Correlation of the Photodetachment Rate of a Scarred Resonance State with the Classical Lyapunov Exponent

T. Timberlake and J.V. Foreman*

Department of Physics, Astronomy, and Geology, Berry College, Mount Berry, Georgia 30149-5004

(Received 4 October 2002; published 13 March 2003)

A metastable resonance state of the periodically driven Gaussian potential well is shown to be scarred on a single unstable periodic orbit of the classical motion. The photodetachment rate of this quantum state is strongly correlated with the Lyapunov exponent of the unstable periodic orbit over a wide range of driving field strengths.

DOI: 10.1103/PhysRevLett.90.103001 PACS numbers: 32.80.Gc, 03.65.Sq, 05.45.Mt

One-dimensional potential wells driven by a periodic field provide a convenient way to study quantum-classical correspondence. Classically, these are the simplest systems that can exhibit Hamiltonian chaos. The fact that these models involve only one spatial dimension makes it very easy to visualize their classical dynamics by creating a strobe plot (a plot of the location of classical trajectories in the phase space after each cycle of the field). Other details of the classical dynamics (Lyapunov exponents, etc.) can be more easily calculated for these models than for higher-dimensional models. The quantum versions of these models also provide a distinct advantage over higher-dimensional models because they are much easier to simulate on a computer. In addition, it is possible to visualize the phase space structure of a quantum state in these systems by constructing the Husimi distribution of the state [1].

One-dimensional time-periodic systems may also provide a convenient way to study atomic stabilization [2]. Atomic stabilization is characterized by a *decrease* in the probability for an electron to ionize as the strength of the driving field is *increased*. Interest in this phenomenon was heightened when stabilization was observed in recent experiments involving periodically kicked Rydberg atoms [3]. Quantum-classical correspondence plays a role in atomic stabilization, as shown by the fact that some stabilized quantum states of the periodically kicked Rydberg atom may be associated with stable regions in the classical phase space of that system [4].

Quantum-classical correspondence may also be related to stabilization in other ways. Some stabilized quantum states may be localized (or scarred) on unstable periodic orbits of the classical motion. Scarred eigenstates of a quantum system, in which the eigenstate has a heightened probability density in the vicinity of an unstable periodic orbit, were originally identified by Heller [5]. Jensen and co-workers provided the first evidence to link scarred eigenstates to stabilization [6]. However, the calculation technique used in their work did not provide decay lifetimes for the quantum states. This made it difficult to compare the properties of the quantum state and those of the classical periodic orbit on which it was scarred. In the present work we seek to provide a quantitative comparison between the photodetachment rate (the reciprocal of the lifetime) of a stabilized quantum state that is scarred on an unstable periodic orbit and the Lyapunov exponent of that periodic orbit.

The model we will investigate is an inverted Gaussian potential interacting with a monochromatic driving field in the radiation gauge. The Hamiltonian of this system in atomic units ($\hbar = 1$, etc.) is

$$H = \frac{1}{2}\left[p - \frac{\epsilon}{\omega}\sin(\omega t)\right]^2 - V_0 \exp[-(x/a)^2], \qquad (1)$$

where $V_0 = 0.63$ a.u., $a = 2.65$ a.u., ϵ is the strength of the driving field, and ω is the field frequency. This system exhibits characteristics of atomic stabilization, because the number of metastable quantum resonance states increases as the field strength is increased [7]. Moreover, these resonance states are scarred on unstable periodic orbits of the classical motion [8].

Figure 1 shows strobe plots of the motion at two different field strengths. We have identified four different periodic orbits for this system for field strengths ranging from $\epsilon = 0.062$ a.u. to $\epsilon = 0.18$ a.u. One periodic orbit is stable and the other three are unstable. As the field strength is increased the locations of the periodic orbits at $t = 0$ move away from each other along the line $p = 0$ in phase space. The stable orbit (orbit A) remains near the origin and is surrounded by an island of regular motion, which becomes smaller as the field strength is increased. One of the unstable orbits remains just outside of this regular region (orbit B), while the other two are located near $x = \alpha$ (orbit C) and $x = 2\alpha$ (orbit D), where $\alpha = \epsilon/\omega^2$ is the classical excursion parameter for a free electron in the field. Orbits B and D are mirror images of each other.

