

Origin of Narrow Resonances in the Diamagnetic Rydberg Spectrum

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Recently, ultranarrow resonances have been observed in the diamagnetic Rydberg spectrum of the lithium atom. We show that they originate from an accidental destructive interference, which, in turn, is due to the chaotic character of the classical behavior. Our numerical simulations show that their statistical properties are well described by a random-matrix model.

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The hydrogen atom in a magnetic field is well known as a prototype for the study of quantum manifestations in a chaotic system (the so-called quantum chaos) [1-5], because theoretical, numerical, and experimental studies on high lying Rydberg states are possible. In the last few years, the bounded energy spectrum of this system has been widely studied [1-5].

Recently, Kleppner and co-workers have experimentally observed the continuous spectrum of this system (more precisely, of the lithium diamagnetic spectrum which is almost equivalent to the hydrogen one) above the ionization threshold [3]. In these conditions, discrete energy levels turn into resonances. Surprisingly, many extremely narrow resonances are observed, with lifetimes of the order of several thousand cyclotron periods. That might appear in contradiction with the chaotic classical behavior: the electron should rapidly diffuse in phase space and ionize in a few cyclotron periods. The experimental observation has been confirmed by the first numerical calculations that can yield accurate results at laboratory field strengths [4, 6-8].

This Letter presents numerical and statistical results to prove that the existence of narrow resonances is an effect of quantum interferences specific to classically chaotic systems and that their probability distribution can be predicted by a random-matrix theory. These narrow resonances are actually the first experimental observation of the so-called Porter-Thomas distribution in a simple quantum system.

In atomic units ($\hbar = |q| = m = 4\pi\epsilon_0 = 1$), the Hamiltonian of the atom in a magnetic field (along the z axis) is

$$H = \frac{p^2}{2} - \frac{1}{r} + \frac{\gamma}{2}L_z + \frac{\gamma^2}{8}\rho^2, \quad (1)$$

where $\gamma = B/B_c$ ($B_c = 2.35 \times 10^5$ T) and L_z is the z component of the angular momentum, which remains a good quantum number.

In the vicinity of the classical ionization threshold, the classical dynamics has been shown to be almost fully chaotic [1, 2].

At large distance from the nucleus, the Coulomb term is negligible and the Hamiltonian (1) reduces to the one of a free electron in a magnetic field. Hence, whereas there is a single classical ionization threshold at $E = 0$ above which almost any trajectory ionizes, there are multiple quantum ionization thresholds at the different Landau levels (energy levels of an electron in a magnetic field):

$$E_N = (N + \frac{1}{2})\gamma, \quad (2)$$

where N is a non-negative integer.

At very high magnetic field, the diamagnetic potential is dominant and shrinks the atom in the ρ plane. Thus the rapid motion in the ρ direction can be adiabatically separated from the slow motion along the z axis; the Hamiltonian is written as $H = H_0 + V_c$ with

$$\begin{aligned} H_0 &= \frac{p^2}{2} - \frac{1}{|z|} + \frac{\gamma}{2}L_z + \frac{\gamma^2}{8}\rho^2, \\ V_c &= -\frac{1}{r} + \frac{1}{|z|}. \end{aligned} \quad (3)$$

This yields a spectrum of H_0 composed of an infinite set of one-dimensional (along z) Rydberg series, each converging to a Landau threshold. All the series, but the lowest one which is discrete, are coupled with the continua of the lower Landau levels through the nonadiabatic term V_c and, thus, are composed of resonances [6]. For lower fields, such an adiabatic separation cannot be made and the Coulomb potential generates a strong coupling between all these series yielding to a chaotic spectrum.

Whatever the magnetic field strength (i.e., adiabatic approximation valid or not), the ionization process strongly depends on the number of open channels, that is, the number of Landau thresholds with lower energy. In the following, we will focus on the energy interval between the first and the second Landau thresholds, where the ultranarrow resonances have been experimentally observed [3]. As only one single channel is then open, the resonances can be thought of as discrete states resulting from the complicated interaction of all the Landau channels, except the first one, coupled to the single continuum

of the first Landau level. The complexity of the spectrum in the chaotic region brings up an interest in a statistical description of the resonances. It is reasonable to assume that the statistical properties of the discrete states (before the coupling with the continuum is taken into account) are not different from those of the discrete states just below the ionization threshold. The latter have been widely studied: they are well described by the Gaussian orthogonal ensemble (GOE) of random matrices [9, 10]. Roughly, this means that the statistical properties of the energy levels are those of the eigenvalues of a set of random matrices, whose matrix elements have independent Gaussian distributions.

