Classical chaos in one-dimensional hydrogen in strong dc electric fields

D. C. Humm and Munir H. Nayfeh
Department of Physics, University of Illinois at Urbana-Champaign, Urbana, Illinois 61801
(Received 11 October 1988; revised manuscript received 2 March 1989)

We analyze the effect of a dc electric field on classical chaos in one-dimensional hydrogen in a microwave field in the n nonmixing regime and also in the inter-n-mixing regime where significant dc field-induced ionization occurs. We study the ac field-induced nonlinear classical resonances, the threshold of chaos, and the number of states trapped in the resonances. In the strong-n-mixing and ionizing regime (unclamping dc field), we find the chaotic dynamics depend sharply on the dc field and the number of states trapped in the resonances, allowing the system to undergo a transition from a regime of classical behavior to a regime of uniquely quantum behavior as the dc field is changed. We show that ionization by classical chaos competes favorably with ionization by tunneling in the transition region, and that tunneling allows very sensitive spectroscopy of this region.

The flourishing of the study of nonintegrable classical systems has stimulated interest in the equivalent quantum systems, especially because quantum mechanics was developed and tested from analogies with and observations of systems that classically are integrable.[1] A great deal of theoretical effort has been expended in an attempt to understand the quantum dynamics of systems which are classically chaotic.[1–6] A wide variety of hypotheses have been advanced. It has been widely stated[3] that the mathematical structure of quantum mechanics is incapable of producing chaos in certain physical situations in which classical mechanics leads to chaos. Since chaos now is accepted by some as the correct deterministic foundation of the laws of classical statistical mechanics, the viability of the standard laws of quantum mechanics as a foundation of quantum-statistical mechanics has been called into question.[1] Computer simulations have shown that, in some situations, quantum-correlation functions decay more slowly than their classical counterparts.[4] Other simulations have exhibited the diffusive energy growth expected for classical chaos, but it stopped after a break time.[3] These results have led to the idea of a quantum "quenching" of chaos. However, studies of other situations have shown that, under certain conditions, there exists a classical limit in which the quantum motion mimics the classically chaotic behavior for a finite time. This classical limit can depend not only on the principal quantum number n but also on whether the frequency of the external driving force is greater than or less than the frequency inherent in the system,[5] and on the number of quantum states "trapped" in a given nonlinear resonance.[4] Other analyses have predicted a profound alteration in the spectrum of the quantum system at the point at which the equivalent classical system becomes chaotic.[4,6]

The interaction of highly excited atomic hydrogen with microwave radiation has been used to study some aspects of this problem.[7,8] However, it has been realized that even the simplest of all atoms is not easily amenable to theoretical calculations of this nature.[9] More recent experiments therefore exploited some properties of the Stark components of the spectrum in external dc electric fields in an attempt to reduce the six degrees of freedom in phase space.[10] Subsequent analysis of the experimental results of this system assumed that the interaction of the Stark components with fields is described in terms of one-dimensional atoms.[5,9,11] However, the validity of the one-dimensionality under high-field strength necessary for triggering classical chaos has since been questioned.[5,12] Moreover, the question of the effect of the dc field, if any, on the chaotic behavior of the hydrogen system has been raised.[13] Because the nature of the effects of dc fields on the system varies considerably as the field strength rises (i.e., from no appreciable mixing of quantum numbers to inter-l-mixing to inter-n-mixing), the dc field is expected to have large effects on the dimensionality and on the chaotic behavior.

Two studies of the effect of strong dc fields on the chaotic behavior of hydrogen atoms were carried out recently.[14,15] One study focused on nonionizing states corresponding to clamping fields in surface electron example, in the limit of very strong dc fields.[14] In the second study,[15] expressions for the static field-dependent action-angle variables were given in terms of complete elliptical functions of the first and second kind. The ac-induced nonlinear resonances and their widths and the threshold for classical chaos were also given in terms of these integrals. Series expansion of these integrals were used to arrive at analytical expressions to second order in the static field strength. It was found that the static field nontrivially modifies the response to the ac field, though the size of the effect was inadequate to explain discrepancies with recent experiment.

Here we examine some aspects of the problem by studying the chaotic dynamics of one-dimensional hydrogen in fields from zero to well within the inter-n-mixing regime and in situations where quantum-mechanical ionization by tunneling is appreciable (corresponding to an unclamping field in the surface electron model). We analyze the problem using a classical one-dimensional Hamiltonian. Although the one-dimensional model has given thresholds essentially identical to those of a twodimensional model,[5] it is not clear whether the model will prove to be appropriate in the presence of strong dc fields where n is fully mixed. In any case we will assume the appropriateness of the model with regard to the studies we are presenting here.

We examine in detail the effect of the dc field on the width and spacing of the classical nonlinear resonances for both clamping and unclamping fields, whose strength covers a wide range of interaction regimes (l-mixing and n-mixing regimes). Our results indicate that in the weaker-field limit, where n mixing is not taking place, the width and the spacings, and hence the threshold of chaos, are insensitive to the field strength. However, in the strong-field regime these are quite sensitive to the field strength. In the clamping case, the resonances widen but their spacings increase more rapidly with the field strength, thus resulting in a higher threshold of chaos. On the other hand, in the unclamping case, the resonances get narrower but their spacings drop much faster than the chaos threshold drops, a feature with advantageous experimental implications.

Another interesting feature: Our results indicate that the width of the resonances in the unclamping case can be narrowed enough using appropriate field strength to allow trapping a very few quantum levels at the threshold of chaos. On the other hand, in the clamping case, with typical microwave frequencies, one cannot help but trap a large number of quantum levels at the threshold of chaos, which indicates the usefulness of the unclamping case in probing and contrasting features of both the classical and the quantum regimes.

