

Torus Quantization in Normal Mode Region for Two Kinetically Coupled Morse Oscillators

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Abstract The results of torus quantization in the normal mode regions for a system of two kinetically coupled Morse oscillators was reported. It is found that the result of the quantization is numerically strongly dependent on the quantizing circuits. For the correct circuits we chose, semiclassical result agrees well with quantum result. It is believed that this relates to the separability of the system.

Key words EBK quantization condition, normal mode, separability, quantizing circuits

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两运动耦合的 Morse 振子系统本征模区域内环量子化

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[摘要] 报道了两个运动耦合的 Morse 振子系统相空间中本征模区域内环量子化的结果. 研究发现, 量子化的结果在数值上很强烈地依赖于量子化回路的选取. 对正确选择的回路, 其半经典结果与量子结果符合得很好. 我们认为这与系统的可分离性有很大关系.

[关键词] EBK 量子化条件, 本征模, 可分离性, 量子化回路

The Hamiltonian of the two kinetically coupled Morse oscillators can be written as the following form

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

where δ is the coupling constant, $\delta \in [-1, 0]$. For smaller $|\delta|$, phase space can be basically classified into two regions, the local mode region and normal mode region. Classical motions in local mode region correspond to motions that one oscillator is important, which means that the energy of one oscillator is higher than the energy of another oscillator. Motions in normal mode region are different in that the energy is equally shared by the two oscillators, i.e. equal amplitude and in phase or with phase π difference. We studied the classical dynamics by studying the bifurcation phenomena for this system^[1]. As a model of a triatomic molecule such as H_2O , the classical dynamics was first studied by Jaffe and Brumer^[2], and later by many others^[3, 4]. We quantized this system by finding quantizing torus numerically in local mode region^[5], where the local mode Surface of Section (SOS) automatically provides the quantizing circuits for the quantization. In this paper we will report the result of normal mode torus quantization, the quantizing circuits need to be chosen specifically for certain coupling parameter values, which differ from the case of local mode torus quantization.

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Torus Quantization in Regular Normal Mode Region for

$$\delta = -0.014$$

1.1 Choosing circuits C_1 and C_2

The EBK quantization conditions for a torus can be written as

$$I_1 = \frac{1}{2\pi} \oint (p_1 dx_1 + p_2 dx_2) = E \left[n_1 + \frac{1}{2} \right], \quad (2)$$

$$I_2 = \frac{1}{2\pi} \oint (p_1 dx_1 + p_2 dx_2) = E \left[n_2 + \frac{1}{2} \right]. \quad (3)$$

where C_1 and C_2 are two topologically independent circuits around the torus in phase space. γ is a system dependent constant. For the two kinetically coupled Morse oscillators, it is given by $\gamma = \omega_0 \sqrt{2D}$.

The circuits C_1 and C_2 taken in (2) and (3) are ideal. For a practical problem, it is difficult to search such ideal circuits. Fortunately, some approximate circuits can also give very good semiclassical results. For example, we took localmode SOSs as circuits C_1 and C_2 in the localmode quantization. Localmode surface of section is not a good circuit for the normalmode quantization, because we found that the semiclassical eigenenergy found is far from the true quantum eigenvalue even though the quantization conditions can be satisfied very well in the circuits chosen. The success in localmode quantization by localmode SOS method comes from the near separability of the wave function in localmode coordinates. DeDebn and Heller^[6] have studied the separability of wave function in “nodal coordinates” and found that the wave function can be written as a product of two functions of nodal coordinates (except for the swallow tail trajectories). Based on this analysis, we introduce two circuits C_1 and C_2 that are the intersections of the normalmode torus with plane XP at $x=0$, $p>0$ and plane xP at $X=X_0$, for both $P>0$ and $P<0$. Where

$$X = (x_1 + x_2) \sqrt{2}, \quad (4)$$

$$P = (p_1 + p_2) \sqrt{2}, \quad (5)$$

$$x = (x_1 - x_2) \sqrt{2}, \quad (6)$$

$$p = (p_1 - p_2) \sqrt{2}, \quad (7)$$

$$X_0 = -\ln(1 - \epsilon_0(n_2)) \sqrt{2}, \quad (8)$$

$$\epsilon_0(n_2) = 2 \left[\left(n_2 + \frac{1}{2} \right) - \left(n_2 + \frac{1}{2} \right)^2 / 2\lambda \right] / \lambda. \quad (9)$$

