# Quantum chaos in a double square well: An approach based on Bohm's view of quantum mechanics

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We study the dynamics of a quantum particle in a double square-well potential within a deterministic framework using Bohm's quantum mechanics. Phase portraits, Fourier spectral analysis, Poincaré sections, and Lyapunov exponents clearly indicate that the particle undergoes periodic, quasiperiodic, and chaotic motions depending on the initial form of the wave packet. We also make a detailed comparison between the predictions of the present approach and those of conventional quantum mechanics for the same problem. [S1063-651X(98)03411-4]

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Quantum chaos is an area of much research activity in spite of a lack of consensus about its very meaning, definition, or even its observability. Because of the lack of a direct correspondence between classical trajectories in phase space and the observables in conventional quantum mechanics, the characterization of chaos in the latter is quite controversial. As we know, classical chaotic behavior is usually defined by the unique property of a nonlinear system which under certain conditions becomes highly sensitive to its initial conditions. When a system is in the chaotic state, initially neighboring phase-space trajectories will separate exponentially as the system evolves in time. This definition, however, seems to be inadequate to study chaos in quantum systems since it presumes that the trajectory of a particle is a well-defined quantity. Hence, the conventional interpretation of quantum mechanics is not appropriate to describe quantum chaos the same way we do in classical mechanics.

A variety of methods have been proposed to identify the criteria by which a quantum system is chaotic [1–3]. One such method is to study the evolution of the mean values of the operators and the structure of the energy spectrum. The energy levels have been found to have different statistical distribution when the corresponding classical system is chaotic (Wigner statistics) or regular (Poisson statistics) [2,3]. Although the energy level spacing statistics of a variety of quantum systems that are chaotic when treated classically are described by Wigner statistics, it was found recently [4] that two systems, namely, the hydrogen atom in magnetic field and a two-dimensional quartic oscillator, which are chaotic classically, have in the quantum regime an energy level spacing distribution drastically different from the expected Wigner distribution. It has also been conjectured [5] that the distribution of the fluctuations of the spectral density of states of a quantum system must be Gaussian if the corresponding classical counterpart is strongly chaotic, or non-Gaussian if the classical system is integrable. Another approach to detect the presence of quantum chaos is to assume that its signature can be inferred directly from the behavior of the wave function [6,7]. For instance, the wave packet of the quantum counterpart of a classical chaotic system was found to spread rapidly over regions where the potential is significantly nonlinear [8], or the wave function develops a highly complex pattern in the chaotic region [9]. In spite of these attempts, finding unambiguous fingerprints of quantum chaos is still very much an open problem. In any event, the field of quantum chaos is usually restricted to the study of quantum systems whose classical limits are chaotic.

An alternate way to deal with quantum dynamics is by using the so-called quantum theory of motion (QTM), which was proposed some time ago by Bohm [10] (and similarly by de Broglie [11,12]) but that only recently has gained some attention [13–15]. Bohm's theory gives exactly the same results as conventional quantum mechanics, yet it goes one step ahead of the Schrödinger equation insofar as making precise statements about the actual trajectories of a single particle (Bohm's postulate). Hence, QTM seems to be a more appropriate framework for investigating quantum chaos. Actually, Bohm and Hiley were the first to put forth the idea of applying QTM to quantum chaos, namely in the problem of a single particle confined in a two-dimensional box [13]. About the same time, Holland [15] also suggested that the concepts of chaos from classical physics could be extended to the particle trajectories of Bohm's mechanics.

In this work we use Bohm's theory to investigate the dynamics of a particle in a double square-well potential, that is, a square barrier embedded in an infinite well. In a recent paper, Parmenter and Valentine [16] argued that a one-dimensional quantum system could not exhibit chaos within the QTM framework. We find that a one-dimensional system can indeed exhibit chaotic behavior, in contrast to Parmenter and Valentine's assertions. To our knowledge, ours is the first application of Bohm's mechanics to the study of quantum chaos in a one-dimensional system. We believe this is also the first comparison between the predictions of QTM and conventional quantum mechanics about the chaotic behavior of a quantum system.