The classical nonlinear oscillator model is

$$H(r,p,t)=p^2/2-Z/r+F_0x+F_1x\cos(\Omega t)\ , \tag{1}$$

where F_0 is the strength of the dc field, F_1 is the amplitude of the microwave field, and Z is the nuclear charge. We can use cylindrical symmetry about the direction of the fields to reduce the dimensionality of the system from six to four dimensions in phase space.

In the case of strong F_0 we will assume one can approximate (see the discussion above) the Hamiltonian of the nonlinear oscillator to

$$H(r,p,t)=p_x^2/2-Z/x+F_0x+F_1x\cos(\Omega t) \tag{2}$$

which reduces the system to two dimensions in phase space. This system, in the absence of the external dc field ($F_0=0$) was extensively analyzed by numerical simulation and the nonlinear resonance overlap method.[9] It describes the system of an electron located over a liquid-helium surface and interacting with an oscillatory field polarized perpendicular to the surface. $Z=1$ for the hydrogen atoms; it is 7.1×10^{-3} for the surface-state electron.[9]

The basic procedure of our numerical calculation is similar to the analytical procedure of Jensen,[9] utilizing action-angle variables and the nonlinear resonances overlap criterion[16,17] to determine chaos thresholds. Similar procedures were also used in the two recent studies mentioned above. The difference between all of these calculations lies in the methods of performing the integrations and function inversions necessary. Berman, Zaslavsky, and Kolovsky[14] took the case of a very strong clamping dc field and dropped the Coulomb term, allowing an exact analytical calculation of the overlap resonance criterion in that limit. Stevens and Sundaram[15] gave expressions for the static field-dependent action-angle variables in terms of complete elliptical functions of the first and second kind and used series expansions of these integrals to arrive at an analytical expression for the resonance criterion to second order in the dc field strength.

In our studies, we perform the necessary integrations and function inversions numerically. Although our calculations are done for specific values of the parameters of the problems, scaling laws ensure the generality of the application of our result. Note that we are not performing a numerical simulation but rather are using numerical methods to calculate the value of the nonlinear resonance overlap criterion.

We now describe the formalism. We use a canonical transformation to transform the Hamiltonian given in Eq. (2) to

$$K=\alpha(I)+F_1x(\theta,I)\cos(\Omega t)\ , \tag{3}$$

where I and θ are the action and angle variables. The constant α is

$$\alpha=\tfrac{1}{2}p_x^2-\frac{1}{x}+F_0x\ . \tag{4}$$

The variables θ and I are chosen such that $x(\theta,I)$ is periodic in θ with a period of 2π. Thus we expand $x(\theta,I)$ in the Fourier series[17]

$$F_1x=\sum_{m=-\infty}^{\infty}V_m(I)e^{im\theta}\ \text{with}\ V_m=V_{-m} \tag{5}$$

which when substituted in Eq. (3) and rearranging the terms while using the fact that $V_m=V_{-m}$ because x is symmetrical about $\theta=0$ gives

$$K=\alpha(I)+\sum_{m=-\infty}^{\infty}V_m(I)\cos(m\theta-\Omega t)\ . \tag{6}$$

The problem is first solved for weak time-dependent fields. The effect of higher intensities will be determined as a distortion to the weak-field solution. If V_m is weak, the microwave field can only affect the system significantly when the phase $m\theta-\Omega t=0$. This condition is called the mth resonance. Thus, when the system is excited to near the mth resonance, it can only interact strongly with this resonance in the weak-field limit, and consequently the expansion in Eq. (6) can be separated as follows:

$$K=\alpha(I)+V_m(I)\cos(m\theta-\Omega t)+f(t)\ , \tag{7}$$

where

$$f(t)=\sum_{n(\neq m)}V_n(I)\cos(n\theta-\Omega t) \tag{8}$$

contributes very little to the interaction in the weak-field limit, and hence can be neglected. The system of Eq. (7) with $f(t)$ neglected can now be solved by making another transformation to get rid of the explicit time dependence. The new variables Δ and ϕ are defined as follows:

$$I - I_m = m\Delta \text{ and } \phi = m\theta - \Omega t \ . \tag{9}$$

The new corresponding generating function is

$$F(\Delta,\theta,t) = (I_m + m\Delta)(\theta - \Omega t/m) \tag{10}$$

with the transformation equations

$$I = \frac{\partial F}{\partial \theta}, \phi = \frac{\partial F}{\partial \Delta} \ . \tag{11}$$

The transformed Hamiltonian becomes

$$K' = \alpha(I) - \Omega I/m + V_m(I)\cos\phi \ . \tag{12}$$

It is to be noted that the new variable $m\Delta$ is just the small change in the action of the mth resonance caused by the weak microwave field. The new variable ϕ measures the phase difference between the phase of the system $m\theta$ and that of the external field Ωt. In order to see the nature of K' further, we can examine it in the limit of very small V_m, that is in the limit of small Δ and ϕ. Taking

$$V_m(I) \simeq V_m(I_m) \ , \tag{13}$$

$$\alpha(I) \approx \alpha(I_m) + \left.\frac{d\alpha}{dI}\right|_{I_m} m\Delta + \frac{1}{2}\left.\frac{d^2\alpha}{dI^2}\right|_{I_m} m^2\Delta^2 \ , \tag{14}$$

$$\frac{d\alpha}{dI} = \frac{d\theta}{dt} = \omega \ , \tag{15}$$

we get

$$K' = C_1\Delta^2 + V_m\cos\phi + C_2 \tag{16}$$

where $C_1 = \frac{1}{2}m^2(d\omega/dI)|_{I_m}$ and $C_1 = \alpha(I_m) - (\Omega/m)I_m$ are constants. Hamiltonian (16) is a pendulum Hamiltonian, where Δ and ϕ can be associated with the angular momentum and the pendulum angle, respectively.

