

Quantum Torus Wave Function

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Abstract For two kinetically coupled identical Morse oscillator system, this paper introduced the concept of quantum torus wave function. Quantum torus wave function comes from the decomposition of a quantum wave function of the system. It reflects the symmetry of the quantum wave function. Physically, it corresponds to a quantizing torus or a quantizing cantorus (when it exists) in phase space. The number of nodes in x and y coordinates in the contour plot being the same as the quantum number in the Einstein-Brillouin-Keller (EBK) quantization conditions is the natural assignment of the given energy level. When quantizing torus or cantorus is destroyed by weak resonances in phase space, using quantum torus wave function to assign energy level is easier and reasonable. This paper also shows the application of quantum torus wave function in the study of dynamical tunneling.

Key words torus, cantorus, assignment, dynamical tunneling

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量子环波函数

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[摘要] 对两个动能耦合的全同 Morse 振子系统引入了量子环波函数的概念. 量子环波函数来源于一个系统量子态的分解, 反映量子波函数的对称性. 物理上对应于相空间中的一个量子化环或量子化康托环 (如存在的话). 等高线图中沿 x 轴和 y 轴的节点数目, 与 EBK 量子化条件中量子数相同, 是给定能级的自然命名. 当量子化环或量子化康托环被相空间中弱谐振带破坏时, 用量子环波函数命名能级更容易, 也是合理的. 这篇文章也显示了量子环波函数在研究动力学隧穿的潜在应用.

[关键词] 环, 康托环, 命名, 动力学隧穿

Spectrum assignment has been an important task for spectroscopists, atomic and molecular physicists. Historically, people used normal mode assignment for low excited states, which is reasonable because the potential energy surface in the lower part can be approximated to harmonic oscillators. With the development of laser techniques, a molecule can be easily excited to states where the harmonic oscillator approximation is no longer valid. An example is the H_2O molecule^[1] which is a normal-local transition in phase-space, so it is not quite accurate to use just a normal mode assignment method, as the classical object corresponding to the given energy level may not be a normal mode character. Kellman et al studied the bifurcation structure^[2] and catastrophe classifications^[3] of a molecular fitting Hamiltonian, from which they assigned local (normal) mode quantum numbers to levels that correspond to local (normal) mode trajectories^[4]. Using physical quantum numbers to assign the energy level for a nonintegrable system, we need to search a classical torus or cantorus^[5,6] in phase space which

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satisfies some quantization conditions. The energy required for the quantization conditions is the semiclassical eigenenergy of the system. The integers in the quantization conditions are the quantum numbers which will be used to assign the given energy level.

One of the important applications of semiclassical quantization is the energy level assignment, but semiclassical quantization is not the only way to assign energy level. When quantum wave function is easy to calculate, for example, for the two kinetically coupled identical Morse oscillators, we can assign the energy level by quantum wave function through desymmetrization of the local mode doublet^[7], a small splitting of two degenerated energy levels by dynamical tunneling^[8]. In this paper, we introduce the concept of quantum torus wave function, which is of course uniform and reflects the effect of classical chaos and dynamics on the quantum state. Quantum torus wave functions come from the desymmetrization of a given energy quantum state; it is different from the traditional desymmetrization method^[7]. We will apply this concept to the energy level assignment and compare with the semiclassical assignment of quantum energy levels.

1 Quantum Torus Wave Function

The Hamiltonian for two kinetically coupled identical Morse oscillators is given by

$$H = \frac{p_1^2}{2m} + \frac{p_2^2}{2m} + \frac{\delta}{m} p_1 p_2 + D(1 - \exp(-\beta x_1))^2 + D(1 - \exp(-\beta x_2))^2, \quad (1)$$

where δ is the coupling parameter, β is called Morse parameter, and D is the dissociation energy for the Morse oscillator. Except for $\delta = 0$ and $\delta = -1$, this is a nonintegrable system, phase space can be classified into regular and irregular regions at higher energy.

