Ericson Fluctuations in the Chaotic Ionization of the Hydrogen Atom in Crossed Magnetic and Electric Fields

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We report exact quantum calculations for the hydrogen atom in crossed magnetic and electric fields. Employing the complex-coordinate-rotation method we are able to extend the calculations of eigenstates far into the continuum region. Calculated photoionization cross sections are found to exhibit strong Ericson fluctuations, a characteristic feature of chaotic scattering. This interpretation is supported by classical trajectory calculations which reveal a fractal dependence of the classical ionization time on the initial conditions.

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Highly excited states of atoms exposed to a uniform magnetic field have proved, in recent years, ideal objects in which to study—both theoretically and experimentally—the novel quantum features that emerge in quantum systems when the underlying classical system undergoes a transition to chaos [1]. As a paradigm of a real nonseparable quantum system with a classically chaotic counterpart, the hydrogen atom in a magnetic field, and, in particular, its *bound-state* spectrum have been analyzed extensively with respect to universal quantum signatures of chaos, such as the changes in the statistics of the fluctuations of energy-level densities from a Poissonian behavior to the behavior predicted by random-matrix theory [2], or the appearance of long-range modulations in the spectra that are related to classical periodic orbits [3]. By contrast, in this Letter we want to direct the attention to a quantum signature of chaos that is to be expected in the *continuous* part of the spectrum, viz., *fluctuations* in quantal cross sections that can be associated with *unbounded* classical trajectories. This phenomenon was first discovered many years ago in nuclear reaction physics by Ericson [4], and an interpretation was given in terms of random-matrix theory; the relation between these "Ericson" fluctuations and classical chaotic scattering was elaborated by Blümel and Smilansky [5], who demonstrated the occurrence of Ericson fluctuations in a model system. Revealing the existence of Ericson fluctuations in the ionization cross section of atoms in external fields and establishing a connection to classical chaotic orbits is the central objective of this paper.

Continuum (i.e., positive-energy) spectra of Rydberg atoms in uniform magnetic fields were computed recently by Delande, Bommier, and Gay [6], who used the complex-rotation method, and O'Mahony and Mota-Furtado [7] and Watanabe and Komine [8], who took a closed-coupling approach. Here we wish to go one step further and look at the continuum spectrum of a system slightly more complicated, namely, the hydrogen atom under the combined action of a magnetic *and* a crossed electric field. The motivation for doing so derives from the fact that above-ionization-threshold spectra of atoms in crossed fields are largely unexplored both experimentally and theoretically: Experiments so far were restricted to states below threshold [9], or could only resolve long-lived states above threshold [10], while theoretical work was confined to either perturbative approaches (weak fields) [11] or, in the nonperturbative regime, to general discussions of the possible existence of a double-minimum potential [12] and quasi-Penning resonances [13]. Another reason for looking at the crossed-field problem is that the electric field enhances ionization and shifts the above-threshold region to energies which are still theoretically feasible.

The Hamiltonian of a hydrogen atom in crossed uniform magnetic and electric fields reads [in atomic units, $\gamma=B/(2.35\times10^5\ \mathrm{T})$, $f=F/(5.14\times10^9\ \mathrm{V/cm})$]

$$H=\tfrac{1}{2}\mathbf{p}^2-1/r+\tfrac{1}{2}\gamma L_z+\tfrac{1}{8}\gamma^2(x^2+y^2)+fx\,. \qquad (1)$$

In contrast to the case of an atom in a single uniform magnetic field (or parallel fields), the z component of the angular momentum, L_z, is no longer conserved for an atom in crossed fields, and thus one deals with a system nonintegrable in *three* degrees of freedom, the only remaining constants of motion being the total energy, E, and the parity with respect to the ($z=0$) plane, π_z.

To account for continuum states we adopted the complex-rotation method [14] (replacement of $\mathbf{r}$ with $\mathbf{r}e^{i\theta}$ in the Hamiltonian and wave functions), which proved so efficient in determining the positive-energy spectrum of the hydrogen atom in a magnetic field [6]. By this transformation, hidden resonances of the Hamiltonian in the continuum, associated with complex eigenvalues, are exposed, while the resonance wave functions are described by $\mathcal{L}_2$-integrable basis functions, with complex arguments. We worked with a Sturmian-type basis set and used semiparabolical coordinates [15]. In this way, the complex-rotated Schrödinger equation is transformed to a generalized complex symmetric eigenvalue problem with sparse matrices and complex energy eigenvalues E. We solved the eigenvalue problem numerically by extending the Lanczos algorithm [16] to complex matrices. Note that, since L_z is no longer a good quantum number, the

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basis set cannot be restricted to states with fixed magnetic quantum number m as is the case for an atom in a pure magnetic field. The crossed-field atom, therefore, requires considerably enlarged basis sets in comparable energy-field regions.

