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Inhibition of Quantum Transport Due to "Scars" of Unstable Periodic Orbits

R. V. Jensen and M. M. Sanders

Department of Applied Physics, Yale University, New Haven, Connecticut 06520

M. Saraceno

Departamento de Fisica, Comisión Nacional de Energia Atomica, 1429 Buenos Aires, Argentina

B. Sundaram

Los Alamos National Laboratory, MS J-569, Los Alamos, New Mexico 87545

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A new quantum mechanism for the suppression of chaotic ionization of highly excited hydrogen atoms explains the appearance of anomalously stable states in the microwave ionization experiments of Koch *et al.* A novel phase-space representation of the perturbed wave functions reveals that the inhibition of quantum transport is due to the selective excitation of wave functions that are highly localized near unstable periodic orbits in the chaotic classical phase space. These "scarred" wave functions provide a new basis for the quantum description of a variety of classically chaotic systems.

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Advances in the study of the chaotic behavior of strongly coupled and strongly perturbed nonlinear oscillators has lead many researchers to the question of how quantum mechanics modifies the chaotic classical dynamics in corresponding quantum systems like atoms or molecules in strong fields.[1] Until Heller's detailed studies of the stadium billiard,[2] highly excited states of chaotic systems were expected to resemble random functions in configuration space.[3] However, Heller found that typical eigenfunctions were often strongly peaked along the paths of unstable classical periodic orbits (PO).[3] In the past year these so-called "scars" of the PO have also been identified in several other systems that are classically chaotic,[4] where the peaking of the quantum probability near PO was found to be even more pronounced in the phase-space (PS) representation of the wave functions. These quantum PS distributions also revealed that the stable and unstable manifolds associated with the PO also play an important role in determining the regular structure of the eigenfunctions. Most recently, scars have also been found for highly excited hydrogen atoms in strong magnetic fields[5] where the scarred wave functions have a clear experimental signature in the regular modulations of the photoabsorption spectrum.[6]

The purpose of this Letter is to show that the wave functions of highly excited hydrogen atoms in strong microwave fields also exhibit surprisingly regular structure that is closely correlated with unstable PO and their associated stable and unstable manifolds. A novel PS representation of the wave functions, which is closely related to the Husimi or coarse-grained Wigner distribution,[7] is introduced, which clearly and simply reveals this underlying structure. Moreover, we show that these scarred wave functions are responsible for some of the large fluctuations in the threshold fields for the onset of ionization in the experimental measurements[8,9] shown in Fig. 1.

The classical description of the electron dynamics in the combined Coulomb and microwave field exhibits a sharp transition from regular behavior to chaos when the perturbing field exceeds a critical threshold which is typically 10%–20% of the binding field.[10] For low scaled frequencies, $n_0^3\Omega < 1$, Fig. 1 shows that the predictions of the onset of chaotic ionization for a one-dimensional model of the experiment, described by the Hamiltonian (in a.u.)

$$H(x,p,t) = p^2/2 - 1/x + xF(t)\cos\Omega t \quad (x>0) \qquad (1)$$

[where n_0 is the princpal quantum number of the initial state, Ω is the microwave frequency, and $F(t)$ is the field

