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Quantum motion of three trapped ions in one dimension

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Abstract. The hyperspherical-coordinate approach is employed to a one-dimensional model of three ions in a Paul trap. It is shown that the eigen wave functions have well-defined η, θ nodal structure indicating a near separability in the hyperspherical coordinates, then two approximate good quantum numbers are introduced to classify the eigenstates. Three important classical periodic motions, including the breathing motion and the (distorted-)symmetric or anti-symmetric stretching motion, are found to dominate the wave function distribution.

PACS. 32.80.Pj Optical cooling of atoms; trapping – 03.65.Ge Solutions of wave equations: bound states – 42.50.Vk Mechanical effects of light on atoms, molecules, electrons, and ions

1 Introduction

Recently, quantum computation based on trapped-ion physics has become a hot topic. One of the choices for realizing the quantum computation is an array of trapped ions in a collinear configuration, which can be achieved experimentally in a linear trap or a Paul trap where the restoring forces are much softer in one principal-axis direction than in the other two orthogonal directions. To understand the dynamics and cooling process of the ultracold ion configuration, one needs to study the quantum mechanics of the trapped ions in one dimension. Some initial steps have already been taken [1,2]. In reference [2] Yin and Javanainen take their approaches to a one-dimensional model of *two* ions in a Paul trap. Their discussion is an offshoot of an experiment of Eichmann [3]. Duan *et al.* [4] extend to one-, two- and three-dimensional cases by obtaining a series solution of this problem. The present study is dedicated to the three-ion problem. As an initial study we will not consider the internal structures of the ions, that is, we shall ignore the internal degree of freedom, as Yin and Javanainen did in reference [2].

On the other hand, the Paul trap becomes a so-called "chaos lab" when more than one charged particle is trapped simultaneously. In the absence of laser cooling the Paul trap is a promising testing ground for ideas in classical and quantum Hamiltonian chaos. While chaos is generally concerned with the classical level, the quantum dynamics of the few-particle Paul trap provides new insights into the question of quantum chaos. References [5–8] show that even the collinear model of the atomic and molecular systems, *e.g.*, the one-dimensional atomic helium and hydrogen molecular ion, provides a rich variety of periodic orbits, a typical situation in nonlinear chaotic systems. Quantization of these orbits yields eigenvalues in good agreement with quantum results [6]. The system studied in this paper is another simple model for the restricted three-body problem, the collinear three trapped ions. The most collinear three-body systems reported previously are chaotic, however our work [9] based on classical treatment shows that the system of three trapped ions with a collinear configuration possesses a pure regular KAM zone. Thus, the corresponding quantum motion, besides providing us with interesting dynamical behavior and formal classical-quantum comparison, may actually be useful in providing new physical insights into the three-body problem.

In the next section we solve the Schrödinger equation in terms of the hyperspherical coordinate approach. The eigensolutions are investigated and two quantum numbers are introduced to classify the eigenstates in section 3. Then there follows a comparison between the classical periodic orbits and the quantum wave functions. In section 4 a brief review and discussion are presented.

2 Model and procedures

We consider three identical ions with mass m and charge e. Let us start with the one-dimensional motion under the harmonic oscillator binding potential with frequency ω_0. For this one-dimensional model (see Fig. 1), the total

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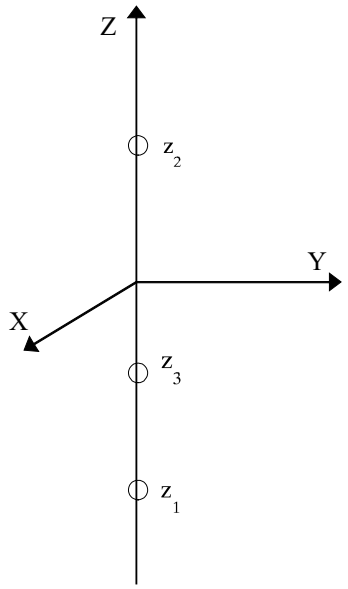

Fig. 1. The one-dimensional model of three Paul trapped ions.

