Irreversibility with quantum trajectories

D. A. Wisniacki*
Departamento de Química C-IX, Universidad Autónoma de Madrid, Cantoblanco, 28049-Madrid, Spain and Departamento de Física "J. J. Giambiagi," FCEN, UBA, 1428 Buenos Aires, Argentina

F. Borondo†
Departamento de Química C-IX, Universidad Autónoma de Madrid, Cantoblanco, 28049-Madrid, Spain

R. M. Benito‡
Departamento de Física, E.T.S.I. Agrónomos, Universidad Politécnica de Madrid, 28040 Madrid, Spain
(Received 5 April 2005; published 27 October 2005)

Irreversibility is an important issue for many quantum processes. Loschmidt echoes, originally introduced as a way to gauge sensitivity to perturbations in quantum mechanics, have turned out to be a useful tool for its investigation. Following the philosophy supporting this idea, and using quantum trajectories as defined in the causal interpretation of quantum mechanics due to Bohm, we introduce in this paper a more informative alternative measure for irreversibility. The method is applied to the Bunimovich stadium billiard, a paradigmatic example of chaotic system, that constitutes an excellent model for mesoscopic devices.

DOI: 10.1103/PhysRevE.72.046219 PACS number(s): 05.45.Mt, 03.65.Ta, 03.65.Yz

I. INTRODUCTION

In the last 20 years, there has been an increasing interest in the study of chaotic phenomena [1], both in dissipative and Hamiltonian systems. These processes are very relevant in a variety of fields in physics. Among them, the late addition of the increasingly developing area of nanotechnology deserves a special mention [2]. For example, the ballistic transport of electrons in semiconductor heterostructures has been recently studied experimentally [3,4]. The corresponding dynamics is often chaotic and the associated motions are classically well characterized in terms of relevant phase space structures, such as attractors, homoclinic tangles, Lyapunov exponents, etc., that have been thoroughly studied. The situation is different for the quantum counterpart, where much less is known, being "quantum chaos" an active field of research [5,6].

Most problems in quantum chaos are of theoretical nature, falling within the category of semiclassical theories [7]. However, they find an immediate application in mesoscopic systems, thanks to recent technical developments that have made possible the manufacturing of micro- and nanostructures, whose dimensions and characteristics allow charge transport without loss of electron phase coherence [8]. Moreover, when the system is confined in all dimensions and the sample is sufficiently clean, the correlations in the energy spectrum against variations of parameters, such as the sample geometry or the intensity of an external field, are very similar to those found in quantum billiards [9].

Important recent topics in the field of quantum chaos are irreversibility and/or sensitivity to perturbations, noise for example. They can be related to the theory of chaos, concept which is classically interpreted as the result of exponential separation of trajectories in phase space [1]. However, in quantum mechanics, and due to the unitary character of this theory, sensitivity to initial conditions is a meaningless concept. For this reason, Peres proposed to consider the sensitivity to perturbations in quantum systems, as a mean to investigate the instability of quantum motion [10]. Such quantity, called *Loschmidt echo (LE)* or *fidelity*, can be defined as

$$M(t) = |\langle\psi|\exp(i\hat{H}t)\exp(-i\hat{H}_0 t)|\psi\rangle|^2 \qquad (1)$$

($\hbar$ is set equal to unity throughout this paper). It measures the ability of a system to return to an initial state $|\psi\rangle$, after a forward evolution with a Hamiltonian $\hat{H}_0$, followed by a (imperfect) reverse evolution with a perturbed Hamiltonian $\hat{H} = \hat{H}_0 + \Sigma$ (reversibility). The perturbation Σ can represent the uncontrolled degrees of freedom of an environment, thus providing a bridge to link induced decoherence effects and LE, as recently established in Ref. [11]. Alternatively, LE can be thought of as comparing the evolution of an initial state under different Hamiltonians (sensitivity to perturbations). In the last five years, many aspects of the LE have been considered in the literature [12–14]. The most interesting result is probably that, for a given range of perturbation strengths, the LE decays exponentially, at a rate given by the smallest quantity between the mean Lyapunov exponent and the level broadening following from the golden rule [12,13]. In the case of quantum computers [15] these issues are of paramount importance, since in this case it is essential to prevent any loss of coherence due to interaction with the environment.