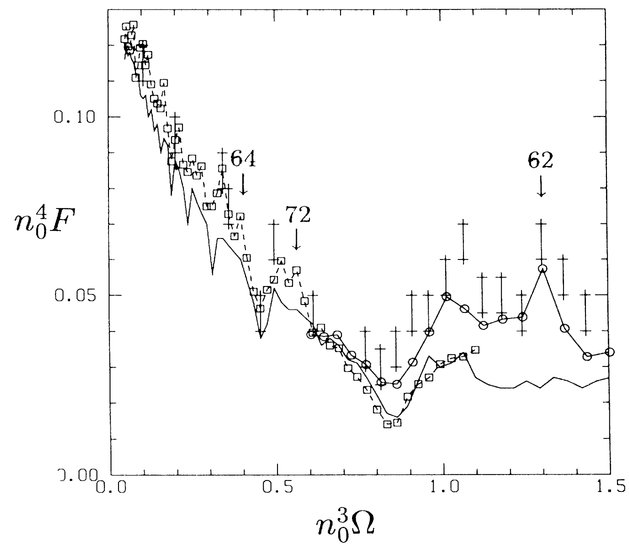


FIG. 1. The experimental measurements (Refs. 8 and 9) of the scaled threshold fields, n_0^4F, for 10% ionization at 9.9 GHz with $n_0=32$ to 90 (squares) and 36 GHz with $n_0=45$ to 80 (circles) are compared with classical (Ref. 10) (solid curve) and quantum (Ref. 11) (crosses) predictions for a one-dimensional model of the experiment.

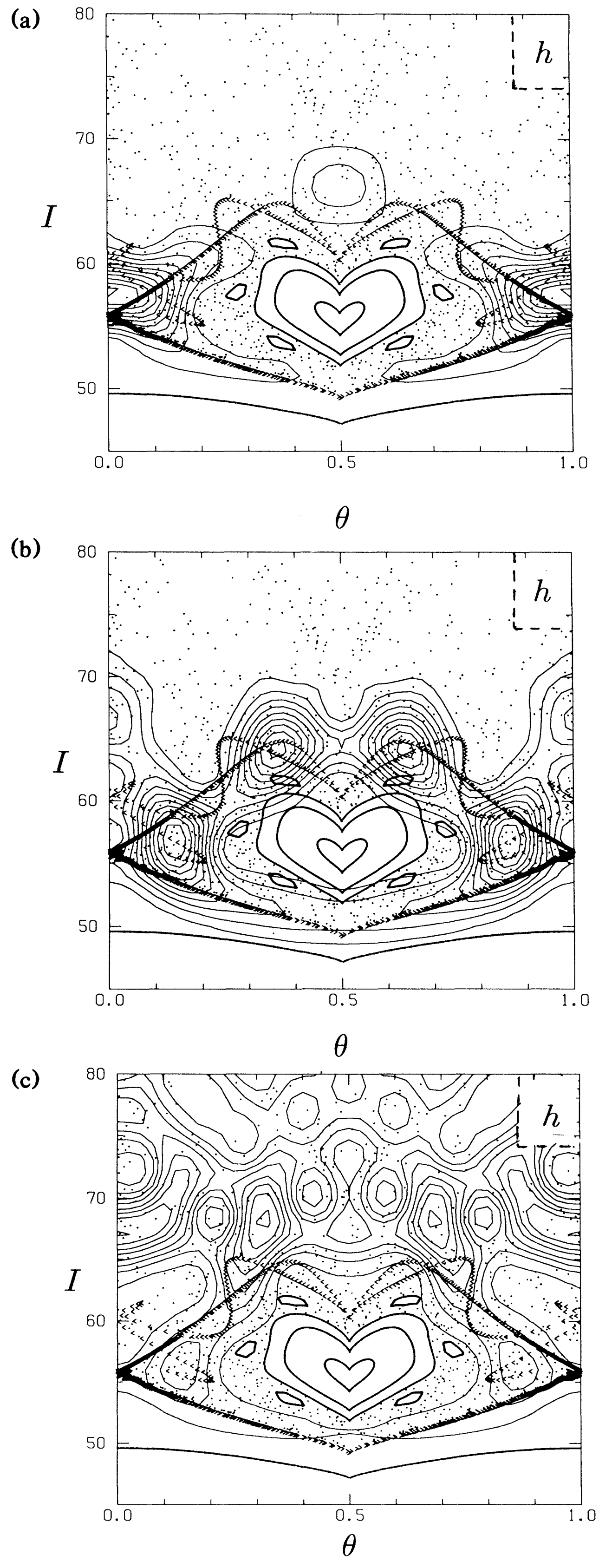
strength which slowly turns on and off as the atoms enter and exit from the cavity], are in remarkably good agreement with the experiment.[8] However, for $n_0^3\Omega > 1$ the thresholds for the onset of ionization in the experiments[9] and the quantum calculations[11] gradually rise above the classical thresholds in rough agreement with the "localization" theory of Casati, Guarneri, and Shepelyansky.[12] In addition, the experimental measurements and quantum calculations exhibit large peaks near resonant frequencies $n_0^3\Omega=\frac{4}{3}$, $\frac{3}{2}$, 2, $\frac{5}{2}$, and $\frac{8}{3}$.[9,11] At low scaled frequencies the prominent peaks at $n_0^3\Omega=1$, $\frac{1}{2}$, and $\frac{1}{3}$ in the classical and experimental ionization thresholds were previously shown[13] to be associated with regular, resonance island structures that persist in the classical PS and stabilize both the classical and the quantum dynamics. However, in Fig. 1 the striking peak near $n_0^3\Omega=\frac{4}{3}$ in the experiment and the quantum calculations does not appear in the classical simulations.