The chaotic behavior of a particle in the double-well potential was discussed recently by Ashkenazy *et al.* [6] and also by Berkovits *et al.* [7] within the context of conventional quantum mechanics. Ashkenazy *et al.* found that the time evolution of an initially Gaussian wave packet in a double square-well potential shows a complex behavior. This was believed to be induced by tunneling through the barrier since such complex behavior for the wave packet was not observed in the absence of the barrier. Such a behavior was then interpreted as a signature of quantum chaos. On the other hand, Berkovits *et al.* [7] tackled the same problem by analyzing the distribution of energy levels about the top of the barrier. They found that the distribution of energies slightly above the barrier is closer to Wigner statistics than for other values of energy, thus indicating that the system is chaotic for energies just above the barrier level. One should note that in the work of Ashkenazy *et al.*, all the energy levels included in their Gaussian packet are below the height of the barrier.

According to QTM, a single quantum-mechanical object consists of a particle of mass $m$ enveloped in a physically real field (the $\psi$ field) which guides the particle according to the *guidance formula* Eq. (1) below. The field satisfies the time-dependent Schrödinger equation (TDSE), and the particle motion is obtained from the equation

$$m\mathbf{v}=\nabla S, \tag{1}$$

where $S(x,t)$ is the phase of the wave function. For a given external potential $V(x)$, the trajectory of a particle and the time evolution of its dynamical variables are determined once its initial $\psi$ field and its initial position are given. The phase $S(x,t)$ of the wave function satisfies the nonlinear differential equation

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

where $Q=-(\hbar^2/2m)\nabla^2 R/R$ is the so-called quantum potential and $R$ is the amplitude of the wave function. Equation (2) can be interpreted as a Hamiltonian-Jacobi equation describing the classical trajectory of a particle of mass $m$ moving in the potential $V+Q$. The equivalent Newtonian form for the equation of motion is

$$m\,\frac{d^2\mathbf{x}}{dt^2}=-\nabla(V+Q)\big|_{\mathbf{x}=\mathbf{x}(\mathbf{t})}. \tag{3}$$

Therefore, in the QTM framework quantum dynamics is similar to classical dynamics, with an important addition: the particle is subjected not only to a classical external potential $V(x)$, but also to a quantum internal potential $Q(x,t)$. The latter depends on both the external potential and the form of the initial wave packet.

Owing to the nonlinear nature of the quantum potential and its time dependence, a particle subjected to a harmonic classical potential $V(x)$ may show a chaotic behavior in the quantum regime, which would not be present had the particle been treated classically [13,16]. Pattanayak and Schive [17], by using a semiquantal approximation for the double-well potential, were able to find quantum chaos for an extended classical potential which effectively included effects of quantum fluctuations, thereby showing that the presence of quantum effects could induce chaos.

One of the primary goals of the present work is to compare the predictions of conventional quantum mechanics with those of Bohm's theory regarding chaotic behavior in the problem of a particle confined to a double square-well potential. In order to make such comparison, we use the same parameters as those in Refs. [6,7], namely the barrier half-width $a=1$ and the half-width of the well $L=55$. In all our calculations we have assumed $\hbar=2m=1$. For the barrier height, however, we take $V=0.1$ in order to enhance the tunneling probability.

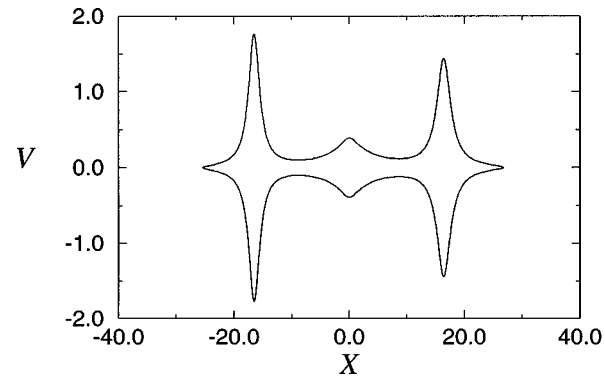


FIG. 1. Phase-space portrait for a quantum particle trapped in a double square-well potential. The system of units is such that $\hbar=2M=1$ and the length unit is the barrier half-width $a$. The initial position was $x_0=3.0$ and the wave function at $t=0$ was given by $\psi(x,0)=u_3^-(x)+iu_3^+(x)$. The system is periodic with period $T=2\pi/\omega$ and angular frequency $\omega=(E_3^+-E_3^-)/\hbar$.

