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The quantum spectra analysis of the circular billiards in wells*

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We use a recently defined quantum spectral function and apply the method of closed-orbit theory to the 2D circular billiard system. The quantum spectra contain rich information of all classical orbits connecting two arbitrary points in the well. We study the correspondence between quantum spectra and classical orbits in the circular, 1/2 circular and 1/4 circular wells using the analytic and numerical methods. We find that the peak positions in the Fourier-transformed quantum spectra match accurately with the lengths of the classical orbits. These examples show evidently that semi-classical method provides a bridge between quantum and classical mechanics.

Keywords: circular billiard, closed-orbit theory, quantum spectra function, Fourier-transformed spectra

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1. Introduction

Various semi-classical calculation methods used in quantum mechanics are of help in understanding the interface between classical and quantum theories. Since the periodic orbit theory was put forward by Gutzwiller,[1] the study of integral and chaos system has got a fresh impetus. The semi-classical method in classical motion has become an indispensable implement to solving some quantum problems. Recently nano-technology is more and more widely used in some fields, micro-junction and its transport [2,3] property are popular topics of theoretical and experimental investigations. Quantum billiard is a good model for the research of the property of quantum transport, and valuable for the research of dynamics property of quantum chaos system.

Many authors have done much work in periodic-orbit theory[4−6] based on the Berry formula. But now we are only beginning to study the open orbit system based on the closed-orbit theory. We calculate the Fourier transform of the quantum spectra by using the energy eigenvalues and eigenfunction of two-dimensional infinite circular well and give the corresponding classical orbits; and we also study 1/2 circular and 1/4 circular well; our calculation shows that there is a good correspondence between quantum spectra and classical orbits.

2. Quantum spectra function and the Fourier transform

We consider the motion of a unit mass billiard, the Hamiltonian of the system is given by

$$H = \frac{P^2}{2} + V(q). \tag{1}$$

The corresponding Schrödinger equation for the particle is

$$H\psi_n(q) = \left[\frac{P^2}{2} + V(q)\right]\psi_n(q) = E_n\psi_n(q). \tag{2}$$

The energy eigenvalues and eigenfunctions are denoted by E_n and ψ_n, where n is the label for the quantum states. Suppose A and B are two arbitrary points in coordinate space. The quantum spectral function is defined as[7]

$$\rho_{AB} = \sum_n \psi_n^*(A)\psi_n(B)\delta(E - E_n). \tag{3}$$

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Similar to closed-orbit theory,[8] the semi-classical expression of $\rho_{AB}(E)$ can be written as a combination of a smooth background term and a sum of sinusoidal oscillating terms,

$$\rho_{AB}(E) = \rho^0_{AB}(E) + \sum_i C_i \sin(S_i + \varphi_i). \quad (4)$$

The first term on the right is a smooth background term. The sum runs over all possible classical orbits from A to B. The amplitude C_i is related to the orbit stability, S_i is the action of the ith orbit such that $S_i = \int_A^B p\mathrm{d}q$ is evaluated along a classical orbit, φ_i is the phase including Maslov phase correction. For billiard systems, we have the expression $S = KL$, $K = \sqrt{2E}$, and L is the length of classical orbit. The Fourier transform of quantum spectral function is

$$\tilde{\rho}_{AB}(L) = \int_{E_{\min}}^{E_{\max}} \rho_{AB}\exp(\mathrm{i}kL)\mathrm{d}E, \quad (5)$$

where $E_{\max}$ and $E_{\min}$ are the lower and higher boundaries, both of them are chosen to meet the calculation precision demand. Substituting Eq.(3) into Eq.(5) we get the Fourier transform formula

$$\tilde{\rho}_{AB}(L) = \sum_m \psi^*_m(x_1, y_1)\psi_m(x_2, y_2)\exp(\mathrm{i}K_m L). \quad (6)$$

