Quantum spectra and classical periodic orbit in the cubic billiard

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Quantum billiards have attracted much interest in many fields. People have made a lot of researches on the two-dimensional (2D) billiard systems. Contrary to the 2D billiard, due to the complication of its classical periodic orbits, no one has studied the correspondence between the quantum spectra and the classical orbits of the three-dimensional (3D) billiards. Taking the cubic billiard as an example, using the periodic orbit theory, we find the periodic orbit of the cubic billiard and study the correspondence between the quantum spectra and the length of the classical orbits in 3D system. The Fourier transformed spectrum of this system has allowed direct comparison between peaks in such plot and the length of the periodic orbits, which verifies the correctness of the periodic orbit theory. This is another example showing that semiclassical method provides a bridge between quantum and classical mechanics.

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With the improvement of the ability to probe the quantum-classical interface experimentally, the study of the connections between the quantized energy eigenvalues of a bound state and the classical motions of the corresponding classical point particle has become more and more important. Advances in lithographic techniques and crystal growth have made it possible to produce very small and clean devices, such as nanodevices. The electron in such devices is confined to two or more spatial dimensions through gate voltage, which can be considered as a quantum billiard. Quantum billiards have attracted much interest in many fields[1−5]. Subsequently, many theoretical methods have been developed, such as periodic orbit theory[6] which providing very direct connections between the energy spectrum and the periodic orbit of the classical system. Many researchers have focused their attention on the two-dimensional (2D) billiard system, such as the square billiard, 2D triangular billiard, circular or annular billiard, etc.[7−12]. As for the three-dimensional (3D) billiard, none has given the exact study. But as we all know, 3D billiard system is more important than the 2D system, because most of the devices are 3D other than 2D. In this paper, taking the cubic billiard as an example, using the periodic orbit theory, we find the periodic orbit of the cubic billiard and study the correspondence between the quantum spectra and the length of the classical orbits. The Fourier transformed spectrum of this system has allowed direct comparison between peaks in such plot and the length of the periodic orbits, which verifies the correctness of these methods and shows the correspondence between the quantum description and the classical description for the 3D billiard system.

Considering a billiard moving in a 3D cubic potential with the sides $L_x = L_y = L_z = a$, the potential is described by

$$V(x,y,z) = \begin{cases} 0, & 0 < x \leq a, 0 < y \leq a, 0 < z \leq a \\ \infty & \text{(other regions)} \end{cases} . \quad (1)$$

The Schrödinger equation for the particle in this quantum well is

$$\frac{1}{2}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right)\psi(x,y,z) = E\psi(x,y,z). \quad (2)$$

By solving the Schrödinger equation, we get the energy eigenvalues and eigenfunctions of this system,

$$E_{(n_x,n_y,n_z)} = \frac{\pi^2\hbar^2}{2ma^2}(n_x^2 + n_y^2 + n_z^2),$$

$$\psi_{(n_x,n_y,n_z)}(x,y,z) = \sqrt{\frac{8}{a^3}}\sin\left(\frac{n_x\pi x}{a}\right) \times \sin\left(\frac{n_y\pi y}{a}\right)\sin\left(\frac{n_z\pi z}{a}\right), \quad (3)$$

where n_x, n_y, $n_z = 1, 2, 3, \cdots$.

In the periodic orbit theory, one of the most important physical quantities is the density of energy states. As in Ref. [6], the energy state density can be split into a smooth, slowly varying part $\rho_0(E)$ and some oscillatory terms which are dominated by the classical periodic orbits whose actions, $S_\gamma(E)$, correspond to periodic orbit or closed paths. Specially, using the quantized energy eigenvalues, labelled collectively as E_n, one has

$$\sum_{n=1}^{\infty}\delta(E - E_n) \equiv \rho(E) = \rho_0(E) + \sum_{p=1}^{\infty}\sum_{\gamma}\rho_{\gamma,p}\cos\left[p\left(\frac{S_\gamma(E)}{\hbar} - \phi_\gamma\right)\right], \quad (4)$$

where each periodic orbit is characterized by a label $\gamma = 1, \cdots, \infty$, p denotes all possible repetitions of such trajectories ($p = 1, \cdots, \infty$), and ϕ_γ is the phase modification in the path integral.