In all cases discussed below, we use a linear combination of the first few states with energy less than the barrier energy as the initial wave function. Let $u_n^+(x)$ and $u_n^-(x)$ denote the even and odd eigenfunctions for the double square-well potential with eigenvalues $E_n^+$ and $E_n^-$, respectively. The position of the particle is determined by simultaneous integration of both the TDSE and the guidance formula, Eq. (1). We performed the numerical integration of Eq. (1) by using a fourth-order Runge-Kutta integration procedure with integration step $\delta t=0.01-0.001$. The integration was performed up to times of $t=1.5\times 10^5$.

Consider the dynamics of a particle initially in the quantum state $\psi(x,0)=u_3^-(x)+iu_3^+(x)$ whose position is located at the right of the barrier, at $x_0=3$. We find that the particle undergoes a periodic behavior, with a period given by $T=2\pi\hbar/(E_3^+-E_3^-)$. The particle is periodically ''tunneling'' since the barrier energy $V>E_3^+>E_3^-$. The phase portrait is shown in Fig. 1. In that case, the largest Lyapunov exponent is zero. A simple explanation for that phenomenon, from the QTM point of view, is that the particle is not only subject to the barrier potential but also to the oscillating quantum potential generated by the $\psi$ field. As a result, the effective potential near the center of the well is no longer constant but oscillating in time, leading to an effective energy barrier that is smaller than the kinetic energy of the particle in the same region. A change in the form of the wave function at $t=0$ leads to a change in the form of the quantum potential and, therefore, to an altogether different dynamics. For instance, by taking $\psi(x,0)=u_1^-(x)+u_2^+(x)+iu_1^+(x)$ and the same initial position $x_0=3$, the particle undergoes a quasiperiodic behavior, as shown in Figs. 2(a)–2(c). The quasiperiodic behavior can be readily seen from the Poincaré plot [Fig. 2(b)], where all the points fall on a closed curve. In that case, the