We are primarily interested in the stability of these periodic orbits as measured by their Lyapunov exponents [9]. The Lyapunov exponent (λ) of an unstable orbit is positive, with larger values of λ indicating a more unstable orbit. We have calculated Lyapunov exponents, as a

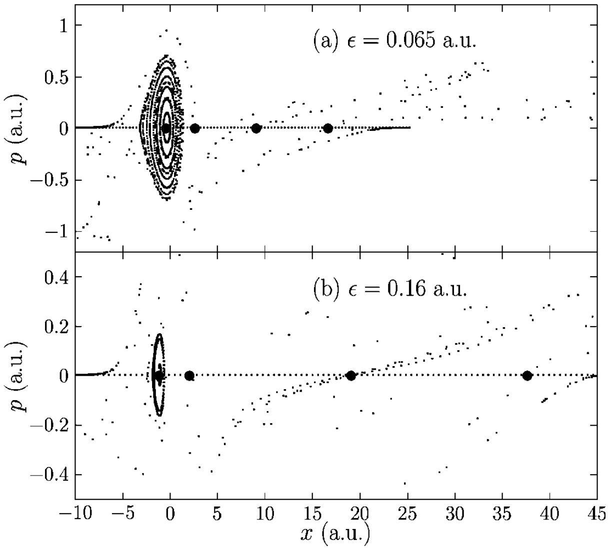

FIG. 1. Strobe plots of the classical motion in the periodically driven inverted Gaussian system. The locations of periodic orbits at $t = 0$ are indicated by filled circles. The orbits are denoted A to D from left to right. Orbit A is stable and is surrounded by an island of regular motion that decreases in size as ϵ is increased. The other orbits are unstable and move away from each other as ϵ is increased.

function of ϵ, for all four periodic orbits for $0.062 \le \epsilon \le 0.18$ a.u. The orbit that lies in the center of the island of regular motion (orbit A) is found to have $\lambda = 0$, as expected for a stable orbit. The antisymmetric pair of orbits (orbits B and D) have the same Lyapunov exponent, which increases slightly as ϵ is increased, indicating that these unstable orbits become more unstable as the driving field becomes stronger. The Lyapunov exponent of orbit C decreases significantly as ϵ is increased from 0.062 to 0.18 a.u., indicating that this unstable orbit is becoming less unstable as the field strength is increased. The continuous curve in Fig. 2 illustrates the behavior of this Lyapunov exponent as a function of ϵ. As we will see, the somewhat counterintuitive behavior of this periodic orbit may be responsible for stabilizing the quantum system against ionization.

To investigate the dynamics of a time-periodic quantum system one usually examines the Floquet states, which play a role in time-periodic systems similar to that played by energy eigenstates in time-independent systems. The Floquet states are eigenstates of the one-period time evolution operator $\hat{U}(0, T)$ [10]. Because an open system can ionize, the eigenvalues of $\hat{U}(0, T)$ will be of the form $e^{-iq_\beta T}$, where $q_\beta = \Omega_\beta - i\Gamma_\beta/2$. The quantity q_β is called the quasienergy of the Floquet state. The quantity Γ_β is the photodetachment rate, and the lifetime of the Floquet state is given by $\tau_\beta = 1/\Gamma_\beta$ in atomic units. Some of the Floquet states will be metastable and localized in phase space. These states are known as resonances.

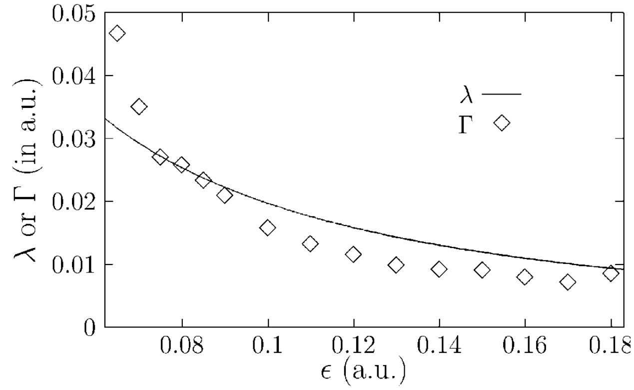

FIG. 2. The continuous line shows the Lyapunov exponent (λ) of orbit C as a function of field strength (ϵ). The data points show the photodetachment rate (Γ) of the resonance state scarred on orbit C at several field strengths.

