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Energy gaps of a trapped ion interacting with a laser field

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Abstract. We consider the secular motion of an ion stored in a Paul trap and interacting with a standing laser field. It is shown that the Schrödinger equation of the system is analogous to the linearized equation of a classically chaotic system. From the mathematical simulation between the two systems we reveal several new properties in the fully quantum treatment. The results lead to some parameter and energy gaps in which the motional ground state does not exist.

1. Introduction

Chaotic behaviour of the ions confined in a Paul trap has become a problem of increasing interest over the last few years. Most of the works are focused on classically chaotic motions of the systems with ion numbers greater than one [1–5]. Chacon *et al* used a semiclassical approximation to show that chaos can occur in the system of a single trapped ion interacting with a sufficiently strong standing laser field [6, 7]. Some quantum signatures associated with the classical chaos have also been found in the systems [8, 9].

Recently, we applied a new perturbation technique to the Melnikov chaotic systems [10] and obtained kinds of analytically chaotic solutions [11, 12]. We also found that the technique can be employed to the perturbed Schrödinger equations [13]. The quantum mechanics of the trapped single ion interacting with a weak laser field is described by the Schrödinger equation with harmonic potential and spatially periodical perturbation. In this paper, we show that this Schrödinger equation is mathematically analogous to the linearized one of a Melnikov chaotic system, by using time in place of the spatial coordinate. Simulation of the chaotic system to the quantum system leads to a new type of wavefunction. The Melnikov chaos criterion corresponds to the formula of energy correction, the sensitive dependence on the initial conditions is associated with sensitivity on the boundary conditions which results in the indetermination of the wavefunction in the fully quantum mechanical treatment. We define stability of the quantum system as the mathematical analogy to the Lyapunov stability and obtain the corresponding boundedness conditions of the wavefunction in total space. The conditions imply that under the laser perturbation there exist some gaps of the parameter region and the corresponding energy gaps in which the motional ground state is unstable. This phenomenon can be observed by measuring the probability of the system in the ground state for different system parameters.

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2. General solutions of the corrected Schrödinger equations

We consider the standard Paul trap setup [14, 15] with a standing laser field of frequency ω_L and wavevector k aligned along the x direction, which couples the internal states of a single two-level ion with mass m to the centre-of-mass motion. To avoid spontaneous emission we suppose that the ion is initially in its internal ground state and the detuning of the laser field is large [8]. Under the rotating wave and the secular approximations, the quantum mechanics of the ion in a frame rotating with the laser frequency is governed by the Hamiltonian [6, 8]

$$H = -\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \frac{1}{2}m\nu^2x^2 + \frac{\hbar\Omega_0^2}{8\Delta}\cos(2kx + 2\phi) \tag{1}$$

where ν is the angular frequency of the effective potential oscillation, Ω_0 is the Rabi frequency, Δ the frequency difference between ω_L and the atomic transition frequency, and ϕ denotes the relative position between the centre of the trap and the standing laser wave. After adopting the dimensionless coordinate ξ and energy λ,

$$\xi = \alpha x \qquad \alpha = \sqrt{m\nu/\hbar} \qquad \lambda = 2E/(\hbar\nu) \tag{2}$$

the corresponding Schrödinger equation reads

$$\Psi_{\xi\xi} + (\lambda - \xi^2)\Psi = \frac{\Omega_0^2}{4\nu\Delta}\cos(2\sqrt{2}\eta\xi + 2\phi)\Psi \tag{3}$$

with $\eta = \frac{k}{\sqrt{2}\alpha}$ being the Lamb–Dicke constant. Setting $(\nu\Delta) \gg \Omega_0^2$, the interaction term denotes a perturbation. We apply the Rayleigh–Schrödinger expansions

$$\Psi = \sum_{i=0}^{\infty}\Psi_n^{(i)} \qquad E = \sum_{i=0}^{\infty}E_n^{(i)} \qquad \text{for} \quad |\Psi_n^{(i)}| \ll |\Psi_n^{(i-1)}|,\ |E_n^{(i)}| \ll |E_n^{(i-1)}| \tag{4}$$