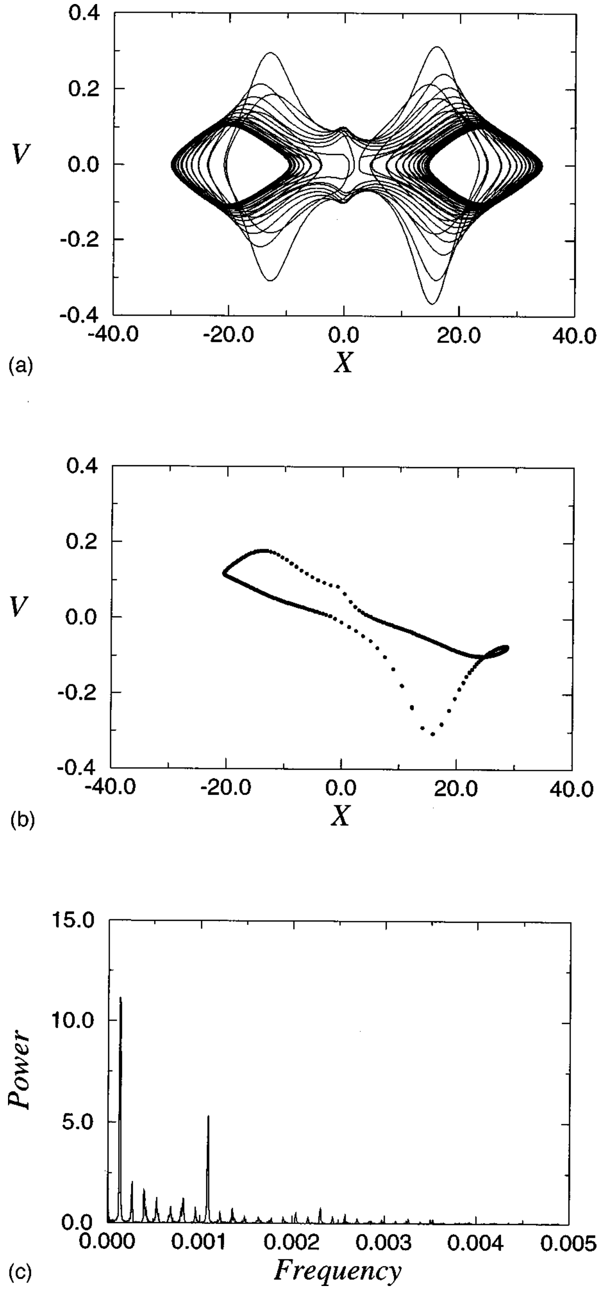


FIG. 2. Particle in a double square-well potential in a quasiperiodic regime. In the system of units used, $\hbar = 2m = 1$, and the length unit is the barrier half-width $a$. (a) Plot of the phase-space trajectory. The initial position was taken as $x_0 = 3.0$ and the wave function at $t = 0$ was given by $\psi(x,0) = u_1^-(x) + u_2^+(x) + iu_1^+(x)$; (b) Poincaré section for the velocity and position using a strobe frequency of $\omega = (E_2^+ - E_1^+)/\hbar$; (c) power spectral density as a function of frequency $f = 2\pi/\omega$ obtained from a time series for $x(t)$. The system is quasiperiodic.

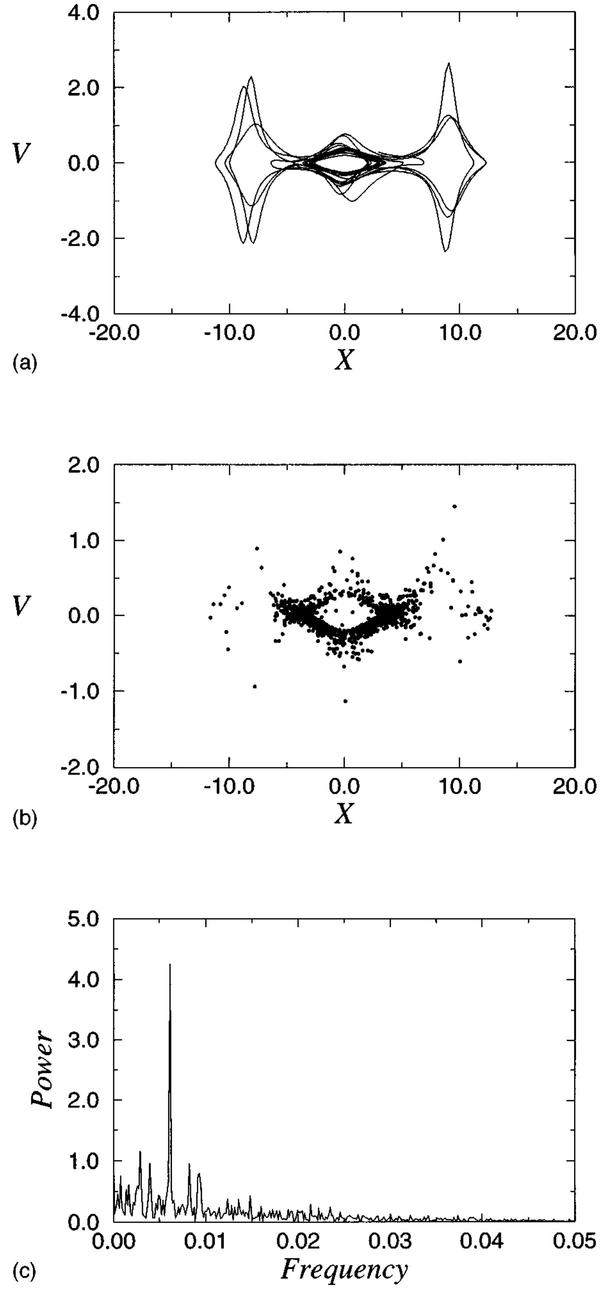


FIG. 3. Chaotic behavior of a particle in a double square well. Again, the units are such that $\hbar = 2m = 1$, and the unit of length is the barrier half-width $a$. (a) Phase-space diagram. We took the initial position $x_0 = 3.0$ and the wave function at $t = 0$ as $\psi(x,0) = \Sigma_{n=1}^4 u_n^+ + iu_5^-(x)$; (b) Poincaré section for the velocity and position using a strobe angular frequency $\omega = (E_5^- - E_1^+)/\hbar$; (c) power spectral density as a function of frequency $f = 2\pi/\omega$ obtained from a time series for $x(t)$. The system is in a chaotic state.

