# Bifurcation Phenomena of Two Kinetically Coupled Morse Oscillators

Yang Shuangbo

(School of Physical Science and Technology, Nanjing Normal University, Nanjing 210097, China)

**Abstract** Starting from two uncoupled Morse oscillators, this paper first studied the bifurcation structures in the local mode region in phase space for two kinetically coupled Morse oscillators. It turns out that local mode resonances $\frac{n}{m}$ coexistence in phase space for a weak coupling parameter relating to the system energy through the inequality equation $\sqrt{\frac{1}{1-}}$ $\frac{n}{m}$ $\sqrt{1-}$. This paper also reports the bifurcation phenomena of symmetric stretch normal mode with both system energy and coupling parameter. At a weak coupling parameter, the symmetric stretch experiences a pitch fork bifurcation at a very low energy domain, then the local mode regions are gradually formed with system energy. For an intermediate high energy, the symmetric stretch normal mode stays stable and unstable alternatively with coupling parameter in the range [-1, 0].

**Key words** bifurcation; Morse oscillator; local mode; normal mode; resonance

**CLC number** O413.1 **Document code** A **Article ID** 1001-4616(2008)01-0052-06

# 两个动能耦合 Morse振子系统的分岔现象

杨双波

(南京师范大学物理科学与技术学院,江苏 南京 210097)

[摘要] 从两个未耦合的 Morse振子出发,首先研究了两个动能耦合的 Morse振子系统局域模区域内的分岔结构.发现对弱耦合参数 ,相空间中局域模谐振$\frac{n}{m}$共存与系统能量 通过不等式 $\sqrt{\frac{1}{1-}}$ $\frac{n}{m}$ $\sqrt{1-}$相关联.同时报导了对称伸缩本征模的分岔现象与能量及耦合常数的关系.在弱耦合参数 下,在非常低的能量区域内,对称伸缩经历一个 pitch-fork分岔.随后,局域模随能量的增加逐渐形成.对中等高能量 ,对称伸缩本征征模在耦合参数范围[-1, 0]内由不稳定到稳定到不稳定等交替变化.

[关键词] 分岔, Morse振子,局域模,本征模,谐振

The classical Hamiltonian for a system of two kinetically coupled Morse oscillators can be written as the following form

$$= \frac{1}{2}p_1^2 + \frac{1}{2}p_2^2 + p_1p_2 + (1-e^{-x_1})^2 + (1-e^{-x_2})^2, \quad (1)$$

where $= \frac{m}{M}\cos$ is the coupling parameter. This Hamiltonian is a good model for the vibrational motions of some type of triatomic molecule, such as $H_2O$, which has a smaller mass ratio between the light atom and the heavier central atom, and the $x_1$, $x_2$ correspond to the displacement from its equilibrium point for each OH bond. The classical motions for this type of molecule have been first studied by Jaffe and Brumer in 1980[1]. They

**Received date:** 2007-05-22.

**Foundation item:** Supported by the National Natural Science Foundation of China (10674073) and Nanjing Normal University (2005102XYY1805)

**Biography:** Yang Shuangbo, born in 1958, professor, majored in atomic, molecular physics and nonlinear physics. E-mail: yangshuangbo@njnu.edu.cn

found that at lower energy the classical motions for $H_2O$ in phase space basically can be classified into local mode and normal mode regions. The higher order resonances will be turned on at higher system energy. Matsushita and Terasaka[2] studied the classical motions for large coupling parameter | | case when the Hamiltonian no longer represents the vibrational motions of a real triatomic molecule. Recently, we quantized this Hamiltonian system by finding quantizing tori[3] in local mode region, and buildling semiclassical wave function[4-5], for both rational and irrational tori. In this paper, we will start from two special cases to illustrate the phase space bifurcation structures of this type of Hamiltonian system. We will use = 0 to explain the bifurcation phenomena in local mode region, and very small to illustrate the bifurcation in normal mode region. The finite coupling and finite system energy cases can be explained from those special cases phenomenologically.

This paper is organized in the following. In section 1, we will discuss the bifurcation phenomena within local mode region. The bifurcation phenomena within normal mode region will be discussed in section 2. We summarize this paper in section 3.

## 1 Bifurcation Phenomena Within Local Mode Regions

### 1.1 Bifurcation with System Energy at = 0

Phase space structures for the two uncoupled Morse oscillators are tori. These tori can be classified into rational and irrational two types. Which torus exists in phase space really depends on the system energy . To determine the existence of any torus in phase space, we will take rational tori to illustrate, because one can find an irrational torus in the very neighborhood of a rational torus with closed winding number.

