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The dynamics of a particle in square and circular billiards is studied within the framework of Bohm's quantum mechanics. While conventional quantum mechanics predicts that the system shows no indication of chaotic behavior for these geometries from either the eigenvalue spectra distribution or the structure of the eigenfunctions, we find that in Bohm's quantum mechanics these systems exhibit both regular and chaotic behavior, depending on the form of the initial wave packet and on the particle's initial position.
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The question of how the properties of nonintegrable classical Hamiltonians are manifested in the corresponding quantum systems has been of great interest in recent years [1–4]. A variety of problems has been considered to investigate the connections between classical and quantum systems under the conditions where classical chaos is present [3,5–12]. In particular, two-dimensional billiards is among the problems most studied [5–7,9,12,13].

The stadium (or noncircular billiard) is a planar table with circular ends of radius a separated by parallel sides of length $2b$. The classical trajectories in such systems are found to be regular (integrable) in the circular limit ($b=0$), and chaotic (nonintegrable) for the noncircular case ($b>0$) [5]. The quantum version of those systems were studied by MacDonald and Kaufman [6]. They found that for the circular billiard the energy level separation was a Poisson-like distribution, while the noncircular billiard presented a Wigner-like distribution, exhibiting mutual repulsion of neighboring levels. They also found that the eigenfunction nodal curves for the stadium exhibited a noncrossing irregular pattern. For the circular billiard, the eigenfunction nodal curves are concentric circles.

A very interesting quantum manifestation of classical chaos first observed in billiards [6,13] is that many of the eigenfunctions of the quantum problem appear to coalesce around the (unstable) classical periodic orbits of the system. These larger than expected probability densities are localized around channels forming simple shapes, the so-called ''scars'' of periodic orbits. The presence of scars is seen as an indication of non-integrability of these systems.

After the seminal work of Bohigas *et al.* [7], it was shown [2,3] that the level spacing statistics in a variety of quantum systems with chaotic classical counterparts is well described by random matrix theory (RMT) [14]. That is, the level spacing distributions for those quantum systems are in excellent agreement with the spacing distribution between consecutive eigenvalues of the random matrix. Although the energy level spacing statistics for a variety of quantum systems that are chaotic when treated classically are described by RMT, it was found recently that two systems which are chaotic classically, namely, the hydrogen atom in a magnetic field and a two-dimensional quartic oscillator, have in the quantum regime an energy level spacing distribution drastically different from the expected Wigner distribution [11]

In spite of some progress in the theoretical developments concerning the signatures of chaos in quantum systems, a rigorous procedure to fingerprint chaos in such systems is still lacking. One fundamental reason for this problem is that chaos in classical mechanics is defined in terms of the exponential divergence of neighboring trajectories, while the very concept of a trajectory is absent in conventional quantum mechanics. One way to cope with this problem is to adopt Bohm's formulation of quantum mechanics [15–17], in which particle trajectories are well-defined and, consequently, the definition of chaos in classical mechanics can be naturally extended to the quantum domain. In fact, Bohm and Hiley [16] were the first to propose the application of Bohm's theory to the problem of quantum chaos. They speculated on the possibility of chaotic behavior for a single particle in a two-dimensional box. Since then some papers have appeared dealing with applications of Bohm's quantum mechanics to the study of chaos [18].

One should note that when a statistical ensemble of particles trajectories is incorporated into Bohm's theory, the results will be identical to those of conventional quantum mechanics. That is, by averaging over the initial positions of the particle, one obtains the same results as those of conventional quantum mechanics. In the averaging procedure there may be contributions from chaotic as well as from nonchaotic trajectories arising from different initial conditions. Bohm's theory has the advantage that it can separate chaotic from non-chaotic behavior arising from distinct initial conditions. Such an insight cannot be inferred from conventional quantum mechanics alone.

In the present paper, we investigate the quantum problems of square and circular billiards within the deterministic framework of Bohm's quantum mechanics. We would like to discover whether or not the statistical properties of the eigenvalue spectra have anything to do with the actual motion of a quantum particle when its dynamics is governed by Bohm's mechanics. That is, we want to know whether the Wigner

(Poisson) distribution of energy levels necessarily implies that the system will behave chaotically (regularly) or other criteria apply.