Our quantum simulations[11] of the experiments use a one-dimensional model of the hydrogen atom in an oscillating electric field that provides a good description of the threshold fields for significant excitation above the cutoff $n_c \sim 95$ which is measured as ionization.[8,9] Insight into the relative stability of $n_0=62$ in the 36-GHz field ($n_0^3\Omega=1.3$) is provided by a detailed examination of the structure of the quasienergy states[14] (QES) (eigenstates of the one-period time evolution operator at full perturbation strength) that are excited at the end of the slow switch on of the microwave field. If the perturbation were switched on suddenly, the perturbed wave function would be determined by the overlap of the initial state with each of the QES. For the parameters of the experiments, ten or more of these QES would be excited at a level of 1% or more. With the slow turn on this number is reduced. For example, five different QES are excited for $n_0=61$, with probabilities of 47.6%, 40.1%, 4.9%, 2.6%, and 1.1%. However, for $n_0=62$ only a single QES is excited with a probability of 97.8%.

If we examine the PS representation of these QES using the Husimi distributions described below, we find that many states exhibit regular structure that is reminiscent of the "scars" of unstable PO found in other chaotic systems. For example, Fig. 2 shows the Husimi distributions in action-angle space for three of the QES that are excited when the microwave perturbation is slowly applied to $n_0=61$. The first state in Fig. 2(a), which is excited with 40.1% probability, is strongly peaked near the unstable PO in the classical PS at $\theta=0$ (mod 1) that is associated with the large resonance island centered at $n^3\Omega=1.0$. In addition, this QES exhibits distinct ridges along the classical stable and unstable manifolds which are embedded in the chaotic region surrounding the stable remnants of the nonlinear resonance. Figure 2(b) shows another state, excited with 47.6% probability, that is largely peaked on an annulus interior to the primary stable and unstable manifolds. [Several other states are excited with probabilities less than 1% (not shown) that are concentrated on annuli interior to the regular islands; however, these states are not scars since they are associated with the quantization of tori[3] surrounding the stable PO.] Because all of these QES are highly localized to the vicinity of the classical PS structure, they do not contribute to the ionization of $n_0=61$. Finally, Fig. 2(c) shows an example of a QES, which is excited with 2.6% probability, that is highly delocalized. Since this QES and those excited with 4.9% and 1.1% probability extend to highly excited states with $n > n_c$, the excitation of these states contributes significantly to the ionization of $n_0=61$.

In contrast, Fig. 3 displays the Husimi distribution for the single QES that is excited when the microwave perturbation is slowly applied to $n_0=62$. This QES is highly localized to the separatrix region near the stable and unstable manifolds associated with the primary classical resonance at $n^3\Omega=1.0$. The remarkable feature of this wave function is that it remains localized in a region of PS where the classical dynamics is unstable and chaotic. Because this scarred QES does not extend to states with $n > n_c$ and because no other delocalized states are excited with probability greater than 1%, a larger microwave field is required to ionize $n_0=62$ than 61.

