

Hydrogen Atoms in Strong Magnetic Fields – in the Laboratory and in the Cosmos

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1. Introduction

Recent years have seen tremendous progress in studies of the properties of hydrogen atoms in strong magnetic fields. Decisive stimulus came from the discovery of huge magnetic fields in astrophysical "laboratories", viz. field strengths of order $\sim 10^7 - 10^9$ T in neutron stars and of order $\sim 10^2 - 10^4$ T in white dwarf stars. At these field strengths the magnetic forces acting on an atomic electron outweigh the Coulomb binding forces even in low-lying states, and thus atomic structure is completely changed. On the other hand, the rapid advancement of high-resolution laser spectroscopy has made it possible to produce atoms in highly excited states, with principal quantum numbers ranging up to $n \cong 520$ (in Ba I) [1], and therefore Rydberg states can be used to investigate the effects of magnetic dominance on atomic structure also in terrestrial laboratories with magnetic fields of a few Tesla, or less.

A detailed description of the astrophysical scenarios which finally led to the conclusive determination of magnetic field strengths up to $5 \cdot 10^8$ T in neutron stars, and an account of theoretical results for atomic level schemes, wavefunctions, transition rates, etc. at these field strengths, where the system becomes highly nonseparable, has been presented elsewhere [2]. Here we present a selection of more recent results. We briefly review, in section 2, the basics of the theory and then concentrate, in section 3, on the wavelength spectrum of the hydrogen atom in magnetic fields of *arbitrary strength*. We then turn to atoms in terrestrial laboratories and discuss, in section 4, the progress that has been made in the theoretical description of magnetized hydrogen Rydberg states. We compare spectroscopic predictions of theory with results of actual experiments, and demonstrate, in section 5, that phenomena which have turned out characteristic of the onset of "quantum stochasticity" in investigations of model Hamiltonian systems are recovered in the quantal properties of highly excited hydrogen atoms (e.g. in the statistics of level sequences and transition strengths in the classically chaotic domain). This highlights the fact that the hydrogen atom in a strong magnetic field is an ideal example of a simple but real physical system displaying all the features which are currently causing so much excitement in the classical and quantum mechanical study of nonintegrable systems.

2. Hydrogenic Atoms in Magnetic Fields of Arbitrary Strength

The Hamiltonian which describes the motion of an electron under the combined influence of a fixed Coulomb potential and a uniform magnetic field $\mathbf{B} = B \cdot \mathbf{e}_z$ reads, (in atomic units, $\beta = B/B_0$ with $B_0 = 2(\alpha m_e c)^2 / (e\hbar) \cong 4.70 \cdot 10^5$ T),

$$H = -\Delta - \frac{2}{r} + 2\beta l_z + \beta^2(x^2 + y^2). \quad (1)$$

The reference magnetic field B_0 is chosen in such a way that at B_0 the cyclotron energy of the electron becomes equal to four times the Rydberg energy, or, equivalently, the Larmor radius equals the Bohr radius. For small or extremely large magnetic field strengths, where either the Coulomb forces dominate the Lorentz forces or vice versa, corresponding

perturbational approaches to solving the Schrödinger equation for the Hamiltonian (1) are of course appropriate. In the *intermediate* (or *strong-*) *field regime*, the electron experiences electric and magnetic forces of comparable strength, and perturbative approaches fail. The mathematical reason for this lies in the fact that the spherical symmetry of the Coulomb potential, on the one hand, and the cylindrical symmetry of the magnetic field on the other, prevent a separation of variables so that closed-form analytical solutions are not possible. Thus the Hamiltonian (1) belongs to the class of nonintegrable Hamiltonians. The absolute sizes of the field strengths at which one lies in this regime depend on the state of excitation of the electron. By considering the equality of Coulomb and Lorentz forces for an electron in a circular Bohr orbit with principal quantum number n one obtains as a rough measure $B_n \cong B_0/(2n^3) \cong (8.7 \text{ T})(30/n)^3$. Therefore for white dwarf and neutron star magnetic fields low-lying states are found to be subjected to a strong-field situation, while at laboratory field strengths studies of the strong-field regime are restricted to Rydberg states.

The nonintegrability of the Hamiltonian (1) implies that one is forced, in the complete quantum theoretical treatment of the problem, to resort to numerical methods. In our calculations we expand the wavefunctions either in terms of spherical harmonics and a complete set of radial functions, or in terms of Landau functions and a complete longitudinal basis. The different expansions are employed depending on whether one approaches the intermediate-field regime from the side of low or intense fields, and overlapping results are expected in the transitional region.