to equation (3) and equate the sum of ith-order terms for both sides, obtaining

$$\Psi_{n,\xi\xi}^{(0)} + (\lambda_n - \xi^2)\Psi_n^{(0)} = 0 \tag{5}$$

$$\Psi_{n,\xi\xi}^{(i)} + (\lambda_n - \xi^2)\Psi_n^{(i)} = \varepsilon_n^{(i)} \qquad i = 1, 2, \ldots, \infty \tag{6a}$$

$$\varepsilon_n^{(i)} = \frac{\Omega_0^2}{4\nu\Delta}\cos(2\sqrt{2}\eta\xi + 2\phi)\Psi_n^{(i-1)} - \frac{2}{\hbar\nu}\sum_{j=1}^{i}E_n^{(j)}\Psi_n^{(i-j)}. \tag{6b}$$

The unperturbed equation (5) describes a harmonic oscillator with the well known solution

$$\Psi_n^{(0)} = N_n H_n(\xi)\mathrm{e}^{-\frac{1}{2}\xi^2} \qquad \text{for} \quad \lambda_n = 2E_n^{(0)}/(\hbar\nu) = 2n + 1 \tag{7}$$

where N_n is the normalization constant and H_n the Hermitian polynomials. Making use of the previous result [13], we construct the general solutions of the ith-order corrected equations (6) as

$$\Psi_n^{(i)} = g_n\int_{A_{ni}}^{\xi} f_n\varepsilon_n^{(i)}\,\mathrm{d}\xi - f_n\int_{B_{ni}}^{\xi} g_n\varepsilon_n^{(i)}\,\mathrm{d}\xi \qquad i = 1, 2, \ldots, \infty \tag{8a}$$

$$f_n = \Psi_n^{(0)} \qquad g_n = \Psi_n^{(0)}\int(\Psi_n^{(0)})^{-2}\,\mathrm{d}\xi \tag{8b}$$

with A_{n_i} and B_{n_i} being the integration constants adjusted by the normalization and the boundary conditions. Note that equations (8) are non-integrable and even g_n is non-integrable for some n. Applying equations (8) and (5) to equations (6), one can directly prove the general solutions. We combine equation (8a) with (8b) to simplify the solutions to the form

$$\Psi_n^{(i)} = \Psi_n^{(0)}\int_{B_{ni}}^{\xi}(\Psi_n^{(0)})^{-2}\left(\int_{A_{ni}}^{\xi}\Psi_n^{(0)}\varepsilon_n^{(i)}\,\mathrm{d}\xi\right)\mathrm{d}\xi \qquad i = 1, 2, \ldots, \infty. \tag{9}$$

The general solutions contain all of the special solutions of equations (6), the bounded and unbounded, which are determined by the constants A_{n_i} and B_{n_i}.

3. The corresponding classically chaotic system

In order to investigate chaotic behaviour of the quantum system, we mathematically construct the Melnikov classically chaotic system

$$\varphi_{tt} + \left(2\ln\frac{\varphi}{2} + 1\right)\varphi = \varepsilon(\varphi, t) \qquad |\varepsilon(\varphi, t)| \ll 1 \tag{10}$$

where $\varepsilon(\varphi, t)$ is a periodical function of time. The similar perturbation expansion

$$\varphi = \sum_{i=0}^{\infty} \varphi^{(i)} \qquad |\varphi^{(i)}| \ll |\varphi^{(i-1)}| \tag{11}$$

of equations (4) leads equation (10) to the set of equations

$$\varphi_{tt}^{(0)} + \left(2\ln\frac{\varphi^{(0)}}{2} + 1\right)\varphi^{(0)} = 0 \tag{12}$$

$$\varphi_{tt}^{(i)} + \left(2\ln\frac{\varphi^{(0)}}{2} + 3\right)\varphi^{(i)} = \varepsilon^{(i)}(\varphi^{(j)}, t) \qquad i = 1, 2, \ldots, \infty \quad j < i. \tag{13}$$

The unperturbed equation (12) has the homoclinic orbit

$$\varphi^{(0)} = 2\mathrm{e}^{-\frac{1}{2}(t-t_0)^2} \qquad \varphi_t^{(0)} = -2(t - t_0)\mathrm{e}^{-\frac{1}{2}(t-t_0)^2}. \tag{14}$$