We performed numerical calculations for $B=21$ T, $F=5140$ V/cm, with a basis set of up to 19600 states, which, for these field strengths, proved sufficient to guarantee convergence of the results for the bound states, long-lived resonances, and the cross section for dipole transitions. Continuum states of course depend, in general, on the complex rotation angle θ. For the purpose of the present investigation we chose a relatively strong magnetic field to keep the basis sizes feasible on small machines (the extension to laboratory field strengths using larger basis sizes is straightforward). The complex rotation angle we used was $\theta=0.08$. Figure 1(a) shows the results for the complex energy eigenvalues obtained at these field strengths. Below the Stark saddle-point energy, $E_{sp}=-2\sqrt{f}$ a.u. $=-438.8$ cm^{-1}, ionization is classically forbidden and quantum states are evidently restricted to the real energy axis with zero (or negligibly small) imaginary parts. Above the saddle point, more and more continuum states are rotated towards negative imaginary parts, revealing a lot of hidden resonances near the real axis. The energy widths Γ of these resonances are given by $\Gamma=-2\,\mathrm{Im}E$.

With the energy eigenvalues and eigenvectors at hand it is a straightforward task to evaluate the cross section for dipole transitions, which can be written in the form [17]

$$\sigma(E)=4\pi\alpha(E-E_0)\mathrm{Im}\left[\sum_j\frac{\langle\Psi_0|D|\Psi_j(\theta)\rangle^2}{E_j(\theta)-E}\right], \qquad (2)$$

where Ψ_0 is the initial state with energy E_0, and $\Psi_j(\theta)$ are final states at (complex) energies $E_j(\theta)$; D denotes the dipole operator for some given polarization, and $\alpha\approx\frac{1}{137}$ is the fine-structure constant. Though the energies $E_j(\theta)$ and the (complex) dipole matrix elements $\langle\Psi_0|D|\Psi_j(\theta)\rangle$ may, in general, depend on the complex rotation angle θ, the cross section $\sigma(E)$ is not affected by this rotation angle in converged spectra. As an example we considered dipole transitions of the crossed-field hydrogen atom from the initial state $|2p0\rangle$ to final states with even z parity, excited by coherent light with linear polarization parallel to the direction of the magnetic field. The spectrum resulting at $B=21$ T, $F=5140$ V/cm is shown in Fig. 1(b). For graphical purposes, infinite or very large values of the photoionization cross section resulting from states with $\Gamma<0.04$ cm^{-1} have been drawn with the widths of these states arbitrarily set to $\Gamma=0.04$ cm^{-1}. It is evident from Fig. 1(b) that up to energies even well above the Stark saddle point the photoionization spectrum is dominated by sharp lines, i.e., long-lived states. Below $E\approx-280$ cm^{-1}, almost no continuum states are excited, which may be interpreted in terms of a stabilizing effect of the magnetic field on states above the Stark saddle energy. At higher energies ($E\gtrsim-280$ cm^{-1}) the continuum is growing, but in contrast to the Stark effect [18] it is not a smooth function of the energy, but exhibits irregular fluctuations. Figure 2(a) shows this part of the spectrum on a larger scale. To make the fluctuations in the continuum signal stand out, we have plotted the part of the spectrum which results from broad resonances with $\mathrm{Im}E<-0.1$ cm^{-1} by the solid curve. The dashed curve represents the complete photoionization cross section. In general the peaks of the fluctuations do not belong to a single resonance, but result from the in-