Except at very high fields ($\beta \geq 0.1$) [3] calculations using the Landau function expansion have confined themselves so far to low-lying states. Calculations using expansions based on the field-free symmetries have been performed for both low-lying and highly excited states, and in this case energies and wavefunctions were obtained by either direct integration [4], or diagonalization of the Hamiltonian matrix in large basis sets. In our own computations in this regime we expanded the wavefunctions in terms of spherical harmonics, $\psi_m = \sum h_l(r) Y_{l,m}(\theta, \phi)$ (m is the magnetic quantum number), and the radial functions in the complete, orthonormal set of functions

$$G_{nl}^{(\zeta)}(r) = \zeta^{3/2} \left[\frac{n!}{(n+2l+2)!} \right]^{1/2} \exp[-\zeta r/2] (\zeta r)^l L_n^{(2l+2)}(\zeta r), \quad (2)$$

where ζ denotes an inverse-length parameter, and the $L_n^{(2\ell+2)}$ are generalized Laguerre polynomials. Matrix elements with respect to this basis can be expressed in closed analytical form and give rise to a banded Hamiltonian matrix which can be diagonalized by efficient standard algorithms. In our calculations we used basis sizes of up to 220000 for determining both eigenvalues and eigenvectors of the first ~ 700 states in given m -parity subspaces in the intermediate-field regime. Convergence was established by varying the size of the basis and the scale parameter ζ .

As a result of our efforts we are able to continuously trace the energy values and oscillator strengths of low-lying states ($n \leq 5$) from zero field up to neutron star magnetic fields (for accurate numerical values we refer the reader to Rösner et al. [4], Forster et al. [5], and Ruder et al. [6]), while we can calculate the energies and oscillator strengths of Rydberg states in laboratory fields of a few Tesla up to the field-free ionization threshold $E = 0$. The following sections present examples of our results.

3. Low-Lying States in Magnetic Fields of Arbitrary Strength

3.1. Wavelength Spectrum of the Hydrogen Atom

The behaviour of the energy values and wavefunctions over the range from laboratory fields up to neutron star magnetic fields has been discussed in great detail elsewhere (Ruder et al. [2]). Here we concentrate on the behaviour of *wavelengths* and present, in Fig. 1, the