where $\epsilon_0(n_2)$ is the zeroth order energy for the second Morse oscillator, then, the quantization conditions become

$$I_1 = \frac{1}{2\pi} \oint P dX = E(n_s + 1/2), \quad (10)$$

$$I_2 = \frac{1}{2\pi} \oint p dx = E(n_a + 1/2). \quad (11)$$

It should be noted that we can set $X_0 = 0$ for states $n_s = 0$ and $n_a < 3$ because these low lying states do not “feel” the nonlinearity of Morse potential at $X = 0$. Above these low lying states we have to take into account the nonlinearity of Morse potential by setting X_0 appropriately like that in (8). For those states which have $n_s = 0$ and $n_a \leq 4$, we can use regular SOS (records data only for $P > 0$ at $X = X_0$ for xP SOS and for $p > 0$ at $x = 0$ for XP SOS) as circuits C_1 and C_2 because it is enough to construct closed curve after the nonlinearity correction in (8). For states of $n_s = 0$ and $n_a > 4$, the regular SOS for C_2 is not a closed curve as shown in figure 1, and the regular SOS method has to be extended to include both $P > 0$ and $P < 0$. By using this type of SOS method, we can solve the quantization problem for normalmode tori.

1.2 The calculation of action I_2

The intersection of a normalmode torus with plane xP for both $P > 0$ and $P < 0$ in phase space are two entan-

gled curves as shown in figure 2(a). The circuit C₂ needed for the quantization corresponds to one of them. In order to separate these “win” curves, we first sort the data in ascending order then use distance and slope as criteria to distinguish which curve the given point belongs to. The algorithm is a continuous separator; even one datum point misassignment will cause the failure of the whole curve separation. Since the errors in numerical computation (significant when the tons becomes highly unstable), the nearby data points which correspond to the intersections of the trajectory with the given SOS at different time can have different errors, if the error is greater than the correct separation, it will bring difficulties to the separation of the twin curves. Another problem is the highly nonuniform distribution of the data points. Gaps are difficult to be filled by data points, even though we have run trajectory as long as to there are 30 000 data points for the “win” curves. Because of these problems, the program of separator has been made complicated to care about every possible individual problem. Finally these “win” curves are effectively separated in the form of (p, x) as shown in figure 2(b). After the separation, the action I₂ can be calculated by interpolation method^[7], similar to the calculation for the local mode torus.