Given equations (10) and (14), the Melnikov function [6, 7, 10] becomes

$$\Delta(t_0) = \int_{-\infty}^{\infty} \varphi_t^{(0)}(t - t_0)\varepsilon^{(1)}(\varphi^{(0)}, t)\,\mathrm{d}t \tag{15}$$

which measures the distance between the stable and unstable orbits in the Poincaré section. Obviously, the function has simple zeros, indicating the existence of chaos for the orbits whose initial conditions are sufficiently near the homoclinic orbit (14). Inserting equations (14) into equations (11) and (13) can easily bring about such an orbit. The insertion leads equations (13) to the form

$$\varphi_{tt}^{(i)} + [3 - (t - t_0)^2]\varphi^{(i)} = \varepsilon^{(i)}(\varphi^{(j)}, t) \qquad i = 1, 2, \ldots, \infty \quad j < i. \tag{16}$$

We are familiar with the general solutions of these equations [11, 12]

$$\varphi^{(i)} = g\int_{A_i}^{t} f\varepsilon^{(i)}(\varphi^{(j)}, t)\,\mathrm{d}t - f\int_{B_i}^{t} g\varepsilon^{(i)}(\varphi^{(j)}, t)\,\mathrm{d}t \tag{17a}$$

$$f = \varphi_t^{(0)} = -2(t - t_0)\mathrm{e}^{-\frac{1}{2}(t-t_0)^2} \qquad g = \varphi_t^{(0)}\int(\varphi_t^{(0)})^{-2}\,\mathrm{d}t \tag{17b}$$

where A_i and B_i are the integration constants determined by the initial conditions. For the integrands $f\varepsilon^{(i)}$ and $g\varepsilon^{(i)}$ with $\varepsilon^{(i)}$ being the periodical function of t, equations (17) are non-integrable. This non-integrability is a common signature of the chaotic system. Because the function g tends to infinity as $t \to \infty$, the solutions in equations (17) are unbounded in the general case. This implies that equations (17) are not the corrected solutions of equation (10), since the unbounded $\varphi^{(i)}$ does not satisfy the inequality in equations (11) and causes divergence of the series. However, the unboundedness of the functions $\varphi - \varphi^{(0)} = \sum_{i=1}^{\infty}\varphi^{(i)}$ and $\varphi_t - \varphi_t^{(0)} = \sum_{i=1}^{\infty}\varphi_t^{(i)}$ is associated with the Lyapunov instability [16] of the homoclinic orbit $(\varphi^{(0)}, \varphi_t^{(0)})$. Fortunately, the unboundedness can be controlled by the necessary and sufficient conditions [7, 11]

$$I_{\pm}^{(i)}(A_i) = \lim_{t\to\pm\infty}\int_{A_i}^{t} f\varepsilon^{(i)}(\varphi^{(j)}, t)\,\mathrm{d}t = 0 \qquad \text{for} \quad i = 1, 2, \ldots, \infty \quad j < i. \tag{18}$$

The case $t \to -\infty$ corresponds to the time reversal of equations (14), because of the time reversal symmetry of equation (12). The necessity of the conditions is evident, because of the unboundedness of g in equations (17) as $t \to \pm\infty$. Given equations (18), we could use the l'Hospital rule to easily derive the small superior limits of $|\varphi^{(i)}|$ and $|\varphi_t^{(i)}|$ for $t \to \pm\infty$ from equations (17). This is the proof of the sufficiency. Combining equation (15) and (17*b*) with equations (18) for $i = 1$ yields the Melnikov chaos criterion $\Delta(t_0) = I_+^{(1)} - I_-^{(1)} = 0$. Therefore, the homoclinic orbit is embedded in a chaotic attractor. According to equations (18), any infinitesimal change of the initial constants A_i may break the boundedness conditions. This is the sensitive dependence of the solution on the initial conditions [7]. Generally, the initial conditions cannot be set experimentally. All of these make the solution (11) with equations (14) and (17) the chaotic one.

