# Semiclassical Wave Function of a Resonance Torus by Evolving State along Periodic Orbits

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**Abstract**: In this paper we show the construction of a semiclassical wave function for a resonance torus with winding number $n/m$, and satisfying the Einstein-Brillouin-Keller (EBK) quantization condition, by evolving a state along periodic orbits on the torus. Numerically, we choose a resonance torus of winding number 29/39, a very close periodic torus convergent to the quantizing torus corresponding to state (8,3), to build wave function.

**Key words**: resonance torus, EBK quantization condition, stability equation, Maslov index

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## 利用沿周期轨道演化态构造谐振环的半经典波函数

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[摘要] 介绍了如何利用沿着环上的周期轨道演化态构造一个环绕数为 $n/m$,且满足 Einstein-Brillouin-Keller 量子化条件的谐振环的半经典波函数. 数值上,我们选择一个环绕数为 29/39 的谐振环(非常接近于量子化环(8,3))构造波函数.

[关键词] 谐振环,EBK 量子化条件,稳定性方程,Maslov 指数

## 0 Introduction

Semiclassical quantization started before the modern quantum mechanics. It was first the Bohr-Sommerfeld quantization for periodic orbit, for example, the quantization of Hydrogen atom by Bohr, and then the torus quantization for integrable system by Einstein, the wave function for integrable torus came much later until in 1958 by Keller, and in 1970's by Maslov and Fedoriuk. We here bring up the question of semiclassical wave function for resonance torus has two main reasons: first of all the numerical implementation of both Keller's method and Maslov-Fedoriuk's method for wave function is scarce in the literature, and especially we can do exact calculation for the resonance torus; second it relates the construction of chaos wave function, for example, the cantorus wave function.

The basic idea of EBK quantization is that eigenstates correspond to invariant tori satisfying EBK quantization conditions:

$$\oint_{C_\alpha} p_1 \mathrm{d}x_1 + p_2 \mathrm{d}x_2 = 2\pi\hbar \left(n_\alpha + \frac{1}{2}\right) \tag{1}$$

$$\oint_{C_\beta} p_1 \mathrm{d}x_1 + p_2 \mathrm{d}x_2 = 2\pi\hbar \left(n_\beta + \frac{1}{2}\right) \tag{2}$$

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where $C_\alpha$ and $C_\beta$ are two topologically independent circuits for the torus; $n_\alpha$ and $n_\beta$ are two integers. Spectroscopists treat $C_\alpha$ and $C_\beta$ as mode of molecular vibration, and assign this mode by quantum numbers $n_\alpha$ and $n_\beta$.

In the previous publication[1], we showed how to construct semiclassical wave function of an invariant torus with irrational winding number by running a single trajectory, where a single trajectory, after running long enough will fill the coordinate space occupied by the torus densely. In this paper, we will demonstrate the construction of semiclassical wave function for a torus with rational winding number (so called resonance torus) by running multiple trajectories on the torus. Each trajectory on the torus is a periodic orbit, and the initial distribution (even locally) of the wave function is required. We take the two uncoupled Morse oscillators as our model of study.

## 1 Formulation for Two Uncoupled Morse Oscillators

The Hamiltonian of the two uncoupled Morse oscillators with dissociation energy $D$ and Morse parameter $\beta$ for each oscillator can be written as

$$H = \frac{p_1^2}{2m} + D(1 - e^{-\beta x_1})^2 + \frac{p_2^2}{2m} + D(1 - e^{-\beta x_2})^2 \tag{3}$$

which can be scaled into the following form

$$\varepsilon = \frac{1}{2}\tilde{p}_1^2 + (1 - e^{-\tilde{x}_1})^2 + \frac{1}{2}\tilde{p}_2^2 + (1 - e^{-\tilde{x}_2})^2 \equiv \varepsilon_1 + \varepsilon_2 \tag{4}$$

by the transformations

$$\varepsilon = \frac{H}{D},\ \tilde{p}_i = \frac{1}{\sqrt{mD}}p_i,\ \tilde{x}_i = \beta x_i,\ \tau = D\gamma t,$$

where $\varepsilon_1$ and $\varepsilon_2$ are the energies for oscillator 1 and oscillator 2 respectively.

$$\gamma = \frac{\omega_0}{\sqrt{2}D},\ \omega_0 = \sqrt{\frac{2D\beta^2}{m}},$$

$\omega_0$ is the harmonic frequency at bottom part of the Morse potential. Eq. (4) is the working equation for the rest of the paper.