Using this model, we are able to predict the statistical properties of the widths. The width of a resonance is given by the Fermi golden rule $\Gamma \propto |\langle c | V_c | i \rangle|^2$, where $|i\rangle$ is the discrete state, $|c\rangle$ the continuum state with the same energy, and V_c the coupling. As $|i\rangle$ has the statistical properties of an eigenvector of a GOE random matrix, $|\langle c | V_c | i \rangle|$ has a Gaussian statistical distribution around zero. Thus, the probability distribution for the widths Γ of the resonances between the first two Landau thresholds is given by the Porter-Thomas distribution [9, 11]:

$$P(\Gamma) = \frac{1}{\sqrt{2\pi\bar{\Gamma}}} e^{-\Gamma/2\bar{\Gamma}}, \quad (4)$$

where $\bar{\Gamma}$ is the mean value. One can easily see that the smallest widths are the most probable. This nonintuitive result means that the strong statistical fluctuations in the random-matrix model tend to compensate one another, the most probable value of any matrix element being zero. It is analogous to a random walk, where the most probable ending point is the starting point.

If there is more than one open channel, the width is the sum of the square moduli of the corresponding matrix elements and, thus, the probability of having a small width decreases as the number of open channels increases.

In order to test this prediction, we have numerically computed the positions and widths of the resonances using the complex coordinate method. Replacing $\mathbf{r} \rightarrow \mathbf{r}e^{i\theta}$, $\mathbf{p} \rightarrow \mathbf{p}e^{-i\theta}$ in the Hamiltonian, one obtains a non-Hermitian operator $H(\theta)$ with a complex spectrum. The resonances of H are the complex eigenvalues of $H(\theta)$, whose real and imaginary parts are respectively the energies and the negatives of the half-width of the resonances and are also θ independent (see Ref. [6] for details). The non-Hermitian operator $H(\theta)$ is numerically expanded in a Sturmian basis, as explained in Ref. [6]. This gives an eigenproblem for a complex symmetric matrix, numerically solved using the Lanczos algorithm.

Using the scaling properties of the Hamiltonian [2], the spectrum at fixed E/γ can be generated with a single diagonalization. This makes it possible [see Eq. (2)] to calculate the resonances associated with a fixed number (one in the present case) of open channels. The size of

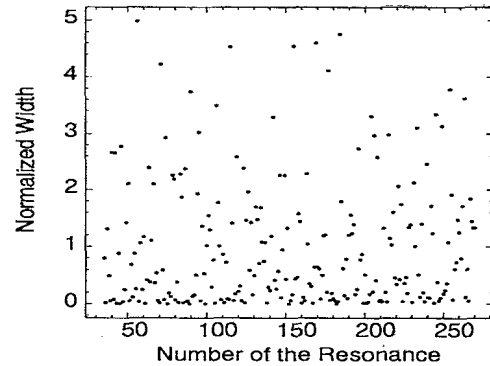


FIG. 1. Normalized widths of the resonances of the diamagnetic Rydberg spectrum vs their number (ordered by decreasing energy). These widths are numerically computed along the $E/\gamma = 0.75$ line. There is a large number of extremely narrow resonances, because of accidental destructive interferences. This is due to the chaotic character of the classical behavior and the fact that there is only one open channel.

the basis sets used is between 10 000 and 23 000.

Our statistical results are based on 275 fully converged resonances of the ($L_z = 0$, even z parity) series, calculated along the line $E/\gamma = 0.75$. The energy ranges from 1.1×10^{-2} to 9.0×10^{-5} in atomic units. In addition, we checked that the same results are also true along the line $E/\gamma = 1$. We numerically found that the widths of the resonances are much smaller than their mean spacing. We then checked that the nearest neighbor spacing distribution of the energies is in good agreement with the Wigner distribution, which characterizes the level repulsion and the strong interaction between resonances [2, 10]. Since this is exactly the property of the bound (discrete) states, we justify this by the assumption that the resonances can be described by random-matrix eigenstates coupled with some continua.