To analyze the resonances of our model, we employ two versions of the complex-scaling method [11]. We identify resonance states and determine their photodetachment rates using the standard complex-scaling method, in which the x coordinate is scaled by a complex factor $e^{i\theta}$. Although the standard complex-scaling technique can provide for very accurate calculation of the photodetachment rates (our results are converged to eight or more decimal places), it provides eigenstates that are functions of the complex scaled coordinate. The transformation back to the real coordinate cannot usually be carried out when the wave functions are represented in a finite basis [12]. To obtain wave functions in terms of the real coordinate we use the exterior complex-scaling technique, in which the complex scaling occurs only for $|x| > x_s$. This technique provides eigenstates that are not scaled within the interior box $|x| < x_s$. The details of our implementation of these methods can be found in Ref. [8]. For $\epsilon \le 0.09$ a.u. we use $x_s = 25$ a.u. and for $\epsilon > 0.09$ a.u. we use $x_s = 50$ a.u.

Once we have identified a resonance state (using standard complex scaling) and calculated its wave function (using exterior complex scaling), we can examine the distribution of that state's probability in phase space by constructing the Husimi distribution of the state [1]. The Husimi distribution is a smoothed probability distribution for a quantum state in phase space. The smoothing of the distribution is necessary because of the restrictions of the uncertainty principle. In practice, one constructs the Husimi distribution by calculating the overlap of the quantum state with a grid of Gaussian wave packets spaced evenly throughout some region of phase space (see Ref. [8] for details on our method for constructing the Husimi distribution of resonance states). The Husimi distribution allows us to identify which resonance states are scarred on unstable periodic orbits of the classical motion. Scarred resonance states have Husimi distributions that are peaked on or near the location of an unstable periodic orbit in the phase space.

At very low field strengths our model has only three resonance states, but this increases to five as the field strength is increased [7]. A previous investigation of this model revealed that many of these states have Husimi distributions that are peaked on unstable periodic orbits [8]. However, for field strengths $\epsilon \leq 0.18$ a.u. there is a stable orbit surrounded by an island of regular motion in the phase space. Many of the resonance states have significant probability in this region. This makes their classification as "scars" uncertain. We find only one state that is peaked only on an unstable periodic orbit, with virtually no probability in the stable region of phase space. This state is a true scar, and it is peaked on orbit C. Figure 3 shows Husimi distributions for this state, as well as the locations of the four periodic orbits, at several field strengths. It is clear that the Husimi distribution becomes more strongly peaked on the unstable periodic orbit as the field strength is increased. At $\epsilon = 0.16$ a.u. it appears that the state is beginning to spread into the regular region surrounding orbit A.

One might expect some properties of this scarred state to be connected to the Lyapunov exponent that measures the stability of orbit C. The strength of the scarring in a scarred state is inversely related to the Lyapunov exponent of the periodic orbit on which it sits [5]. The Husimi distributions in Fig. 3 clearly show the strengthening of the scar as ϵ increases (and the Lyapunov exponent of orbit C decreases). In addition, a quantum wave packet that is initially centered on an unstable periodic orbit will spread away from that orbit at a much faster rate than one centered on a stable orbit [13]. In fact, for a wave packet initially centered on an unstable periodic orbit, the correlation of the wave packet with its initial state decays at a rate given by the Lyapunov exponent of the periodic orbit [5]. In a bounded system, such a wave packet would reflect off of the phase space boundaries and eventually form a standing wave. This standing wave would have a photodetachment rate of zero and there would be no correlation between the properties of this wave function and the Lyapunov exponent of the periodic orbit. In an open system, however, the outgoing portions of the wave function are not reflected by a boundary and never form standing waves. In our calculations the outgoing portions of the wave function are absorbed by the effective potential induced by the complex-scaling procedure. Under these circumstances the photodetachment rate of a scarred state might be closely related to the Lyapunov exponent of the periodic orbit. Indeed, some broad resonance states are known to be associated with unstable periodic orbits and their widths (Γ) are thought to be related to the Lyapunov exponent of the periodic orbit [14]. The association between scarring and stabilization mentioned previously makes the likelihood of a correlation between the photodetachment rate and the Lyapunov exponent even greater.