The Hamiltonian in (1) is invariant under the exchange of these two Morse oscillators, so the quantum wave function should be either symmetric or antisymmetric; a common eigenstate for both Hamiltonian operator (1) and exchange operator \hat{p}_{12} . Let us introduce the unitary exchange operator $U(\hat{p}_{12})$ which satisfies

$$\phi(x_2, x_1) = U(\hat{p}_{12})\phi(x_1, x_2) = \pm\phi(x_1, x_2). \quad (2)$$

The eigenvalues of $U(\hat{p}_{12})$ are equal to ± 1 , which agrees with the definition of either symmetric or antisymmetric of the system quantum wave function. Now, let us consider the bound states; its wave function can be written as superposition of the zeroth order wave functions from two uncoupled Morse oscillators, i.e.,

$$\phi(x_1, x_2) = \sum_{n_1=0}^{n_{\max}} \sum_{n_2=0}^{n_{\max}} C(n_1, n_2) \phi_{n_1}(x_1) \phi_{n_2}(x_2), \quad (3)$$

where

$$C(n_2, n_1) = \pm C(n_1, n_2). \quad (4)$$

$\phi_{n_1}(x_1)$, $\phi_{n_2}(x_2)$ are bound states for 1-dim. Morse potential, and n_{\max} is the number of bound states in the Morse potential well. Note that (4) is a necessary and sufficient condition for the wave function (3) to be symmetrized. This means if the coefficient matrix is either symmetric or antisymmetric, then we can show that the system wave function will be also either symmetric or antisymmetric. On the other hand, the wave function in (3) can be decomposed into the following form

$$\begin{aligned} \phi(x_1, x_2) &= \sum_{n_1=0}^{n_{\max}} \sum_{n_2=0}^{n_1} C(n_1, n_2) \phi_{n_1}(x_1) \phi_{n_2}(x_2) + \sum_{n_1=0}^{n_{\max}} \sum_{n_2=n_1}^{n_{\max}} C(n_1, n_2) \phi_{n_1}(x_1) \phi_{n_2}(x_2) - \\ &\sum_{n_1=0}^{n_{\max}} C(n_1, n_1) \phi_{n_1}(x_1) \phi_{n_1}(x_2) = \phi_1^t(x_1, x_2) + \phi_2^t(x_1, x_2) - \sum_{n_1=0}^{n_{\max}} C(n_1, n_1) \phi_{n_1}(x_1) \phi_{n_1}(x_2), \end{aligned} \quad (5)$$

where

$$\phi_1^t(x_1, x_2) = \sum_{n_1=0}^{n_{\max}} \sum_{n_2=0}^{n_1} C(n_1, n_2) \phi_{n_1}(x_1) \phi_{n_2}(x_2), \quad (6)$$

$$\phi_2^t(x_1, x_2) = \sum_{n_1=0}^{n_{\max}} \sum_{n_2=n_1}^{n_{\max}} C(n_1, n_2) \phi_{n_1}(x_1) \phi_{n_2}(x_2), \quad (7)$$

are called quantum torus wave functions. They look like semiclassical torus wave functions constructed from classical trajectories. In this sense, (6) and (7) correspond to two physical tori. In the following, we will prove the symmetry relations between these two quantum torus wave functions.

2 Symmetry Relation of the Quantum Torus Wave Function

These two quantum torus wave functions are related to each other by the following relation

$$U(\hat{p}_{12}) \psi_1'(x_1, x_2) = \pm \psi_2'(x_1, x_2), \quad (8)$$

$$U(\hat{p}_{12}) \psi_2'(x_1, x_2) = \pm \psi_1'(x_1, x_2), \quad (9)$$

where the plus sign refers to the symmetric quantum state of the system, and the minus sign indicates that the quantum state of the system is antisymmetric. To prove these relations, we will take the symmetric state in (8) as an example, and the antisymmetric state case can be done similarly.

Consider the left hand side of the first equation in (8), which can be written as

$$U(\hat{p}_{12}) \psi_1'(x_1, x_2) = \sum_{n_2=0}^{+\infty} \sum_{n_1=0}^{n_2} C(n_1, n_2) \psi_{n_1}(x_1) \psi_{n_2}(x_2). \quad (10)$$

Comparing (7) and (10), both involve the same matrix elements which are in the upper triangle including the diagonal part of the two dimensional coefficient matrix for a given eigenenergy. So

$$U(\hat{p}_{12}) \psi_1'(x_1, x_2) = \psi_2'(x_1, x_2). \quad (11)$$

It should be noted that the two quantum torus wave functions are exact decomposition of the antisymmetric quantum wave function, because the last term in (5) is zero. For symmetric beam mode quantum wave function, the diagonal elements of the coefficient matrix are usually very small compared to the largest matrix element which is off diagonal, so the two quantum torus wave functions are an approximate decomposition of the symmetric wave function. This method of desymmetrization does not work for normal mode states as the largest matrix element is usually on the diagonal of the coefficient matrix.

