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Resonances in the Diamagnetic Rydberg Spectrum: Order and Chaos.

K. DUPRET (*), J. ZAKRZEWSKI (*)(**) and D. DELANDE (*)

(*) *Laboratoire Kastler-Brossel, Tour 12, Etage 1, Université Pierre et Marie Curie 4 Place Jussieu, 75005 Paris, France*

(**) *Instytut Fizyki, Uniwersytet Jagielloński ulica Reymonta 4, 30-059 Kraków, Poland*

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Abstract. – Statistical properties of resonances of the hydrogen atom in a static, experimentally available magnetic field are studied. We show that the relevant parameter is the number of open channels. A rough agreement with a random matrix model is observed, but significant deviations due to the long-range Coulomb potential are reported and explained.

The hydrogen atom in a magnetic field has been widely used [1] as a prototype of quantally chaotic system [2]. Although the statistical properties of its bound spectrum are in general well described by predictions of the Random Matrix Theory (RMT) [1], it has been shown recently that deviations from these predictions exist in the immediate vicinity of the ionization threshold [3]. Above the ionization threshold, the continuum of states is rich in resonances. The system has a remarkable property: it evolves from a bound regular, then chaotic system to a fully open chaotic system by increasing a single parameter, the energy. It thus fills the gap between traditional quantum chaos and quantum chaotic scattering. In this letter, we present extensive results on the statistical properties of resonances occurring at experimentally accessible magnetic-field values.

Kleppner and coworkers [4] experimentally observed complicated spectra with narrow resonances coexisting with broad ones. As shown before [5], for one open channel and at high magnetic field, the distribution of the resonance widths is well described by the Porter-Thomas distribution. Here we extend considerably that preliminary analysis both to experimentally accessible magnetic-field values and to the high range of energies enabling multichannel decay, and we show that the relevant parameter for the statistical properties is the number of open channels.

In atomic units ($\hbar = |q| = m = 4\pi\varepsilon_0 = 1$), the Hamiltonian is

$$H = \frac{p^2}{2} - \frac{1}{r} + \frac{\gamma^2}{8}\varrho^2, \tag{1}$$

where γ denotes the magnetic field (along the z-axis) in units of $2.35 \cdot 10^5$ T. The paramagnetic term $\gamma L_z/2$ is dropped since we consider $L_z = 0$ odd-parity spectra. The classical dynamics of this system depends on the scaled energy, $\varepsilon = E\gamma^{-2/3}$, and is almost fully chaotic for $\varepsilon > -0.12$. All the resonances studied in this letter are consequently in the chaotic regime.

The diamagnetic potential $\gamma^2 \varrho^2/8$ confines the motion in the direction transverse to the magnetic field. Hence, just below the ionization threshold, the electron can explore the region around the z-axis far from the nucleus, where the adiabatic-like separation holds [4]:

$$H \simeq H_{\text{sep}} = H_z + H_\varrho = \frac{p_z^2}{2} - \frac{1}{|z|} + \frac{p_\varrho^2}{2} + \frac{\gamma^2 \varrho^2}{8}. \tag{2}$$

The spectrum of H_{sep} is

$$E(n_z, n_\varrho) = \left(n_\varrho + \frac{1}{2}\right)\gamma - \frac{1}{2n_z^2} \tag{3}$$

with n_z and n_ϱ integers ($n_z > 0$).

A given Rydberg series (fixed value of n_ϱ) is coupled by the nonadiabatic term $V_{\text{NA}} = 1/|z| - 1/\sqrt{\varrho^2 + z^2}$ to the other Rydberg series and to the continua of the lower n_ϱ series. The spectrum of H is thus composed of an infinite set of one-dimensional (along z) Rydberg series of resonances, each converging to a Landau ionization threshold (see fig. 2 of ref. [6]) $E_{\text{ion}}(n_\varrho) = (n_\varrho + 1/2)\gamma$.

