exact values of secular frequencies for $f_1=0$ and different values of f_2 are compared with the results of this paper and the results of Lindstedt-Poincare approximation. As is seen in the table, the results of this paper are much more closer to the exact values than those of the Lindstedt-Poincare method.

V. CONCLUSION

In this paper we have derived the equations of ion motion in a nonlinear ion trap. The nonlinear ion trap is generated by superposition of weak multipole fields on the pure quadrupole field. Only hexapole and octopole field superpositions are considered. The computed equations of ion motion are nonlinear Duffing-like equations. We have used the homotopy perturbation method for calculating the coupled secular frequencies as well as axial secular frequencies of the ions in a nonlinear ion trap. The results of this paper are compared with the exact results and the results of the Lindstedt-Poincare method for axial secular frequencies.

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