From K' we can determine the phase and the angular momentum of the system near a resonance. A separatrix divides two kinds of motions where on one side the pendulum always swings in the same direction, while on the other side it swings back and forth. Moreover, each separatrix is symmetric and its width is given in terms of the maximum Δ. Since Δ maximizes for $\phi = 0$, one can show that near the mth resonance,

$$(I - I_m)_{\max} = 2\left[V_m\left[\left.\frac{d\omega}{dI}\right|_{I_m}\right]^{-1}\right]^{1/2} \ . \tag{17}$$

We can now discuss the case in which the amplitude of the microwave field F_1 is not weak and the term $f(t)$ in Eq. (7) becomes significant. First, the width of the resonances given by Eq. (17) will increase since V_m is proportional to F_1. Second, the $f(t)$ term acts as an additional time-dependent perturbation embodying the interaction between the otherwise noninteracting resonances.

What happens to this system when we include the time-dependent perturbation $f(t)$? Trajectories far away from the separatrix are affected very little. Trajectories near the separatrix are strongly affected, because the time-dependent external force can push them to one side of the separatrix or the other, changing their motion completely. For trajectories very close to the separatrix, the side of the separatrix they end up on in the next cycle depends not at all on which side of the separatrix they start on, but rather which way the force happens to be pushing them along the way. Since different trajectories take different amounts of time to complete a cycle, especially near the separatrix, this pushing can be completely different for two very close trajectories. Very close to the separatrix, the trajectories get all twisted up. Two trajectories that are nearly the same to start with may end up going in opposite directions, and two that are different to start with may end up going in the same direction.

If one simulates this motion on a computer, it looks irregular and disordered. Researchers have searched through their computer results for some kind of correlation and order in this motion but found none. All correlations that have been examined die out within a fairly short time. It appears that a random motion has arisen from a deterministic system. This is called "chaos."

As the external field is increased, the system undergoes a change from a situation in which most orbits are regular to one in which most are chaotic. A reliable estimate to this threshold of chaos is the external field at which two adjacent resonances overlap.[17] This estimate has proven correct in varying situations.[16] The transition to global chaos happens within a factor of about 2 in ac field of the resonance overlap estimate in the problem with no dc field.[9]

The pendulum approximation is not as good when the transition to global chaos has occurred for all resonances but one is trying to see if the $m=1$ separatrix extends down low enough to encompass states of low I (otherwise, those states will still be stable, even if global chaos occurs). In this case, we compute the actual separatrix of the Hamiltonian K', following Jensen.[9]

To estimate the threshold of chaos, we need to calculate $V_m(I_m)$ and $d\omega/dI$ and I_m. We use the following procedure. First, we need to be able to compute $I(\alpha)$. Given W, the generating function for the transformation to action angle coordinates,[18] we have $H_0(x,p_x) = H_0(x,\partial W/\partial x) = \alpha$, the initial energy, or one can calculate α and I_m by taking [from Eq. (4)]

$$\frac{1}{2}\left[\frac{\partial W}{\partial x}\right]^2 - \frac{1}{x} + Fx = \alpha \ ,$$

or (18)

$$\frac{\partial W}{\partial x} = \pm\left[2\left[\alpha + \frac{1}{x} - Fx\right]\right]^{1/2} \ .$$

Then $I(\alpha)$ is simply

$$I(\alpha) = \frac{1}{2\pi}\oint P_x dx = \frac{1}{2\pi}\oint \frac{\partial W}{\partial x}dx \tag{19}$$

which, upon substitution from Eq. (18), gives

$$I(\alpha) = \frac{1}{\pi}\int_0^{x_{\max}}\left[2\left[\alpha + \frac{1}{x} - Fx\right]\right]^{1/2} dx \ . \tag{20}$$

This integration is performed numerically, using Simpson's rule with Richardson extrapolation, after singularities in the integrand at $x=0$ and x_{max} have been removed by a transformation of variables. Between 41 and 121 integration points were used and the results were checked for independence of the number of integration points above a given number.

At resonance $m\theta=\Omega t$ so $d\alpha/dI=\omega=\Omega/m$. We compute $d\alpha/dI$ using

$$\frac{d\alpha}{dI}\approx\frac{(\alpha+\delta)-(\alpha-\delta)}{I(\alpha+\delta)-I(\alpha-\delta)},$$

with $\delta\sim10^{-5}|\alpha|$. We guess α until $d\alpha/dI$ comes within one part in 10^5 of Ω/m, giving α_m and I_m. We can then compute

$$\left.\frac{d\omega}{dI}\right|_{I_m}=\left.\frac{d^2\alpha}{dI^2}\right|_{I_m}\approx\frac{[(\alpha_m+2\delta)-\alpha_m]/[I(\alpha_m+2\delta)-I(\alpha_m)]-[\alpha_m-(\alpha_m-2\delta)]/[I(\alpha_m)-I(\alpha_m-2\delta)]}{I(\alpha_m+\delta)-I(\alpha_m-\delta)}.$$

Finally, we wish to obtain $V_m(I)$. First, we can obtain θ as a function of x from

$$\theta=\left(\frac{\partial W}{\partial I}\right)_x\approx\frac{W(x,\alpha+\delta)-W(x,\alpha-\delta)}{I(\alpha+\delta)-I(\alpha-\delta)},$$

where $W(x,\alpha\pm\delta)$ is obtained by numerical integration of Eq. (18). Then

$$\frac{d\theta}{dx}\approx\frac{\theta(x+\delta)-\theta(x-\delta)}{(x+\delta)-(x-\delta)}.$$