The deterministic interpretation of Bohm's quantum mechanics [15] arises when we express the wave function in the form $\psi = R\ \exp(-iS/\hbar)$ and rewrite the Schrodinger equation as conditions on both the phase $S(\mathbf{r},t)$ and amplitude $R(\mathbf{r},t)$. The real and imaginary parts of the equations can be separated, yielding a pair of equations for the squared amplitude $\rho = R^2$ and phase S,

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \left(\frac{\rho \nabla S}{M} \right) = 0, \tag{1}$$

$$\frac{\partial S}{\partial t} + \frac{(\nabla S)^2}{2M} + V + Q = 0, \tag{2}$$

where M is the mass of the particle and $Q = -(\hbar^2/2M)/(\nabla^2 R/R)$ is the so-called *quantum potential*. The first equation represents the usual conservation of probability. The similarity between Eq. (2) and the Hamilton-Jacobi equation led Bohm to define the momentum of the quantum particle, just as in classical mechanics, as $M\mathbf{V} = \nabla S$ [15]. The velocity of the particle is then given in terms of the wave function by

$$\mathbf{V}(x,y,t) = \frac{\hbar}{2Mi}(\psi^* \nabla \psi - \psi \nabla \psi^*)/(\psi^* \psi). \tag{3}$$

The particle is assumed to have a well-defined position and a velocity, given by Eq. (3), which upon integration yields the trajectories. The presence of the quantum potential indicates that the particle is guided by a wave that is the solution to the Schrodinger equation, just as in the pilot wave picture proposed earlier by de Broglie [19,20]. In this way, the quantum dynamics is completely understood as the motion of a particle experiencing forces from both classical and quantum potentials. Newton's second law, modified by the presence of the quantum force, can be written as

$$M\frac{d^2\mathbf{r}}{dt^2} = -\nabla(V+Q)|_{\mathbf{r}=\mathbf{r}(\mathbf{t})}. \tag{4}$$

Hence, quantum mechanics can be described in a way similar to classical mechanics, and it seems reasonable to use the same criteria to characterize the dynamical state of the system. The quantum trajectories of the particle are obtained by first solving the time dependent Schrodinger equation, then by determining the quantum potential, and finally by integrating the modified Newton's equation, Eq. (4). An equivalent, but more practical, way to accomplish that is by integrating the guidance formula Eq. (3) directly, for a given initial position (x_0, y_0).

Let us first consider a particle in a two-dimensional square box of side L. The wave function can be built from components of the set of eigenfunctions of the energy,

$$u_{mn}(x,y) = (2/L)\sin(k_x x)\sin(k_y y), \tag{5}$$

where $k_I = n_I \pi/L$. The complete time dependent solution will involve a linear combination of these eigenstates:

$$\psi(x,y,t) = \sum_{m,n} C_{mn} u_{mn}(x,y)\exp(-iE_{mn}t/\hbar), \tag{6}$$

where C_{mn} are complex coefficients, and $E_{mn} = (\hbar^2/2M)(k_x^2 + k_y^2)$ are the energies of the system. At this point, we would like to mention that a *qualitative* discussion on the dynamics of a particle in a two-dimensional box was given earlier by Bohm and Hiley [16]. They noticed that from Eqs. (3) and (6) the expression for the velocity of the particle in the box contains a large number of small terms involving combinations of sines and cosines. As time evolves, these terms change rapidly, and more so the higher the quantum numbers m and n. Although the ratio of the frequencies for the x and y components is rational, it will approach the case of incommensurability in the limit of large quantum numbers. Consequently, the expression for the velocity consists of many terms having complex phase relations with one other. Bohm and Hiley argued that the particle motion would be, in a way, similar to a Lissajous figure. They claimed that in a real box (where irregularities are present) the frequencies and wave numbers would be related incommensurably, and the particle motion would be chaotic-like. We shall see below that the motion of the particle in the (ideal) box can be quite complex even when we consider an initial wavepacket consisting of just a few eigenfunctions with low quantum numbers, and that chaotic behavior is manifested even if the walls have no irregularities.

We now discuss the results of our calculations for the particle in the square box. As the initial wavepacket, we consider linear combinations involving only a few of the lowest eigenfunctions. In all of our numerical analysis, we set $\hbar = 2M = 1$. The linear size of the box is taken as $L = 1$. The integration of Eq. (3) is carried out by using a fourth order fixed step Runge-Kutta routine with an integration step $\delta t = 0.001$. We find that the particle dynamics is strongly dependent on the form of the initial wavepacket. Notice that because of the absence of any position dependent phase factor in the eigenfunctions of the particle in a square box [Eq. (6)], if a particle was in a single eigenstate it would remain at rest for all times. Consider the following initial wavepacket, $\psi(x,y,0) = u_{11}(x,y) + u_{12}(x,y) + iu_{21}(x,y)$, with the particle initially at $(x_0, y_0) = (0.8, 0.5)$. The trajectory of the particle in the (x,y)-plane is depicted in Fig. 1(a).