We can find the symmetry property of the symmetrized quantum wave function by looking at the coefficient matrix corresponding to an eigenenergy. A symmetric matrix represents a symmetric state and an antisymmetric matrix corresponds to an antisymmetric state. The manifestation of the symmetry property of the quantum wave function on the quantum torus wave function is reflected by (8), (9), (5) and (2). This means if the symmetrized quantum wave function is symmetric, then the two quantum torus wave functions are related by exchanging the two coordinate variables; otherwise if the symmetrized quantum wave function is antisymmetric, the two quantum torus wave functions are related by exchanging the two coordinate variables along with a phase π changes. So the quantum torus wave functions can approximately replace the symmetrized quantum wave function.

Quantum torus wave functions correspond to not only the classical tori in phase space, they may also correspond to the classical cantori in the chaotic region of the phase space. We can see that the quantum torus wave functions of most states for nonintegrable system are very much like the wave functions of classical tori. Other useful property for quantum torus wave function method is that it can show us the tunneling pair of the classical tori in phase space for a given quantum state. In discussion section, we will show the strong character on the quantum torus wave functions for strongly tunneling states. Because of the strongly tunneling effect, it is hard to assign integer quantum numbers to these states by the quantum torus wave functions.

Another character of quantum torus wave function is that it automatically exhibits either the beam mode or the normal mode property of the corresponding classical torus without doing numerical search, which makes the level assignment easier.

3 Result of Level Assignment

Using quantum torus wave functions to assign energy level is actually to count the numbers of nodes in x_1 and x_2 (or some other appropriate curvilinear coordinates) directions of the quantum torus wave functions. In this

section we will give examples of level assignment for states whose classical correspondence are tori and for states that correspond to either a quantizing cantorus or a destroyed quantizing cantorus by resonance in phase space. For torus we will choose states within approximate polyad number of 8 (total number of quanta=8) for a system of coupling constant $\delta = -0.014$. For cantorus we will assign state (13, 1) and state (10, 0) for coupling $\delta = -0.0728$. Other parameters we use in Hamiltonian (1) are given by $\omega_0 = \sqrt{2D\beta^2/\hbar} = 7.2916 \times 10^{14} \text{ s}^{-1}$, $D = 44505.216 \text{ cm}^{-1}$, $\beta = 2.175 \times 10^8 \text{ cm}^{-1}$.

3.1 Assignment of level corresponding to classical torus for a system of coupling constant $\delta = -0.014$

Semiclassically to assign a quantum state is to search a classical torus in phase space which satisfies the EBK quantization conditions

$$\oint_{C_1} p_1 dx_1 + p_2 dx_2 = 2\pi \hbar \left(n_1 + \frac{1}{2} \right), \quad (12-1)$$

$$\oint_{C_2} p_1 dx_1 + p_2 dx_2 = 2\pi \hbar \left(n_2 + \frac{1}{2} \right), \quad (12-2)$$

for a two-degree of freedom system, where C_1 and C_2 are two topologically independent circuits for the torus. For the local mode torus, the circuits C_1 and C_2 are usually taken as the contours made by the torus in Surface Of Section (SOS) at $x_2 = 0$, $p_2 > 0$ and in SOS at $x_1 = 0$, $p_1 > 0$ respectively. n_1 and n_2 are two integers (n_1, n_2) is the primitive assignment for the quantum state, which does not distinguish the symmetric and anti-symmetric quantum states. This weakness can be avoided by quantum torus wave function assignment method.