The Hamiltonian for two uncoupled Morse oscillators can be written as[6]

$$= \sqrt{2}I_1 - \frac{1}{2}I_1^2 + \sqrt{2}I_2 - \frac{1}{2}I_2^2. \tag{2}$$

The frequencies of these two Morse oscillators are given by

$$\left.\begin{aligned} {}_1(I_1, I_2) &= \frac{}{I_1} = \sqrt{2} - I_1 \\ {}_2(I_1, I_2) &= \frac{}{I_2} = \sqrt{2} - I_2 \end{aligned}\right\}. \tag{3}$$

The winding number of a torus with action $I_1$ and action $I_2$ is defined as

$$= \frac{{}_1}{{}_2} = \frac{\sqrt{2} - I_1}{\sqrt{2} - I_2} = \frac{n}{m}, \tag{4}$$

where $n$ and $m$ are integers which can be represented as the numbers of intersection points that a periodic orbit on the torus intersects with SOS at $x_1$ = constant and SOS at $x_2$ = constant. From (2) and (4) we get

$${}_1 = \sqrt{2}I_1 - \frac{1}{2}I_1^2 = \frac{1 - (\frac{n}{m})^2(1 - )}{1 + (\frac{n}{m})^2}, \tag{5}$$

$${}_2 = \sqrt{2}I_2 - \frac{1}{2}I_2^2 = \frac{ + (\frac{n}{m})^2 - 1}{1 + (\frac{n}{m})^2}, \tag{6}$$

$$I_1 = \sqrt{2}(1 - \sqrt{1 - {}_1}), \tag{7}$$

$$I_2 = \sqrt{2}(1 - \sqrt{1 - + {}_1}) = \sqrt{2}(1 - \sqrt{1 - {}_2}), \tag{8}$$

where is the total energy of the system and ${}_i (i = 1, 2)$ is the energy for the $i^{th}$ Morse oscillator.

For a torus with winding number $n/m$ to exist, it is necessary that ${}_1$ 0 and ${}_2$ 0. From equation (5) and equation (6) we get the inequality relations in the following

$$1 - (\frac{n}{m})^2(1 - ) \quad 0, \tag{9}$$

$$+\left(\frac{n}{m}\right)^2-1 \quad 0. \tag{10}$$

The solution of the inequality equations is given by

$$\sqrt{\frac{1}{1-}} \quad \left(\frac{n}{m}\right) \quad \sqrt{1-}\ . \tag{11}$$

Inequality equation (11) is our starting point to analyze the bifurcations in localmode region for 0 in the following subsection

**Example** For = 3/4, we get 2 $n/m$ 1/2, then the following resonance tori (and many more in between any two of them) will be turned on

$$\frac{1}{2}\ \frac{2}{3}\ \frac{3}{4}\ \frac{4}{5}\ \frac{5}{6}\ \frac{6}{7}\ \frac{7}{8}\ \frac{8}{9}\ \frac{9}{10}$$

$$\frac{2}{1}\ \frac{3}{2}\ \frac{4}{3}\ \frac{5}{4}\ \frac{6}{5}\ \frac{7}{6}\ \frac{8}{7}\ \frac{9}{8}\ \frac{10}{9}$$

1.2 Result for 0, small

We usually can not see a bifurcation in phase space for = 0 even though it is there. To visualize bifurcation in phase space, we need to turn on coupling 0, so that all the resonance tori are broken up into resonance zone of certain area. Within certain range of coupling parameter, phase space bifurcation structures are dominated by system energy as we showed in section 1.1. In figure 1(a), we show phase space structures for a system of coupling constant = − 0.07 and system energy = 0.6051. We can find that all the resonances in the interval [2/3, 1/1] are turned on, for example, [1] 2/3, [2] 3/4, [3] 4/5, [4] 5/6, in this figure, the resonances that are outside that range are either too weak to be seen or have not been turned on until at a higher energy. The winding number $_L$ of the localmode in this surface of section is > 0/1, because the energy of the system is less than the dissociation energy of a Morse oscillator, which can be seen from equation (4) or equation (11). In Figure 1(b) and Figure 1(c), we show the selected portion of phase space structures and emphasize the resonances for coupling = − 0.014 and a higher energy = 0.98. We find that all the resonances in the interval [1/6, 1/1] have been turned on, for example, the [1] 2/3, [2] 3/5, [3] 1/2, [4] 1/3, [5] 1/4, [6] 1/5, [6] 1/6, , the resonances within [0/1, 1/6] will be turned on when the system energy approaches to dissociation energy = 1. The general way to estimate which resonances will be turned on for a given system energy is the inequality relation shown in equation (11). In addition to changing the size of resonance zone, the coupling constant can also cause the annihilation of certain resonances, which will become obvious in strong coupling region. Phase space structures are related to the symmetry of the system, for this ABA type molecule, all the resonances in the localmode region in phase space appear in pairs. For example, the resonances in the interval [1/1, 6/1] will be turned on when the resonances in the interval [1/6, 1/1] are turned on