As mentioned above, two basic ingredients in the idea of LE are irreversibility and sensitivity to perturbations. However, the calculation of LE's relies only on magnitudes evalu-

*E-mail address: wisniacki@df.uba.ar
†E-mail address: f.borondo@uam.es
‡E-mail address: rosamaria.benito@upm.es

ated at the end of the propagation process, thus not being able to provide any information about the involved history and associated mechanism. In fact, it has been discussed very recently [14] that maximum return probabilities can happen at times different from the total time elapsed forward, indicating that there may exist better definitions of the echo time than the original one.

In this paper, we propose a method to study irreversibility that, keeping the same basic philosophy under the LE, brings some solution to the abovementioned drawback. For this purpose, we use quantum trajectories, as defined in the de Broglie-Bohm (BB) formulation of quantum mechanics [16]. This complementary quantum theory of motion [17], developed in the 1960s trying to overcome the interpretative difficulties encountered in the standard theory, combines both the accuracy of the standard quantum description with intuitive explanations derived by the causal trajectory formalism, thus providing a powerful tool to understand the physics underlying microscopic phenomena [18]. This method has also an important additional advantage, since within its framework it is very easy to consider realistic perturbations, such as noise. This is particularly interesting in connection with billiards since, as stated before, they constitute ideal model for the transport of electrons in mesoscopic systems [5].

The organization of the paper is as follows. In the next section we briefly describe the model and methods used in our theoretical treatment. The results and discussion are given in Sec. III, and we present some concluding remarks in the last section.

II. MODEL AND CALCULATIONS

The fundamental equations in the BB theory are derived by introducing the wave function in polar form, $\psi(\mathbf{r},t) = R(\mathbf{r},t)e^{iS(\mathbf{r},t)}$, into the time-dependent Schrödinger equation, thus obtaining two real equations

$$\frac{\partial R^2}{\partial t} + \boldsymbol{\nabla} \cdot \left(R^2 \frac{\boldsymbol{\nabla} S}{m} \right) = 0, \tag{2a}$$

$$\frac{\partial S}{\partial t} + \frac{(\boldsymbol{\nabla} S)^2}{2m} + V - \frac{1}{2m}\frac{\boldsymbol{\nabla}^2 R}{R} = 0, \tag{2b}$$

which are the continuity and "quantum" Hamilton-Jacobi equations, respectively. Here, the last term in the left-hand side of Eq. (2b) is the so-called quantum potential. This is a nonlocal function given by the quantum state, which, together with V, determines the total forces acting on the system. Similarly to what is done in the usual Hamilton-Jacobi theory, a quantum equation of motion can then be defined from (2b) as

$$m\dot{\mathbf{r}} = \boldsymbol{\nabla} S, \tag{3}$$

from which the corresponding quantum trajectories can be obtained by numerical integration with a suitable method, once $\psi(t)$ is known.

As mentioned in Sec. I, these orbits can be used to define our measure of irreversibility in the following way. Starting from an ensemble of suitable initial conditions, i.e., reproducing the probability density distribution given by $|\psi|^2$ [19], we propagate them forward in time until a final value t_f. At that point we propagate the same trajectories backwards, but introducing a perturbation in the process consisting of kicks given at equally spaced intervals of time Δt. To avoid confusion, we will denote the "new" reversed time by τ. The effect of the kick consists of a displacement of the particle to a new position, randomly chosen within a given circle around the original landing point obtained in the integration. In this process we assume that the pilot wave function does not change during the kick. This is an approximation, but let us remark that approximate computational schemes have already been used in the literature [20], in connection with quantum trajectories in other dynamical problems. Although not absolutely rigorous, they have the advantage of providing an economic alternative to obtain a practical and yet accurate description of quantum processes.

Finally, the distance in configuration space d between both orbits is monitored as a function of τ. In this way we can compute a comparison, followed in time, of both unperturbed and perturbed dynamics of the system. From this, information about the mechanisms of irreversibility can be obtained. The idea behind this procedure is to mimic a thermal environment (noise) whose effective action is to interact with the particle in an averaged way, but leaving the pilot wave function unchanged by the kicks. Notice that this perturbation is a much realistic effect than the shape distortions considered so far in billiard models [21].