We take the rotating-wave approximation, reasonably assuming that $C_i K$ changes slowly in the integral range, and the Fourier transform of Eq.(4) is approximately given by

$$\tilde{\rho}_{AB}(L) \approx \tilde{\rho}^0_{AB}(L) + \sum_i \bar{k}_i c_i \left[-\frac{\exp(-\mathrm{i}\varphi_i)}{2i}\right] \Delta(L - L_i), \quad (7)$$

where

$$\Delta(x) \equiv \int_{k_{\min}}^{k_{\max}} \exp(\mathrm{i}xk)\mathrm{d}k$$

is a function with a peak at $x = 0$, and

$$\tilde{\rho}^0_{AB}(L) = \int_{E_{\min}}^{E_{\max}} \tilde{\rho}^0_{AB}(E)\exp(\mathrm{i}\sqrt{2E}L)\mathrm{d}E,$$

$\bar{k}_i$ is the average value of k in the interval $[k_i, k_{i+1}]$.

3. Quantum spectra for the two-dimensional circular well

The two-dimensional circular well billiard system can be modelled by a particle of unit mass moving inside a circular infinite well of radius R. The potential may be described by

$$V(r,\theta) = V(r) = \begin{cases} 0 & \text{if } r < R \\ \infty & \text{if } r \geq R \end{cases}. \quad (8)$$

The Schrödinger equation for the particle in the quantum well is

$$-\frac{\hbar^2}{2}\left(\frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\frac{\partial^2}{\partial \theta^2}\right)\psi(r,\theta) = E\psi(r,\theta). \quad (9)$$

We assume a separable solution $\psi(r,\theta) = R(r)\Theta(\theta)$, and obtain the angular equation and radial equations, respectively,

$$\frac{\mathrm{d}^2\Theta_{(m)}(\theta)}{\mathrm{d}\theta^2} = -m^2\Theta_{(m)}(\theta), \quad (10)$$

and

$$\frac{\mathrm{d}^2R(r)}{\mathrm{d}r^2} + \frac{1}{r}\frac{\mathrm{d}R(r)}{\mathrm{d}r} - \frac{m^2}{r^2}R(r) = -k^2R(r), \quad (11)$$

where $k = \sqrt{2\mu E/\hbar^2}$, m^2 is the separable variable constant to be determined.

The angular equation has normalized solutions of the form

$$\Theta_{(m)}(\theta) = \frac{1}{\sqrt{2\pi}}\mathrm{e}^{\mathrm{i}m\theta}, \quad m = 0, \pm1, \pm2, \pm3, \ldots \quad (12)$$

When written as $z = kr$, the radial equation becomes

$$\frac{\mathrm{d}^2R'(z)}{\mathrm{d}z^2} + \frac{1}{z}\frac{\mathrm{d}R'(z)}{\mathrm{d}z} + \left(1 - \frac{m^2}{z^2}\right)R'(z) = 0, \quad (13)$$

and solution of Eq.(13) is an integer order Bessel function.

We have determined the energy eigenvalues of Eq.(13) projecting to the circular boundary, $J_m(kR) = 0$,

$$E_{(m,n_r)} = \frac{\hbar^2 k^2_{(m,n_r)}}{2\mu} = \frac{\hbar^2}{2\mu R^2}\left[a_{(m,n_r)}\right]^2, \quad (14)$$

where $a_{(m,n_r)}$ is the n_rth zero of the regular Bessel function. The normalized radial wavefunctions have the forms $J_{(m,n_r)}(kr) = N_{(m,n_r)}J_{(m,n_r)}(kr)$ and $\left[N_{(m,n_r)}\right]^2\int_0^R\left[J_{(m,n_r)}(kr)\right]^2 r\mathrm{d}r = 1$, where $k = \frac{a_{(m,n_r)}}{R}$. Therefore, the billiard eigenfunctions in circular well are

$$\psi(r,\theta) = \frac{1}{\sqrt{2\pi}}\mathrm{e}^{\mathrm{i}m\theta}J_{(m,n_r)}(kr). \quad (15)$$