Hamiltonian reads

$$H_0 = \frac{1}{2m}\sum_{i=1}^{3}(p_{zi}^2 + m^2\omega_0^2 z_i^2) + \frac{e^2}{4\pi\epsilon_0}\left(\frac{1}{|z_1 - z_2|} + \frac{1}{|z_2 - z_3|} + \frac{1}{|z_3 - z_1|}\right). \quad (1)$$

Let us review the classical formulas first. By setting $z_2 > z_3 > z_1$ (as shown in Fig. 1), and introducing a coordinate of the center of mass, $Z_{\rm c}$, and relative coordinates, u_1 and u_2,

$$\begin{aligned} Z_{\rm c} &= \frac{1}{3}(z_1 + z_2 + z_3), \\ u_1 &= z_2 - z_3, \\ u_2 &= z_3 - z_1, \end{aligned} \quad (2)$$

where both u_1 and u_2 vary from 0 to ∞, we can separate the center-of-mass motion from the relative motions and focus on the latter. Scaling the length u_1 and u_2 by the equilibrium distance d_0 and the time by $1/\omega_0$ as

$$\begin{aligned} \xi_i &= u_i/d_0, \\ \tau &= \omega_0 t, \end{aligned} \quad (3)$$

where $d_0 = [\frac{5e^2}{16\pi m\epsilon_0\omega_0^2}]^{1/3}$, the Hamiltonian scaled by $[m\omega_0^2 d_0^2]^{-1}$ for the relative motion is

$$H = p_1^2 + p_2^2 - p_1 p_2 + V(\xi_1, \xi_2)\,, \quad (4)$$

where p_i denotes the momentum associated with the new coordinate ξ_i, $i = 1, 2$, and the potential

$$V(\xi_1, \xi_2) = \frac{1}{3}(\xi_1^2 + \xi_2^2 + \xi_1\xi_2) + \frac{4}{5}\left(\frac{1}{\xi_1} + \frac{1}{\xi_2} + \frac{1}{\xi_1 + \xi_2}\right). \quad (5)$$

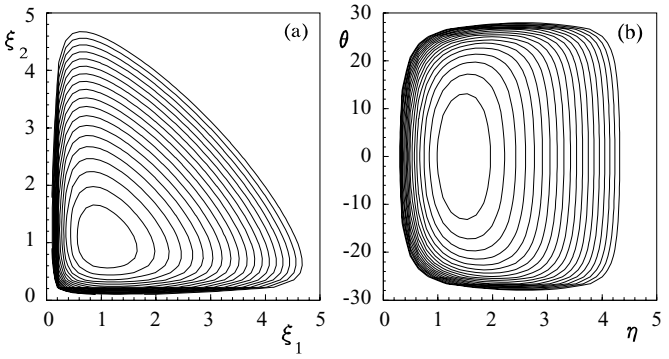

Fig. 2. The equipotential curves of the potential V in (a) ξ_1,ξ_2 coordinates and (b) η, θ coordinates. The potential minimum is located at $\theta = 0, \eta = \sqrt{2}$ or $\xi_1 = \xi_2 = 1$.

We may also introduce the Jacobi coordinates R, r as

$$\begin{aligned} Z_{\rm c} &= \frac{1}{3}(z_1 + z_2 + z_3), \\ R &= z_2 - z_1 \qquad (0 \le R < \infty), \\ r &= z_3 - \frac{1}{2}(z_1 + z_2) \qquad (|r| \le R/2). \end{aligned} \quad (6)$$

In terms of the scales of $d_0/\sqrt{2}$ and $1/\omega_0$, the Hamiltonian for the relative motion becomes

$$H = \frac{1}{2}P_R^2 + \frac{3}{8}p_r^2 + \frac{R^2}{2} + \frac{2}{3}r^2 + \frac{2\sqrt{2}}{5}\left(\frac{1}{R} + \frac{R}{\left(\frac{R}{2}\right)^2 - r^2}\right). \quad (7)$$