The widths are then normalized by dividing them by a moving average value. Figure 1 displays the normalized widths (with average value equal to 1) versus the numbers of the resonances (numbered by decreasing energy). The density of small widths is obviously very large, as expected. To get a quantitative comparison, we plot in Fig. 2 the cumulative probability distribution of the normalized widths compared to the Porter-Thomas distribution. The agreement is very good, especially for the smallest values [for which $P(\Gamma) \propto \sqrt{\Gamma}$], which are characteristic of the number of open channels (if there were more than one open channel, the slope at the origin would be finite). Thus, we prove that the statistical properties of the resonances are well described by a random-matrix theory.

This leads us to a physical interpretation as quantum interferences in a chaotic system. Indeed, the quantum chaotic aspect of the system finds its expression in the mixing of an important number of discrete states, which become resonances due to the coupling with the continua. Thus, because of the strong fluctuations of the states with

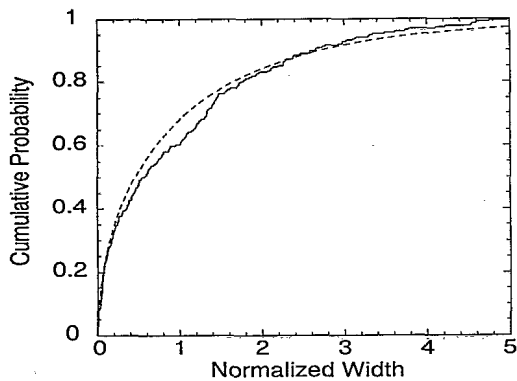


FIG. 2. Cumulative probability of the normalized widths (solid line) compared with the cumulative probability obtained from the Porter-Thomas distribution (dashed line) (data as in Fig. 1). The agreement is very good, especially for the smallest values. The infinite slope at the origin (square root behavior) is characteristic of only one open channel. The narrow resonances are by far the most probable.

the magnetic field and the energy, the matrix elements for ionization also display strong fluctuations, with a Gaussian statistical distribution. When only one channel is open, as the magnetic field is changed, this matrix element fluctuates around its most probable value of zero and, for some specific values of γ , accidentally cancels. There, we have a discrete state embedded in a continuum. In a very small range of magnetic field around the cancellation, there is a narrow resonance. This is the very origin of the ultranarrow resonances experimentally observed. This phenomenon has already been observed by Friedrich and Wintgen [12] for low excited states. Let us stress again that the random-matrix theory predicts that, although this phenomenon is accidental, it is not rare, and even the most probable.

Such narrow resonances are a manifestation of a classical chaotic behavior in a quantum system. It is a quantum phenomenon because it involves only a very small number (in fact, only one) of open channels. If many channels are open, a narrow resonance exists only if many matrix elements are simultaneously small, which is unlikely to happen. Also, the phenomenon requires strong fluctuations of the eigenstates when a parameter is changed and does not exist in a regular system. As far as we know, the narrow resonances observed in the diamagnetic Rydberg spectrum above threshold are probably the most dramatic manifestation of the intrinsic strong fluctuations in a quantum chaotic system.

From a classical point of view, the ionization width originates from the different ionizing trajectories. When the electron escapes in the z direction, its de Broglie wavelength is comparable to the transversal extension of the trajectory (in other words, only one quantum channel is open) and all the classical ionizing trajectories *interfere*. Because of the chaotic behavior, the trajectories, and consequently their interferences, are very sensitive

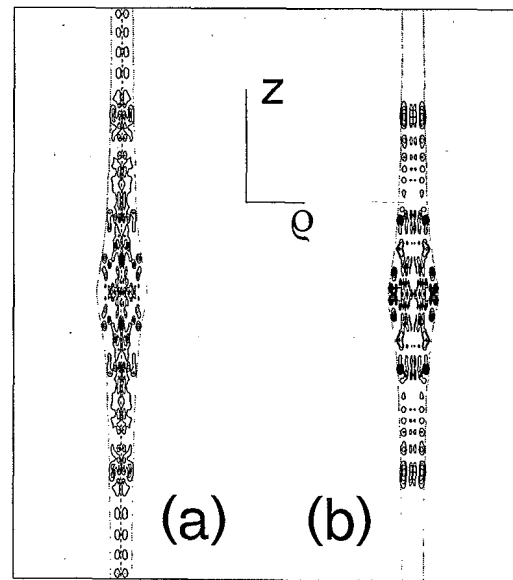


FIG. 3. Probability density (contour plots) for two resonances of the diamagnetic Rydberg spectrum: (a) Broad resonance, normalized width = 3.7, $E = 3.98 \times 10^{-4}$, $\gamma = 5.31 \times 10^{-4}$; (b) narrow resonance, normalized width = 1.3×10^{-4} , $E = 4.00 \times 10^{-4}$, $\gamma = 5.33 \times 10^{-4}$. The dashed lines represent the frontiers of the classically accessible space. The flow of probability along the z axis is clearly more important for the large resonance than for the narrow one. The small widths are due to quantum destructive interferences.

to any change of magnetic field. For some specific value of γ , it can be accidentally completely destructive.