Now we can use these to compute the Fourier component $V_m(I_m)$ by integrating $V(x(\theta,I))=Fx(\theta,I)$ times $\cos m\theta$. This is transformed to

$$V_m(I_m)=\int Fx\cos[m\theta(x,I_m)]\frac{d\theta(x,I_m)}{dx}dx,$$

which we integrate numerically, giving $V_m(I_m)$. Then we have I_m, $V_m(I_m)$, and $(d\omega/dI)|_{I_m}$, and we can substitute into Eq. (17) to get the positions and widths of the resonances and see at what field strength they overlap, the criterion we use for the threshold of chaos. All calculations were performed using a desktop microcomputer with a numeric coprocessor.

We now present the results of these calculations. First we studied the effect of the dc field on the spacing and width of the classical nonlinear resonances. Figure 1 gives these for the second and third nonlinear resonances (as an example) for a number of dc fields strengths at constant ac field strength below that necessary to induce classical chaos. The results show that the spacing increases as the clamping field strength increases, and decreases as the unclamping field strength increases, with the size of the effect being larger the higher the order of the resonance.

As one increases the ac field strength, the system undergoes a transition to chaos near a certain threshold, which we estimate using the resonance overlap technique. Figure 2 gives the ac field (for a 30-GHz ac field) threshold of chaos so computed as a function of the initial action of the electron (the action in units of $\hbar$ is approximately equal to the quantum number n) for a number of different values of the dc field. Figure 3 is a log-log plot, but 36 is subtracted from the action to bring out some features of the curves for unclamping fields which would otherwise be difficult to see. This subtraction is purely for convenience of exposition.

Figure 2 includes a wide range of dc fields ranging from -240 V/cm to 1 kV/cm and in the portion of the spectrum from $n=39$ to 1036. The ratio of the external field frequency to the natural frequency of the atom, which does not change when the problem is scaled to other frequencies, extends from 0.27 to 25 in the $E_{dc}=0$ case. This range is narrower for both clamping and unclamping fields. The lower limit remains similar, but the upper limit drops. In the extreme cases of $E_{dc}=1000$ and -240 V/cm, the upper limit of this ratio drops to less than 2. For other threshold curves, the upper limit of the frequency ratio can be determined by counting the number of resonances. The order of a resonance m is equal to the frequency ratio Ω/ω at its center.

The wide range of this ratio shows the wide range of application of the curves in Fig. 2. The region graphed is the interesting one, where the internal and external frequencies are of nearly the same order of magnitude and so interact. Small external frequencies are essentially dc, and large ones can be described by a single-photon excitation to the continuum. Scaling laws make Fig. 2 useful for other frequencies, further extending its range of applicability.

Before we set out to discuss the present results we discuss the accuracy of our numerical procedure by compar-

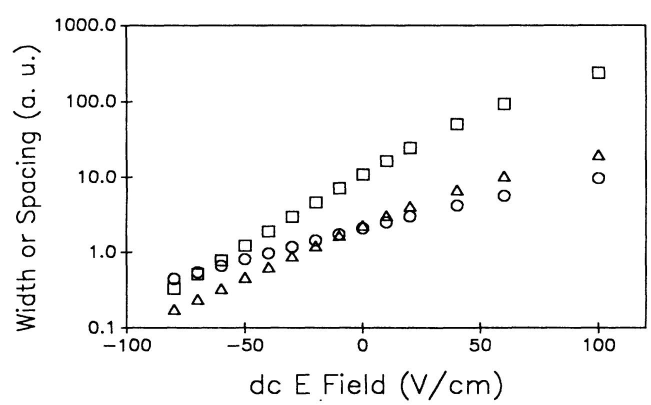

FIG. 1. Width and spacing of $m=2$ and 3 nonlinear resonances as a function of applied dc field of an ac field of amplitude 0.2 V/cm and frequency 30.5 GHz. □, spacing; ○, width of $m=1$; △, width of $m=2$.

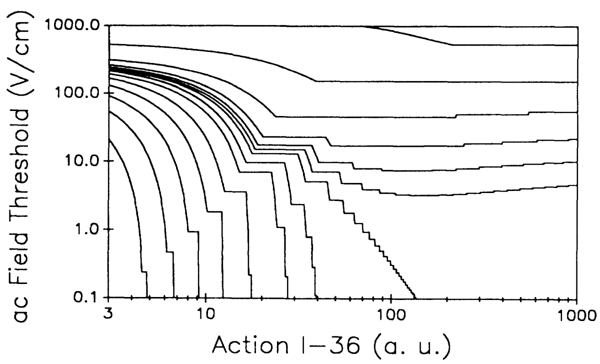

FIG. 2. Chaos thresholds. From the lower left corner to the upper right: $E_{dc}=-240$, -200, -160, -120, -80, -40, -20, 0, 10, 20, 40, 100, 300, and 1000 V/cm.

ing the zero static field results with the results of Jensen.[9] He performed both an analytical resonance overlap calculation and a numerical simulation of the interaction in the absence of the static field. Our results agree very well with his analytical results as they utilize the same method. His analytical and our numerical results agree very well with his numerical simulation except in the region with initial electron quantum number much smaller than those in the $m=1$ nonlinear resonance where there is a discrepancy of approximately a factor of 2.