Furthermore, defining a set of hyperspherical coordinates:

$$\begin{aligned} R &= \eta\cos\theta, \\ r &= \frac{\sqrt{3}}{2}\eta\sin\theta, \end{aligned} \quad (8)$$

with the conditions of $\eta \ge 0$ and $|\theta| \le \frac{\pi}{6}$, one gets the Hamiltonian

$$H = \frac{1}{2}\left(p_\eta^2 + \frac{p_\theta^2}{\eta^2}\right) + \frac{\eta^2}{2} + \frac{2\sqrt{2}}{5\eta}f(\theta), \quad (9)$$

where

$$f(\theta) = \frac{1}{|\cos\theta|} + \frac{1}{|\cos(\theta - \pi/3)|} + \frac{1}{|\cos(\theta + \pi/3)|}. \quad (10)$$

The equipotential contour of the potential V as a function of ξ_1 and ξ_2, and of η and θ, respectively, is plotted in Figure 2.

From equation (9), we write the Schrödinger equation of the system as (in the following, we let $m = \hbar = 1$)

$$\left[-\frac{1}{2}\left(\frac{1}{\eta}\frac{\partial}{\partial\eta}\left(\eta\frac{\partial}{\partial\eta}\right) + \frac{1}{\eta^2}\frac{\partial^2}{\partial\theta^2}\right) + \frac{1}{2}\eta^2 + \frac{2\sqrt{2}}{5\eta}f(\theta)\right] \times\Phi(\eta, \theta) = E\Phi(\eta, \theta)\,. \quad (11)$$

Since the three ions are identical particles, the quantum Hamiltonian is invariant when the positions of any two ions are changed. Then the wave functions could be classified into either symmetric or antisymmetric, and the region for the variable θ should be changed into $-\pi$ to π. To obtain the eigensolution of the Schrödinger equation, we expand the wave function by a set of basis functions:

$$\Phi(\eta,\theta,\omega)=\sum_{nm} C^{\omega}_{nm}\phi^{\omega}_{n,m}(\eta,\theta), \tag{12}$$

where

$$\phi^{\omega}_{n,m}(\eta,\theta)=N_{nm}(\sqrt{\omega}\eta)^{|m|}e^{-\omega\eta^2/2}L_n^{|m|}(\omega\eta^2)X_m(\theta), \tag{13}$$

and

$$X_m(\theta)=\frac{1}{\sqrt{\pi}}\begin{cases}\cos m\theta, & \text{for the even parity,}\\ \sin m\theta, & \text{for the odd parity.}\end{cases} \tag{14}$$

Here, $N_{nm}=\sqrt{\frac{2\omega n!}{(n+|m|)!}}$, ω is a variational parameter, and $L_n^{|m|}$ the Laguerre polynomials. This basis function $\phi^{\omega}_{n,m}(\eta,\theta)$, satisfying the equation

$$\left[-\frac{1}{2}\left(\frac{1}{\eta}\frac{\partial}{\partial\eta}\left(\eta\frac{\partial}{\partial\eta}\right)+\frac{1}{\eta^2}\frac{\partial^2}{\partial\theta^2}\right)+\frac{\omega^2}{2}\eta^2\right]\phi^{\omega}_{nm}(\eta,\theta)=$$
$$\epsilon_{nm}\phi^{\omega}_{nm}(\eta,\theta), \tag{15}$$

is the eigen wave function of a coplanar harmonic oscillator of frequency ω with the energy $\epsilon_{nm}=(2n+|m|+1)\omega$. Considering the exchange symmetry of the identical particles, we reach

$$\Phi(\eta,\theta)=\Phi(\eta,\theta\pm\pi/3), \tag{16}$$

then the angular quantum number m has to be

$$m=\begin{cases}3(2l+1), & \text{for the even parity, } l=0,\pm1,\pm2,\ldots,\\ 6l, & \text{for the odd parity, } l=\pm1,\pm2,\ldots\end{cases} \tag{17}$$