Because of the energy conservation, we have

$$E = \frac{1}{2}\mu\dot{r}^2 + \frac{L^2}{2\mu r^2}. \quad (16)$$

When $\dot{r} = 0$ in the inner turning point[6] (the distance of closest approach to the origin), we have

$$E = \frac{L^2}{2\mu R_{\min}^2}$$

or

$$\frac{R_{\min}}{R} = \sqrt{\frac{L^2}{2\mu E R^2}}. \tag{17}$$

On combining Eq.(17) and Eq.(14) we see that

$$1 \geq \frac{R_{\min}}{R} = \sqrt{\frac{L^2}{2\mu E R^2}} = \sqrt{\frac{m^2\hbar^2}{\hbar^2\left[a_{(m,n_r)}^2\right]}} = \frac{|m|}{a}, \tag{18}$$

where $a \equiv a_{(m,n_r)}$.

4. Calculation results

We take the following values of the parameters: $R = 1$, $E_{\max}$=100000 for the sake of convenience. In general, $A(x_1,\ y_1)$ and $B(x_2,\ y_2)$ are two arbitrary points inside this well, and we chose $A(0.7, 2\pi/3)$, $B(0.6,\ 0)$.

The results are shown in Fig.1 where we have evaluated $\rho(L)$ using the $500a_{mn_r}$ lowest energy values. Figure 1 is the Fourier transform $|\tilde{\rho}_{AB}(L)|^2$ which changes with L where $k_{mn_r} = \frac{a_{mn_r}}{R}$, and the complete spectrum corresponds to one set of the m=0 solutions, but is doubly degenerate for each value of $m \geq 1$.

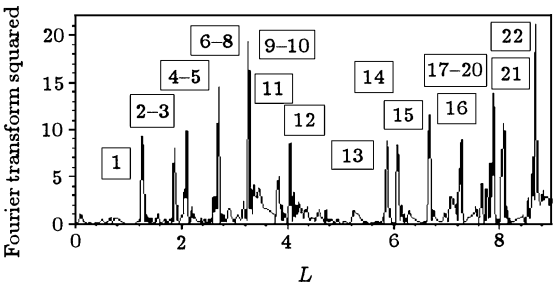


Fig.1. Correspondence of quantum spectra and classical orbit numbers in circular well.

4.1. The correspondence between quantum spectra and classical orbits in circular well

Schematic figures show that the correspondence between the peak position and the length of classical orbits going from A to B. For a classical particle moving in a circular well, if it leaves A, it may pass through various possible paths to get to point B. It moves in a straight line before it collides with the wall.[9,10] The process of collision obeys the law of reflection. We searched for all possible classical orbits limited in length $L \leq 9$, the results are shown in Fig.2.

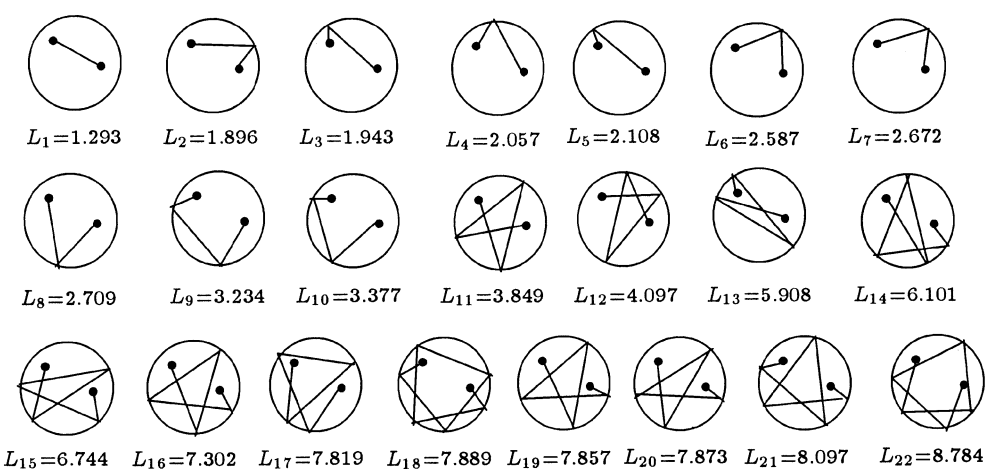


Fig.2. Classical orbit numbers in circular well.