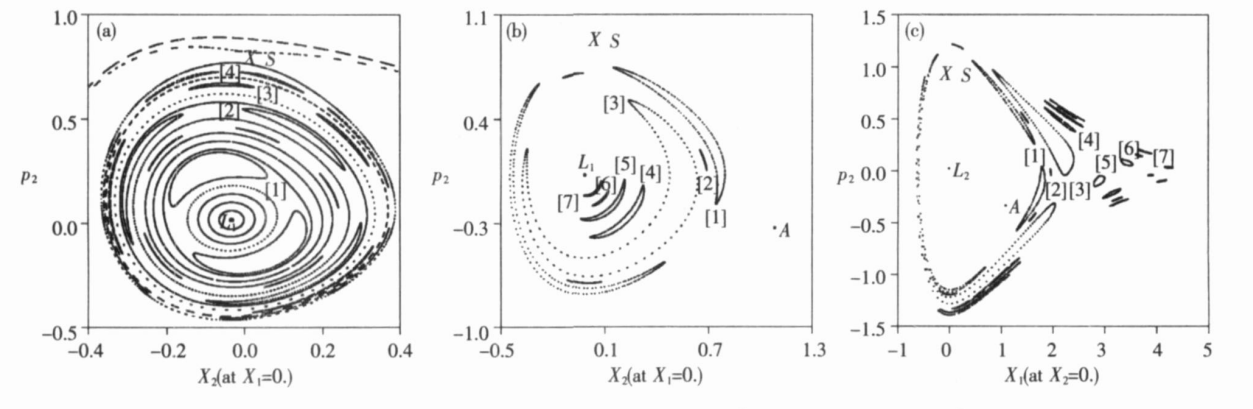


**Fig.1 Resonances in local mode region (a) $\varepsilon$=0.605, $\delta$=−0.07; (b), (c): $\varepsilon$=0.98, $\delta$=−0.014**

## 2 Bifurcation Within Normal Mode Region

### 2.1 Bifurcation with Coupling Parameter for Very Low Energy

At very low energy, the Hamiltonian in equation (1) can be approximated by two uncoupled Harmonic oscillators, one of which represents the symmetric combination of the two local modes, and the other represents the antisymmetric combination of the two local modes. The winding number $_N$ of a torus in phase space is only related to the coupling constant , i.e., $_N = \sqrt{(1+\ )/(1-\ )}$. When the coupling constant is very small, phase space structure basically corresponds to a 1/1 resonance. It corresponds to different resonance as the coupling becomes stronger. The uncoupled Harmonic oscillator approximation will be failed for a higher energy because of the nonlinearity of the Morse oscillator. This nonlinearity of the Morse oscillator and the strong coupling between different Morse oscillator will generate different resonances coexistence in phase space.

### 2.2 Effect of System Energy on the Phase Space Structures—the Local Mode Region Formation Process

As shown in Figure 2, the phase space at very low energy is filled by normal mode tori centered on either symmetric stretch periodic orbit or antisymmetric stretch periodic orbit. As we increase system energy, we will see that the symmetric stretch periodic orbit becomes an unstable periodic orbit and two new stable periodic orbits come out through pitch fork bifurcation. The local modes start to be formed by expending normal modes as we continuously increase the system energy. In a SOS, we will see two different regions divided by a separatrix called the local-normal separatrix. By increasing system energy, we will see that higher order resonances appear, but the phase space is still dominated by local mode and a 1/1 resonance normal mode regions.