That particular choice of initial conditions led the particle to pass through the center of the box on every turn. One should notice that the particle never hits the walls; this is due to the presence of a strong repulsive quantum potential near the walls. A different choice of the initial position can give rise to an entirely new trajectory, depending on whether or not that point lies inside the basin of attraction of the original attractor. On the other hand, a change in the initial wavefunction will generate an altogether different quantum potential and, consequently, an entirely new trajectory for the particle. The type of motion shown in Fig. 1(a) can be characterized by looking, for example, at the Poincaré section, plotted in Fig. 1(b). The distribution of points on that curve indicates that the motion is quasi-periodic. This is confirmed by both the power spectrum $F(\omega)$ shown in Fig. 1(c), where only a few sharp peaks are present, and by the fact that largest Lyapunov exponent is zero.

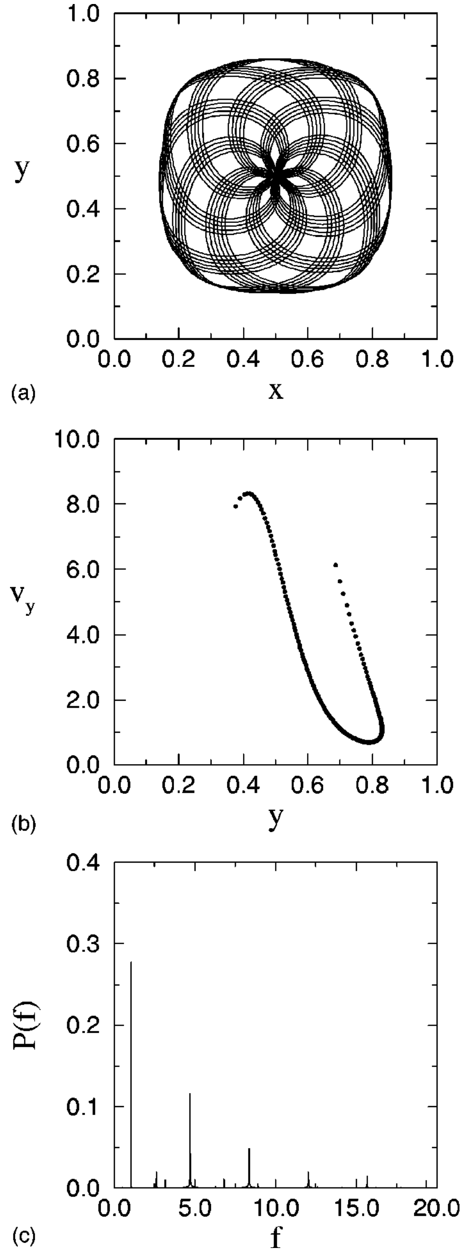

FIG. 1. Quantum particle trapped in a two-dimensional box of sides L. The system of units is such that $\hbar = 2M = 1$ and the length unit is the linear size L of the box. The wave packet for $t=0$ was chosen to be $\psi(x,y,0) = u_{11}(x,y) + u_{12}(x,y) + iu_{21}(x,y)$ and the initial position of the particle was (0.8, 0.5). (a) Actual trajectory of the particle in the (x,y) plane; (b) Poincaré plot in the (y,v_y) plane; (c) power spectrum $P(f)$ for the time series of $x(t)$. The power spectrum is shown in arbitrary units.