Polyad number p is the total number of quanta, i.e., $p = n_1 + n_2$ for two-degree of freedom system. p is constant but n_1 and n_2 vary. It is precisely defined for integrable system, where the Hamiltonian is block diagonal and the dimension of the submatrix for the Hamiltonian is p . In the regular region of phase space and the weak coupling, we still can talk about polyad number approximately. For polyad

Table 1 The comparison of two assignment methods

\mathcal{E}_q	\mathcal{E}_s	Semical Assign	Quant Assign
0.645 676 385	0.645 673 8	(8, 0) (0, 8)	(8, 0) (0, 8) ⁻
0.672 116 122	0.672 115 2	(7, 1) (1, 7)	(7, 1) (1, 7) ⁻
0.690 971 407	0.690 952 1	(6, 2) (2, 6)	(6, 2) (2, 6) ⁻
0.702 948 885	0.701 759 1	(5, 3) (3, 5)	(5, 3) (3, 5) ⁻
0.701 157 120	0.701 759 1	(5, 3) (3, 5)	(5, 3) (3, 5) ⁺
0.707 679 781	0.707 557 3	(0, 8) _N	(4, 4) ⁺

number $p = 8$, the states are $(8, 0) (0, 8)^{\pm}$, $(7, 1) (1, 7)^{\pm}$, $(6, 2) (2, 6)^{\pm}$, $(5, 3) (3, 5)^{\pm}$, and $(4, 4)^{\pm}$. The “ \pm ” represents that the state is symmetric for “+” and antisymmetric for “-”. In table 1, we showed semiclassical assignment and quantum torus wave function assignment. For quantum torus wave function assignment, each pair of quantum torus wave functions is an assignment to a given state. Semiclassical assignment comes from the quantizing actions in (12) satisfied by a quantizing torus. Quantum torus wave function assignment is shown in Figure 1(a-f).

We showed both $(5, 3) (3, 5)^{-}$ and $(5, 3) (3, 5)^{+}$ states because the splitting between the symmetric and antisymmetric states is very large ($\approx 80 \text{ cm}^{-1}$). The $(5, 3) (3, 5)^{+}$ state has a strong normal mode character; it resembles $(8, 0)_N$ state where the number of symmetric stretch quanta is $n_s = 8$ and the number of antisymmetric stretch quanta $n_a = 0$, which can be seen from the quantum wave function itself and the corresponding quantum torus wave functions. But it should be noted that we could not find the quantizing torus of state $(8, 0)_N$ in normal mode region in phase space. The quantum wave function $(5, 3) (3, 5)^{+}$ and the wave function $(4, 4)^{+}$ construct a conjugate pair of the normal mode state for this polyad $p = 8$. The difference is that a quantizing torus $(8, 0)_N$ does not exist in normal mode region, but the state $(0, 8)_N$ for $(4, 4)^{+}$ does exist in normal mode region in phase space.

3.2 Assignment of level corresponding to classical cantorus

A cantorus is a chaotic remnant of a classical torus in phase space; it is the barrier to transport when torus is destroyed. If the cantorus satisfies the EBK-like quantization conditions as (12), then we say that the cantorus is a quantizing cantorus. The integers n_1 and n_2 in (12) is a semiclassical assignment to the quantum state.