A number of interesting features present themselves in Fig. 2. Distinct plateaus are evident in all of the curves. This is due to the nature of the overlap of the nonlinear resonances, the criterion we use for the threshold of chaos. Each nonlinear resonance covers a certain extent in action, which expands when the ac field is increased and contracts when the ac field is decreased. When adjacent resonances overlap, the threshold of chaos is passed for that region of action. Each plateau in the threshold of chaos curve is simply the extent of a nonlinear resonance at the threshold of chaos, where it first overlaps with its neighbor.

As an example, let us examine the curve for a zero dc electric field. The first resonance is centered at $I=60$ ($I-36=24$). The center of a resonance does not change with ac field, only the width. Near the center of the resonance, the chaos threshold is simply the threshold for the overlap of the first and second resonances. If the electron starts at an action enough smaller than the center of the first resonance, however, then the initial action of the electron will be outside the first resonance when the first and second resonances overlap. Chaos will occur within the first and second resonances, but the electron, being outside of that region, will not feel it. The ac field must increase further to make that first resonance reach out to the initial position of the electron. Thus, the chaos threshold becomes larger, and continues to increase as the initial action gets smaller and smaller, as the first resonance has to extend further and further to reach the initial action of the electron. Thus, the chaos threshold rises as the initial action is decreased for the region below the first resonance. As the initial action of the electron is increased above the center of the first resonance, the threshold remains determined by the overlap of the first and second resonances for a time, then the electron rises above the first resonance. The second and third resonances are already overlapping, and for a short time the chaos threshold is determined by how far the second resonance has to reach to find the initial action of the electron. The chaos threshold continues to decrease as the initial action increases, until the initial action is close enough to the center of the second resonance that the threshold is determined only by the threshold of overlap of the second and third levels. The second plateau occurs here, and more and more plateaus occur as the initial action is increased. Note that the width of each plateau in action gives the width of that particular nonlinear resonance (first plateau means first resonance, etc.) at its threshold of chaos. When measured in units of $\hbar$, it gives the number of quantum states contained within that resonance at the threshold of chaos, which we will examine in more detail later.

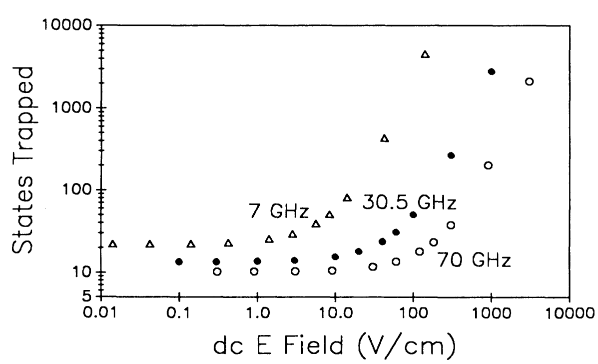

FIG. 3. Number of states trapped in the $m=1$ resonance.

Another feature worth discussing is the effect of the dc field on the number of nonlinear resonances and the ionization threshold of the electron. We note that there are two drastically different regimes in Fig. 2, that of clamping field and unclamping dc field, and the boundary between them at zero dc field. In the unclamping region at the lower left, thresholds for the system with $E_{dc}=-240$, -200, -160, -120, -80, -40, and -20 V/cm are plotted. These thresholds drop with increasing initial action. This occurs because the resonances get much closer to each other as the action increases, making it much easier for them to overlap, and lowering the threshold. Although the resonances also get smaller as the action increases, the effect of getting closer predominates. Because the thresholds drop as the action increases, all the way up to ionization, the chaos threshold is also an ionization threshold. Once the ac field has crossed the threshold of chaos for the initial action, it has crossed the threshold of chaos for all greater actions, and the system moves irregularly in the action, eventually reaching a large enough action to ionize. The above considerations also apply to the case of zero dc field. However, an important qualitative difference between the unclamping and zero-field cases can be observed in Fig. 2. While the zero-field curve drops off in a linear fashion on the log-log plot, while going through many higher and higher m resonances, the unclamping curves curve sharply downward as the action increases, approaching vertical lines, with the resonances piling up. This occurs because the action can go to infinity for the zero-field case, while in the unclamping case, there is a maximum action. Any value of the action above this maximum is not defined. Above this maximum action, the system ionizes classically due to the dc field even in the absence of an ac field (the ac field ionization threshold goes to zero). One would expect the chaos threshold to go to zero at this point, approaching a vertical line on the log-log plot, and it does. For example, the $E_{dc}=-20$ V/cm curve goes to zero at $I=76.5$, very close to where it meets the x axis in Fig. 2.

In contrast, for clamping fields the threshold curves, plotted at the upper right in Fig. 3 for $E_{dc}=10$, 20, 40, 100, 300, and 1000 V/cm, reach a minimum and then start increasing with increasing action. This minimum marks the boundary between two regimes, a regime in which the Coulomb field dominates over the external dc field, and a regime in which the external dc field dominates over the Coulomb field. When the Coulomb field dominates, the situation is similar to the case of zero dc field. When the dc field dominates, the nonlinear resonances get further apart as the action rises, and so the threshold rises. Although the resonances also get larger, the effect of getting farther apart predominates.