From the asymptotic solution of a general linear partial differential equation, Maslov and Fedoriuk gave the semiclassical wave function of schödinger equation as the following form[2]

$$\psi(\tilde{x}_1, \tilde{x}_2, \varepsilon) = \sum_{r=1}^{n} \varphi(\tilde{x}_{10}, \tilde{x}_{20}) \sqrt{\left|\frac{J^r(0, \tilde{x}_{20})}{J^r(\tau, \tilde{x}_{20})}\right|}\, e^{\frac{i}{\hbar\gamma}S^r(\tau, \tilde{x}_1, \tilde{x}_2) - i\frac{\mu^r(\tau)\pi}{2}} \tag{5}$$

where $\varphi(\tilde{x}_{10}, \tilde{x}_{20})$ is the initial distribution of the amplitude of the semiclassical wave function; $S^r(\tau, \tilde{x}_1, \tilde{x}_2) = S_0(\tilde{x}_{10}, \tilde{x}_{20}) + \int_0^\tau (\tilde{p}_1\dot{\tilde{x}}_1 + \tilde{p}_2\dot{\tilde{x}}_2)\mathrm{d}t$, and $S_0(\tilde{x}_{10}, \tilde{x}_{20})$ is the initial phase distribution. $\mu^r(\tau)$ is called the Maslov index which can be calculated by the number of times that the trajectory has passed through caustics at time $\tau$. The superscript $r$ means at time $\tau$ the trajectory is in $r$th branch[3]. The number $n$ in the sum is the total number of branches, for example, $n = 4$ for the two uncoupled Morse oscillators. The Jacobian $J^r$ represents the evolution of a cluster of trajectories and is given by

$$J^r(\tau, \tilde{x}_{20}) = \frac{\partial(\tilde{x}_1, \tilde{x}_2)}{\partial(\tau, \tilde{x}_{20})} = \dot{\tilde{x}}_1\frac{\partial\tilde{x}_2}{\partial\tilde{x}_{20}} - \dot{\tilde{x}}_2\frac{\partial\tilde{x}_1}{\partial\tilde{x}_{20}} \tag{6}$$

The partial derivatives in Eq. (6) relate to the stability of the classical trajectory, which will be determined by stability equations in 1.2. The Jacobian $J^r$ equal to zero where the classical turning points or caustics are reached, and then Eq. (5) diverges. So the semiclassical wave function in Eq. (5) is a primitive type. Eq. (5) corresponds to a quantum state if the trajectories are on an EBK quantizing torus, or the single valuedness condition of Eq. (5) is satisfied on each topologically independent circuit on the torus. The $J^r(0, x_{20})$ in Eq. (5) is the initial value of $J^r(\tau, \tilde{x}_{20})$, and is given by

$$J'(0,\tilde{x}_{20}) = \frac{\partial(\tilde{x}_1,\tilde{x}_2)}{\partial(\tau,\tilde{x}_{20})}\Bigg|_{\tau=0} = \dot{\tilde{x}}_{10} \tag{7}$$

### 1.1 Initial distribution of phase and amplitude

By taking initial phase equal to zero at the equilibrium point of each Morse oscillator, one gets

$$\begin{aligned} S_0^{(j+)}(\tilde{x}_j,I_j) = \int_0^{\tilde{x}_j}\tilde{p}_{j+}\mathrm{d}\tilde{x}_j = \sqrt{2}\Bigg\{\Big[\sqrt{\varepsilon_j} - \sqrt{1-\varepsilon_j}\tan^{-1}\Big(\sqrt{\frac{\varepsilon_j}{1-\varepsilon_j}}\Big)\Big] \\ - \Big[\sqrt{\varepsilon_j-(\mathrm{e}^{-\tilde{x}_j}-1)^2} + \sin^{-1}\Big(\frac{\mathrm{e}^{-\tilde{x}_j}-1}{\sqrt{\varepsilon_j}}\Big) \\ - \sqrt{1-\varepsilon_j}\tan^{-1}\Big(\frac{\varepsilon_j+\mathrm{e}^{-\tilde{x}_j}-1}{\sqrt{1-\varepsilon_j}\sqrt{\varepsilon_j-(\mathrm{e}^{-\tilde{x}_j}-1)^2}}\Big)\Big]\Bigg\} \end{aligned} \tag{8}$$