The recognition that the quantum dynamics is dominated by the excitation of highly structured wave functions may provide an explanation for the remarkable experimental observation,[9] that the ionization threshold at $n_0^3\Omega=1.3$ and for several other relatively stable states does not appear to depend on the value n_c as it is varied from ≈ 95 to ≈ 160. If an "exponentially localized"



wave function[12] gradually extended over more and more excited states as the perturbing field is increased, then the threshold for 10% ionization would be a strong function of n_c. However, in the case of $n_0 = 62$ a highly localized QES is excited that does not spread significantly with increasing field. In this case ionization only occurs when the field is strong enough that delocalized states are also excited to an appreciable level. Consequently, the excitation of highly excited states above either value of n_c sets in abruptly.

To produce these figures we introduced a very simple and effective method for representing the wave functions in the classical action-angle space that should be useful in many other problems.[15] Since the dominant features of the classical dynamics are usually most apparent in the space of the unperturbed action-angle variables, it is desirable to have representation of the wave function in action-angle space. Unfortunately, since quantum mechanics is not invariant under canonical transformations,[16] the Wigner or Husimi distributions, which are usually defined in position-momentum space,[7] cannot be easily transformed from one space to the other.

These difficulties are circumvented using the following prescription. If the wave functions of the perturbed system, $\psi(x,t) = \sum_{n=0}^{\infty} a_n(t)\phi_n(x)$, are expanded in terms of the unperturbed eigenfunctions, $\phi_n(x) = \langle x | n \rangle$ with quantum numbers n that correspond to the unperturbed classical action variables, then a Husimi distribution of $\psi(x,t)$ in action-angle space can be generated by choosing appropriate functional forms for the distributions for the unperturbed eigenstates. In particular, the coherent states that define the Husimi distributions for the one-dimensional hydrogen atom may be chosen to be Poisson wave packets

$$|I,\theta\rangle = \sum_{n=0}^{\infty} [A_n(\alpha) I^{\alpha n} e^{-\alpha I}]^{1/2} e^{i2\pi n\theta} |n\rangle , \qquad (2)$$

where α is a "squeezing" parameter that determines the relative width of the wave packet in θ vs I consistent with the uncertainty principle[17] and $A_n(\alpha) = \alpha^{(\alpha n+1)}/2\pi\Gamma(\alpha n+1)$ is the normalization factor. Then the Husimi distribution of a single unperturbed eigenstate in action-angle space is

$$\rho_n(I,\theta) = |\langle n | I,\theta\rangle|^2 = A_n(\alpha) I^{\alpha n} e^{-\alpha I} ,$$

which is peaked at an action $I = n$ with a width $\Delta I = [(\alpha n+1)/\alpha^2]^{1/2}$ and is uniformly distributed in θ. With this definition, the Husimi distributions in action-

FIG. 2. The level contours (solid curves) of the Husimi distributions in action-angle (I,θ) space are superimposed on a Poincaré section (Refs. 10 and 13) (dots) of the classical dynamics for three of the QES that are excited for $n_0 = 61$ with $n_0^3\Omega = 1.24$ and $n_0^4 F = 0.05$. The lines of arrows show the primary stable and unstable manifolds and their homoclinic oscillations. The relative size of Planck's constant, h, is indicated by the boxed area.