two largest Lyapunov exponents are equal to zero. The Fourier spectral analysis shows a sharply defined peak distribution, as depicted in Fig. 2(c). If the initial wave function has the form $\psi(x,0) = \Sigma_{n=1}^4 u_n^+(x) + iu_5^-(x)$, the particle undergoes a chaotic behavior for the same initial position, as shown in Figs. 3(a)–3(c). The Poincaré plot consists of points that are now scattered in the phase-space plane, and the power spectrum shows the typical sharp peaks in a background of a broadband distribution, features which are similar to those found in classical chaotic systems. The largest Lyapunov exponent calculated numerically from the time series of $x(t)$ using the algorithm of Eckmann *et al.* [18] is found to be positive $(\lambda = 0.10 \pm 0.02)$, typical of a chaotic state. By keeping in mind that the energy levels included in the wave packet are lower than the barrier height, one can see that the above result is different from that of Berkovits *et al.* [7], which claims that quantum chaotic behavior should happen only for energies just above the barrier level.

In order to make a comparison with the results of Ashkenazy *et al.* [6], we now elect to represent the initial state of the particle as a Gaussian wave packet initially placed on the left of the barrier at position $x_0$, with an average momentum $k_0$, and a spread governed by $\sigma_0$. Thus, we set $\psi(x,0) = \exp[ik_0x-(x-x_0)^2/2\sigma_0^2]$. By taking $k_0=0.1$, $\sigma_0=5$, $x_0=-25$, and $V=5$ for the barrier height, the same parameters used in Ref. [6], we find that a particle initially located at the center of the packet undergoes a quasiperiodic motion and *not* a chaotic motion as predicted by those authors.

We should point out that from the QTM point of view there is a classical analog to the problem discussed in the present work. It is the problem of a particle trapped in a quartic potential well in the presence of an external oscillatory force field. The potential energy of the model is given by

$$V(x)=ax^4-bx^2+cx\,\cos(\omega_0 t), \tag{4}$$

where $a,b$ are positive constants, $c$ is a constant, and $\omega_0$ is the frequency of a forcing field. The oscillatory field in the classical case plays a role similar to that of the quantum potential for the corresponding quantum case. The effect of the forcing field is to alter the shape of the double-well and effectively to produce oscillations in the height of the barrier. In fact, the classical problem defined by Eq. (4) has already been studied by Reichl and Zheng [19] and it shows similarities in its dynamical behavior with the quantum double square-well potential discussed here. The system undergoes periodic, quasiperiodic, and chaotic behaviors for an appropriate choice of the parameter in the potential. The Poincaré plots are similar to those found in the quantum problem.

To summarize, we have shown that within Bohm's interpretation of quantum mechanics, a particle in a one-dimensional square double-well potential can undergo chaotic motion, contrary to claims found in the literature that precluded quantum chaos in one-dimensional systems [16]. In addition, based on our definition of chaos we obtain results that are different from those of Refs. [6] and [7]. In one instance, we find quantum chaos behavior even when the energy levels used in the wave packet are lower than the barrier height, contrary to Ref. [7]. The wave packets were built from the ground state and a few low-lying excited states of the double-well, all of which involve a finite $\hbar$. The essential ingredients for our results are the finiteness of $\hbar$, the confining walls, and the Bohmian trajectories. We believe, however, that the barrier is unimportant for the occurrence of chaos in the well. That is what happens in the quantum square billiard, the two-dimensional version of the single well, where we find instances of chaotic Bohmian trajectories even in the absence of internal barriers [20]. We are still investigating the problem of what happens to the trajectories in the semiclassical limit. In the case where the initial wave function is a Gaussian packet, we find quasiperiodic motion instead of the chaotic motion reported in Ref. [6].

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