The functions defined in equation (13), with their m value given by equation (17), construct a sub-space of the Hilbert space for $|\theta|<\pi$, then they are orthogonal in the region of $|\theta|<\pi/6$ as well. Thus, we have

$$\Phi(\eta,\theta=\pm\pi/6)=0. \tag{18}$$

It is easy to derive the matrix elements:

$$\langle n'm'|\eta^2|nm\rangle=\delta_{m',m}[-\sqrt{(n+1)(n+|m|+1)}\delta_{n',n+1}$$
$$+(2n+|m|+1)\delta_{n',n}-\sqrt{n(n+|m|)}\delta_{n',n-1}]/\omega, \tag{19}$$

$$\langle n'm'|\frac{1}{\eta}f(\theta)|nm\rangle=\frac{(-)^{\frac{|m'|-|m|}{2}}}{\pi}\sqrt{\frac{\omega n'!n!}{(n+|m|)!(n'+|m'|)!}}$$
$$\times\sum\frac{\Gamma\left(n-k-\frac{|m'|-|m|}{2}+\frac{1}{2}\right)}{(n-k)!}$$
$$\times\frac{\Gamma\left(n'-k-\frac{|m|-|m'|}{2}+\frac{1}{2}\right)}{(n'-k)!}$$
$$\times\frac{\Gamma\left(k+\frac{|m'|+|m|}{2}+\frac{1}{2}\right)}{k!}$$
$$\times\langle m'|f(\theta)|m\rangle, \tag{20}$$

where the value k varies from 0 to $\min(n,n')$. To calculate the matrix element of the function $f(\theta)$, we use the following integration:

$$\int_{-\frac{\pi}{6}}^{\frac{\pi}{6}}\frac{X_{m'}(\theta)X_m(\theta)}{\cos(\theta\pm\pi/3)}\mathrm{d}\theta=\int_{-\frac{\pi}{6}\pm\pi/3}^{\frac{\pi}{6}\pm\pi/3}\frac{X_{m'}(\theta)X_m(\theta)}{\cos\theta}\mathrm{d}\theta.$$

In this integration, the value of the angular quantum number m, and the boundary conditions of equation (18) have been considered. Thus we derive the matrix element for the function $f(\theta)$:

$$\begin{aligned}\langle m'|f(\theta)|m\rangle&=6\int_{-\pi/6}^{\pi/6}X_{m'}(\theta)X_m(\theta)f(\theta)\mathrm{d}\theta\\&=12\int_0^{\pi/2}\frac{X_{m'}(\theta)X_m(\theta)}{\cos\theta}\mathrm{d}\theta\\&=\Pi\frac{(-)^{(|m|+|m'|)/2+1}12}{\pi}\sum\frac{1}{2k-1},\end{aligned} \tag{21}$$

where Π denotes the parity, and k in the summation changes from $(|m'-m|)/2+1$ up to $(|m'|+|m|)/2$. The matrix element involving the mutual Coulomb potential for one-dimensional three-body systems is generally not integrable but can be numerically calculated in other coordinates [5]. We overcome this difficulty by the use of the angular basis functions with the choice of the angular quantum numbers by considering the boundary conditions and the symmetry of the system. This will ensure the correctness of our calculated results.

3 Eigensolutions and their classification

We solve for both the even and odd parity eigenvalues of the Schrödinger equation by diagonalizing the Hamiltonian in a Hilbert space of the 850 basis states (with $N_b=2n+m$ up to 102). In our practical calculations the variational parameter ω is chosen to be 3.9 to minimize the energy of the ground state. In Figure 3 we plot the contour of the norm of the eigen wave functions of some lower energy states. It is shown clearly that the distribution of the wave functions can be classified according to their nodal lines along both of the η and θ directions.