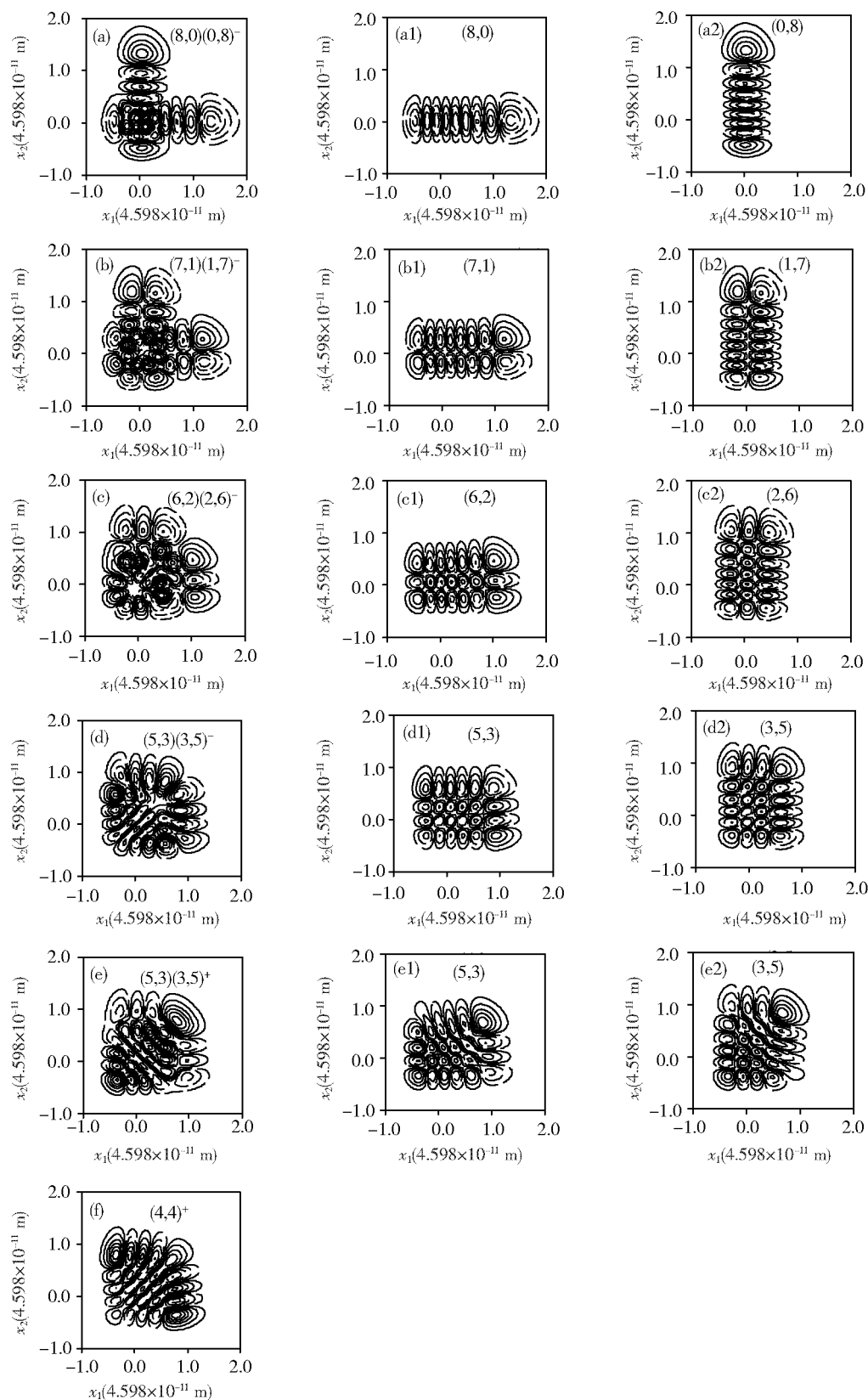


Fig.1 Quantum torus wave function assignment for states within polyad $P=8$

Quantum state $(13\ 1)\ (1\ 13)^+$ at coupling $\delta = -0.072\ 8$ and $\hbar = 0.712$ is quantized^[9] semiclassically, it corresponds to a Golden-Mean cantorus (the winding number of the cantorus is golden-mean) in phase space. The semiclassical energy obtained by the quantization is given by $\mathcal{E}_s = 0.749\ 888\ 33/D$, which differs from the average quantum energy $\bar{\mathcal{E}}_q$ on the local mode doublet $(13\ 1)\ (1\ 13)^\pm$ by $\mathcal{E}_s - \bar{\mathcal{E}}_q = -5.053 \times 10^{-5}/D$ or about

-2.25 m^{-1} . The spacing of quantum energy levels for the two adjacent local mode doublets around energy \mathcal{E}_s is about $2.949 \times 10^{-3} [D]$ or 131.26 m^{-1} . The contour plots for the wave function $(13, 1)(1, 13)^+$ and its quantum torus wave functions are shown in Figure 2(a) row. Even though the classical motions in phase space for this state is chaotic, its quantum torus wave function is regular. In Figure 2(b) row we show the contour plots for state $(10, 0)(0, 10)^+$ and its corresponding quantum torus wave function at coupling $\delta = -0.0728$. The quantizing cantorus in phase space is destroyed by 4/7 strong resonance, so semiclassical assignment is not in existence for this state. Quantum torus wave function for this state shows the strong dynamical tunneling