For a 3D billiard system, i.e., a particle which is free inside an infinite well of arbitrary shape, with the area A, circumference L, and $\psi = 0$ on the boundary, the smooth part $\rho_0(E)$ can be written as[13]

$$\rho_0(E) = \frac{A}{4\pi}\left(\frac{2m}{\hbar^2}\right) - \frac{L}{8\pi}\sqrt{\frac{2m}{\hbar^2 E}} \rightarrow \frac{A}{4\pi} - \frac{L}{8\pi}\frac{1}{\sqrt{E}}. \quad (5)$$

For simplicity, we often set $\hbar^2/2m = 1$.

A particular way to visualize the possible classes of classical closed orbits is presented by geometrical method. Make use of the fact that the 3D cube can be tiled with a cubic lattice. Consider a specific cubic billiard, by repeated folding, any point in the original cubic can be connected to the corresponding point in another "identified" partner and the resulting path inside a specific cubic billiard can be obtained by repeatedly folding the two cube until they overlap. Thus all the length of the periodic orbits can be found by this symmetric method, as shown in Fig. 1.

Taking the point $(0, 0, 0)$ as an example, the corresponding coordinates are

$$x_p = p(2a), \quad y_q = q(2a), \quad z_r = r(2a), \quad (6)$$

in which $2p$, $2q$, and $2r$ count the number of the hits on the vertical, horizontal and the back-forth planes respectively before it returns to the starting point. The length of the classical orbit is

$$L(p, q, r) = \sqrt{(x_p - 0)^2 + (y_q - 0)^2 + (z_r - 0)^2}$$
$$= 2a\sqrt{p^2 + q^2 + r^2}. \quad (7)$$

Using this method, we find all the possible periodic orbits with the length of $L/a \leq 40$. Some of the periodic orbits are given in Fig. 2. Figure 2(a) is the period orbit with the length of $L/a = 2$, $p = 1$, $q = 0$, $r = 0$, which shows that the orbit impacts with the vertical planes twice before it returns to the starting point. Figure 2(b) is one with the length of $L/a = 2.828$ and $p = 1$, $q = 0$, $r = 1$, which shows that the orbit impacts with the vertical planes and back-forth planes twice before it returns to the starting point $\cdots$. Figure 2(d) is the one with the length of $L/a = 4.899$, $p = 2$, $q = 1$, $r = 1$, the orbit impacts with the horizontal planes and

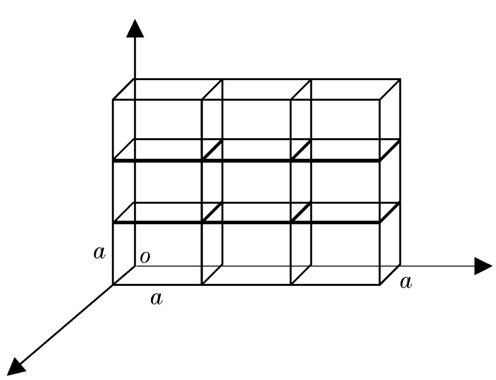

Fig. 1. Geometrical description of the construction of the path lengths corresponding to various periodic orbits in the cubic billiard.