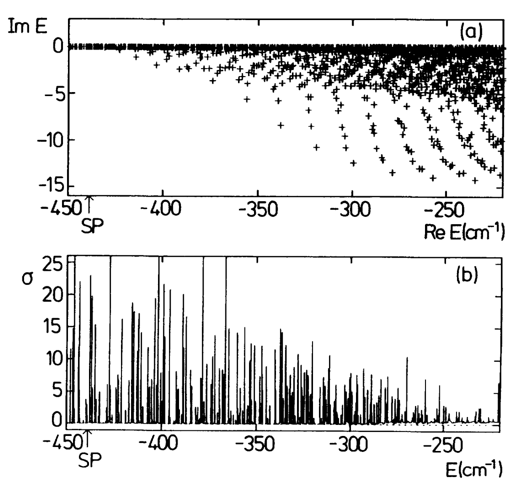

FIG. 1. Spectra of the hydrogen atom in a crossed magnetic and electric field with $B=21$ T, $F=5140$ V/cm. (a) Positions of resonances with even z parity in the complex energy plane. (b) Photoionization cross section (in a_0^2) for excitation of the $|2p0\rangle$ state using light with linear polarization parallel to the magnetic field axis. (SP: position of the Stark saddle point).

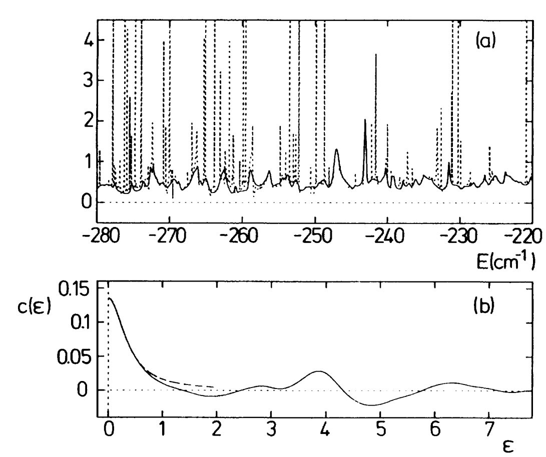

FIG. 2. (a) Enlargement of Fig. 1(b) in the energy range -280 to -220 cm^{-1}. The solid curve is the cross section produced by all resonances with $\mathrm{Im}E<-0.1$ cm^{-1}; the dashed curve represents the complete cross section including the long-lived states. (b) Autocorrelation function calculated from the above spectrum. The dashed curve is a Lorentz curve fitted with a coherence width of $\Gamma=0.37$ cm^{-1}.

terference of many states.

Fluctuations of this type were first discussed by Ericson for nuclear cross sections in the continuum region [4], and were experimentally observed in these systems [19]. The basic ideas of Ericson are the following: (a) If many resonances with widths exceeding the mean level spacing are excited coherently and (b) if the phases of these resonances are distributed randomly, they produce statistical fluctuations in the cross section as a function of energy. It was shown recently that Ericson fluctuations also appear in simple quantum systems with few degrees of freedom, if the corresponding classical scattering system possesses irregular dynamics ("chaotic scattering") [5].

According to Ericson, the fluctuations provide information on the lifetime of the excited compound nucleus when analyzed via the autocorrelation function

$$C(\varepsilon)=\frac{1}{\bar{\sigma}^2}\int_{E_1}^{E_2}[\sigma(E+\varepsilon)-\bar{\sigma}][\sigma(E)-\bar{\sigma}]dE\,, \qquad (3)$$

where $\bar{\sigma}$ is the average cross section in the energy interval $E_1 \le E \le E_2$ under consideration. For small displacements ε the autocorrelation function assumes a Lorentzian shape $C(\varepsilon)\sim(\Gamma^2+\varepsilon^2)^{-1}$, where Γ is the coherence energy ($\sim$ reciprocal lifetime) of the intermediate state. We have analyzed the continuum signal of the crossed-field atom [solid curve in Fig. 2(a)] accordingly. The autocorrelation function is shown in Fig. 2(b). It can indeed be fitted for small ε by a Lorentzian shape, with $\Gamma=0.37$ cm^{-1}, corresponding to a lifetime of $T_{\rm ion}=590\,000$ a.u. This is about 8 times the cyclotron time of a free electron in a magnetic field $B=21$ T. We have deliberately extended the horizontal scale in Fig. 2(b) to larger values of ε, where the autocorrelation function oscillates around zero, to demonstrate the striking similarity between the atomic autocorrelation function and the nuclear autocorrelation function determined in Ref. [19]. While the phenomenon there occurred on energy scales of tens of keV, here we can observe it on scales of 10^{-5} Ry. This evidently points to the universality of the phenomenon. Whether or not physical importance can be attributed to the oscillations in the autocorrelation function remains to be investigated.