The width of the lowest plateau in the clamping field case is a special case. This lowest plateau marks the transition region between the Coulomb field domination and external field domination. It actually spans the width of *two* nonlinear resonances in action, these two being the first nonlinear resonances that overlap. Because these two overlap with each other before they overlap with either of their other neighbors, the chaos threshold is the same within both of them. In every other case, when a resonance first overlaps with a neighbor, *that* neighbor has already overlapped with *its* other neighbor. The dc field also influences the chaos threshold and the width of the thresholds in action. We observe significant variations from curve to curve within each regime. As the unclamping field is increased, the thresholds decrease more sharply, and the plateaus get narrower and start at lower action (red shift). The narrowing of the plateaus gets very extreme at strong unclamping fields, where the electron is quite close to the classical dc ionization threshold. In these cases, the number of quantum states contained in a single nonlinear resonance gets very small ($\ll 1$). The effect of quantum-mechanical tunneling also becomes important. We will discuss both of these effects in detail later. This is due to the nonlinear resonances getting closer and closer to each other as the unclamping field is increased. As the clamping field gets stronger, it dominates the Coulomb field at lower action, causing the chaos threshold to stop decreasing and start increasing sooner, until the clamping field is reached at which the first plateau is the lowest. The widths and heights of the plateaus also increase as the clamping field is increased and the resonances get further apart.

It is interesting to inspect the nature of the results with regard to the degree of mixing of the n quantum number that is caused by the external dc field. The threshold curves diverge the most at the lower right of Fig. 2, showing a drastic dependence on the dc field curve there, in contrast to the upper left, where the curves are similar. This strong effect of the dc field on classical chaos occurs in the region of strong n mixing, where the Stark shift due to the external dc field is much larger than the energy spacing between levels of adjacent n. There are some interesting consequences to this strong dependence on the dc field, which we will discuss in more depth in relation to the number of quantum states contained by a given nonlinear resonance. Previous experiments have all been performed in the region of weak n mixing, where the Stark shift is on the order of or smaller than the spacing between levels of adjacent n. In Fig. 3 this region covers a diagonal path along the threshold curve for $E_{dc}=0$, a very narrow path for larger actions which widens out somewhat for smaller actions. For example, the Stark shift is equal to the energy difference between adjacent levels for $n=40$ (action$=40\ \hbar$) and $E_{dc}=\pm 34$ V/cm, $n=60$ and ± 4.5 V/cm, and $n=90$ and ± 0.59 V/cm. The strong n mixing case would occur for each specific case when E_{dc} becomes much larger than each of these values, respectively.

Finally, we note that Fig. 2 describes the specific case in which the external frequency is 30.5 GH. We have performed the calculations for other frequencies and the results are similar. In fact, the curves in Fig. 2 are universal, because of the scaling properties of the classical differential equation from which they are derived. If $\Omega=30.5$ GHz is changed to Ω', Fig. 3 scales are as follows: $I'=(\Omega'/\Omega)^{-1/3}I$, $F'_{ac}=(\Omega'/\Omega)^{4/3}F_{ac}$, $F'_{dc}=(\Omega'/\Omega)^{4/3}F_{dc}$. For a description of surface state electrons or hydrogen-like ions, Fig. 3 can also be scaled with Z: $\Omega'=\Omega$, $I'=(Z'/Z)^{2/3}I$, $F'=(Z'/Z)^{1/3}F$.

It is clear from this figure that the effect of electric field is nontrivial.[15] For example in the case of interaction of $n=66$ with 30 GHz, we find that a presence of 10 V/cm lowers the threshold of chaos by 30% in agreement with other recent results.[15] On the other hand, the presence of 20 V/cm would lower the threshold more dramatically. Such nontrivial response is directly associated with field emission (ionization) effects.

We now discuss the question of the number of states trapped in the nonlinear resonances and the dependence of this number on the magnitude and the sign of the external dc field. There are good theoretical reasons to believe that the number of quantum states trapped in the first nonlinear resonance determines whether the system is in the classical or purely quantum limit, at least in the low-frequency region (below the first resonance).[4] The system is expected to behave classically when the number of states trapped is $\gg 1$, and nonclassically when the number of states trapped is $\lesssim 1$. With this in mind, we plot in Fig. 3 the number of states trapped in the first resonance for a clamping dc field, and in Fig. 4 the same for an unclamping field. These quantities can be read off the Fig. 2 graph; they are simply the widths of the first nonlinear resonances for the different dc fields. The action measured in units of $\hbar$ is equal to the principal quantum number n in the Wilson-Sommerfeld semiclassical theory of quantum mechanics; it is approximately equal for large n in the Wentzel-Kramers-Brillouin (WKB) approximation.[18] Thus the width of a resonance is a good approximation for the number of states trapped. It is clear that the unclamping field allows one to go from the classical limit to the uniquely quantum limit. The graphs show that this limit can be reached with easily available microwave frequencies and dc fields. Another advantage of the unclamping dc field system is that, by reducing the inherent frequency of the one-dimensional (1D) system, it may allow one to more easily reach the regime in which the externally imposed microwave frequency is greater than the inherent system frequency. Uniquely quantum effects which do not occur in the low-frequency regime have been predicted for this high-frequency regime by a quantum-mechanical numerical simulation of the system,[5] including the quenching of classical chaos by the quantum system. It appears that the dc field allows one to quickly and easily examine the system for various values of the number of trapped states, down to the quantum regime, and helps one to reach a new regime in the frequency as well. Note that if the hypothesis of the quantum quenching of chaos is true, then the application of the unclamping field, a field trying to rip the electron away from the atom or surface, might actually be a stabilizing factor because it brings the system into the quantum regime, a surprising result.

The unclamping field has many advantages as an experimental method to study quantum chaos. There is, however, an important experimental limitation. We are detecting the presence of chaos by measuring either the onset of ionization or enhanced linewidths in the spectrum. If the dc field is too high, then the atoms will ionize by quantum-mechanical tunneling before they ionize by classical chaos, obscuring both the enhanced line widths and the chaos-produced ions. We have done some estimations to see if there are dc fields which reach the quantum regime without producing enough tunneling to obscure the observation of chaos effects.