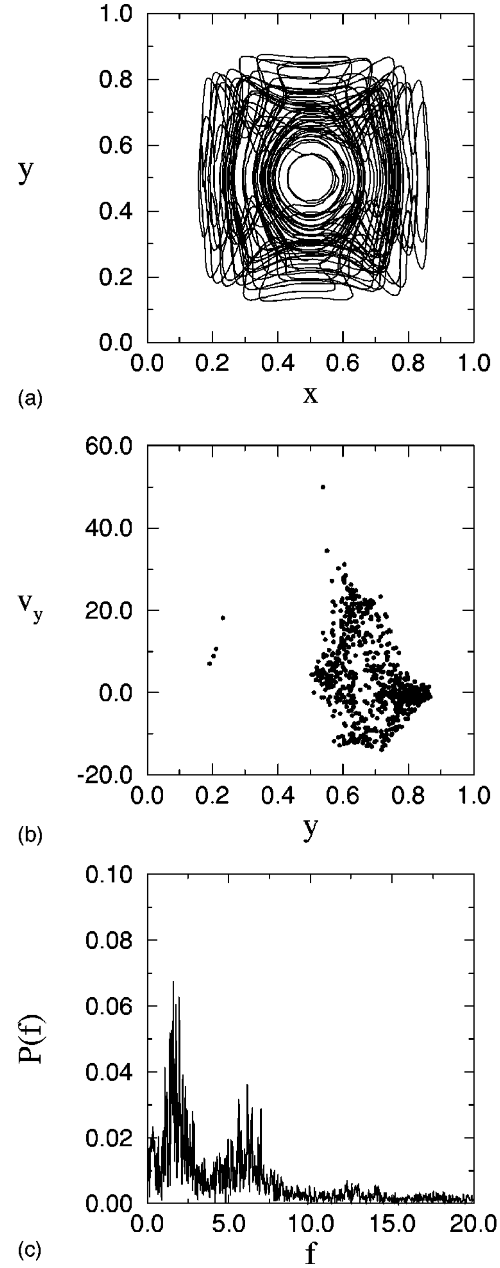

FIG. 2. Quantum particle moving in the square box whose linear size is L. The initial wave packet is $\psi(x,y,0) = u_{12}(x,y) + iu_{21}(x,y) + u_{23}(x,y)$, with starting position at (0.5, 0.25) in units of the box size L. In the system of units used, $\hbar = 2M = 1$. (a) Actual particle's trajectory in the (x,y) plane; (b) phase portrait in the (y,v_y) plane; (c) power spectrum $P(f)$ from the time series of $x(t)$ showing a broadband, which indicates chaotic motion.

Figure 2(a) shows a new particle trajectory resulting from using $\psi(x,y,0) = u_{12}(x,y) + iu_{21}(x,y) + \gamma u_{23}$ as the initial wave packet, $(x_0,y_0) = (0.5,\ 0.25)$ as the initial position, with $\gamma = 1$. The particle's trajectory looks quite irregular, even for such a simple wave function. The scattered points in the Poincaré section plot [Fig. 2(b)] and the broad spectrum shown [Fig. 2(c)] indicate that the motion of the particle is chaotic. As the coefficient γ is lowered towards zero the power spectrum gets less noisy (the largest positive Lyapunov exponent gets smaller), indicating that the particle motion is less chaotic, until γ reaches zero, when the particle describes a circular motion about the center of the box. These results are in disagreement with the criteria previously used to characterize quantum chaos, based on the distribution of nodes [6] or on the distribution of energy states [6,7].

We have also studied the case of a particle in a circular billiard. The analysis is similar to the case of the square billiard. We found that the particle can have either regular or chaotic types of motion, depending on the initial wave packet and initial position, just like in case of the square billard. Therefore, the details of our calculations for the particle in the circular billiard will not be reported here, since the outcomes are qualitatively the same as those of the square billiard.

To summarize, we have discussed the dynamics of a quantum particle in square and circular billiards. We find that for both geometries the motion of the particle can be either regular or chaotic, depending on the initial form of the wave packet and on the particle's initial position. This is a surprising result, even from Bohm's point of view, in that a linear combination containing only a few eigenfunctions is already sufficient to produce very complex trajectories. We conclude that the dynamics of the particle, as described by Bohm's quantum mechanics, is not determined by the distribution of the eigenvalue spectra: In both cases investigated, the level spacing follows a Poisson-like distribution, which would suggest regular behavior, yet we found instances where the motion is clearly chaotic. Moreover, the chaotic nature of Bohmian trajectories is not dictated by whether or not the underlying classical Hamiltonian counterpart is chaotic. In the two cases we studied, the classical versions are not chaotic, yet we find instances where the Bohmian orbits do show chaos. That can be understood from the fact that in Bohm's picture the wave function introduces an additional interaction, the quantum potential, into the system. It follows that by studying Bohmian trajectories one cannot distinguish systems with chaotic classical counterparts from systems with nonchaotic classical analogues.

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