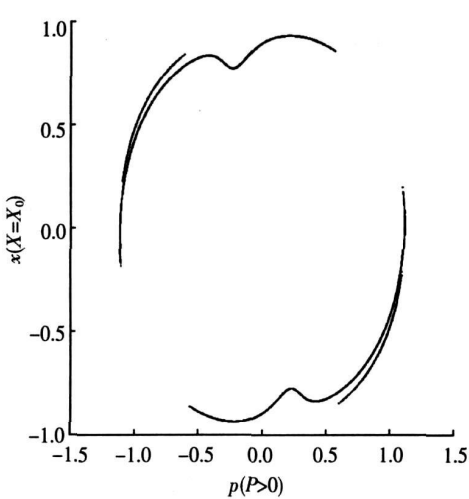


Fig.1 The intersection of a normal mode torus with a plane at X=X₀ for P>0

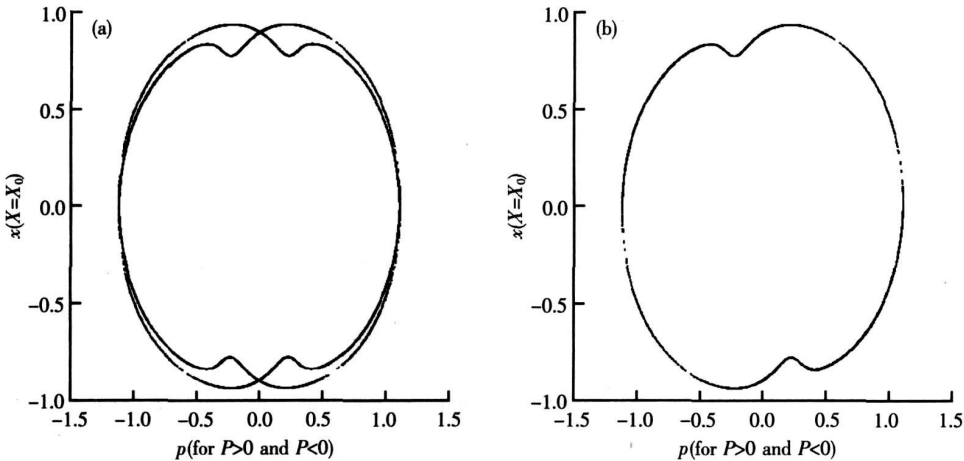


Fig.2 (a) the intersection of a normal mode torus with a plane at X=X₀ for both P>0 and P<0; (b) one of the separated curves

Table 1 The semiclassical results in normal mode region for two kinetically coupled morse oscillators at δ= - 0.014

(n _s , n _a)	ε _s	en _f	en _x	dn _s	dn _a	ε _q	ε _s - ε _q
(0 0)	0.085650	0.1E-05	0.8E-05	0.2E-06	0.2E-05	0.860392	3.89E-04
(0 1)	0.169933	0.5E-05	0.3E-04	0.1E-04	0.3E-05	0.169810	1.23E-04
(0 2)	0.252420	0.6E-05	0.2E-05	0.9E-06	0.8E-07	0.252736	3.17E-04
(0 3)	0.333023	0.2E-04	0.4E-05	0.2E-03	0.5E-06	0.333009	1.44E-05
(0 4)	0.411695	0.2E-03	0.3E-05	0.7E-03	0.8E-06	0.411973	2.79E-04
(0 5)	0.488566	0.9E-05	0.3E-04	0.2E-04	0.1E-06	0.488571	4.87E-06
(1 5)	0.559675	0.7E-05	0.3E-04	0.2E-04	0.2E-05	0.559081	5.94E-04
(0 6)	0.563468	0.8E-04	0.2E-03	0.2E-03	0.1E-05	0.563637	3.07E-05
(0 7)	0.636469	0.9E-04	0.5E-05	0.2E-03	0.3E-05	0.636481	1.24E-05
(0 8)	0.707557	0.5E-04	0.8E-06	0.1E-03	0.8E-06	0.707680	1.23E-04
(0 9)	0.776759	0.9E-04	0.8E-04	0.2E-03	0.3E-06	0.776733	2.62E-05
(0 10)	0.844016	0.9E-04	0.8E-04	0.2E-03	0.7E-06	0.844080	6.43E-05
(0 11)	0.909332	0.3E-03	0.3E-04	0.3E-03	0.8E-06	0.909325	6.63E-06
(0 12)	0.972711	0.9E-03	0.4E-03	0.2E-02	0.5E-05	0.972833	1.23E-04

1.3 The results of semiclassical quantization in normal mode region

The method to search a normal mode tons that satisfies quantization conditions (10) and (11) is similar to the method used in local mode quantization with different initial conditions in the following

$$X = - \ln(1 - \sqrt{\varepsilon(1-f)})/\sqrt{2},$$

(12)

$$x = -X,$$

(13)

$$P = \sqrt{g},$$

(14)

$$p = P.$$

(15)

where

$$f = \frac{p_1^2}{2\varepsilon},$$

$$\varepsilon = \frac{2}{\lambda} \left[\left(n_1 + \frac{1}{2} \right) - \frac{1}{2\lambda} \left(n_1 + \frac{1}{2} \right)^2 + \left(n_2 + \frac{1}{2} \right) - \frac{1}{2\lambda} \left(n_2 + \frac{1}{2} \right)^2 \right].$$

ε is the zeroth order energy for the system. The numerical results for coupling parameter $\delta = -0.014$, dissociation energy $D = 8.84 \times 10^{-12}$ erg = $44505.216 \text{ cm}^{-1}$, and the harmonic frequency at the bottom part of the Morse potential $\omega_0 = 7.2916 \times 10^{14} \text{ s}^{-1}$ are summarized in the Table 1. The number of iterations for getting each of these states is less than 10 except for the state (0,0) which used 22 iterations. Since the number of data points needed for generating a C_2 curve is large, this program is slower.

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