The width of a state due to tunneling (or, equivalently, the inverse of the tunneling lifetime) is determined by the tunneling integral τ, given by

$$\tau=\int_a^b \sqrt{2(V-E)}\,dx \ .$$

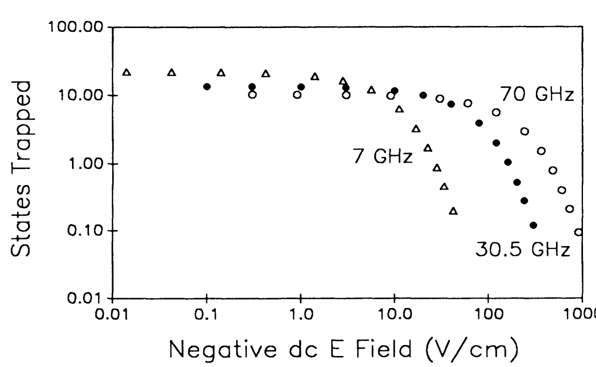

FIG. 4. Number of states trapped in the $m=1$ resonance as a function of negative dc electric field.

Parameters a and b are the inner and outer boundaries of the classically forbidden region. The tunneling integral τ is simply the imaginary part of the wave function's accumulated phase in the classically forbidden approximation region.[16] In the WKB approximation (which will be sufficiently accurate for our purposes provided $n \gg 1$ and $\tau > 1$), the width of a state due to tunneling Γ depends only on τ and the energy separation between adjacent states (inverse of the density of states). It is closely approximated by (full width at half-maximum)

$$\Gamma\frac{dn}{dE}=\frac{1}{2}e^{-2\tau}$$

for $\tau > 1$.[18,19] This expresses Γ as a fraction of the state spacing or, equivalently, the characteristic period of the system divided by the tunneling lifetime. When $\tau=1.5$, the system on average goes through 40 cycles before ionizing by tunneling, and that number increases very rapidly as τ increases. Since one would generally expect, in usual experimental situations involving this type of system, a system ionizing by chaos to do it within about 40 cycles,[9] then when $\tau=1.5$ one would expect the chaos lifetime to be similar to or shorter than the tunneling lifetime, and so the observed effects of chaos (including ionization and widening of line widths) would be at least as strong as those of tunneling if the tunneling signal is observable. The $\tau > 1.5$ limitation on observing chaos is a conservative one. The criterion makes the most conservative estimate of the effect of classical chaos on the quantum spectrum; chaos broadens the lines, which it must do if it creates ionization within a certain period of time. Of course, chaos is likely also to have other effects on the spectrum,[6,12,20] in which case chaos would be even easier to detect.

We calculated τ as a function of the unclamping dc field for the three frequencies 7, 30.5, and 70 GHz, with initial electron energy at the bottom of the $m=1$ and 2 resonances at the threshold of global chaos. It is plotted in Fig. 5. We used a parabolic approximation to the potential at the top of the barrier being tunneled through. Comparison with numerical integration showed this parabolic approximation, best for small τ, to give τ within 5% even for the largest τ, and within 1% for the region of interest. The $m=1$ criterion gives a direct comparison between ionization by chaos and ionization by tunneling directly from the initial state. The $m=2$ criterion is more conservative, because if the electron area tunnels from $m=2$, it must have first experienced chaos to reach $m=2$. Thus, all ionization would have some chaos component, if $\tau > 1.5$ from the $m=2$ resonance with an ac field of strength equal to the threshold of chaos. The tunneling integral τ, like Ω, F_0, and F_1, scales as a function of frequency, as it is entirely classical except for a *factor* of h; the scaling law is given in the caption of Fig. 5.

Of course, the question in which we are interested is not how high a dc field can be reached without tunneling obscuring the results, but rather how a few trapped states can be reached without tunneling becoming a problem. With that in mind, we combine Figs. 4 and 5 and plot in Fig. 6 the tunneling integral τ as a function of the number of states trapped in the $m=1$ resonance at the

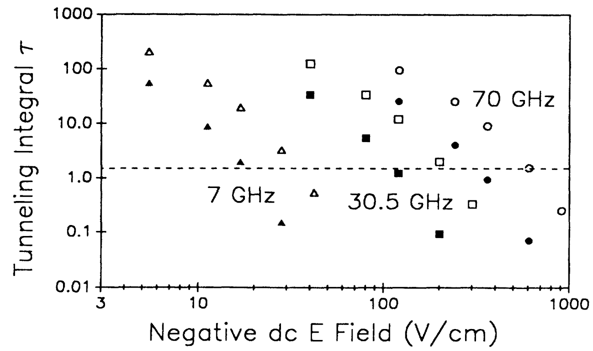

FIG. 5. Tunneling integral τ as a function of negative dc electric field, for states at the bottom of the $m=1$ resonance (open symbols) and the bottom of the $m=2$ resonance (filled symbols) for three ac field frequencies at the threshold of classical chaos. Scaling: $\tau'=(\Omega'/\Omega)^{-1/3}\tau$ at constant Z, and $\tau'=(Z'/Z)^{2/3}\tau$ at constant Ω. Below $\tau=1.5$, ionization by chaos would be obscured by ionization by tunneling.