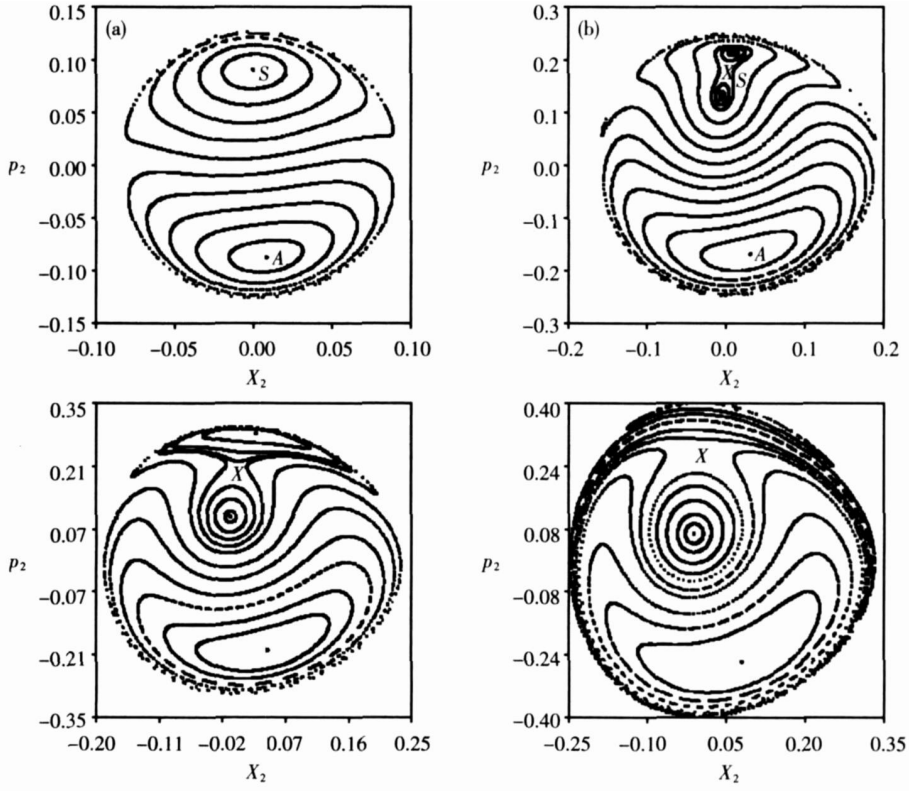


**Fig.2 Local mode formation process $\delta$=−0.014 (a) $\varepsilon$=0.008; (b) $\varepsilon$=0.031; (c) $\varepsilon$=0.044 8; (a) $\varepsilon$=0.08**

### 2.3 Bifurcation Phenomena of Symmetric Stretch Normal Mode

In section 2.2, we discussed the pitch fork bifurcation of symmetric stretch normal mode periodic orbit with system energy at very weak coupling parameter = − 0.014, which is what has happened for $H_2O$ molecule. In this section, we will illustrate, through phase space portrait, the bifurcation phenomena of symmetric stretch normal mode with coupling parameter for a fixed system energy = 0.5. Figure 3(a) (b) are symmetric stretch

and antisymmetric stretch normal mode SOS at coupling $= -0.1$ and energy $= 0.5$. Where $P_s = (p_1 + p_2)/\sqrt{2}$ and $P_a = (p_1 - p_2)/\sqrt{2}$ are momenta for symmetric stretch and antisymmetric stretch normal mode respectively, $X_s = (x_1 + x_2)/\sqrt{2}$ and $X_a = (x_1 - x_2)/\sqrt{2}$ are corresponding symmetric stretch and antisymmetric stretch normal mode coordinates. The symmetric stretch normal mode S corresponds to the most outside curve in Figure 3(a), and it is inside the center of the antisymmetric stretch SOS as shown in Figure 3(b). $L_1$, $L_2$, and $A$ in Figure 3(a) are local modes and antisymmetric stretch normal mode respectively.