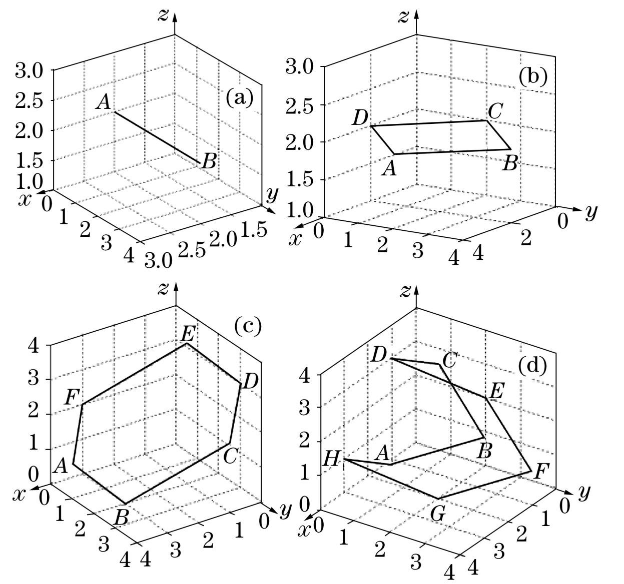

Fig. 2. Some classical periodic orbits of the cubic billiard with the length of $L/a \leq 40$. (a) $p = 1$, $q = 0$, $r = 0$; (b) $p = 1$, $q = 0$, $r = 1$; (c) $p = 1$, $q = 1$, $r = 1$; (d) $p = 2$, $q = 1$, $r = 1$.

back-forth planes twice and the vertical planes four times before it returns to the starting point. It is obvious that the more the number of hits, the more complex the shape of the orbits.

We are most interested in the oscillatory term of Eq. (4). The quantized energies and the primitive actions are given by

$$E_n = \frac{\hbar^2 k_n^2}{2m} \rightarrow k_n^2,$$
$$S_\gamma(E = k^2) = \hbar k L_\gamma, \quad (8)$$

where k_n is the wavenumber and L_γ is the length of the primitive periodic orbit.

Using these formulas and Eq. (4), we write the equivalent density of states in k-space (ignoring the unimportant factor of 1/2) as

$$\sum_{n=1}^{\infty}\delta(k - k_n) \equiv \rho(k)$$
$$= \rho_0(k) + \sum_{p=1}^{\infty}\sum_{\gamma}\rho_{\gamma,p}\cos[p(kL_\gamma - \phi_\gamma)]. \quad (9)$$

By taking the Fourier transform of the above equation, we have

$$\rho(L) = \sum_{n=1}^{\infty}\int_{-\infty}^{+\infty}\delta(k - k_n)\mathrm{e}^{ikL}\mathrm{d}k = \sum_{n=1}^{\infty}\mathrm{e}^{ik_n L}, \quad (10)$$

which can be evaluated by using the bound state energy spectrum, actually the corresponding wavenumbers k_n.

For the semi-classical oscillatory term, after taking the Fourier transformation, we get

$$\rho(L) = \sum_{p=1}^{\infty}\sum_{\gamma}\rho_{\gamma,p}\delta(L - pL_\gamma). \quad (11)$$

Table 1. Correspondence between the Positions of the Peaks in the Quantum Spectra and the Lengths of the Classical Periodic Orbits

	1	2	3	4	5	6	7	8
Position of the Peak of the Quantum Spectra	8.0	8.250	8.490	8.720	8.940	14.0	14.140	14.280
Length of the Classical Periodic Orbit	8.0	8.246	8.485	8.718	8.944	14.0	14.141	14.283
	9	10	11	12	13	14	15	16
Position of the Peak of the Quantum Spectra	14.420	14.560	14.700	15.000	27.930	28.070	28.140	28.350
Length of the Classical Periodic Orbit	14.422	14.560	14.697	14.967	27.929	28.068	28.142	28.348
	17	18	19	20	21	22	23	24
Position of the Peak of the Quantum Spectra	28.490	28.700	28.910	28.990	36.110	36.280	36.810	36.920
Length of the Classical Periodic Orbit	28.492	28.698	28.912	28.988	36.112	36.278	36.811	36.922

It exhibits a series of δ function like sharp peaks at multiples of the lengths of the primitive closed paths, i.e., at $L = pL_\gamma$. Thus, if we evaluate the Fourier transform $\rho(L)$ of the wavenumber spectrum via Eq. (10), we should find a series of sharp peaks corresponding to the lengths of classical periodic orbits. For evaluating Eq. (10) numerically, we use a finite number of wavevectors, namely

$$\rho_N(L) = \sum_{n=1}^{N} \mathrm{e}^{ik_n L}. \tag{12}$$

For the 3D cubic billiard system, the wavenumbers are

$$k_n = k_{(n_x,n_y,n_z)} = \sqrt{\frac{2m}{\hbar^2} E(n_x, n_y, n_z)} = \frac{\pi}{a}\sqrt{n_x^2 + n_y^2 + n_z^2}. \tag{13}$$