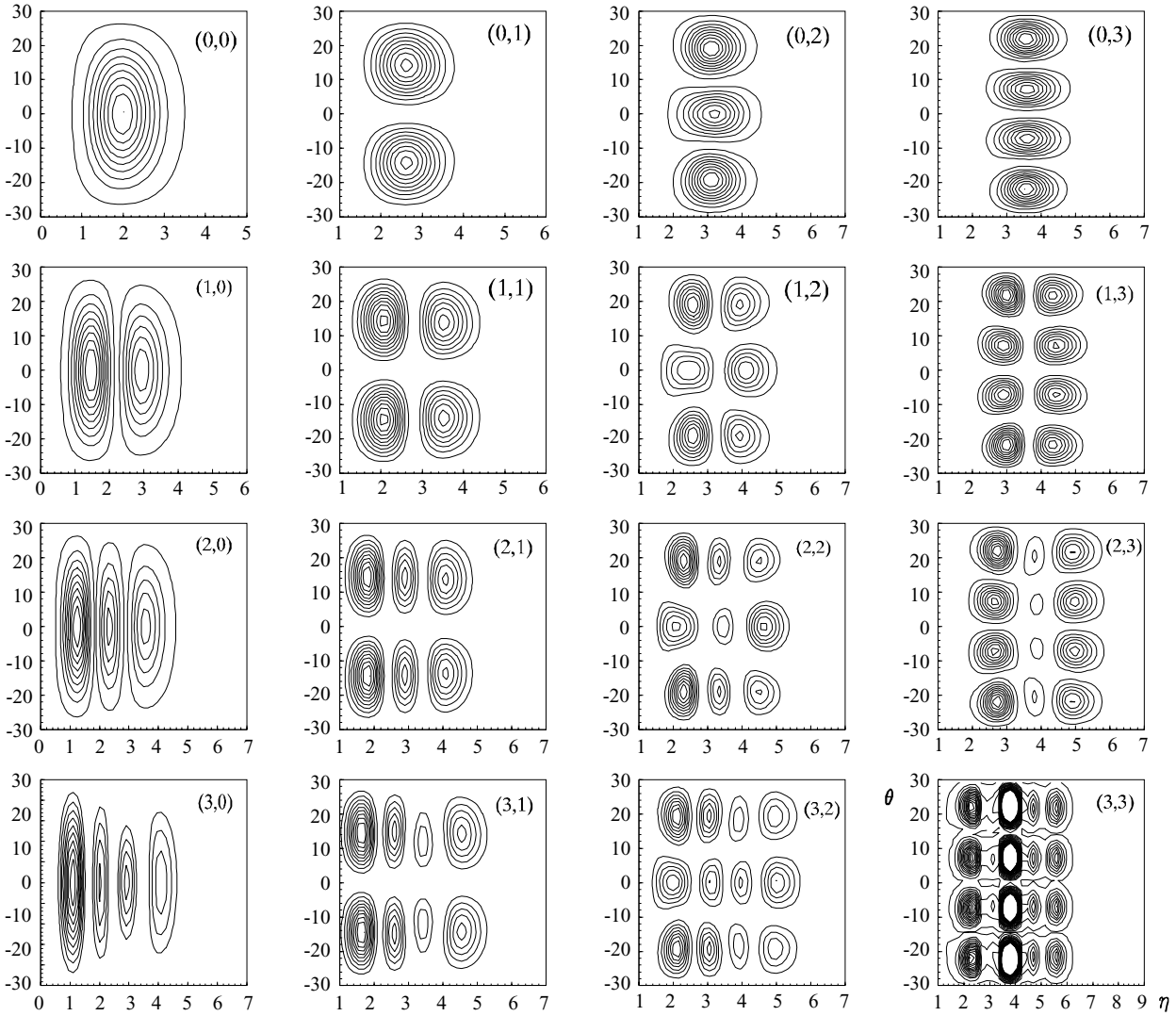

Fig. 3. Distributions of the wave functions in the η, θ coordinates. We label the states with the numbers of nodal lines along the η and θ directions.