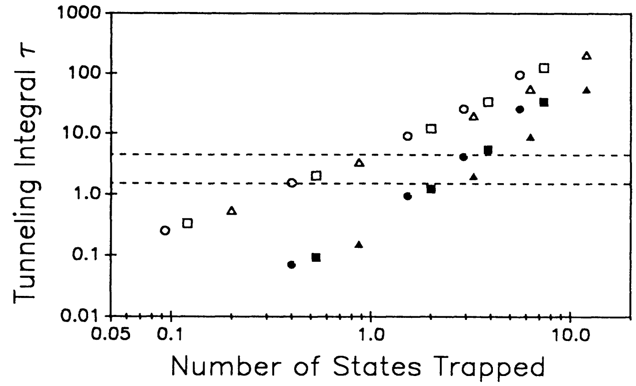

FIG. 6. Tunneling integral τ as a function of the number of states trapped in the $m=1$ nonlinear resonance, from the bottom of the $m=1$ (open symbols) and $m=2$ (closed symbols) resonances at the threshold of classical chaos. The triangles are 7 GHz, the squares 30.5 GHz, and the circles 70 GHz. The dotted lines delineate the area within which resonant ionization spectroscopy is possible without chaos being obscured by tunneling. Notice that it stretches from fewer than one state trapped to more than one state trapped.

threshold of chaos. Comparing with tunneling from the initial state, one clearly reaches the quantum regime at $\tau=1.5$, with about 0.45 states trapped at 30.5 GHz. The $m=2$ criterion puts one in the very beginning of the quantum regime at $\tau=1.5$, with about 2 states trapped at 30.5 GHz. Note that the number of states trapped at $\tau=1.5$ is fairly insensitive to frequency.

If one is trying to obtain an ionization spectrum, instead of just looking at ionization by chaos, then there is also a maximum τ criterion. For a typical experimental setup, the atom must ionize by tunneling within a few microseconds in order to be detected. This criterion gives a maximum τ of about 4.5 for detection at 7 GHz (the τ criterion, calculated from above, is slightly larger for the other frequencies plotted). This maximum τ criterion, as well as the minimum, is plotted in Fig. 6. Although the band of observable spectra is fairly narrow in τ, it spans a wide range in the number of states trapped. If one looks at the spectrum low in the first resonance, one can go down to about 0.5 states trapped, and if one looks high in the first resonance, one can see the spectrum for as many as five states trapped. Since agreement with classical chaos predictions has been observed for as few as 20 states trapped,[11] one would expect five states to show at least some classical chaos character. Thus, the spectrum measurement would span the region from the clearly quantum mechanical to the classical.

In conclusion, we find the unclamping field to be a promising technique for bringing the system, be it selectively excited hydrogen atom or surface state electron, from the classical regime to the uniquely quantum regime. Ionization by classical chaos can compete favorably with ionization by tunneling in usual experimental situations, and tunneling allows very sensitive measurements of the quantum spectrum.

[1]J. Ford, in *The New Physics,* edited by S. Capelin and P. C. W. Davies (Cambridge University Press, Cambridge, MA, 1986).

[2]For examples, see *Stochastic Behavior in Classical and Quantum Hamiltonian Systems,* Vol. 93 of *Lecture Notes in Physics,* edited by G. Casati and J. Ford (Springer-Verlag, Berlin, 1979); *Chaotic Behavior in Quantum Systems,* edited by G. Casati (Plenum, New York, 1985).

[3]G. Casati, J. Ford, I. Guarneri, and F. Vivaldi, Phys. Rev. A **34**, 1413 (1986).

[4]G. P. Berman, G. M. Zaslavsky, and A. R. Kolovsky, Phys. Lett. **87A**, 152 (1982).

[5]G. Casati, B. Chirikov, D. Shepelyansky, and I. Guarneri, Phys. Rep. **154**, 79 (1987).

[6]I. C. Percival, J. Phys. B **6**, L229 (1973); N. Pomphrey, *ibid.* **7**, 1909 (1974).

[7]J. E. Bayfield and P. M. Koch, Phys. Rev. Lett. **33**, 258 (1974).

[8]P. M. Koch, in *Fundamental Aspects of Quantum Theory,* edited by V. Gorini and A. Frigerio (Plenum, New York, 1986).

[9]R. V. Jensen, Phys. Rev. A **30**, 386 (1984).

[10]J. E. Bayfield and L. A. Pinnaduwage, Phys. Rev. Lett. **54**, 313 (1985).

[11]R. V. Jensen and S. M. Susskind, in *Photons and Continuum States of Atoms and Molecules,* edited by N. K. Rahman, C. Guidotti, and M. Allegrini (Springer-Verlag, Berlin, 1987), p. 13.

[12]M. H. Nayfeh, D. C. Humm, and M. S. Peercy, Proceedings of the Symposium on the Hydrogen Atom, Pisa, Italy, 1988, edited by F. Bassani, T. W. Hänsch, and M. Inguscio (unpublished).

[13]R. V. Jensen, Phys. Rev. Lett. **54**, 2057 (1985).

[14]G. P. Berman, G. M. Zaslavsky, and A. R. Kolovsky, Zh. Eksp. Teor. Fiz. **88**, 1551 (1985) [Sov. Phys.—JETP **61**, 925

(1985)].
[15]M. J. Stevens and B. Sundaram, Phys. Rev. A **36**, 417 (1987).
[16]B. V. Chirikov, Phys. Rep. **52**, 263 (1979).
[17]G. M. Zaslavsky and B. V. Chirikov, Usp. Fiz. Nauk. **105**, 3 (1971) [Sov. Phys. Usp. **14**, 549 (1971)].
[18]H. Goldstein, *Classical Mechanics,* 1st ed. (Addison-Wesley, Reading, MA, 1959), p. 288.
[19]L. I. Schiff, *Quantum Mechanics,* 3rd ed. (McGraw-Hill, New York, 1968), p. 268.
[20]D. A. Harmin, Phys. Rev. A **26**, 2656 (1982).
[21]O. Bohigas, M. J. Giannoni, and C. Schmit, Phys. Rev. Lett. **52**, 1 (1984).