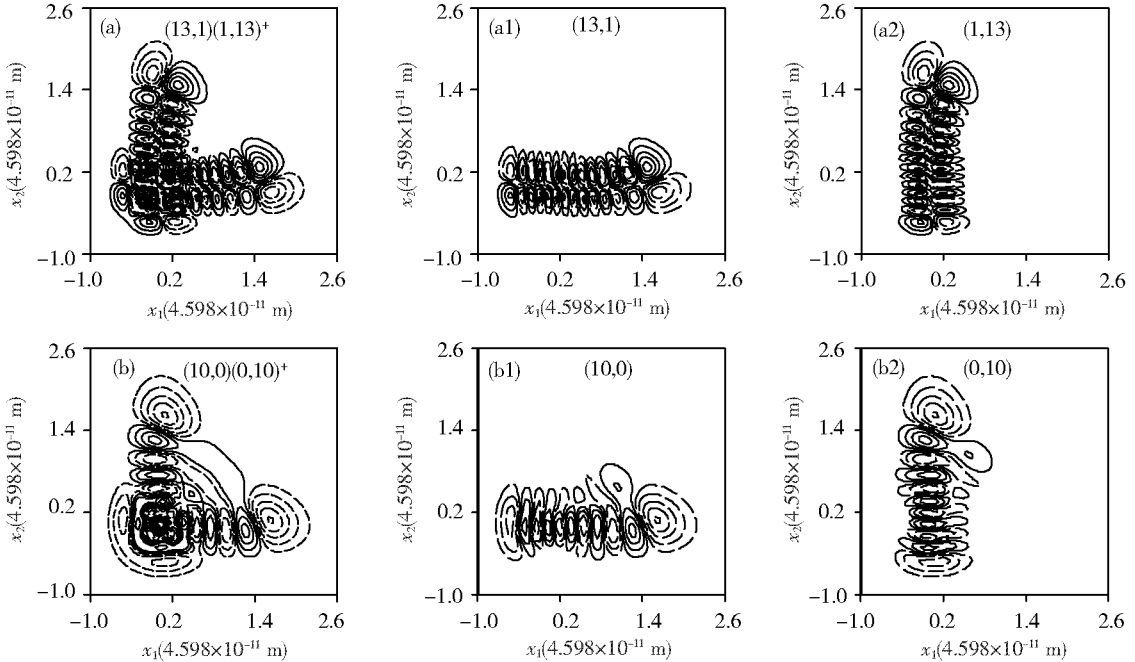


Fig.2 Quantum torus wave function assignment for states corresponding to classical cantorus in (a) row and destroyed cantorus by 4/7 strong resonance in (b) row

3.3 Discussion on dynamical tunneling between different types of tori

Using quantum torus wave function method we can find the tunneling pair for a given quantum state. In the regular region of the spectra, the tunneling pair usually is (n_1, n_2) and (n_2, n_1) only, tunneling with other tori can be neglected, but in the irregular region, tunneling with other tori can be dominant. In Figure 3(a) row, we show the number 91 symmetric quantum state at $\delta = -0.014$ and its desymmetrization by quantum torus wave function method. The desymmetrized wave functions are approximately torus character ($\approx (9, 3)$ and $\approx (3, 9)$) in the sense that we can not assign integer quantum numbers to them. However, semiclassically this state can be quantized primarily very well by torus quantization with $n_1 = 9$ and $n_2 = 3$. The difference between semiclassical energy \mathcal{E}_s and average quantum energy $\bar{\mathcal{E}}_q$ on local mode doublet (number 91 and number 92 states) is given by $\mathcal{E}_s - \bar{\mathcal{E}}_q = 1.534 \times 10^{-5} [D] = 0.683 \text{ m}^{-1}$ only. The reason that the desymmetrized wave function differ from torus wave function is due to the weak tunneling of torus state $(9, 3)$ or $(3, 9)$ with other type torus state $(15, 0)$ or $(0, 15)$. The desymmetrized wave functions for number 93 state are approximately two tori states $(15, 0)$ and $(0, 15)$. Once again, the difference from the exact tori states comes from the tunneling with tori states $(9, 3)$ and $(3, 9)$, and the quantizing tori for states $(15, 0)$ and $(0, 15)$ exist in phase space. The energies for the two tunneling doublets (4 energy levels) are given by

$$\begin{aligned} \mathcal{E}_q^{91} &= 0.9367652534586932 [D], & \mathcal{E}_q^{92} &= 0.9367677689242470 [D], \\ \mathcal{E}_q^{93} &= 0.9368004040634637 [D], & \mathcal{E}_q^{94} &= 0.9368005279069438 [D]. \end{aligned}$$

States for \mathcal{E}_q^{91} and \mathcal{E}_q^{93} are symmetric, and states for \mathcal{E}_q^{92} and \mathcal{E}_q^{94} are antisymmetric. Because the tunneling be-