4. Energy gaps of the quantum system

Now we make a comparison between the classically chaotic system (16) and the quantum one (6). At first we see that after setting $\xi \to (t - t_0)$ the linearized equations (16) of the chaotic system (10) are similar to the corrected Schrödinger equations (6). Particularly, for $\lambda_n = \lambda_1 = 3$, equations (6) possess the same form as equations (16). Secondly, the eigenstate $\Psi_n^{(0)}$ ($\Psi_1^{(0)}$) in equation (7) and its corrections $\Psi_n^{(i)}$ ($\Psi_1^{(i)}$) in equations (8) are similar to (agree with) the homoclinic solution (14) and its corrected solutions (17) of the chaotic system respectively, which implies equations (4) with equations (7) and (8) becoming the indeterminate wavefunction. Consequently, we have the necessary and sufficient conditions for the boundedness of equations (8) as

$$I_{n\pm}^{(i)}(A_{ni}) = \lim_{x\to\pm\infty} \int_{A_{ni}}^{\xi} f_n \varepsilon_n^{(i)} \, \mathrm{d}\xi = 0 \qquad \text{for} \quad i = 1, 2, \ldots, \infty. \tag{19}$$

It is the mathematical analogy to the boundedness conditions (18) of the chaotic system. The necessity of the conditions is exhibited by the unbounded g_n in equations (8) as $x \to \pm\infty$. Under these conditions, one can use the l'Hospital rule to prove the boundedness of equations (8). This displays the sufficiency of the conditions. The necessity and sufficiency show that once equations (19) are broken, we get unbounded corrections (8) and divergent wavefunction (4). The divergence means that it does not represent a real physical state. The unboundedness destroys the expansion conditions in equations (4) and shows it not to be a solution of the system (3). These are in complete agreement with the classical case. As in the Lyapunov definition, the unboundedness of the corrected solution ($\sum_{i=1} \Psi_n^{(i)} = \Psi_n - \Psi_n^{(0)}$) in the total space $x \in (-\infty, \infty)$ can be defined as instability of the initial state $\Psi_n^{(0)}$ under the perturbations. The corresponding boundedness conditions have been given in equations (19). Associating with the Melnikov chaos criterion $\Delta(t_0) = I_+^{(1)} - I_-^{(1)} = 0$, from the conditions we have the corresponding criterion for the quantum system as

$$\Delta_n^{(i)}(E_n^{(i)}) = I_{n+}^{(i)} - I_{n-}^{(i)} = \int_{-\infty}^{\infty} f_n \varepsilon_n^{(i)} \, \mathrm{d}\xi = 0 \qquad \text{for} \quad i = 1, 2, \ldots, \infty. \tag{20}$$

Substituting equations (6*b*) and (8*b*) into equations (20) yields the formulae of the energy corrections,

$$\int_{-\infty}^{\infty} \Psi_n^{(0)} \left[\frac{\Omega_0^2}{4\nu\Delta} \cos(2\sqrt{2}\eta\xi + 2\phi) \Psi_n^{(i-1)} - \frac{2}{\hbar\nu} \sum_{j=1}^{i} E_n^{(j)} \Psi_n^{(i-j)} \right] \mathrm{d}\xi = 0 \qquad i = 1, 2, \ldots. \tag{21}$$