In a conventional spectroscopy experiment [4], the resonances appear as local structures in the photoionization cross-section while, in a scattering experiment, they show as complex poles of the S-matrix, the real part being the position of the centre of the resonance and -2 times the imaginary part being its width. We have numerically computed the positions of these resonances in the complex plane using the complex coordinate method. Replacing $\boldsymbol{r} \to \boldsymbol{r} \exp[i\theta]$, $\boldsymbol{p} \to \boldsymbol{p} \exp[-i\theta]$ in the Hamiltonian, one obtains a non-Hermitian operator $H(\theta)$ whose eigenvalues coincide with the resonances of H [6]. Numerical diagonalization of $H(\theta)$ in a huge Sturmian basis using the Lanczos algorithm [6] allows us to compute at low cost the few resonances of interest in a narrow energy band [7].

We have studied several ranges of values of the magnetic-field strength and obtained—except for global scaling factors—the same results. We present here the data around $B = 6$ T, the value used in current experiments. We have analysed fully converged sets of resonances in the energy intervals $[(n - 0.5)\gamma, (n - 0.3)\gamma]$ for $n = 1, 2, 3$ and 4. In each interval, we studied both the level spacing (difference in the real parts of consecutive resonances) and the width distributions.

Consider the energy range between the first and the second ionization threshold ($n_\varrho = 0$ channel is open only). There, we have found numerically that the ratio of the average width to the average level spacing is independent of γ and the energy with the value

$$\frac{\overline{\Gamma}}{\overline{\Delta E}} = 0.23 \pm 0.01. \tag{4}$$

Such a behaviour can be understood from a semiclassical analysis. The coupling between the Rydberg series by the nonadiabatic term V_{NA} is important only close to the nucleus. There, both the density probability of the Rydberg electron and the spacing between Rydberg states scale as $1/n_z^3$. Therefore, the density of nonadiabatic matrix elements is constant over a Rydberg series, which explains why eq. (4) holds. Similarly, in the energy region where more ionization channels are open, nonadiabatic matrix elements will be only weakly dependent on the channel considered. The neat result is that the average partial ionization rates to the various channels are almost equal. Thus for n open channels, we expect $\overline{\Gamma}/\overline{\Delta E} = 0.23n$ (from eq. (4)).

The numerical calculations show an unexpected difficulty when at least two channels are open. In addition to the set of resonances lying close to the real axis, there is a small number of broad resonances having widths larger by one or two orders of magnitude. These broad resonances do not have any experimental relevance as their optical excitation probabilities are vanishingly small. They remind us of the «shadow» poles observed in the Floquet analysis of a hydrogen atom ionization [8].

The number of those resonances is small (few percents at maximum) but their widths are so large that they influence the average width $\overline{\Gamma}$. In order to obtain reliable width distributions, we deleted them from the samples. This has almost no effect on the unfolding of the real parts of the energy levels and consequently does not affect the spacing distribution. For the widths, it has the effect of cutting the tail without affecting the distribution of small widths, which is of major importance for experimental purposes. On the average, we checked that $\overline{\Gamma}/\overline{\Delta E} \approx 0.23n$ but with an accuracy worse than for eq. (4).

To obtain the statistical properties of resonances we unfold the spectrum, *i.e.* we normalize the level spacings and widths with respect to their mean values. The unfolding of the real part of the energies is done in the standard way [2]. The determined $\overline{\Gamma}/\overline{\Delta E}$ ratio is then used to unfold the widths. The results are shown in fig. 1 and 2 for the cumulative level spacing distribution $N(s) = \int_0^s P(x)\mathrm{d}x$ and the cumulative width distribution $N(\Gamma)$.