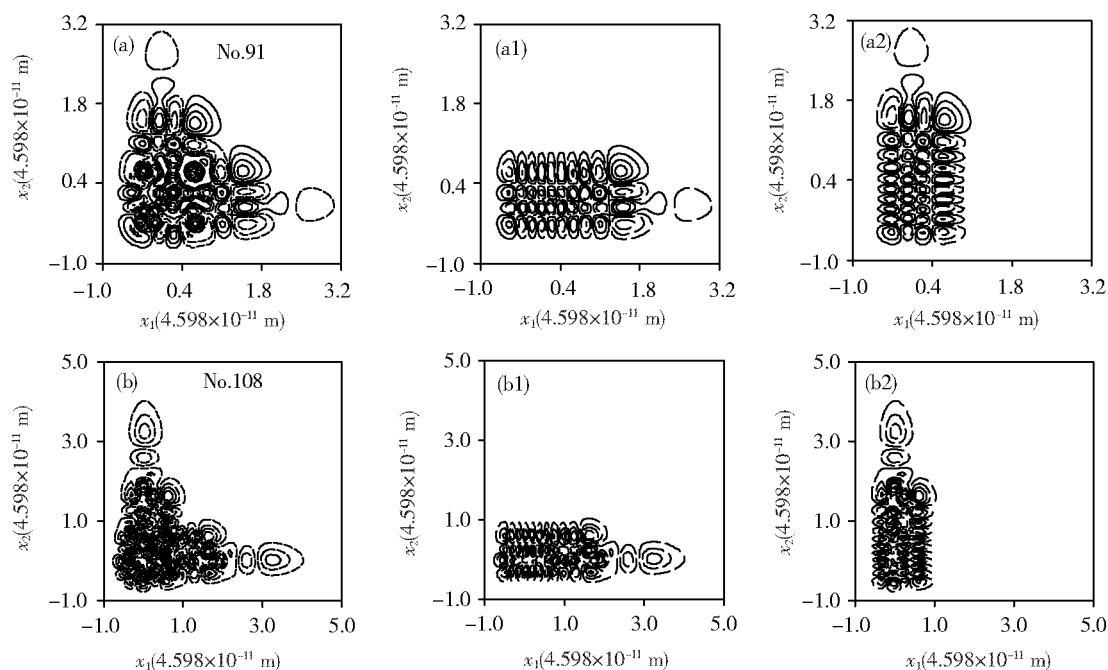


Fig.3 Quantum wave functions and its decomposition by quantum torus wave function method for state No.91 in (a) row and state No.108 in (b) row

tween torus (9 3) and torus (3 9) are strong , tunneling between torus (9 3) (or (3 9)) and torus (15 0) are weak , so the tori character in the desymmetrized wave function are still in existence . Another example is shown in Figure 3 (b) row , where we show the number 108 symmetric wave function at $\delta = - 0.014$ and its desymmetrized wave functions by quantum torus wave function method . Obviously , these are far from tori wave functions . Semiclassically , we found that quantizing tori corresponding to states (10 3) and (3 10) are barely destroyed by weak resonance 9 / 14 . The semiclassical energy \mathcal{E}_s for quantizing periodic orbit 9 / 14 is given by $\mathcal{E}_s = 0.985\,897\,185 [D]$, which differ from the average quantum energy $\bar{\mathcal{E}}_q$ on local mode doublet (level number 108 and level number 109) by $\mathcal{E}_s - \bar{\mathcal{E}}_q = - 2.451\,5 \times 10^{-5} [D] \approx - 1.09\,\text{cm}^{-1}$. The EBK type quantum numbers n_1 and n_2 can be obtained from the nearby cantorus and its separatrices , which gives $n_1 = 9.990\,79$ and $n_2 = 3.005\,92$. Desymmetrized wave functions come from the tunneling between the cantorus for (10 3) and the cantorus for (17 0) , cantorus for state (17 0) is in the strongly chaotic region , many resonances around in phase space . The energies for the four energy levels corresponding to two local mode doublets are very close and are given by

$$\begin{aligned}\mathcal{E}_q^{106} &= 0.985\,864\,091\,724\,236\,5 [D] , & \mathcal{E}_q^{107} &= 0.985\,864\,188\,552\,198\,9 [D] , \\ \mathcal{E}_q^{108} &= 0.985\,921\,612\,410\,902\,5 [D] , & \mathcal{E}_q^{109} &= 0.985\,921\,836\,237\,718\,5 [D] .\end{aligned}$$

Quantum wave functions and their desymmetrized wave functions for these four states are very similar ; this means that the tunneling between cantorus for state (10 3) and cantorus for state (17 0) is very strong , making their wave functions severely mixed up .