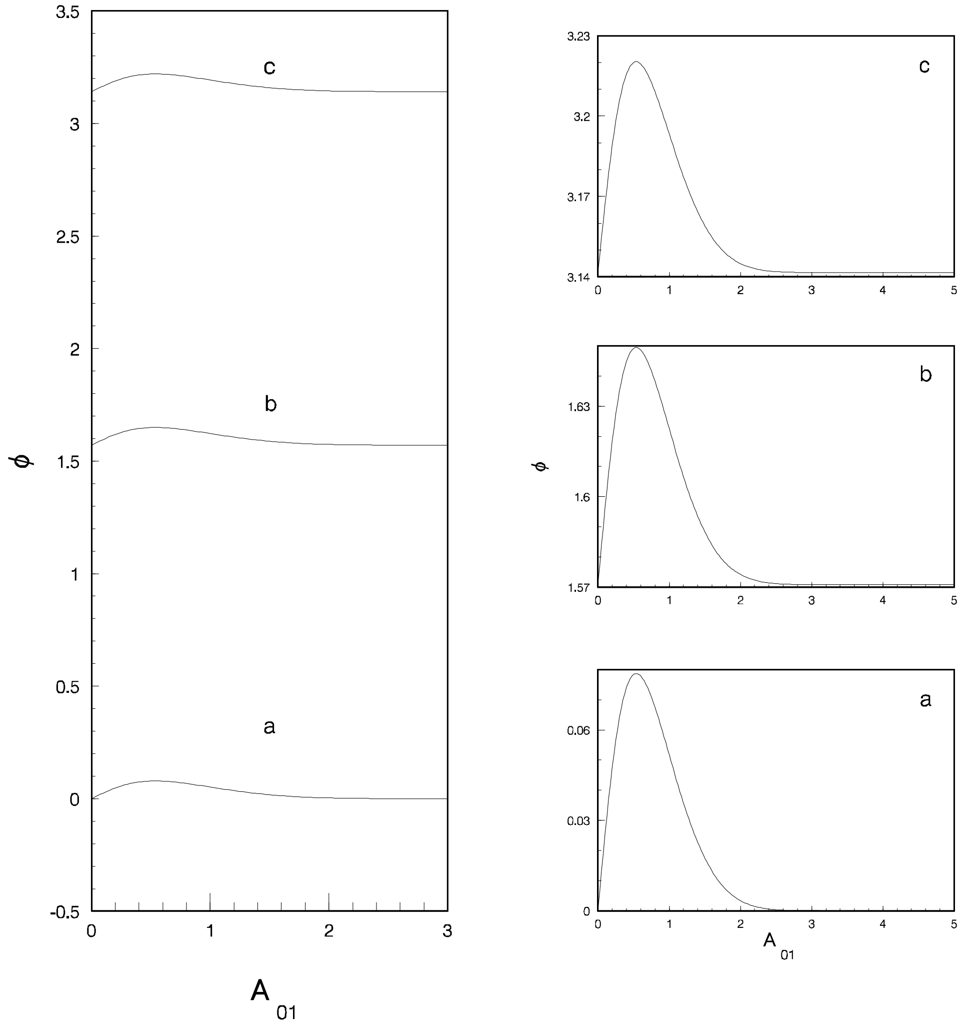

Figure 1. The boundedness curves for the Lamb–Dicke parameter $\eta = 1/(2\sqrt{2})$ from equation (24). The curves on the right-hand side are the amplification of ones on the left-hand side, which show the curves falling only on the parameter intervals $\phi \in [0, 0.08)$, $[\pi/2, 1.65)$ and $[\pi, 3.22)$. Therefore, the motional ground state cannot exist in the gaps $\Delta\phi_1 \in [0.08, \pi/2)$ and $\Delta\phi_2 \in [1.65, \pi)$.

Let us take the motional ground state $\Psi_0^{(0)}$ and its first-order correction $\Psi_0^{(1)}$ as an example. Applying equations (7) for $n = 0$ to the formulae (21) produces the first-order correction to the energy $E_0^{(0)}$ of the ground state,

$$E_0^{(1)} = \int_{-\infty}^{\infty} \frac{\hbar\Omega_0^2}{8\sqrt{\pi}\Delta} \cos(2\sqrt{2}\eta\xi + 2\phi)\mathrm{e}^{-\xi^2}\,\mathrm{d}\xi = \frac{\hbar\Omega_0^2}{8\Delta}\cos(2\phi)\mathrm{e}^{-2\eta^2}. \tag{22}$$

The substitution of equations (6*b*), (8*b*) and (22) into equations (19) for $i = 1$, $n = 0$ gives

$$I_{0\pm}^{(1)} = \frac{\Omega_0^2}{4\sqrt{\pi}\nu\Delta}\int_{A_{01}}^{\pm\infty} F(\xi)\,\mathrm{d}\xi = 0 \tag{23a}$$

$$F(\xi) = [\cos(2\sqrt{2}\eta\xi + 2\phi) - \cos(2\phi)\mathrm{e}^{-2\eta^2}]\mathrm{e}^{-\xi^2}. \tag{23b}$$