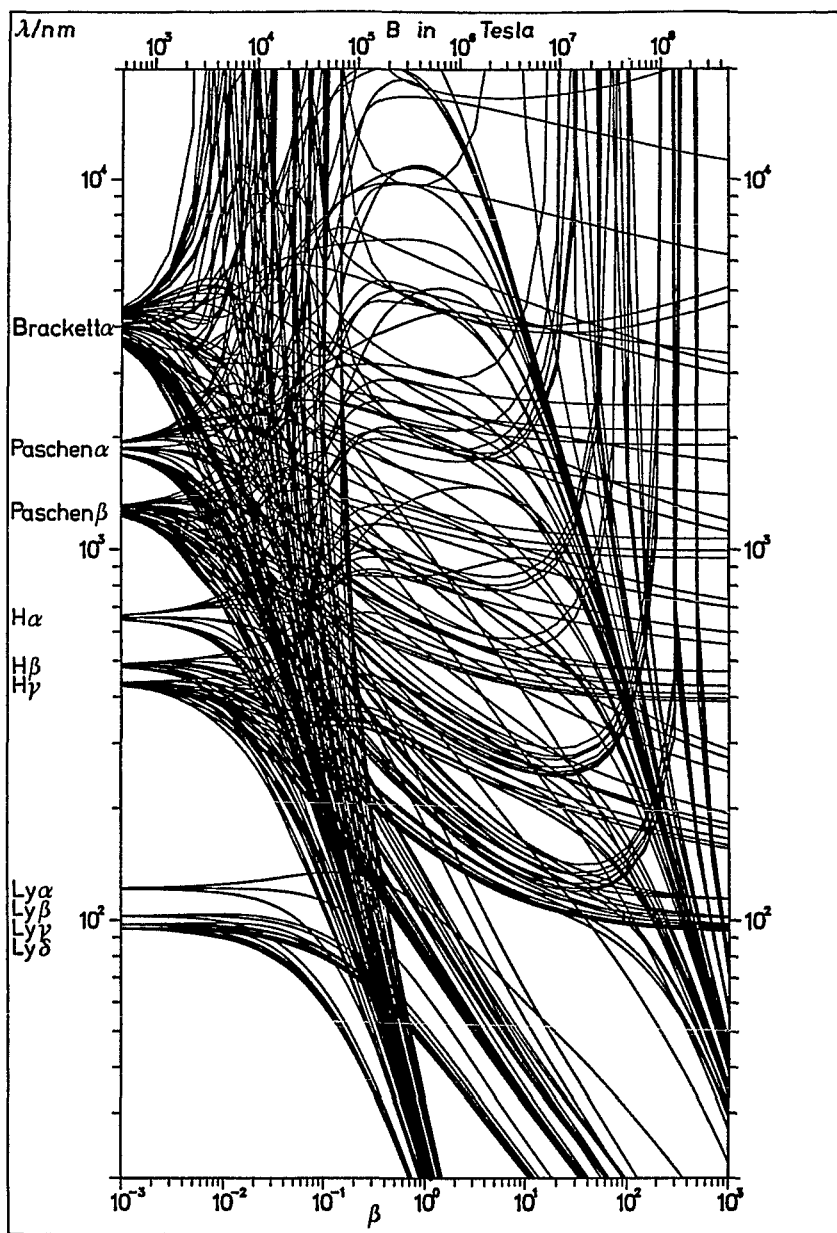


Fig. 1: The wavelength spectrum of the hydrogen atom from the soft X-ray range (20 nm) up to the far infrared (10000 nm) as a function of the magnetic field strength in the interval 470 T to $4.7 \cdot 10^8$ T. Effects of the finiteness of the proton mass are taken into account. The two rapidly declining bunches of lines correspond to cyclotron-like transitions of electrons (left-hand bunch) and protons (right-hand bunch), respectively. Note the occurrence of "stationary" lines in the intermediate region.

spectrum of the hydrogen atom between 20 nm and 10000 nm as a function of β in the range $10^{-3} \leq \beta \leq 10^3$ which we have computed from our energy values for a total of 364 transitions between states with $n \leq 5$. This is the most comprehensive compilation of the hydrogen spectrum to date.

One recognizes, at small field strengths, the splittings of the unperturbed lines into three equidistant Zeeman components. For larger β these components continue splitting by the quadratic Zeeman effect. The onset of the quadratic Zeeman effect is shifted to smaller β values with increasing wavelengths. Beyond this region ($\beta \approx 10^{-2}$), where the perturbation theory treatment breaks down, the lines are completely torn apart by the magnetic field within one β decade and the spectrum becomes totally distorted. Since the energy levels of states with different m and different z parity are allowed to cross, the wavelengths of corresponding transitions go to infinity at certain values of β .

Order reappears only in intense fields, indicative of the fact that in the limit $B \rightarrow \infty$ the level scheme approaches that of the one-dimensional Coulomb problem, which consists of tightly bound levels and levels whose energies equal those of the field-free H atom. As a consequence numerous lines tend to the wavelengths of the unperturbed hydrogen series at the right-hand side of Fig. 1.

Clearly, any attempt to observe, and resolve, a line spectrum of hydrogen at a given magnetic field strength in the intermediate regime is doomed to failure. An element of order is, however, brought in even in this domain by several transitions whose wavelengths go through minima and maxima in certain intervals of the magnetic field strength, that is they are less sensitive to variations of the magnetic field than the many fast running components. An inhomogeneous field with a variation of, say, a factor of two (as is the case for a dipolar field) around extrema of wavelengths will therefore filter out exactly these stationary components, thus opening the possibility of observing, in this instance, a clearly arranged spectrum with few well resolved features. Speculative as this may sound, nature has indeed provided us with a cosmic laboratory to test this hypothesis, and in fact this has opened a totally new era of stellar atomic spectroscopy, namely the "spectroscopy of stationary lines".