Further investigation to the higher-energy states supports this conclusion. This results in a classification scheme. We simply use the numbers n_η and m_θ of the nodal lines in the two directions to label these states. Thus the parity of a state is just the same as even or odd m_θ of the state.

In Table 1 we present the eigenenergies. From the data in this table, we may easily find a formula to fit roughly the energies as

$$E(n_\eta, m_\theta) \approx A(2n_\eta + 3m_\theta + 4) + \frac{B}{2n_\eta + 3m_\theta + 4} + C, \tag{22}$$

where the fitting parameters $A = 0.972$, $B = 0.364$, and $C = 1.732$.

In order to gain insight into the physical quantum wave function distributions, we redraw the states of Figure 3 in Figure 4 in terms of the ξ_1 and ξ_2 coordinates. Through the analysis of the nodal structures we may find the modes of internal motion among these quantum states [10,11]. From these pictures and the data in Table 1 one may conclude:

i) The energy for the ground state is 5.71093, 1.71093 larger than that of the system in the absence of the mutual Coulomb interaction, for which its zero-point vibration energy should be $[2n+3(2l+1)+1] = 4$. The wave function of the ground state $(0, 0)$ locates near the region of $\theta = 0$ and $\eta = 2$, a little larger than the minimum of the potential, *i.e.* $\theta = 0$ and $\eta = \sqrt{2}$. Evidently, the motion of this state is a small oscillation around a valley of the potential. There is no nodal line in the wave function, as we expected.

ii) Let us consider the sequence of the $(n_\eta, 0)$ states. The wave functions of these states locate along the line of $\theta = 0$ (or $\xi_1 = \xi_2$). In classical mechanics, this corresponds to a periodic-orbit so-called "breathing" or symmetric stretching motion if one stands at the position of the third ion z_3.

Table 1. Eigenenergies of the collinear three Paul trapped ions.

	$m_\theta = 0$	1	2	3	4	5
$n_\eta = 0$	5.71093	8.54578	11.42628	14.33613	17.26436	20.20556
1	7.62493	10.49609	13.39127	16.31056	19.24445	22.18951
2	9.55409	12.45244	15.35785	18.28605	21.22501	24.17374
3	11.49483	14.41405	17.32573	20.26267	23.20596	26.15826
4	13.44493	16.38028	19.29506	22.24048	25.18722	28.14310
5	15.40297	18.35054	21.26627	24.21960	27.19404	
6	17.36778	20.32429	23.23971	26.20007	29.17491	
7	19.33811	22.30101	25.21561			
8	21.31266	24.28025	27.25287			
9	23.29041	26.26160	29.23677			
10	25.27064	28.24473				