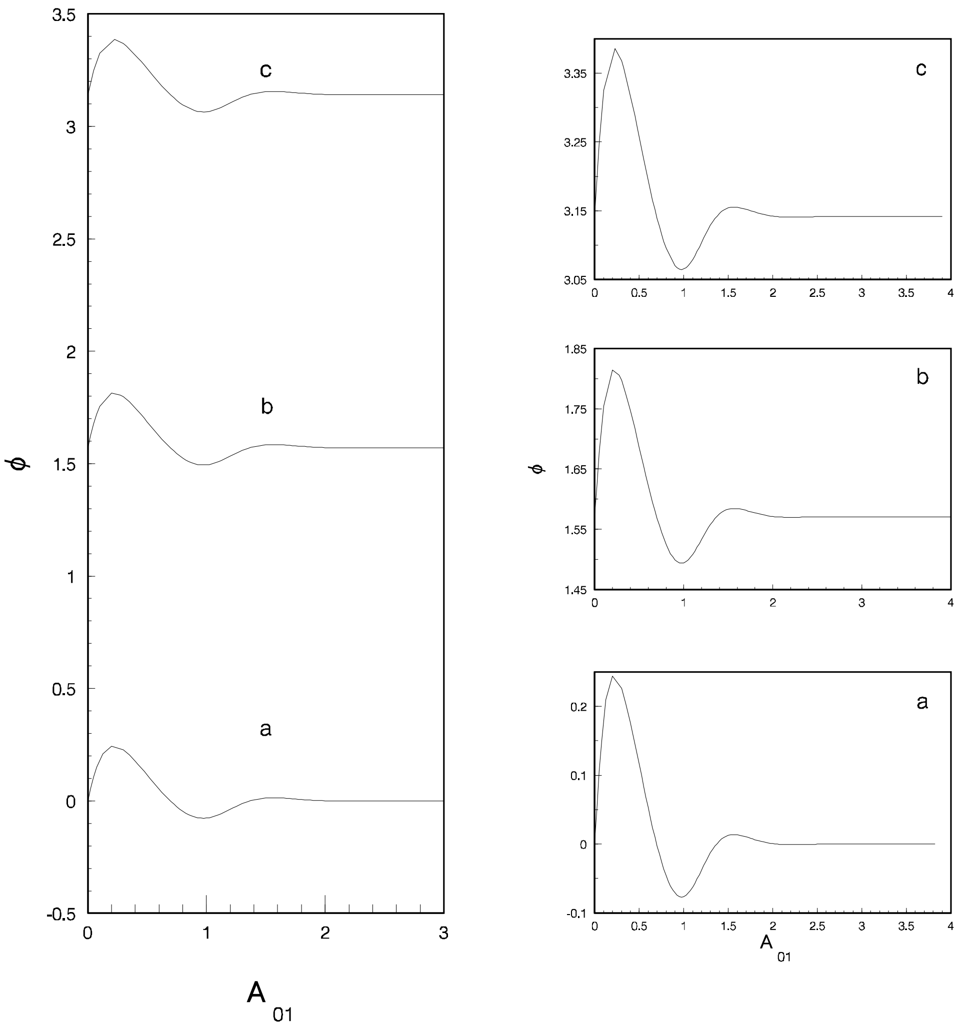

Figure 2. The boundedness curves for the parameter $\eta = 5/(2\sqrt{2})$, which reveal the width of the instability gaps decreasing to $\Delta\phi_3 \in [0.24, 1.5)$ and $\Delta\phi_4 \in [1.82, 3.07)$ for the given Lamb–Dicke parameter η.

A careful calculation leads them to the simplified form

$$\begin{aligned}\int_{A_{01}}^{\pm\infty} F(\xi)\,\mathrm{d}\xi &= \int_{A_{01}}^{0} F(\xi)\,\mathrm{d}\xi + \int_{0}^{\pm\infty} F(\xi)\,\mathrm{d}\xi \\ &= -\int_{0}^{A_{01}} F(\xi)\,\mathrm{d}\xi - \sin(2\phi)\int_{0}^{\infty}\sin(2\sqrt{2}\eta\xi)\mathrm{e}^{-\xi^2}\,\mathrm{d}\xi = 0. \end{aligned} \tag{24}$$

This is the boundedness condition of the first-order solution $\Psi_0^{(1)}$, under the laser perturbation.