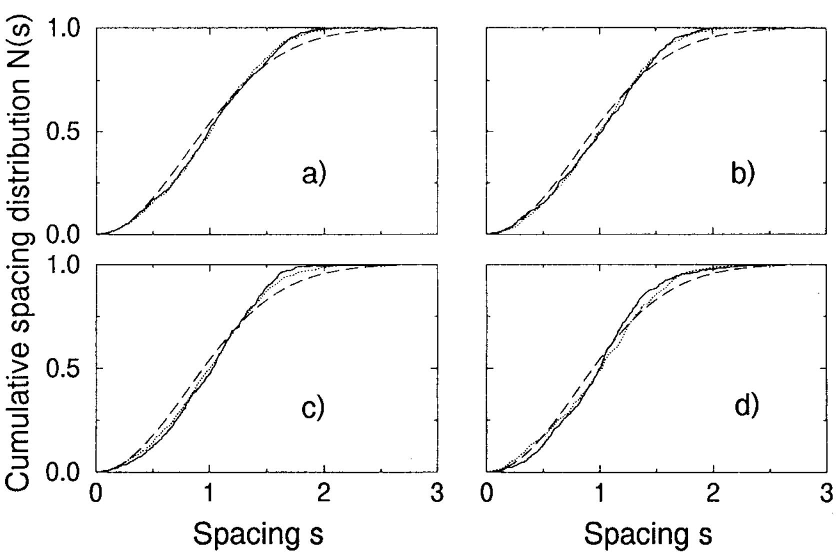

Fig. 1. – Cumulative level spacing distribution of the resonances of the hydrogen atom in a magnetic field. Each set corresponds to a fixed number of open channels and is composed of about 700 resonances computed for magnetic fields close to 6 T. The solid line represents the numerical result, the dashed line is the prediction of random matrix theory and the dotted line is the prediction of our model. The agreement is excellent. Note the lack of large level spacings compared to the random matrix prediction. *a*), *b*), *c*) and *d*) refer respectively, to 1, 2, 3 and 4 open channels.

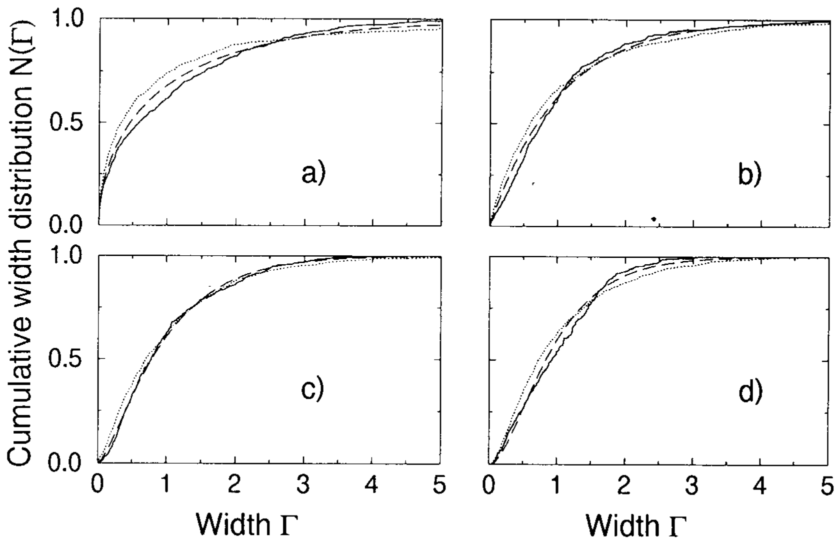

Fig. 2. – Cumulative width distribution for the same data as in fig. 1. Note the $\Gamma^{(n+1)/2}$ dependence near the origin, well reproduced by the random matrix model (dashed line) and by our improved model (dotted line). When the number of open channels increases from 1 (*a*)) to 4 (*d*)), the probability of having small widths decreases, although not very rapidly (see text).

RMT can be modified to include coupling to the continuum, represented by an anti-Hermitian random matrix [9]. The model then predicts in the limit $\overline{\Gamma} \ll \overline{\Delta E}$ that the resonance spacing distribution is the same as for the discrete spectra and that the width distribution is

$$P_n(\Gamma) = \frac{1}{(2\overline{\Gamma})^{n/2}\,\Gamma(\frac{n}{2})}\,\Gamma^{(n/2)-1}\exp\left[-\frac{\Gamma}{2\overline{\Gamma}}\right], \tag{5}$$

where n is the number of open channels, $\overline{\Gamma}$ is the average width *per channel* and Γ is the gamma-function (not to be confused with the width Γ). Equation (5) gives the so-called Porter-Thomas distribution [5, 10] for $n = 1$.

These predictions are plotted in the figures as dashed lines. The numerical spacing distribution is roughly the same for the 4 cases, with a systematic lack of large spacings as compared to the prediction of RMT. The only change is near $s = 0$ where the number of small spacings increases with the number of open channels. This is related to the increase of $\overline{\Gamma} / \overline{\Delta E}$, which makes the observation of eigenvalues with almost the same real parts, but different imaginary parts more probable. On the contrary, the width distribution strongly depends on the number n of open channels and shows a good agreement with random matrix model prediction, eq. (5), especially for small widths. In particular, for one channel open, these results confirm earlier study performed at higher magnetic field [5] showing agreement with the Porter-Thomas distribution and thus an abundance of small widths—$P(\Gamma)$ diverges then as $1/\sqrt{\Gamma}$ at the origin.

