

Correlation of Photodetachment Rate and Lyapunov Exponent for a Scarred Resonance State

Todd K. Timberlake and John V. Foreman*

Department of Physics, Astronomy, & Geology
Berry College, Mount Berry, GA 30149-5004

*current address: Dept. of Physics, Duke University, Durham, NC, 27708

Dynamical Chaos in Classical and Quantum Systems
Novosibirsk, Russia August 4-9, 2003

ABSTRACT: We have investigated a model one-dimensional open quantum well driven by an intense monochromatic laser field. This model exhibits behavior similar to atomic stabilization. In particular, new quasi-bound resonance states are created as the strength of the driving field is increased. Previous work has shown that at least one of the newly created resonance states is scarred on an unstable periodic orbit of the classical system. We will present the results of calculations showing that the photodetachment rate for this scarred resonance state is strongly correlated with the Lyapunov exponent of the unstable classical orbit with which it is associated. This correlation holds over a large range of field strengths. In fact, the behavior of the two quantities as a function of field strength is very similar and the numerical values of the two quantities are close at all of the field strengths that we investigated. The photodetachment rate of the resonance state associated with the stable classical region increases as the stable classical region gets smaller. However, the photodetachment rate does not increase monotonically. Instead it displays sudden jumps as the field strength is increased. These jumps may be related to avoided crossings in the Floquet spectrum.

The Model and Previous Results

The model we investigate is an inverted Gaussian potential well driven by a monochromatic field. In the radiation gauge the Hamiltonian (in atomic units) is

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

where $V_0 = 0.63$ a.u., $a = 2.65$ a.u., and $\omega = 0.0925$ a.u. We investigate the classical and quantum dynamics over a range of values of the driving field strength ϵ .

This model is known to exhibit signs of stabilization against ionization in this parameter regime. In particular, as ϵ is increased the number of metastable quantum resonance states increases [1]. At least one of the resonance states in the system is known to be scarred on an unstable periodic orbit [2]. The goal of our investigation is to determine the relationship between the stability of the quantum resonance states (as measured by the photodetachment rate, or reciprocal lifetime) and the stability of the classical structures with which these quantum states are associated (as measured by the Lyapunov exponent of an unstable orbit or the phase space area of a stable classical island).

Classical Dynamics

The classical dynamics of this system is illustrated in the strobe plots in **Figure 1**. These plots show the location of classical trajectories at times $t = nT$, where n is an integer and $T = 2\pi/\omega$. We have identified four periodic orbits with period T . These orbits are designated A-D from left to right and they all lie on the line $p = 0$. **Orbit A** is stable for $\epsilon < 0.18$ a.u. and it is surrounded by a region of stable motion in the phase space. This region grows smaller as ϵ is increased. The other three orbits are all unstable. **Orbit B** remains near the origin for all ϵ . **Orbit C** is located near $x = \epsilon$ and **Orbit D** is located near $x = 2\epsilon$, where $\epsilon = \epsilon^2$ is the classical excursion parameter for a free particle in the field.

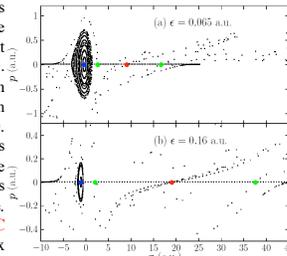


Figure 1

Figure 2 shows the trajectories of three of the four periodic orbits with period T for $\epsilon = 0.09$ a.u. **Orbit A**, the stable orbit, remains close to the origin throughout its entire path. **Orbit B** extends in the positive x -direction, but not in the negative direction. **Orbit C** is symmetric about $x = 0$. **Orbit D** (not shown) is identical to **Orbit B** reflected about the line $x = 0$.