The system that we have chosen to study is a two degrees of freedom model consisting of a particle of mass $1/2$ enclosed in a desymmetrized stadium billiard of radius $r=1$ and area $1+\pi/4$ (see Fig. 1). This choice and that for $\hbar$ made after Eq. (1) define units of length and time that will be used to make nondimensional all magnitudes reported in this paper. Dirichlet boundary conditions are imposed at the boundaries, i.e., only odd-odd symmetry eigenfunctions are considered. The stadium billiard is known to be classically ergodic. Moreover, experiments in stadium shape microwave cavities have been performed [5,22], and conductance measurements in semiconductor billiard-shaped devices have been carried out [23].

III. RESULTS AND DISCUSSION

To gauge the performance of our method, we examine a simple situation with chaotic dynamics that has been considered extensively in the past [24]. It consists in following the dynamics of a wave packet along an unstable periodic orbit. The corresponding wave function is initially given as the harmonic oscillator coherent state

$$\psi(x,y,t=0) = (2\alpha/\pi)^{1/4} e^{-\alpha(x-x_0)^2-\alpha(y-y_0)^2} e^{i(P_x^0 x + P_y^0 y)}, \tag{4}$$

with $\alpha=16$, $(x_0,y_0,P_x^0,P_y^0)=(1,1/2,96/\sqrt{5},-48/\sqrt{5})$, an energy value of $E=2304$, and a period $T=0.0466$. This corresponds to a packet with its center on the diagonal orbit, running from the upper left to the lower right corners of the billiard, that would have diamond shape in the full version of the stadium. The time evolution of this state, calculated by projection into the system eigenstates followed by application of the evolution operator [25], is shown in Fig. 1.

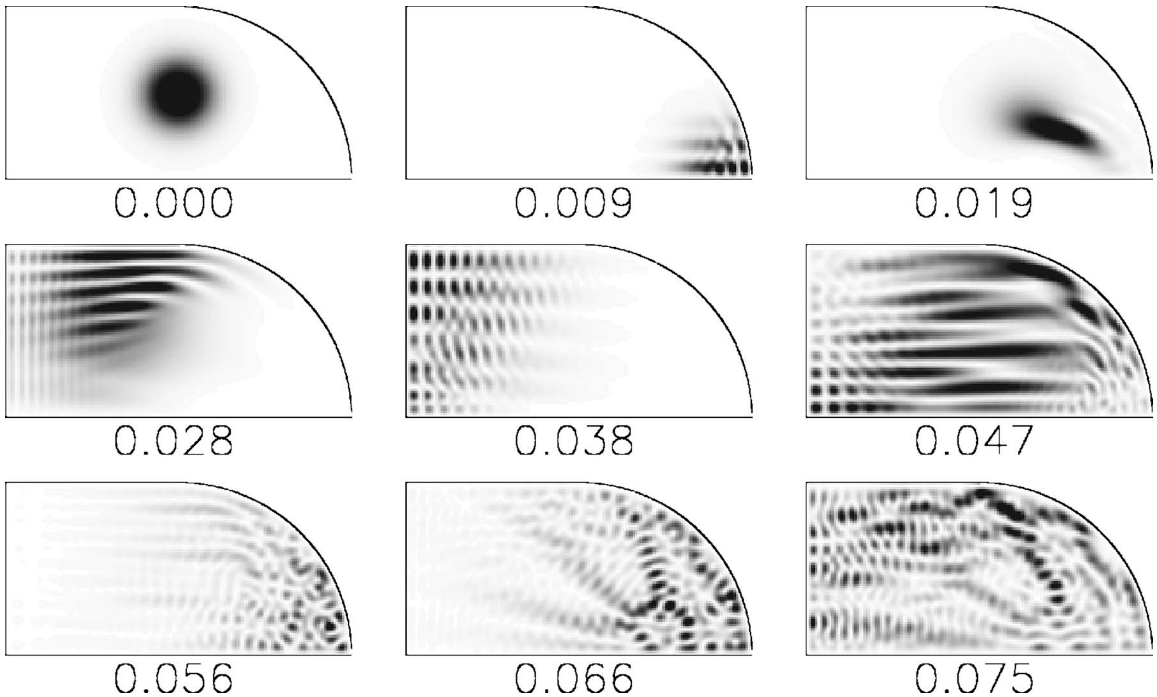

FIG. 1. Time evolution of the probability density, $|\psi(x,y,t)|^2$, corresponding to a wave packet initially centered on the diagonal of a desymmetrized stadium billiard with $r=1$, area $1+\pi/4$, and Dirichlet boundary conditions. The elapsed time is indicated below each panel.