These destructive interferences appear when one looks at the wave functions in (ρ, z) plane. Figure 3 displays contour plots of the probability density of two resonances, a broad and a narrow one. The adiabatic separation between the slow motion along the z axis and the rapid perpendicular motion can be noticed in the structure of nodes along the z axis (for large z). As only the first Landau channel is open, the wave functions associated with all the other thresholds are bounded. Thus, one can observe that the number of transversal nodes decreases when z becomes large, in correspondence with closures of the channels. Then, the width of the resonance depends on the flow of probability contained in the first Landau channel, which may become very low because of destructive interferences. Furthermore, as Fig. 4 shows (these are two sharp resonances with normalized widths of the same order $\sim 10^{-4}$), there is no simple regular structure in the internal part of the wave functions. This shows that the wave functions of the narrow resonances are not localized ("scarred") in the vicinity of some simple periodic orbits [13]. Of course, it cannot be excluded that such states are scarred by more complicated classical structures, or that their existence and shapes can be predicted using a semiclassical approach. However, no such simple theory has been presently worked out. On

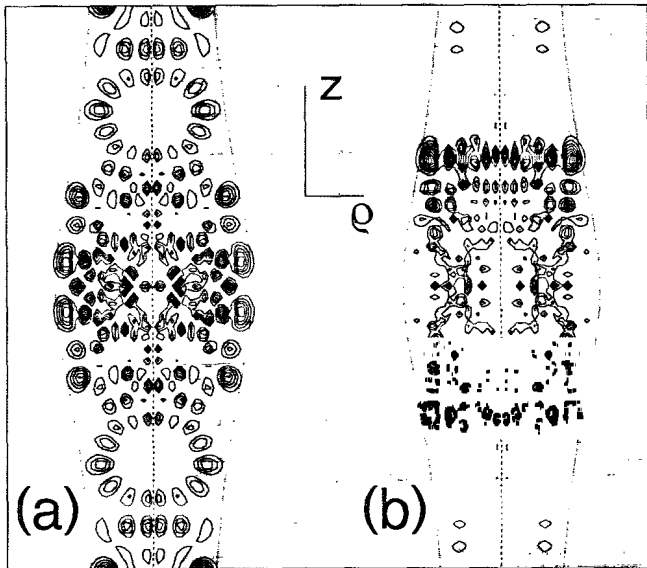


FIG. 4. Probability density (contour plots) for two narrow resonances of the diamagnetic Rydberg spectrum (with normalized widths $\sim 10^{-4}$) near the nucleus. (a) $E = 4.00 \times 10^{-4}$, $\gamma = 5.33 \times 10^{-4}$; (b) $E = 2.00 \times 10^{-4}$, $\gamma = 2.67 \times 10^{-4}$. There are no simple regular structures and no scars of simple classical periodic orbits in the wave functions.

the other hand, the random-matrix theory, based on a pure quantum approach, is able to give quantitative predictions on the statistical properties of the resonances.

Finally, the high accuracy of our simulations allows us to extend our results at laboratory fields. Thus, for a magnetic field of 6.10 T and for an energy of 7 cm^{-1} , the mean value of the widths of the resonances should be $2 \times 10^{-2} \text{ cm}^{-1}$, the probability of having a width lower than 10^{-3} cm^{-1} is 0.17, and the probability of having a width lower than 10^{-4} cm^{-1} is 0.05. These predictions are in good agreement with the experimental spectra, especially the number of narrow resonances are well described by the random-matrix model. This is the first observation of the Porter-Thomas distribution in a simple system with only a few parameters. This simplicity

of the hydrogen atom in a magnetic field provides a very good understanding of quantum chaos and gives hope of attaining physical sight of more complicated systems.

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(a) Deceased.

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