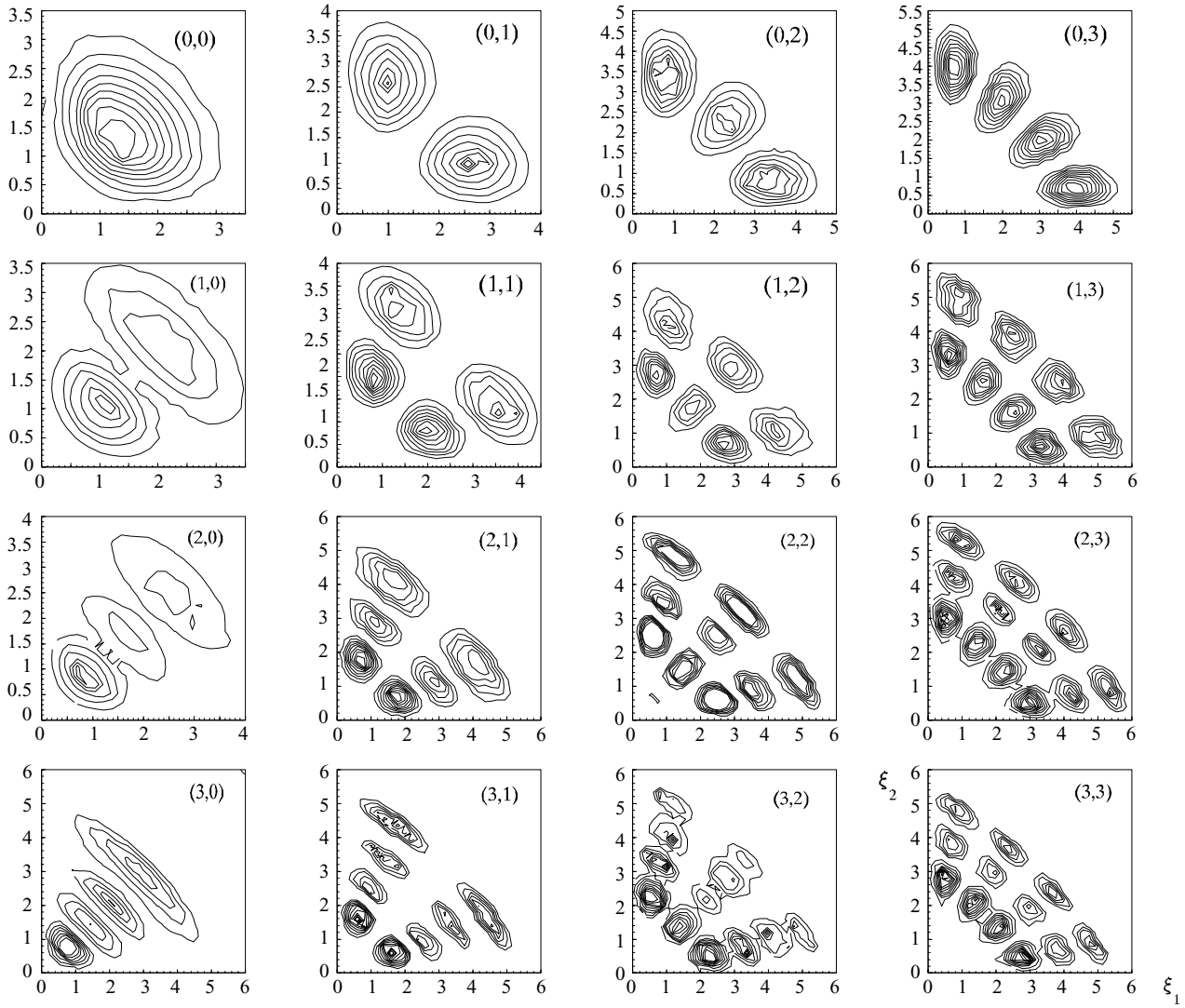

Fig. 4. The same as Figure 3 but in the ξ_1, ξ_2 coordinates.

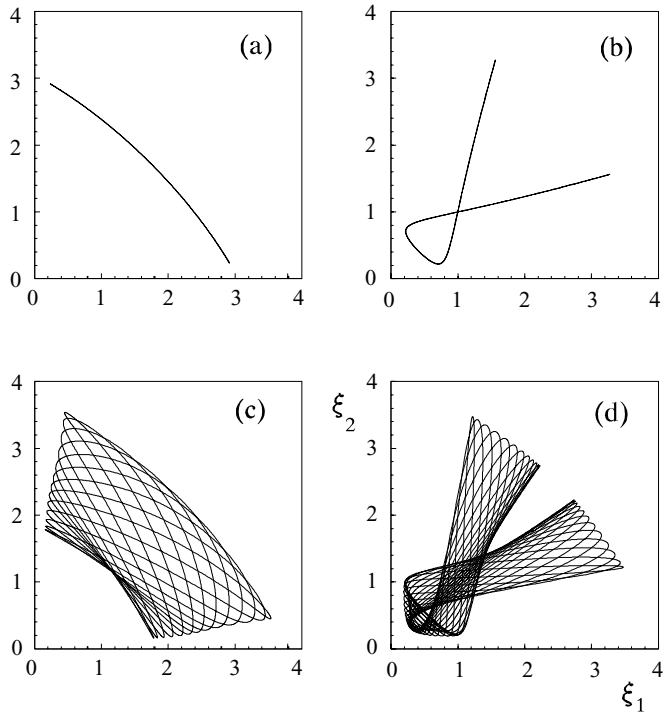

Fig. 5. Classical (quasi)periodic trajectories at energy = 5.7: (a) the anti-symmetric stretching motion; (b) the distorted symmetric stretching motion; (c) the quasi-anti-symmetric stretching motion; (d) the more general distorted symmetric stretching motion.