We find that every peak position corresponds to one or several orbits from A to B in Fig.1. Table 1 gives the correspondence values.

Table 1. The position of the peaks of the Fourier transform and the classical orbits leading from A to B.

Number	1	2	3	4	5	6	7	8	9	10	11
The location of peak	1.297	1.904	1.904	2.104	2.104	2.690	2.690	2.690	3.298	3.298	3.843
The length of orbit	1.293	1.896	1.943	2.057	2.108	2.587	2.672	2.709	3.234	3.377	3.849
Number	12	13	14	15	16	17	18	19	20	21	22
The location of peak	4.102	5.879	6.105	6.724	7.297	7.869	7.869	7.869	7.869	8.087	8.870
The length of orbit	4.097	5.908	6.101	6.744	7.302	7.819	7.889	7.857	7.873	8.097	8.874

4.2. The correspondence between quantum spectra and classical orbits in 1/2 circular well

The solution in 1/2 circular well is $\Theta_m(\theta) \propto \sin(m\theta), m > 0$, but angular partition of solution $\Theta_m(\theta) \propto \cos(m\theta)$ is not satisfying 1/2 circular boundary condition. Using the same open orbit method, we evaluate the correspondence between the Fourier transform spectra and classical orbits in 1/2 circular well. We compare the quantum peak position with classical orbits. The results are showed in Figs.3, 4 and in the Table 2.

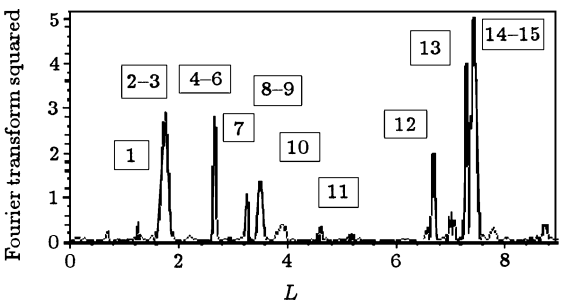


Fig.3. Correspondence of quantum spectra and classical orbit numbers in 1/2 circular well.

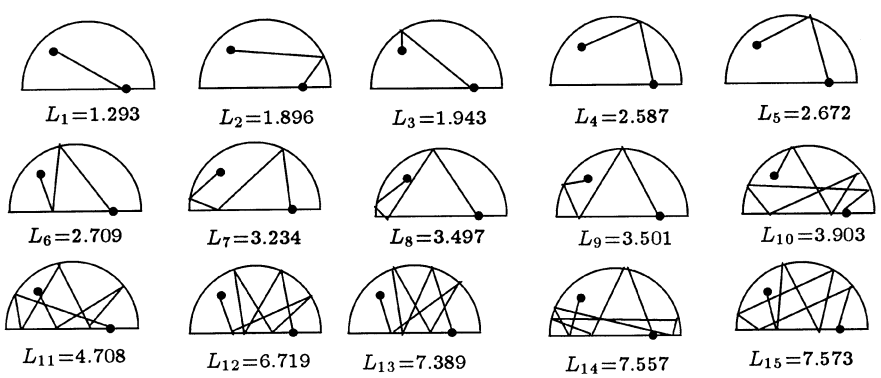


Fig.4. Classical orbit numbers in 1/2 circular well.

Table 2. The position of the peaks of the Fourier transform and the classical orbits leading from A to B.