In conditions (24) we show that the boundedness of the corrected wavefunction of the motional ground state depends on the system parameters η, ϕ and the boundary constant A_{01} in the first-order approximation. From equation (24) we draw the ϕ versus A_{01} graphs for figure 1: $\eta = 1/(2\sqrt{2})$, figure 2: $\eta = 5/(2\sqrt{2})$ and figure 3: $\eta = 5/\sqrt{2}$, respectively. Figure 1 displays the curves associated with boundedness to be restricted in the interval

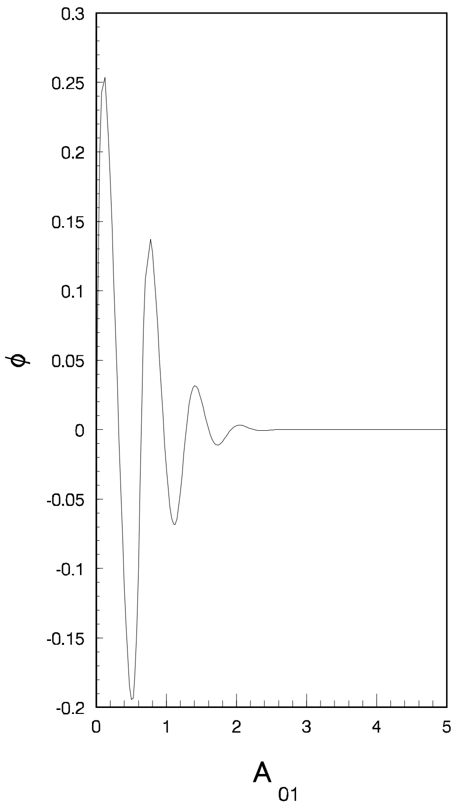

Figure 3. The boundedness curve for the parameter $\eta = 5/\sqrt{2}$ that displays the curve density tending to a large value in the parameter region $0 \leqslant A_{01} < 2.2$, and $-0.2 < \phi < 0.3$ as the parameter η increases to a large value. The quantum motion of the system sensitively depends on the system parameters and boundary constant in this region.

$\phi \in [0, 0.08)$, $[\pi/2, 1.65)$ and $[\pi, 3.22)$ for an arbitrary A_{01} value. This implies that for the parameter $\eta = 1/(2\sqrt{2})$ the correction to motional ground state is unbounded in the parameter gaps $\Delta\phi_1 \in [0.08, \pi/2)$ and $\Delta\phi_2 \in [1.65, \pi)\ldots.$ Figure 2 shows the width of the gaps decreasing to $\Delta\phi_3 \in [0.24, 1.5)$ and $\Delta\phi_4 \in [1.82, 3.07)$ with the increase of the Lamb–Dicke parameter η. Combining these with equation (22) we can obtain the corresponding energy gaps $(-0.082, 0.082)$ and $(-0.02, 0.02)$, respectively corresponding to $\eta = 1/2\sqrt{2}$ and $\eta = 5/2\sqrt{2}$, as in figure 4. The unboundedness means that the corrected motional ground state cannot exist in these gaps. This phenomenon can be observed by measuring the probability of the ion in the ground state [17, 18] for different ϕ values. Combining figure 2 with 3 we see that in some parameter regions the curve density will become very large as the parameter η increases to a large value. Clearly, only for the parameters lying on the curves is the corrected wavefunction bounded so that the motional ground state is stable under the laser perturbation. Any infinitesimal departure of the boundary constant and the system parameters from the curves may cause unboundedness and instability. This is the sensitive dependence of the quantum system to the boundary conditions and the system parameters.

In the distribution region of the curve in figure 3, one value of ϕ may correspond to multi-values of A_{01}. This implies degeneracy of the corrected states, since equations (9) may give multi-states for these A_{01} and equation (22) only gives one value of energy for this ϕ. The meaning of the parameters η and ϕ are familiar to us. Fixing a set of parameters η and ϕ, the boundedness of the corrected solution $\Psi_0^{(1)}$ to the ground state $\Psi_0^{(0)}$ are uniquely determined by the constant A_{01}. What is the boundary constant A_{01}? Mathematically, the general solution $\Psi_0^{(1)}$ of the second-order differential equations (6) for $n = 0$ and $i = 1$