The packet initially moves following the classical path, showing just a slight dispersion, as dictated by the Ehrenfest theorem. After the first rebound at the lower right corner (taking place at $t\simeq 0.009$), the packet spreads in a fan-type pattern ($t\sim 0.019$), experiencing the well known defocalization effect originated by the self-focal point of the orbit [24]. Afterwards, the dispersed wave collides with the upper left corner, giving rise to a noticeable series of horizontal fringes ($t\simeq 0.028-0.047$), formed by the maxima and nodal lines of the wave function. For subsequent times other rebounds take place, originating at $t\geqslant 0.066$ a complicated structure in the distribution of the quantum probability density.

These patterns dictate the topology of the corresponding quantum trajectories [19], which have been computed by integration of Eq. (3) using a Gear stiff method with tolerance control. The initial conditions were selected so as to reproduce the probability density associated with Eq. (4). Notice that the time values considered here are relatively short. Accordingly, the accumulated errors are not very severe and the quantum trajectories are completely reversible in the absent of perturbation.

In Fig. 2 we show the distance $\bar{d}$ computed for $\Delta t=0.001$ and averaged over 20 such trajectories propagated up to a final time of $t_f=0.02$, for different values of the perturbation strength (parametrized by the kicking radius ξ). Notice that the origin of the reversed time, $\tau=0$, corresponds to the final point of the forward propagation t_f. As can be seen, the behavior of the four curves is the same. In the range of the lowest times considered, $t\leqslant 0.008$, they grow very slowly and linearly. After that, the averaged distance increases dramatically in a cubic fashion for times up to the order of $t\sim 0.01$. And finally, for $0.015<t<0.020$, the values of $\bar{d}$ stabilize oscillating slightly around some sort of plateaus.

More interesting is the relationship existing between these results and the dynamics of the original packet shown in Fig. 1. When doing this, it is important to realize that $t_f=0.02$ is a relatively short time for the dynamics that we are considering here. Actually, in this time, the packet has only had time to return once to the vicinity of the initial position. By taking this into account, it follows that the first part of the $\bar{d}$ versus τ plots (showing a linear behavior) corresponds to a period of time in which the particle moves (flies back under the effect of the perturbation) from the center of the stadium to just before the bounce with the circular boundary. In this part of the travel the packet is in a semiclassical regime, in which

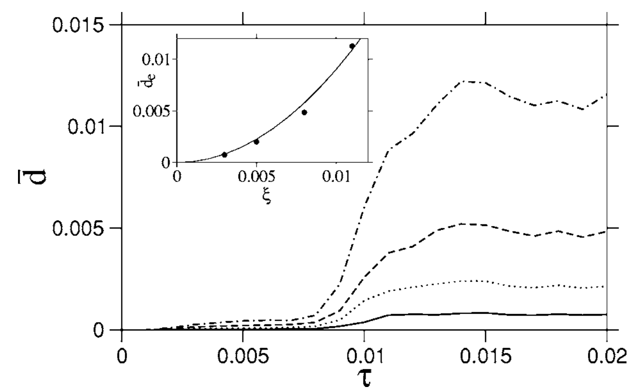

FIG. 2. Averaged distance between forward and reversed quantum orbits as a function of the reverse time τ for different values of the perturbation strength parameter ξ: 0.003 (full line), 0.005 (dotted line), 0.008 (dashed line), and 0.011 (dashed-dotted line). A value of $t_f=0.02$ was used in the calculations. A fitting to a quadratic expression of the averaged distance at the echo (observed for $t>0.015$) is shown in the inset.