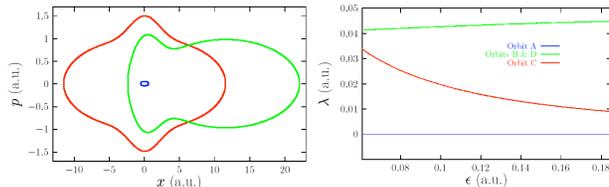


Figure 2

The stability of the periodic orbits can be determined quantitatively by calculating the Lyapunov exponent of each orbit. The larger the Lyapunov exponent, the more unstable the periodic orbit. **Figure 3** shows the Lyapunov exponent λ as a function of the field strength ϵ for Orbits A-D. The Lyapunov exponent of **Orbit A** is zero in the range of field strengths shown in the diagram, as expected for a stable orbit. The Lyapunov exponents of **Orbits B & D** (which are always equal) increase slightly as ϵ is increased. However, the Lyapunov exponent of **Orbit C** decreases as ϵ is increased indicating that the orbit becomes less unstable as the driving field gets stronger.

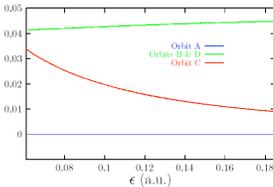


Figure 3

Quantum Resonance States

Resonance states of a time-periodic system are eigenstates of the one-period time evolution operator, or Floquet operator. We construct the Floquet operator numerically by first calculating the eigenstates of the undriven system. These eigenstates serve as a basis, and each basis state is evolved over one cycle of the driving field to provide a column of the Floquet matrix. Because the system can ionize we must use a special calculation technique, known as complex coordinate scaling (CCS), to accurately determine the eigenvalues and eigenstates using a finite basis [3].

We used two versions of CCS. In ordinary CCS the x -coordinate is scaled by a complex factor of unit modulus. This technique allows for easy identification of resonances because all non-resonance eigenvalues of the Floquet matrix form a spiral inside the unit circle, as shown in **Figure 4a**. Ordinary CCS also provides accurate Floquet eigenvalues, from which the photodetachment rates of the resonance states can be determined. Unfortunately, ordinary CCS does not provide accurate eigenstates. For this purpose we use exterior coordinate scaling, in which the coordinate is scaled only for $|x| > x_c$. Plotting the eigenvalues from the exterior CCS calculations (**Figure 4b**) allows us to match the accurate exterior CCS eigenstates with the accurate ordinary CCS eigenvalues.

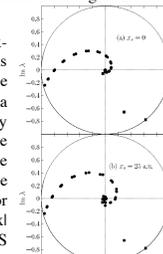


Figure 4

To investigate the phase-space structure of the resonance states we constructed Husimi distributions [4], which are smoothed probability distributions. This enabled us to identify one particular state which appeared to be scarred on **Orbit C** over a range of field strengths, as shown in **Figure 5**. Most of the other resonance states were not true scars because they had significant probability in the stable region of the phase space [5]. Note that the scarred state is a light-induced state that does not exist for $\epsilon = 0$. This scarred state becomes the longest-lived resonance state at high field strengths.

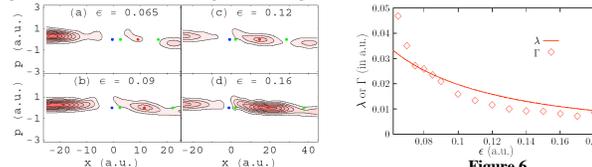


Figure 5

Correlation of Γ and λ

Figure 6 shows the photodetachment rate (Γ) of the scarred state, as well as the Lyapunov exponent (λ) of **Orbit C**, as a function of ϵ . Note that the lifetime of the resonance is $\tau = 1/\Gamma$. The two quantities exhibit similar behavior and numerical values over the range of field strengths we studied.

The correlation between Γ and λ is illustrated in **Figure 7**. The data for the full range of field strengths we investigated is shown in **Figure 7a**. There is a strong correlation ($R = 0.953$), and the best-fit line is found to be $\Gamma = 1.505\lambda - 0.010$ a.u. **Figure 7b** shows the data for a restricted range of field strengths. In this range Γ and λ appear to be linearly related with correlation coefficient $R = 0.993$ and best-fit line $\Gamma = 1.496\lambda - 0.013$ a.u. This restricted range may provide a more reliable measure of the correlation because at lower field strengths the scarred state is just beginning to form, while at higher field strengths it is beginning to spread into other regions of phase space.