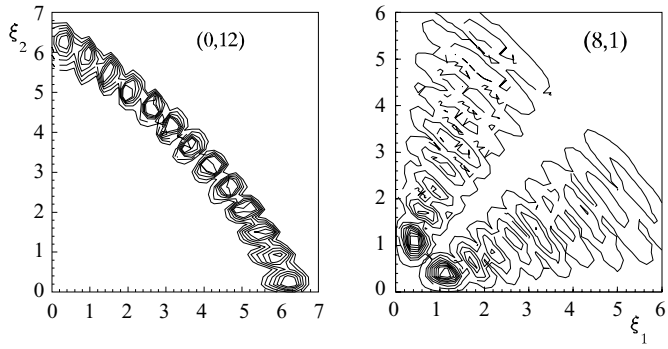

Fig. 6. The distributions of the wave function for the $(0, 12)$ and $(8, 1)$ states, which correspond to the classical periodic orbits shown in Figures 5(a) and (b).

iii) The classical study [9] shows that the classical motion of the system is not chaotic but regular, and all of the trajectories locate on a KAM torus. The study also shows that the KAM torus is dominated by two periodic orbits. One is the anti-symmetric stretching and the other a distorted symmetric stretching (see Fig. 5(a) and (b)). If one investigates the $(0, m_\theta)$ and $(n_\eta, 1)$ families, it will be found that as the quantum number m_θ or n_η increase, the wave function distributions of these two kinds of states will primarily overlap the location of these two classical periodic orbits. Two examples of these two families are shown in Figure 6.

iv) More general modes of quantum motion corresponding to the classical motion on a KAM torus (see Fig. 5(c) and (d)) should be the other quantum states with n_η and m_θ greater than 1, corresponding to classical symmetric and anti-symmetric quasiperiodic orbits (Fig. 5(c) and (d)). In fact, as the system is excited to higher states, the four modes corresponding to the four classical quasi-periodic orbits mentioned above will appear in the distributions of the wave functions (as an example, see Fig. 6)

4 Summary and discussion

We have carried out a systematic study of a one-dimensional model of the trapped three-ion system in a static potential well, which would apply to a "linear" Paul ion trap. For the quantum solutions we emphasize the following conclusions:

1) The hyperspherical-coordinate method we employed here could be applicable to most one-dimensional models of three-body Coulomb systems, since the integration (19) can be applied with only a slight modification. This will overcome the difficulty of the singularity of the numerical integration at the two-body collision.

2) The quantum states can be classified in the scheme of the nodal numbers in the two η and θ directions. The mode of the motion of a quantum state is governed by its nodal structure, which is determined by the symmetry and the energy of the system. Different states are characterized by different modes of motion. Higher states are generally dominated by more complicated modes, especially for the states with their quantum number n_η, m_θ more than 2.

3) The phenomenon of density enhancement of the probability density distributions of a high-energy eigenstate along a periodic orbit is called scarring [12], which is the trace of the classical chaos in the corresponding quantum states. In general, the classical motion of collinear three-body Coulomb systems is chaotic [5–7], the motion of the two Paul trapped ions in all three dimensions is chaotic too [13]. However, for the present model, we can only find the regular motion classically [9], which is in agreement with the distributions of the wave function.

It should be pointed out that the classical motion of a collinear trapped three-ion system in the Paul-trap rf driving fields becomes chaotic [14]. It should be more interesting to study its corresponding quantum motion. Another further study is the semiclassical quantization of the classical KAM torus or the periodic orbits. The results will be reported elsewhere.

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