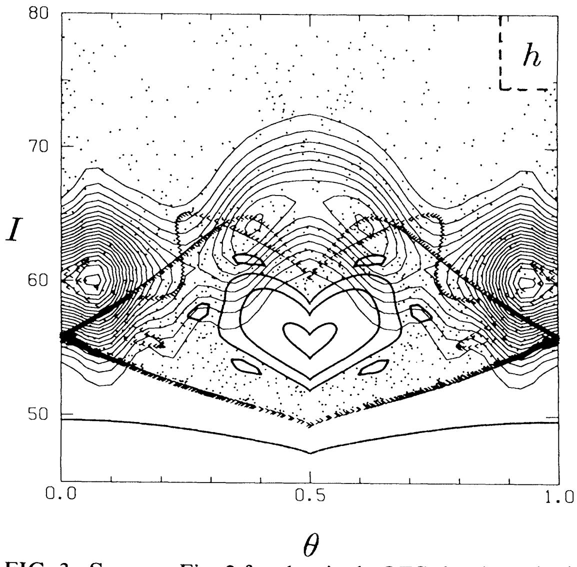


FIG. 3. Same as Fig. 2 for the single QES that is excited for $n_0=62$ with $n_0^3\Omega=1.3$ and $n_0^4F=0.05$.

angle space for the QES displayed in Figs. 2 and 3 are given by

$$\rho(I,\theta)=\left|\sum_{n=0}^{\infty}a_n\langle I,\theta|n\rangle\right|^2, \tag{3}$$

where the coefficients a_n are supplied by the numerical solutions.[18]

Our analysis of these numerical "experiments" indicates that the stable peak in the ionization thresholds measured by Koch and co-workers[9] near $n_0^3\Omega=\frac{4}{3}$ is due to the excitation of a single QES that corresponds to a localized scar in phase space. To assess the broader significance of our results, we first studied the dependence of the ionization probability of $n_0=62$ to small changes in the microwave frequency and found that at a fixed field the excitation above $n_c=95$ exhibits a broad minimum centered at $n_0^3\Omega=1.3050$ that appears to extend smoothly from $n_0^3\Omega\simeq1.28$ to 1.32. We also examined the dependence of the excitation of the single scarred QES to the shape and length of the microwave pulse and found little change when the turn-on, turn-off, and total duration was varied by a factor of 2. So the appearance of a relatively stable state in both the experiments and the quantum calculations near $n_0^3\Omega=1.3$ is no accident.[19]

Secondly, we found that the sharp peaks in the ionization thresholds for $n_0=64$ and $n_0=72$ in the 9.9-GHz field,[8] that could not be explained by the classical theory, also appear to be caused by the excitation of single QES that are highly localized in the chaotic classical phase space. In fact, the Husimi distributions of many different QES for $n_0^3\Omega=0.4$ to 2.8 and $n_0^4F=0.05$ to 0.07 appeared to exhibit regular structure that was often closely associated with PO and their associated manifolds. Coupled with similar results for other time-dependent and time-independent quantum systems,[4,5] it appears that scarred wave functions should be a ubiquitous feature of most quantum systems that are classically chaotic in atomic, molecular, solid-state, and nuclear physics and that these scars should have interesting, observable effects on the quantum dynamics as has already been demonstrated for hydrogen atoms in strong magnetic fields[5,6] and now for highly excited hydrogen atoms in intense microwave fields.

Finally, we note that, although a number of different theories have recently been proposed based on the wave-packed dynamics in the vicinity of unstable periodic orbits[3,20] and on the representation of the quantum Green's function in terms of semiclassical sums over the classical PO introduced by Gutzwiller,[21] the detailed understanding of the physical mechanisms that cause some wave functions to exhibit scars is still lacking. The empirical results presented here provide another illustration of this phenomena that should serve to stimulate further experiments and classical and quantum analyses of this simple, physical system.

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[17]The phase-space distributions for the QES are not very sensitive to the choice of α as long as $1 \ll \alpha \ll n_0$. Figures 2 and 3 were generated with $\alpha = 10$ or 20.

[18]Since the equation of evolution for $\rho(\theta, I, t)$ reduces to the classical Liouville equation with corrections of order $\hbar$, this quantum distribution function is properly identified with the classical phase-space distribution in the limit $\hbar \rightarrow 0$.

[19]Although the quantum simulations of the experiment of J. E. Bayfield *et al.* [Phys. Rev. Lett. **63**, 364 (1989)] also exhibit a stable peak near $n_0^3 \Omega = 1.3$, this structure appears to be absent from the experimental measurements, possibly due to the presence of a small static field or noise in the waveguide.

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