Number	1	2	3	4	5	6	7	8	9
The location of peak	1.297	1.904	1.904	2.690	2.690	2.690	3.298	3.498	3.503
The length of orbit	1.293	1.896	1.943	2.587	2.672	2.709	3.234	3.497	3.501
Number	10	11	12	13	14	15			
The location of peak	3.890	4.707	6.709	7.369	7.559	7.569			
The length of orbit	3.903	4.709	6.719	7.389	7.557	7.573			

4.3. The correspondence between quantum spectra and classical orbits in 1/4 circular well

The solution in 1/4 circular well is $\Theta_m(\theta) \propto \sin(m\theta)$, $m > 0$ and m is even in order to satisfy the required boundary condition. We evaluate the correspondence between the Fourier transform spectra and classical orbits in 1/4 circular well. The results are shown in Figs.5 and 6 and in Table 3.

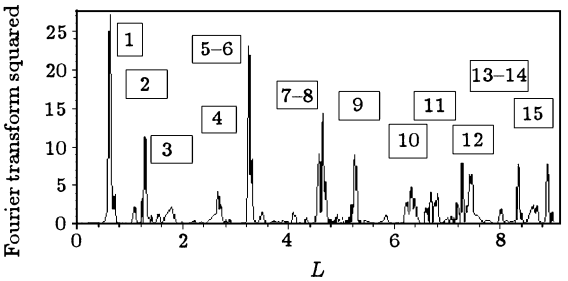


Fig.5. Correspondence of quantum spectra and classical orbit numbers in 1/4 circular well.

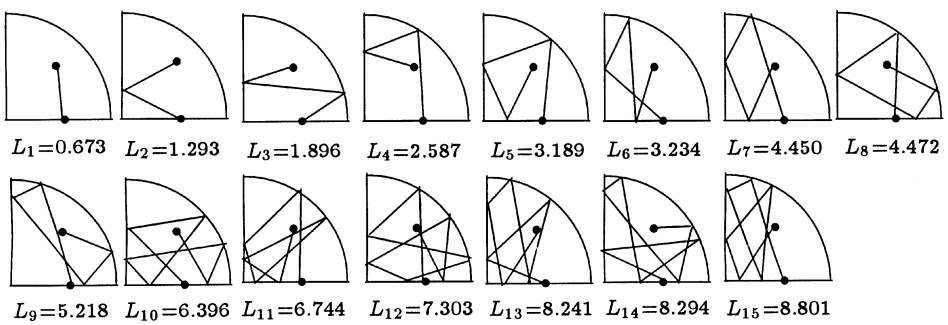


Fig.6. Classical orbit numbers in 1/4 circular well.

Table 3. The position of the peaks of the Fourier transform and the classical orbits leading from A to B.

Number	1	2	3	4	5	6	7	8	9
The location of peak	0.669	1.287	1.860	2.602	3.209	3.209	4.456	4.456	5.220
The length of orbit	0.673	1.293	1.869	2.587	3.189	3.234	4.450	4.472	5.218
Number	10	11	12	13	14	15			
The location of peak	6.380	6.801	7.320	8.236	8.236	8.818			
The length of orbit	6.396	6.744	7.303	8.241	8.294	8.801			

Comparing the Fourier transform spectra with classical orbits we find good correspondence between the Fourier transform spectra and classical orbits for circular, 1/2 circular or 1/4 circular wells. Every peak corresponds to one or several classical orbits.

5. Conclusion

We study the correspondence between quantum spectra and classical orbits of billiards in circular, 1/2 circular and 1/4 circular wells. It is proved that there is an intrinsic link between the quantum property and classical orbits for an integral system. The closed-orbited theory can be used to explain the atomic structure in magnetic field, transport property of semi-conductor in micro-cavity, and design of micro-junction.[11] Especially, quantum transport of electrons depends on the shape of the well, so our study about dynamic property in a series of billiard systems may have value in the future.

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