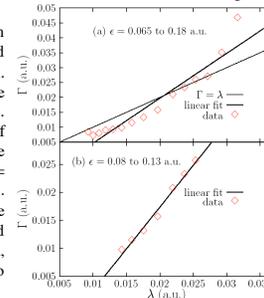


Figure 7

Quantum-Classical Correspondence in the Stable Island

The Husimi distributions of a different resonance state show that it is associated with the stable island surrounding **Orbit A**, as shown in **Figure 8**. This state resembles the ground state of the undriven system, and it is continuously connected to the ground state as $\epsilon \rightarrow 0$. Note that the Husimi distribution of this state is somewhat distorted for $\epsilon = 0.08$ a.u., but that it returns to its original shape by $\epsilon = 0.1$ a.u. This is due to an avoided crossing in the Floquet spectrum between this state and another resonance state around $\epsilon = 0.08$ a.u. By $\epsilon = 0.13$ a.u. this state is starting to spread outside of the (now very small) stable island.

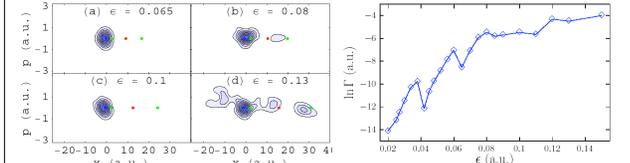


Figure 8

Figure 9

Figure 9 shows the natural logarithm of the photodetachment rate ($\ln \Gamma$) for this stable island state as a function of ϵ . The predominant trend is that $\ln \Gamma$ (and thus $\ln \tau$) increases as ϵ increases. This is to be expected since the size of the stable island decreases as ϵ increases (see **Figure 1**), which would lead to increased tunneling of the resonance state out of the stable island and into the chaotic sea where it can ionize. However, $\ln \Gamma$ does not increase monotonically. Instead there are several sudden jumps in the plot, indicating rapid changes in the photodetachment rate of the resonance state as ϵ is increased. We are not yet certain of the cause of these jumps, but preliminary evidence indicates that they may be associated with avoided crossings in the Floquet spectrum.

Conclusions

- (1) At least one quantum resonance state of our model is scarred on an unstable periodic orbit of the classical motion.
- (2) The photodetachment rate of this scarred state is strongly correlated with the Lyapunov exponent of the unstable periodic orbit on which the state is scarred. This represents a new form of quantum-classical correspondence.
- (3) Since the scarred state becomes the longest-lived resonance state at high field strengths, and since the lifetime of this state increases as the field strength is increased, we conclude that this model exhibits stabilization against ionization. This stabilization can be termed "non-classical" because the quantum state is not associated with a stable classical structure.
- (4) Our results indicate that even this "non-classical" stabilization may be related to properties of the classical dynamics in our model.
- (5) Additionally, the resonance state associated with the stable region of phase space shows behavior that corresponds to the shrinking of the stable region as the field strength is increased, but with occasional deviations that may be due to avoided crossings in the Floquet spectrum.

References

- [1] N. Ben-Tal, N. Moiseyev, and R. Kosloff, *J. Chem. Phys.* **98**, 9610 (1993).
- [2] T. Timberlake and L. E. Reichl, *Phys. Rev. A* **64**, 033404.
- [3] N. Moiseyev, *Phys. Rep.* **302**, 211 (1998).
- [4] K. Husimi, *Proc. Phys. Math. Soc. Jpn.* **22**, 264 (1940).
- [5] E. J. Heller, *Phys. Rev. Lett.* **53**, 1515 (1984).

Acknowledgments

The authors would like to thank Dr. Linda Reichl for her guidance and assistance on a previous project that laid the groundwork for this project. We would also like to thank Berry College and the Berry College Office of Student Work for their financial support.