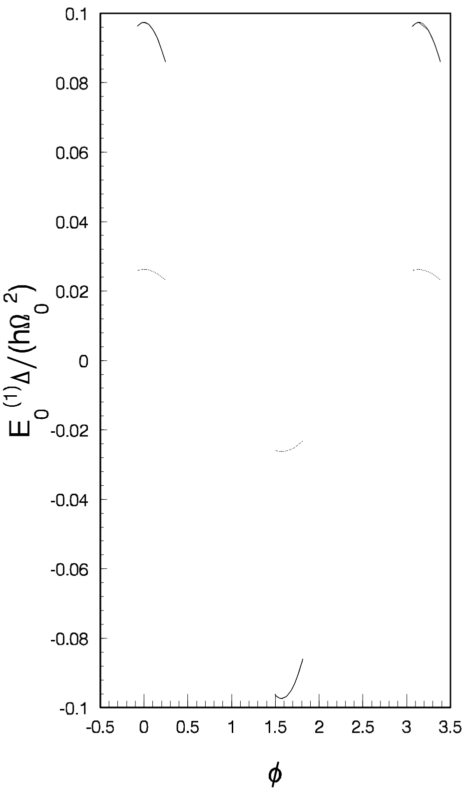

Figure 4. The plot of the energy correction versus laser phase from equations (22) and (24). The solid curves correspond to $\eta = 1/(2\sqrt{2})$ and the dotted curves to $\eta = 5/(2\sqrt{2})$. The corresponding energy gaps are $(-0.082, 0.082)$ and $(-0.02, 0.02)$, respectively.

contains the two arbitrary constants A_{01} and B_{01}, which depend on the physically definite conditions. For the considered spatial problem with boundary $x = \pm\infty$, the definite conditions are just the boundary conditions (19) and a normalization condition. However, in the example $n = 0$, $i = 1$, we see that the A_{01} cannot be solely determined from the corresponding boundary condition (24), while the normalization condition can only give the constant B_{01} for any A_{01} value. The indetermination of the boundary constant A_{01} and the sensitivity of the system on the constant leads to the indeterminate wavefunction (4) with equations (7) and (8). From equations (8) we see that any infinitesimal change of the boundary constant A_{ni} could be infinitely amplified, since the factor g_n tends to infinity as $x \to \pm\infty$. Only when the boundedness conditions (19) are strictly held, do we have the bounded solutions $\Psi_n^{(i)}$ and the stable eigenstates $\Psi_n^{(0)}$. Although the boundary constant A_{ni} is indeterminate, we can adjust the controllable parameters η and ϕ to fit the conditions (19) for arbitrary A_{ni}. Figures 1, 2 and 4 exhibit the suitable regions for the adjustment as $\phi \approx l\pi/2$ for $l = 0, 1, 2, \ldots$ and the considered case. Once the conditions are fitted, the ion is stably confined and behaves regularly in the trap. However, such quantum motion sensitively depends on the boundary conditions and the system parameters.

5. Conclusions and discussions

In conclusion, we have investigated the quantum motion of a trapped ion interacting with a standing laser field. We find that the Schrödinger equation of the system is similar to the linearized equation of a classically chaotic system and that their solutions possess the same form after using time instead of the spatial coordinate. We define the stability of the quantum system as the mathematical analogy to the Lyapunov stability of the classical system. The corresponding solution and the necessary and sufficient boundedness conditions are obtained. The conditions imply the sensitive dependence of the system on the boundary conditions and system parameters and contain formulae of the energy corrections. In order to obtain the required quantum states, we must adjust the control parameters to fit the corresponding boundedness conditions. Taking the motional ground state as an example, we demonstrate that there exist some parameter gaps and energy gaps in which the ground state is unstable under the laser perturbation. The advances for cooling a single trapped ion to a motional ground state [17] could lead to an experimental observation of this phenomenon.

Although the results formally contain any ith-order corrections to the eigenstates and eigenenergy with arbitrary quantum number n, the cases $i > 1$ and $n > 0$ are mathematically complicated. The non-integrability of the corrected solutions necessitates numerical calculations. The above-mentioned results can be directly extended to the system with two trapped ions [19]. By using the perturbation technique, we will extend the results to the time-dependent case in further work.

Acknowledgments

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