The comparison shows that the RMT catches the essential part of the physics of ionization in this system: firstly, a state is on the average equally coupled to the different open Landau channels (the average width increases linearly with the number of open channels); secondly, the partial ionization rates have *independent* statistical fluctuations given by the Porter-Thomas distribution. The appearance of a narrow resonance is only possible if all the partial ionization rates are by chance simultaneously small, which is less probable as the number of open channels increases. This rules out the possibility that narrow resonances are due to localization in the vicinity of a periodic orbit. Then all the partial-ionization rates should be small, but strongly correlated and the behaviour near $\Gamma = 0$ should be different.

What remains to be explained is the lack of large spacings in numerical data. Such a behaviour we observed already for the level spacings just below the first ionization threshold [3]. There, the $n_\varrho = 0$ Rydberg series has a much higher density of states than all the other n_ϱ series converging to higher thresholds. Thus, the nonadiabatic coupling is not strong enough to completely mix the various series. We modelled this situation by considering a Hilbert space composed of two subspaces baptized «regular» and «chaotic». The model Hamiltonian is a diagonal matrix in the regular subspace with equally spaced eigenvalues (this represents the $n_\varrho = 0$ series discussed above). In the chaotic subspace (which represents the strongly mixed $n_\varrho = 1, 2 \ldots$ series), it is a random matrix. The coupling of the regular states to the chaotic ones is taken constant throughout the regular series. This simple model has two parameters—the ratio of the dimensions of the regular and chaotic subspaces and the strength of the coupling—and reproduces quantitatively the lack of large spacings (see ref. [3] for details).

Above the ionization threshold, the situation is similar. Between the $(n_\varrho - 1)$-th and the n_ϱ-th threshold, the n_ϱ Rydberg series has a density of states much higher than the other series. Hence, the same kind of deviations in the spacing distribution is expected and indeed observed in fig. 1. We adapt the previous model by allowing a random matrix type of decay [9] to the regular subspace which represents the coupling of the Rydberg series to the continua. The strength of the decay is imposed by the value of the ratio $\overline{\Gamma}/\overline{\Delta E}$. The numerically determined spacing and width distributions are shown in fig. 1 and 2 as dotted lines. The agreement is very good. The three important features: level repulsion, lack of large spacings and power law for small widths are *quantitatively* reproduced. We emphasize that the same parameters are used for all the fits, which proves the relevance of the model. Furthermore, the parameters used are the same as for the study of bound states in ref. [3].

These results have important consequences. The ionization thresholds being equally spaced, one Rydberg series has always a much higher density of states than the other ones, whatever the value of the energy. If the average width is not much larger than the mean spacing, the lack of large level spacings will exist independently of the high degree of excitation of the atom. Around the first ionization thresholds—either above or below—the semiclassical limit is thus *never* reached. It is only when a large number of Landau channels are open ($\overline{\Gamma} \gg \overline{\Delta E}$) that the hole at large spacings will eventually disappear.

In the experiments [11], the spectra are recorded at low energy, when only few channels are open. Hence, our calculations and the associated model are able to understand and predict the observations. For example, at 6 T, the density of resonances in the middle of each Landau channel is of the order of 40 resonances/cm^{-1}, a value a little larger than the experimental observation [4]. The difference probably comes from the small excitation probability of highly excited Rydberg states, not visible in the experiment. The average width is thus expected to be of the order of 0.006 cm^{-1} which makes the observation of widths of the order of 0.001 cm^{-1} a probable event. This fully explains the experimental results of ref. [4] where numerous small widths have been observed: they are not due to some hidden symmetry or localization phenomenon, but simply to accidental destructive interferences and fluctuations common to all chaotic systems. At higher energies, in the range [25, 30 cm^{-1}], there are 5 open channels. We can predict that the average width will be of the order of 0.04 cm^{-1}, and that the probability of having a width smaller than 0.01 cm^{-1} is of the order of

5%. Observing such a phenomenon [11] is thus not exceptional. It is only when about 10 channels are open that the probability of observing very narrow resonances is really small. As far as we know, no such observation has ever been reported.

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