$$\begin{aligned} S_0^{(j-)}(\tilde{x}_j,I_j) = \int_0^{\tilde{x}_{\max}}\tilde{p}_{j+}\mathrm{d}\tilde{x}_j + \int_{\tilde{x}_{\max}}^{\tilde{x}_j}\tilde{p}_{j-}\mathrm{d}\tilde{x}_j = \\ -S_0^{(j+)} + \sqrt{2}\Bigg\{\pi(1-\sqrt{1-\varepsilon_j}) + 2\Big[\sqrt{\varepsilon_j} - \sqrt{1-\varepsilon_j}\tan^{-1}\Big(\sqrt{\frac{\varepsilon_j}{1-\varepsilon_j}}\Big)\Big]\Bigg\} \end{aligned} \tag{9}$$

where

$$\varepsilon_j = \sqrt{2}I_j - \frac{1}{2}I_j^2 \tag{10}$$

$I_j = \frac{1}{2\pi}\oint\tilde{p}_j\mathrm{d}\tilde{x}_j$ is the action of the Morse oscillator $j$,

$$\tilde{x}_{\max} = -\ln(1-\sqrt{\varepsilon_j}) \tag{11}$$

is the right turning point of the Morse oscillator $j$, $\tilde{p}_{j+}$ corresponds to $\tilde{p}_j > 0$, and $\tilde{p}_{j-}$ corresponds to $\tilde{p}_j < 0$. The amplitude for each Morse oscillator is given by

$$A_{j+} = \left|\frac{\partial^2 S_0^{(j+)}}{\partial\tilde{x}_j\partial I_j}\right|^{\frac{1}{2}} = \left|\frac{\partial\tilde{p}_{j+}}{\partial I_j}\right|^{\frac{1}{2}} = \Big[\frac{1-\varepsilon_j(I_j)}{\varepsilon_j(I_j)-(1-\mathrm{e}^{-\tilde{x}_j})^2}\Big]^{\frac{1}{4}} = \left|\frac{\partial^2 S_0^{(j-)}}{\partial\tilde{x}_j\partial I_j}\right|^{\frac{1}{2}} = A_{j-} \equiv A_j \quad j = 1,2 \tag{12}$$

The periodic trajectories are taken from a resonance torus with winding number $n/m$. On the Surface of Section (SOS) at $\tilde{x}_1 = 0$, $\tilde{p}_1 > 0$, the amplitude distribution is given by

$$\varphi(0,\tilde{x}_2) = \Big(\frac{1-\varepsilon_1}{\varepsilon_1}\Big)^{\frac{1}{4}}\Big[\frac{1-\varepsilon_2}{\varepsilon_2-(\mathrm{e}^{-\tilde{x}_2}-1)^2}\Big]^{\frac{1}{4}} \tag{13}$$

The phase distribution for different trajectories on the torus on this SOS, from Eq. (8), (9) and by taking into account the phase change at the right turning point, is given by

$$S_0(0,\tilde{x}_2) = S_0^{(2+)}(\tilde{x}_2,I_2),\quad \tilde{p}_2 > 0 \tag{14}$$

$$S_0(0,\tilde{x}_2) = S_0^{(2-)}(\tilde{x}_2,I_2) - \frac{\hbar\gamma\pi}{2},\quad \tilde{p}_2 < 0 \tag{15}$$