not much dispersion (irreversibility) should be expected; this agrees perfectly well with our numerical findings. On the contrary, in the interval τ=0.008–0.012 the now perturbed dynamics include the bounce with the circle. Here, a lot of interference of the packet with itself happens, and a great dispersion due to the perturbation takes place. This corresponds to the big, cubic growth observed in the computed $\bar{d}$. An addition, for $\tau \sim 0.02$ we are at the echo, and our results can then be compared with those that would be obtained from the usual LE theory [12,13]. This is done in the inset to the figure, where the functional form of $\bar{d}$ at the echo averaged along the plateau ($\bar{d}_e$) as a function of the magnitude of the perturbation (ξ) is shown. As is seen, in this case, in which we have a noise-type perturbation, this dependence is quadratic with a very good accuracy, thus indicating that we are in a regime controlled by the Fermi golden rule [13]. Accordingly, we can conclude that noise-type perturbations like ours should be considered as generic from the point of view of the LE. It is important to note here that for billiard-shaped deformation perturbations, a linear dependence of LE with the magnitude of the perturbation is found [21]. This effect was explained as a result of the fact that the particular billiard deformations used in that work do not destroy the localization effect on short periodic orbits, as is the case for more random perturbations, such as the one considered here.

To conclude this section, let us examine what happens when longer t_f times are considered, thus allowing a more complicated dynamics to enter into play. To help in the interpretation of the resulting curves, let us first indicate that they should not be expected to be identical, in the interval $\tau \leq 0.02$, to those previously shown in Fig. 2. The reason for this is clear. For the new values of t_f, the origin of the reverse time τ for the back-integrated trajectories is further apart from that used in the calculations of Fig. 2. The results corresponding to t_f=0.04 and 0.06 are shown in Fig. 3. When examined in detail, the same conclusions as for the case of Fig. 2 are obtained. Namely, all curves consist of several very different pieces, in which what happens is either of very little dynamical significance (plateaus or slowly increasing curves), or it consists in very big cubic growths of $\bar{d}$. Moreover, these important growths always take place at the times values at which the particle collides with the boundaries, being the dynamics of the system there much more sensitive to the effect of the perturbation that we have introduced.

Another interesting point worth discussing for the longer times considered now is the dependence of the distance at the echo, $\bar{d}_e$, with the value of the perturbation strength. The results are shown in the insets to Fig. 3, where a quadratic behavior is also observed in both cases. Here the fitting is not as good as in the case with t_f=0.02. The reason for that is very clear, since in the results in Fig. 3 there are no plateaus, helping us to average out the oscillations which are known to disappear when a proper average over initial wave packet is performed.

Let us finally remark that there are, however, some differences between the results of Fig. 3 and those in Fig. 2. As can be seen, the plateaus in Fig. 3 are not completely flat, but rather they show a conspicuous decreasing behavior that, for

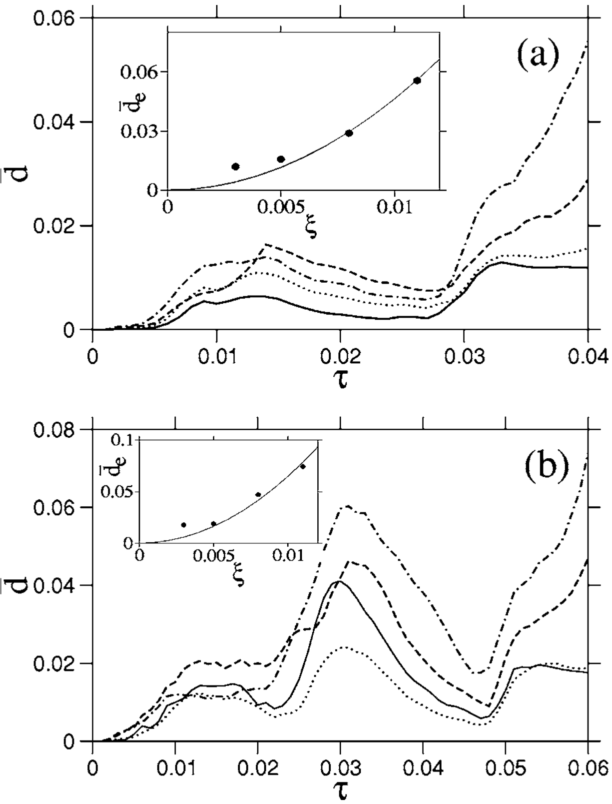

FIG. 3. Averaged distance between forward and reversed quantum orbits as a function of the reverse time, τ, for the same values of the perturbation strength considered in Fig. 2 and values of t_f =0.04 (a) and 0.06 (b).

example, in the case of Fig. 3(b) is quite important in the range $0.03 < \tau < 0.047$. The reason for this behavior can be understood if one considers that in these ranges of the reverse time, the packet is traveling from the upper left to the lower right corners, where it takes place a dynamics influenced by the self-focal point. This creates a quantum potential that forces the packet to return close to the original unperturbed path, which makes the separation $\bar{d}$ to go down.