To confirm our interpretation of the structures in the photoionization cross section of the cross-field atom in terms of Ericson fluctuations we also analyzed the classical dynamics of the system. Of course, the crossed-field atom is not a generic scattering system, with an asymptotically free incoming and outgoing electron. Rather, the electron is located very close to the nucleus at the moment of excitation ($t=0$), and the classical trajectories do not depend on certain impact parameters, as for scattering, but on the starting direction of the electron, parametrized, e.g., by spherical coordinate angles ϑ and φ. The ensuing motion of the electron is in general very complicated due to the nonintegrable nature of the Hamiltonian (1), but for ionizing trajectories the Coulomb potential can be neglected as $r\rightarrow\infty$, and asymptotically we have free motion along the z axis and a cycloidal motion in the (x,y) plane [12(a)], with the center of the cycloid moving parallel to the y axis according to $y(t)=-(t-T_{\rm ion})F/B$. Fitting ionizing trajectories $\mathbf{r}(t)$ with this asymptotic motion, one can interpret $T_{\rm ion}$ as the classical ionization time, depending on the starting angles ϑ and φ. As an example, Fig. 3 shows this dependence in the ($z=0$) plane ($\vartheta=90°$) at scaled energy $\tilde{E}=E\gamma^{-2/3}=-0.6$ and scaled field strength $\tilde{F}=f\gamma^{-4/3}=0.25$, corresponding to $E\approx-260$ cm^{-1}, $F\approx5140$ V/cm at $B=21$ T. For $\varphi<120°$ and $\varphi>240°$ the ionization time grows rapidly, indicating the presence of bounded or extremely long-lived trajectories. By contrast, in the interval $120°<\varphi<240°$ [Fig. 3(a)] the classical ionization time exhibits large fluctuations in some regions. Magnifications of parts of these regions [Figs. 3(b) and 3(c)] reveal the existence of fractal structures in the classical ionization time as a function of the starting angle φ. This fractal dependence is not restricted to the ($z=0$) plane; we have observed similar structures as a function of ϑ as well. The features strikingly resemble fractal structures seen in model systems of chaotic scattering [5,20].

To distinguish between photoionization and scattering problems we adopt the term "chaotic ionization" in the case of the crossed-field atom, but the connection to chaotic scattering is quite obvious. There is also a deep connection between the classically chaotic ionization of

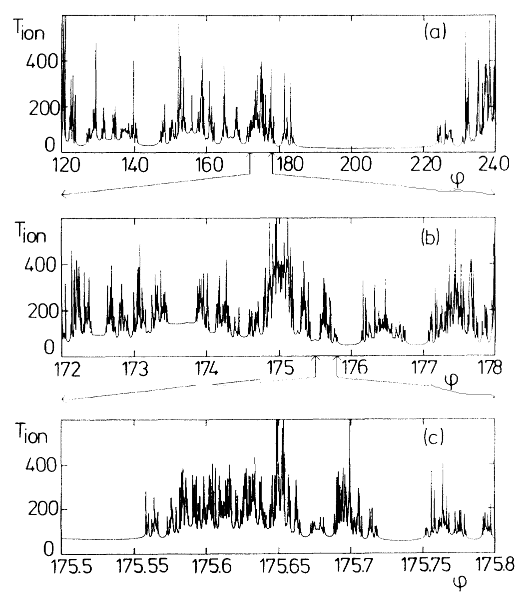

FIG. 3. Classical ionization time (in γ^{-1} a.u.) of an electron in the crossed-field atom starting at the nucleus in the ($z=0$) plane with azimuth φ for scaled energy $\tilde{E}=-0.6$ and scaled field strength $\tilde{F}=0.25$ in successively smaller φ intervals. The fractal structure is evident from the enlargements.

the crossed-field atoms and the observation of Ericson fluctuations in the quantum mechanically calculated photoionization cross section. If we change the ratio of the external field strengths a decrease of fractal structures in the classical ionization time is accompanied by a decrease of fluctuations in the continuum part of the photoionization cross section.

In conclusion, we have performed exact quantum-mechanical calculations for the hydrogen atom in crossed magnetic and electric fields by numerical diagonalization of the Hamiltonian in a complete Sturmian-type basis set. Using complex rotation we could extend the calculations to energies far above the Stark saddle point. The continuum part of the photoionization cross section exhibits Ericson fluctuations in energy–field-strength regions where classical trajectory calculations point to chaotic ionization. The features resemble structures observed in chaotic scattering systems. The universality of Ericson fluctuations in quantum systems with classical chaotic counterparts is thus strongly supported by our investigations in a real quantum system with few degrees of freedom.

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