### 1.2 Jacobian determinant for each periodic trajectory

The partial derivatives in Eq. (6) can be determined by[1]

$$\Big(\frac{\partial\tilde{x}_1}{\partial\tilde{x}_{20}}\Big)_{\tilde{x}_{10},\tau} = u_{13} + u_{14}\Big(\frac{\partial\tilde{p}_{20}}{\partial\tilde{x}_{20}}\Big) \tag{16}$$

$$\Big(\frac{\partial\tilde{x}_2}{\partial\tilde{x}_{20}}\Big)_{\tilde{x}_{10},\tau} = u_{33} + u_{34}\Big(\frac{\partial\tilde{p}_{20}}{\partial\tilde{x}_{20}}\Big) \tag{17}$$

where

$$\Big(\frac{\partial\tilde{p}_{20}}{\partial\tilde{x}_{20}}\Big) = \mp\frac{\sqrt{2}(\mathrm{e}^{-\tilde{x}_{20}} - \mathrm{e}^{-2\tilde{x}_{20}})}{\sqrt{\varepsilon_2-(1-\mathrm{e}^{-\tilde{x}_{20}})^2}} \tag{18}$$

with " − " sign for $\tilde{p}_{20} > 0$ and " + " sign for $\tilde{p}_{20} < 0$ obtained from Eq. (4). $u_{13}, u_{14}, u_{33}, u_{34}$ are elements of stability matrix, which have been discussed in detail in [1]. It is easy to show that (see [1]) $u_{13}(\tau) \equiv 0, u_{14}(\tau) \equiv 0$, because they are equal to zero initially and their time derivatives are also equal to zero initially. Then, one gets

$$\left(\frac{\partial \tilde{x}_1}{\partial \tilde{x}_{20}}\right)_{\tilde{x}_{10},\tau} = 0 \tag{19}$$

and the Jacobian determinant becomes

$$J'(\tilde{x}_{20},\tau) = \dot{\tilde{x}}_1\left(u_{33} + u_{34}\frac{\partial \tilde{p}_{20}}{\partial \tilde{x}_{20}}\right) \tag{20}$$

where $u_{33}$ and $u_{34}$ are determined by the combination of stability equations of classical trajectory and the equations of motion in the following set

$$\dot{\tilde{x}}_1 = \tilde{p}_1,\ \dot{\tilde{p}}_1 = 2(e^{-2\tilde{x}_1} - e^{-\tilde{x}_1}),$$
$$\dot{\tilde{x}}_2 = \tilde{p}_2,\ \dot{\tilde{p}}_2 = 2(e^{-2\tilde{x}_2} - e^{-\tilde{x}_2}),$$
$$\dot{u}_{33} = u_{43},\ \dot{u}_{43} = 2(e^{-\tilde{x}_2} - 2e^{-2\tilde{x}_2})u_{33},$$
$$\dot{u}_{34} = u_{44},\ \dot{u}_{44} = 2(e^{-\tilde{x}_2} - 2e^{-2\tilde{x}_2})u_{34}$$

with the initial conditions $u_{33}(0) = u_{44}(0) = 1, u_{34}(0) = u_{43}(0) = 0, \tilde{x}_1(0) = 0$ and $\tilde{p}_1(0) > 0$, $\tilde{x}_2(0)$, $\tilde{p}_2(0)$, the values of $\tilde{x}_2(0)$, $\tilde{p}_2(0)$, $\tilde{p}_1(0)$ will be determined from the periodic trajectory on the resonant torus.

### 1.3 Energy distribution to these two morse oscillators

For a periodic orbit of winding number $\nu = \omega_1/\omega_2 = n/m$, the total energy $\varepsilon$ of the system is distributed to these two Morse oscillators by[4]

$$\varepsilon_1 = \sqrt{2}I_1 - \frac{1}{2}I_1^2 = \frac{1 - \left(\frac{n}{m}\right)^2(1-\varepsilon)}{1 + \left(\frac{n}{m}\right)^2},$$

$$\varepsilon_2 = \sqrt{2}I_2 - \frac{1}{2}I_2^2 = \frac{\varepsilon + \left(\frac{n}{m}\right)^2 - 1}{1 + \left(\frac{n}{m}\right)^2}.$$