IV. CONCLUDING REMARKS

In this paper we have presented a method to study irreversibility in quantum processes. This method is similar in spirit to the Loschmidt echo introduced by Peres [10], but it is constructed in terms of causal quantum trajectories, which allows one to obtain information about the history and mechanisms involved in the involved perturbation process.

As an example, our method has been applied to study the dynamics of a particle moving in the vicinity of a totally unstable periodic orbit of the stadium billiard in the presence of noise, a model which is quite adequate for electrons in mesoscopic cavities. Our main results can be summarized in the following way. First, we have found that the corresponding dynamics is very sensitive to the perturbation when the particle is bouncing at the boundaries, points in which the trajectories separate from each other cubically in time, on average. Second, the noise-type perturbation that has been used in the present work behaves in a totally generic way, as is indicated by the fact that the Fermi golden rule regime is found.

We should remark that in our calculation times beyond the Ehrenfest time have not been considered. For these longer times, large interference effects in the pilot wave guiding the quantum trajectories, and then the complexity of the associated quantum potential, are much higher and widespread over all configuration space. This point is very interesting and deserves further investigation, which will imply an enormous computational effort if a reasonable average over initial conditions is to be maintained. The same comment applies for the consideration of larger perturbations than those considered here, for which a Lyapunov regime is expected. In this case, smaller times steps will be necessary to reasonably guarantee the accuracy along the whole evolution process. Despite the fact that these two points have not been considered, the results presented in this work are relevant and interesting, since they clearly show which are the building blocks responsible for the irreversibility effect observed in the dynamics of the system under study.

Finally, let us conclude by presenting a brief comment on the comparison of our results and those corresponding to the case of an integrable dynamical behavior. For this purpose we have performed some preliminary calculations for the diagonal periodic orbit of a rectangular billiard of the same area. Our results indicate that the values of the averaged trajectories separation is always greater than in the chaotic case considered in this paper. This is in agreement with the results obtained by Prosen and Znidarik [26] for the standard LE. Moreover, the results for $\bar{d}$ do not show the existence of any plateau, as opposed to what happens in the case of the stadium. These points deserve further investigation and will be the subject of a future publication [27].

ACKNOWLEDGMENTS

This work was supported by MCyT (Contract BQU2003-8212), MECD (Contract SAB2000-0340), UPM (Contract AL05-PID-0018) in Spain, and CONICET and Fundación Antorchas in Argentina.