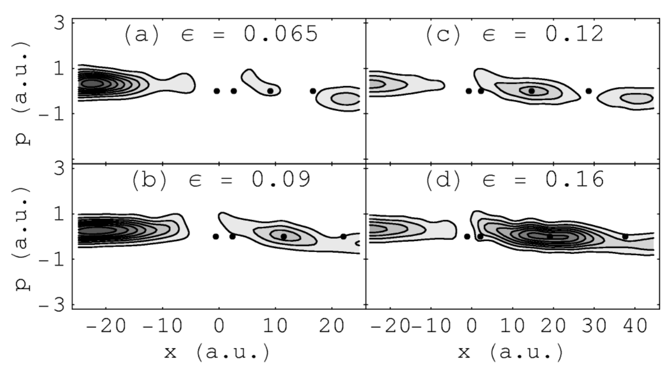

FIG. 3. Husimi distributions of the scarred resonance state for several field strengths. The locations of the periodic orbits are shown as filled circles. The orbits are denoted A to D from left to right.

Figure 2 shows the photodetachment rate (Γ) of the state that is scarred on orbit C, as well as a plot of the Lyapunov exponent (λ) of orbit C, for several field strengths. The photodetachment rate decreases as the field strength is increased, which means that the lifetime of the state increases as ϵ increases. So this scarred resonance state exhibits the characteristics of atomic stabilization. In fact, for $\epsilon \geq 0.13$ a.u. this state has the longest lifetime of any resonance state in the system. Furthermore, the behavior of the photodetachment rate as a function of ϵ is very similar to the behavior of the Lypunov exponent of orbit C.

We have analyzed the correlation between the photodetachment rate of this scarred resonance state and the Lyapunov exponent of orbit C. The correlation plot is shown in Fig. 4(a). Note that the data for low field strengths appear in the top right of the plot, while the data for high field strengths is in the bottom left. It is clear that there is a strong positive correlation. Figure 4(a) also shows the line $\Gamma = \lambda$ and the line of best fit whose equation is given by $\Gamma = 1.505\lambda - 0.010$ a.u. The correlation coefficient for this fit is $R = 0.953$, indicating a probability of only 4×10^{-8} that these two quantities are uncorrelated. If we restrict the range of field strengths to those between $\epsilon = 0.08$ a.u. and $\epsilon = 0.13$ a.u. we find that the relationship between Γ and λ is very linear, as shown in Fig. 4(b). The line of best fit for this restricted range of field strengths is $\Gamma = 1.496\lambda - 0.013$ a.u. and the correlation coefficient is $R = 0.993$.

At this point we can only speculate as to why the relationship between Γ and λ is so linear for field strengths between $\epsilon = 0.08$ a.u. and $\epsilon = 0.13$ a.u., but appears to be different for field strengths outside this range. This particular resonance state does not exist at very low field strengths [8]. It may be that for low field strengths the resonance has not fully formed and its association with the unstable periodic orbit is relatively weak. This might explain why the photodetachment rate