This can be understood in another way . Suppose the equal weighting of the tori (10 3) , (3 10) , (17 0) , and (0 17) for any state from the number 106 to the number 109 , we can construct the set of states by superposition of quantum states ϕ_q^{106} , ϕ_q^{107} , ϕ_q^{108} , and ϕ_q^{109} in the following

$$\phi_1 = \frac{\phi_q^{106} + \phi_q^{108} + \phi_q^{107} + \phi_q^{109}}{2} , \tag{13}$$

$$\phi_2 = \frac{\phi_q^{106} + \phi_q^{108} - \phi_q^{107} - \phi_q^{109}}{2} , \tag{14}$$

$$\phi_3 = \frac{\phi_q^{106} - \phi_q^{108} + \phi_q^{107} - \phi_q^{109}}{2} , \tag{15}$$

$$\phi_4 = \frac{\phi_q^{106} - \phi_q^{108} - \phi_q^{107} + \phi_q^{109}}{2}. \quad (16)$$

As shown in Figure 4(a–d), numerical calculation shows that ϕ_1 is torus state (10 3), ϕ_2 is torus state (17 0), ϕ_3 is torus state (3 10), and ϕ_4 is torus state (0 17). The deviation from integrable torus state comes from the tunneling among them.

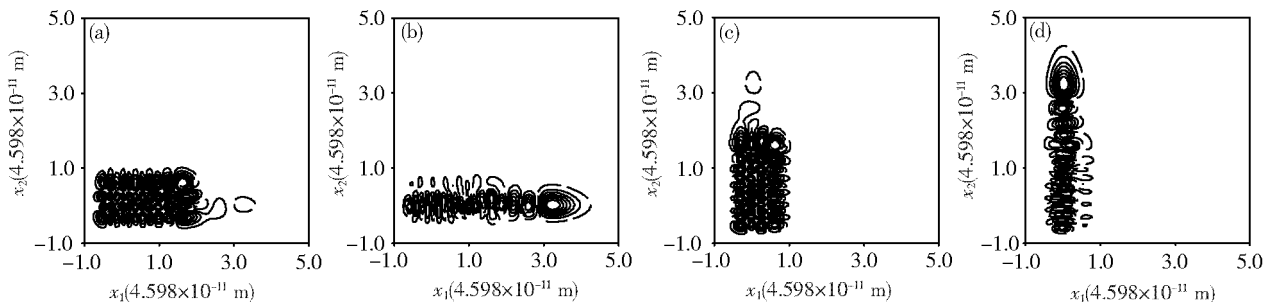


Fig.4 The 4 different superposition states for the states No.106, No.107, No.108, No.109

4 Conclusion

Starting from a quantum wave function, this paper introduced the concept of quantum torus wave function for an ABA type triatomic molecule. Quantum torus wave function comes from the decomposition of a single quantum state, which is different from the traditional desymmetrization method where a couple of quantum states (usually the local mode doublet) are involved. Except for the similarities to the semiclassical wave function of classical torus, quantum torus wave function also reflects the symmetry property of the given quantum wave function. One of the applications of the quantum torus wave function is the level assignment. By using quantum torus wave function we can accurately assign energy levels. For example, the $(5, 3)(3, 5)^{\pm}$ quantum states at coupling $\delta = -0.014$. It is more reasonable to assign state $(5, 3)(3, 5)^{+}$ as $(8, 0)_N$, which means $n_s = 8$ and $n_a = 0$ because it is similar to state $(4, 4)^{+}$ that is assigned as $(0, 8)_N$ normal mode state by semiclassical quantization method. But state $(5, 3)(3, 5)^{-}$ is more like a local mode torus state. Semiclassically, we can only assign $(5, 3)(3, 5)^{\pm}$ states as $(5, 3)(3, 5)$ state. It has been shown in this paper that the quantum torus wave function corresponds to not only the classical torus but also classical cantorus in phase space. We have also demonstrated the application of quantum torus wave function method in dynamical tunneling studies.

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