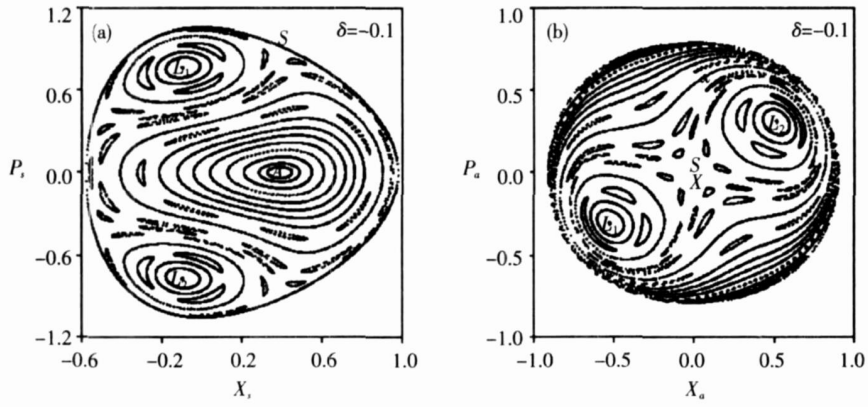


**Fig.3 Normal mode SOS, $\varepsilon$=0.5, $\delta$=−0.1**

The symmetric stretch normal mode stays unstable until the local modes are gone in phase space at coupling $-0.3$. Then it will become stable and unstable alternatively with coupling parameter . For example, the symmetric stretch normal mode is stable for coupling parameter $[-0.4, -0.3]$, unstable for $[-0.55, -0.45]$, stable for $[-0.65, -0.6]$, unstable for $[-0.8, -0.7]$, and stable for $[-1.0, -0.9]$. The symmetric stretch normal mode will stay stable if it is far from any resonance when the local modes have gone; in other words, it stays stable if there are more tori around it. It becomes unstable only when resonance is in contact with it, because the separatrix is consisted of stable and unstable manifolds of unstable fixed points. So, the symmetric stretch normal mode is unstable when it is close to an unstable periodic orbit.

## 3 Summary

In summary, phase space structures are normal mode tori centered on symmetric stretch and antisymmetric stretch periodic orbits at very low energy. The symmetric stretch periodic orbit experiences a pitch fork bifurcation at energy around $= 0.031$ and coupling $= -0.014$. The local mode regions then start to be formed gradually with system energy. Higher order resonances set into local mode region at higher energy for a fixed coupling parameter and different order of resonances overlap with coupling for a fixed system energy, then the tori between them are all destroyed. These phenomena first happen in local mode regions.

Phase space structures change with coupling. The normal mode region grows and the local mode regions shrink until all the local mode regions are gone with coupling. A sequence of bifurcations then takes place in phase space with coupling, which is reflected by the annihilation and creation of resonances. The resonances with larger winding number will first be turned on at small coupling parameter, and the resonance with small winding number will be turned on at larger coupling parameter for a fixed system energy.

For a fixed small coupling parameter, phase space structures change with system energy. The resonances with larger winding number (but less than or equal to one) in one of the local mode regions will be first turned on at smaller system energy. The smaller the winding number of the resonance, the higher the system energy is required to turn on that resonance. The 0/1 resonance will not be turned on until the system energy reaches the dissociation energy of the system.

There exist two special cases for this two kinetically coupled Morse oscillators. One is zero coupling limit

All the classical motions are local mode motions. Another case is coupling equal to -1. Phase space then is occupied by normal mode tori. Both of these two cases belong to integrable system with very simple phase space structures-the tori.

**Acknowledgements** The author appreciate the helpful discussion with Professor Michael E. Kellman of University of Oregon.

## [References]

[1] Jaff C, Brumer P. Local and normal modes: A classical perspective[J]. J Chem Phys, 1980, 73(11): 5646-5658.

[2] Matsushita T, Terasaka T. Mass dependence of the Kolmogorov-Arnold-Moser stability and lower resonances in the kinetically coupled two-degree-of freedom Morse system[J]. Chem Phys Lett, 1983, 100: 138-144.

[3] Yang shuangbo. Torus quantization in local mode region for two kinetically coupled Morse oscillators[J]. Journal of Nanjing Normal University: Natural Science, 2007, 30(1): 33-38.

[4] Yang shuangbo. Semiclassical wave function of resonance torus by evolving state along periodic orbits[J]. Journal of Nanjing Normal University: Natural Science, 2006, 29(2): 35-39.

[5] Yang shuangbo, Kellman M E. Addendum to direct trajectory method for semiclassical wave functions[J]. Phys Rev A, 2002, 65(3): 034103-1-034103-4.

[6] Yang Shuangbo, Kellman Michael E. Perspective on semiclassical quantization: How periodic orbits converge to quantizing tori[J]. Phys Rev A, 2002, 66(5): 052113-1-052113-11.

[责任编辑: 顾晓天]