## 2 Numerical Results of Resonance Torus with Winding Number 29/39

The parameter values used for the calculation in this paper are given by $D = 44\ 505.216\ \text{cm}^{-1}$, $\omega_0 = 7.291\ 6 \times 10^{14}\text{s}^{-1}$, and from which we get

$$(\hbar\gamma)^{-1} = \left(\frac{\hbar\omega_0}{\sqrt{2}D}\right)^{-1} = 16.257\ 734\ 126\ 174\ 46$$

Considering the quantizing torus corresponding to state (8,3) with $n_1 = 8$ and $n_2 = 3$, and its close periodic torus (resonance torus) convergent with winding number $\nu = 29/39$ for the two uncoupled Morse oscillators. Each trajectory on the periodic torus is a periodic orbit of winding number $\nu = 29/39$. The difference between the winding number of the periodic torus and the winding number of the EBK quantizing tous is $|\nu_{\text{torus}} - \nu| \approx 1.064 \times 10^{-4}$; the difference between the EBK energy for the quantizing torus and the BS-EBK[4] energy for the periodic torus is given by $\Delta\varepsilon \approx 5.24 \times 10^{-9}D$. Semiclassical wave function and its contour plot shown in Fig. 1 and Fig. 2 are constructed by 40 periodic orbits on the resonance torus 29/39, and by running each periodic orbit for a period. We have also constructed the four branches of this semiclassical wave function in a slice along $\tilde{x}_1$ direction with $\tilde{x}_2$ fixed, and their superposition by 100 periodic orbits on the torus. The inexact quantization of this resonance torus is too weak to see with the naked eye in the wave function.

## 3 Summary and Discussion

We showed in this paper that a quantum state can be constructed from periodic orbits on the EBK quantizing torus for two uncoupled Morse oscillators. The number of periodic orbits needed to build the quantum state is de-

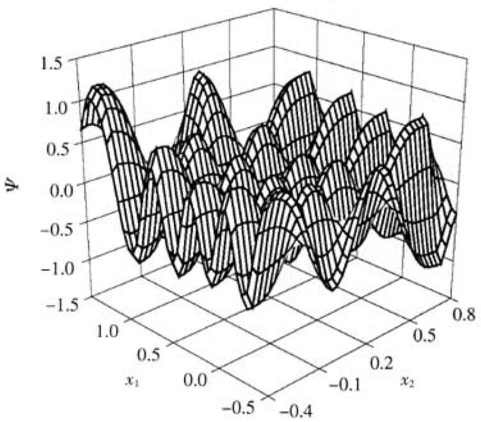


Fig.1 Semical wave function constructed from a resonance torus 29/39 which is a periodic torus convergent to an EBK quantizing torus corresponding to state (8,3) of two uncoupled Morse oscillators

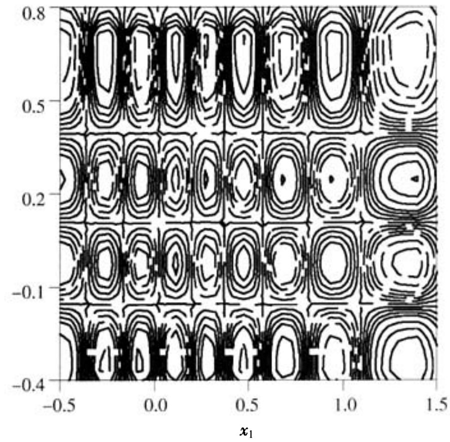


Fig.2 Contour plot of semical wave function

termined by the length of the periodic orbit and the distribution of the periodic orbits on the torus, so that the periodic orbits fill the coordinate space occupied by the quantizing torus densely after running for a period of time. In the chaotic region of a nonintegrable system, for example, the system of two kinetically coupled Morse oscillators, tori are destroyed by resonance, and chaotic sea prevail. The chaotic remnants of the classical tori called cantori are embeded inside the chaotic sea. Like torus, we use quantizing periodic orbits to approach a quantizing cantorus. Instead of using periodic orbits like that for the two uncoupled Morse oscillators, in building semiclassical wave function of a cantorus for the two kinetically coupled Morse oscillators, we run trajectories on the manifold of the cantorus to calculate the phase factors, the amplitude factors are obtained from the real density distribution of the clasical trajectories initially distributed widely inside chaotic sea[5].

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