[1] A. J. Lichtenberg and M. A. Lieberman, *Regular and Chaotic Dynamics* (Springer-Verlag, New York, 1992).
[2] K. Richter, *Semiclassical Theory of Mesoscopic Quantum Systems* (Springer-Verlag, Berlin, 2000); R. A. Jalabert, in *New Directions in Quantum Chaos*, edited by G. Casati, I. Guarneri, and U. Smylanski (IOS Press, Amsterdam 2000).
[3] T. M. Fromhold, P. B. Wilkinson, F. W. Sheard, L. Eaves, J. Miao, and G. Edwards, Phys. Rev. Lett. **75**, 1142 (1995); P. B. Wilkinson, T. M. Fromhold, L. Eaves, F. W. Sheard, N. Miura, and T. Takamasu, Nature (London) **380**, 608 (1996).
[4] Y. Takagaki and K. H. Ploog, Phys. Rev. E **62**, 4804 (2000).
[5] H.-J. Stöckmann, *Quantum Chaos: An Introduction* (Cambridge University Press, Cambridge, 1999).
[6] F. Haake, *Quantum Signatures of Chaos* (Springer-Verlag, Berlin, 2001).
[7] M. Brack and R. K. Bhaduri, *Semiclassical Physics* (Perseus Books, Reading, MA, 1997).
[8] C. M. Marcus, A. J. Rimberg, R. M. Westervelt, P. F. Hopkins, and A. C. Gossard, Phys. Rev. Lett. **69**, 506 (1992).
[9] B. D. Simons and B. L. Altshuler, Phys. Rev. Lett. **70**, 4063 (1993); E. J. Heller, M. F. Crommie, C. P. Lutz, and D. M. Eigler, Nature (London) **369**, 464 (1994).
[10] A. Peres, Phys. Rev. A **30**, 1610 (1984).
[11] F. M. Cucchietti, D. A. R. Dalvit, J. P. Paz, and W. H. Zurek, Phys. Rev. Lett. **91**, 210403 (2003).
[12] R. A. Jalabert and H. M. Pastawski, Phys. Rev. Lett. **86**, 2490 (2001).
[13] Ph. Jacquod, P. G. Silvestrov and C. W. J. Beenakker, Phys. Rev. E **64**, 055203(R) (2001).
[14] M. Hiller, T. Kottos, D. Cohen, and T. Geisel, Phys. Rev. Lett. **92**, 010402 (2004).
[15] M. A. Nielsen and I. L. Chuang, *Quantum Computation and Quantum Information* (Cambridge University Press, Cambridge, 2000).
[16] D. Bohm, Phys. Rev. **85**, 166 (1952); **85**, 180 (1952).
[17] P. R. Holland, *The Quantum Theory of Motion* (Cambridge University Press, Cambridge, 1993).
[18] B. K. Dey, A. Askar, and H. Rabitz, J. Chem. Phys. **109**, 8870 (1998); C. L. Lopreore and R. E. Wyatt, Phys. Rev. Lett. **82**, 5190 (1999); D. Nerukh and J. H. Frederick, Chem. Phys. Lett. **332**, 145 (2000); E. Gindensperger, C. Meier, and J. A. Beswick, J. Chem. Phys. **113**, 9369 (2000); A. Donoso and C. C. Martens, *ibid.* **115**, 6309 (2002).
[19] D. A. Wisniacki, F. Borondo, and R. M. Benito, Europhys. Lett. **64**, 441 (2003).
[20] S. Garashchuk and V. A. Rassolov, J. Chem. Phys. **118**, 2482 (2003); Chem. Phys. Lett. **376**, 358 (2003); J. B. Maddox and E. R. Bittner, J. Chem. Phys. **119**, 6465 (2003).
[21] D. A. Wisniacki, E. G. Vergini, H. M. Pastawski, and F. M. Cucchietti, Phys. Rev. E **65**, 055206(R) (2002).
[22] S. Sridhar, Phys. Rev. Lett. **67**, 785 (1991); J. Stein, and H.-J. Stöckmann, *ibid.* **68**, 2867 (1992); H.-D. Gräf, H. L. Harney, H. Lengeler, C. H. Lewenkopf, C. Rangacharyulu, A. Richter, P. Schardt, and H. A. Weidenmüller, *ibid.* **69**, 1296 (1992).
[23] A. S. Sachrajda, R. Ketzmerick, C. Gould, Y. Feng, P. J. Kelly, A. Delage, and Z. Wasilewski, Phys. Rev. Lett. **80**, 1948 (1998); B. Huckestein, R. Ketzmerick, and C. H. Lewenkopf, *ibid.* **84**, 5504 (2000); C. Dembowski, B. Dietz, T. Friedrich, H.-D. Gräf, A. Heine, C. Mejía-Monasterio, M. Miski-Oglu, A. Richter, and T. H. Seligman, *ibid.* **93**, 134102 (2004).
[24] E. J. Heller, in *Chaos and Quantum Physics*, edited by M. J. Giannoni, A. Voros, and J. Zinn-Justin (Elsevier, Amsterdam, 1991).
[25] D. Wisniacki, F. Borondo, E. Vergini, and R. M. Benito, Phys. Rev. E **62**, R7583 (2000).
[26] T. Prosen and M. Znidarik, J. Phys. A **35**, 1455 (2002).
[27] D. Wisniacki, F. Borondo, and R. M. Benito (in preparation).