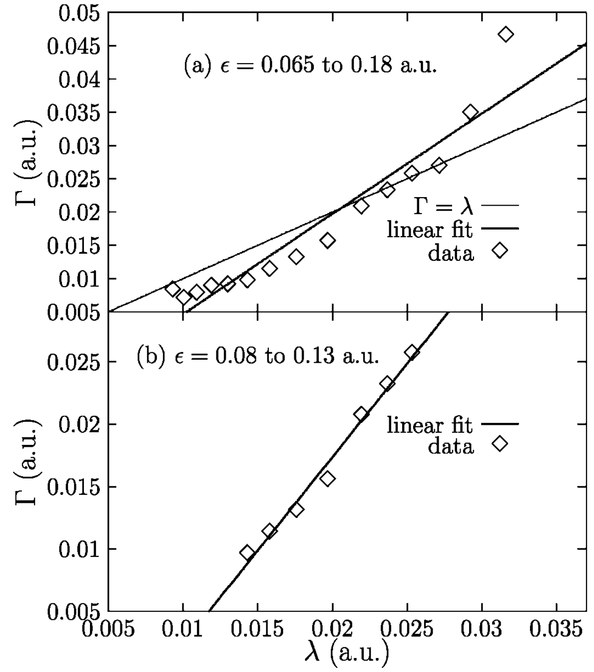

FIG. 4. Correlation between the photodetachment rate (Γ) of the scarred resonance state and the Lyapunov exponent (λ) of the unstable orbit on which it is scarred. The correlation over the full range of field strengths ($\epsilon = 0.065$ to 0.18 a.u.) is shown in (a). Also shown in (a) is the line $\Gamma = \lambda$ and the line of best fit, given by $\Gamma = 1.505\lambda - 0.010$ a.u. with correlation coefficient $R = 0.953$. The correlation over a restricted range of field strengths ($\epsilon = 0.08$ to 0.13 a.u.) is shown in (b), along with the line of best fit for this set of data ($\Gamma = 1.496\lambda - 0.013$ a.u. with correlation coefficient $R = 0.993$). Note that the points in the upper right of the plot correspond to low field strengths, while the points in the lower left correspond to high field strengths.

is higher at low field strengths than it would be if the linear relationship continued below $\epsilon = 0.08$ a.u. At high field strengths we see that the photodetachment rate seems to level off, rather than continuing to decrease. This may be because the resonance state is beginning to spread onto other periodic orbits at these high field strengths.

In summary, we have found a very strong correlation between the photodetachment rate of a scarred resonance state and the Lyapunov exponent of the unstable periodic orbit on which the resonance state is scarred. This implies a close quantum-classical correspondence, at least for a resonance state that is scarred on a single unstable periodic orbit, even though the system is not in the semiclassical regime. We would like to be able to extend this analysis to other resonance states in this system, but this cannot be done easily since the other resonance states are peaked on multiple orbits including the stable orbit. Lowering the value of $\hbar$ used in the model might lead to more resonance states that are peaked on a single unstable orbit. This might also reduce the quantum fluctuations that could lead to differences between the photodetachment rate and the Lyapunov exponent. It is possible that in the semiclassical limit ($\hbar \rightarrow 0$) the photodetachment rate and Lyapunov exponent will coincide.

The authors would like to thank Berry College and the Berry College Office of Student Work for providing financial support for this research.

*Current Address: Department of Physics, Duke University, Durham, NC 27708.

[1] K. Husimi, Proc. Phys. Math. Soc. Jpn. **22**, 264 (1940).
[2] Q. Su, J. H. Eberly, and J. Javanainen, Phys. Rev. Lett. **64**, 862 (1990).
[3] C. O. Reinhold, J. Burgdörfer, M. T. Frey, and F. B. Dunning, Phys. Rev. Lett. **79**, 5226 (1997).
[4] S. Yoshida, C. O. Reinhold, P. Kristöfel, J. Burgdörfer, S. Watanabe, and F. B. Dunning, Phys. Rev. A **59**, R4121 (1999).
[5] E. J. Heller, Phys. Rev. Lett. **53**, 1515 (1984).
[6] R. V. Jensen, M. M. Sanders, M. Saraceno, and B. Sundaram, Phys. Rev. Lett. **63**, 2771 (1989); R. V. Jensen and B. Sundaram, Phys. Rev. Lett. **65**, 1964 (1990); B. Sundaram and R. V. Jensen, Phys. Rev. A **47**, 1415 (1993).
[7] N. Ben-Tal, N. Moiseyev, and R. Kosloff, J. Chem. Phys. **98**, 9610 (1993).
[8] T. Timberlake and L. E. Reichl, Phys. Rev. A **64**, 033404 (2001).
[9] W. Schweizer, R. Niemeier, H. Friedrich, G. Wunner, and H. Ruder, Phys. Rev. A **38**, 1724 (1988); S. De Souza-Machado, R. W. Rollins, D. T. Jacobs, and J. L. Hartman, Am. J. Phys. **58**, 321 (1990).
[10] J. H. Shirley, Phys. Rev. **138**, B979 (1965).
[11] N. Moiseyev, Phys. Rep. **302**, 211 (1998).
[12] A. Csótó, B. Gyarmati, A. T. Kruppa, K. F. Pál, and N. Moiseyev, Phys. Rev. A **41**, 3469 (1990).
[13] N. Moiseyev and A. Peres, J. Chem. Phys. **79**, 5945 (1983).
[14] H. S. Taylor and J. Zakrewski, Phys. Rev. A **38**, 3732 (1988); M. L. Du, A. K. Kazansky, and V. N. Ostrovsky, Phys. Rev. A **42**, 4381 (1990).