Using Eq. (12), we calculate the Fourier transformed quantum spectra $\rho_N(L)$ (using the lowest eigenvalues $N = 10000$). Figure 3 plots the results of $|\rho_N(L)|^2$ versus $L/a \leq 40$ (for simplicity, we set $a = 4.0$). In Table 1, we list part of the positions of peaks in Fig. 3 and the lengths of the classical periodic orbits. The results show the classical result and the quantum result agree well with each other, which verifies the correctness of the periodic orbit theory. It also shows the correspondence of the quantum and classical description of the 3D cubic billiard system. From Fig. 3 we can see that when the length of the periodic orbit is short, the number of the periodic orbits is small, and so does the peak of the quantum spectra; however with the increase of the length of the orbits, the number of the periodic orbit increases greatly and more and more peaks appear. However, if we limit the length of the orbit to a small region, we will find that each peak corresponds to one periodic orbit. In order to show this clearly, we give an inset plot in each figure. In Fig. 4, we plot the Fourier transformed quantum spectra $|\rho_N(L)|^2$ of the 2D square billiard using the lowest eigenvalues $N = 3000$ versus $L/a \leq 40$. From Figs. 3 and 4, we found that the quantum spectra of the cubic billiard are more complex than that of the square billiard, because the number of the periodic orbits in cubic billiard is much more than that in the square billiard within the same length of the orbits.

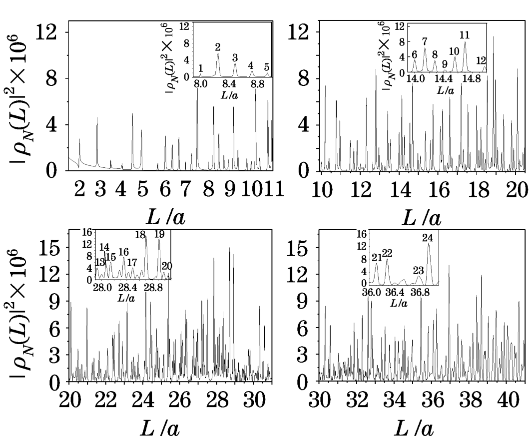

Fig. 3. Fourier transformed quantum spectra $|\rho_N(L)|^2$ of the 3D cubic billiard (using the lowest eigenvalues of $N = 10000$) versus $L/a \leq 40$.

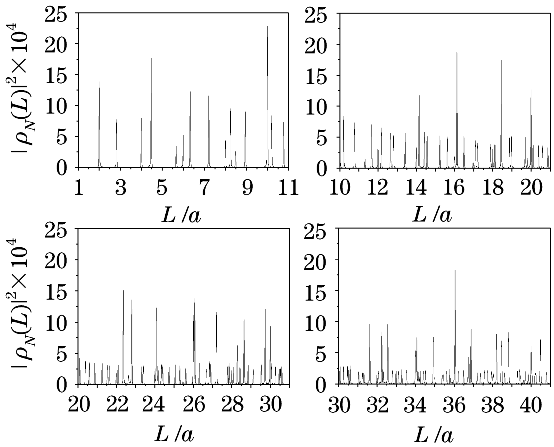

Fig. 4. Fourier transformed quantum spectra $|\rho_N(L)|^2$ of the 2D square billiard (using the lowest eigenvalues of $N = 3000$) versus $L/a \leq 40$.

In conclusion, by solving the Schrödinger equation of the 3D billiard, we get the energy eigenvalues and eigenfunctions of this system. Using periodic orbit theory, we find the periodic orbits of this system within a certain length. Then we calculate the quantum spectra of the 3D billiard. In order to show the correspondence between the quantum spectra and the classical periodic orbits, we make a Fourier transformation to the spectra. The Fourier transformed spectrum of this system has allowed direct comparison between peaks in such plot and the length of the periodic orbits, which verifies the correctness of the periodic orbit theory in 3D systems. It also shows the correspondence between the quantum description and the classical description for the same system. The correspondence we have studied is quite general and should also exist in other systems, and it may shed light on the transport property of semiconductor, which depends on the shape of the potential well[14,15]. In the future, we will use the quantum Gaussian wave packet method[16] and other methods to analyze the dynamics of this system.

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