3.2 Spectroscopy of Stationary Lines

The spectrum of the white dwarf star known as *Grw + 70°8247* had been an unsolved puzzle for more than four decades. The circular polarization of its optical continuum [7] had given a clue to the existence of a strong magnetic field in the vicinity of this object, and Angel [8] first proposed a tentative identification of a few of the features in terms of stationary lines using variational energy values of Praddaude [9] available at that time. On the basis of our very accurate computations of the energy values and transition rates of the hydrogen atom in magnetic fields of arbitrary strength it became possible to positively identify all observed features as stationary hydrogen lines in a magnetic field whose value was pinned down to between 17000 and 35000 T [10-12]. No other previously known white dwarf had a magnetic field even one tenth this value. Fig. 2 demonstrates the excellent agreement between the wavelength positions of the extrema of stationary components of H_β , H_γ and absorption features in the blue part of the spectrum of *Grw + 70°8247*. In particular, the sharp blue edges and "red-shaded" extensions of the features at 3650 Å and 4135 Å are well accounted for by the minimum character of the corresponding stationary components. Thus for the first time *low-lying states exposed to a strong-field situation* were actually observed in nature. In the meantime a second object has been found (PG 1031+234, Schmidt et al. [14]), in the spectrum of which stationary components of hydrogen lines, in a field ranging up to ~ 50000 Tesla, have positively been identified. Here the observed phase modulations of the spectrum yield additional information from which the morphology of the magnetic field of this star can be extracted.

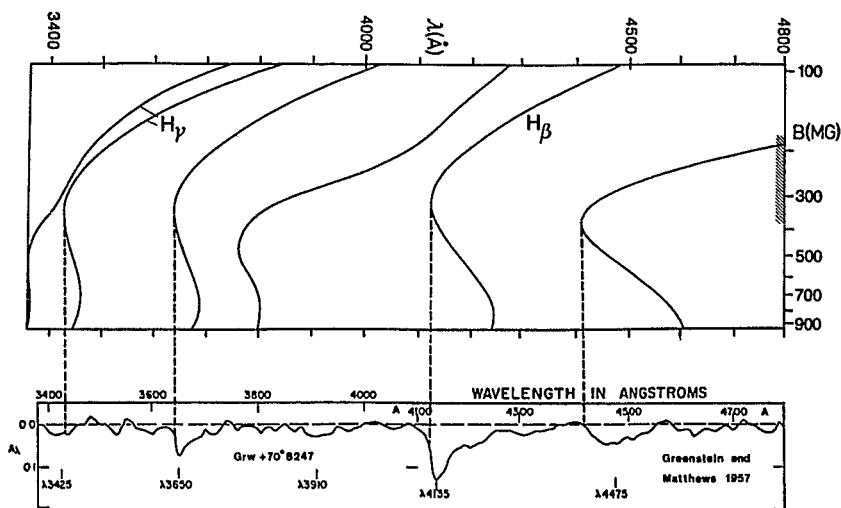


Fig. 2: Stationary H_β and H_γ transitions of the hydrogen atom in magnetic fields from 100 to 900 million Gauss in comparison with the short-wavelength part of the spectrum of Grw+70°8247 taken by Greenstein and Matthews [13]. All the features are explained in a consistent way in terms of stationary Balmer transitions of hydrogen in an extended magnetic field whose strength varies from ~ 170 to ~ 350 million Gauss (see the corresponding hatching along the B ordinate). Such a variation is present, e.g., in a dipolar magnetic dipole field.

4. Highly Excited States in Strong Laboratory Fields — Comparison between Experimental and Theoretical Spectra

For many years research of magnetized Rydberg atoms was characterized by the situation that experimental work concentrated on non-hydrogenic atoms (e.g. Ba, Na, Li) while most of the theoretical papers were devoted to hydrogenic systems. Semiclassical and quantal calculations were performed to account for the nature of the quasi-Landau-resonances observed experimentally around and above the field-free ionization threshold, but so far no detailed quantitative comparisons were possible for the rich and complicated line structure seen in experimental spectra of magnetized Rydberg atoms. Quite recently this situation has changed in that, on the one hand, actual experiments have been performed with highly excited *hydrogen* and *deuterium* atoms in 4 – 6 T fields by the Bielefeld group (Holle et al. [15]), and, on the other, the computer codes developed over the last years allow an almost routine calculation of highly accurate energy values and wavefunctions of one-electron systems in uniform laboratory magnetic fields up to shortly below the field-free ionization threshold. To illustrate the state of the art, Fig. 3 provides a comparison between the experimental and theoretical spectra in the range -24 cm^{-1} to -12 cm^{-1} at 5.96 T. The agreement between theory and experiment can be considered excellent; moreover, theory reveals where neighbouring lines were no longer resolved in the experiment. The broad experimental feature around -13 cm^{-1} , e.g., is found to be composed of ~ 10 lines of different intensities. Obviously this calls for increased experimental efforts to refine resolution and actually check the theoretical spectra also in these ranges of energy.

All in all we have compared successfully more than 1000 lines so far in the π and σ spectra in the strong-field regime, and this certainly can be considered a hallmark of modern quantitative spectroscopy in magnetic fields.

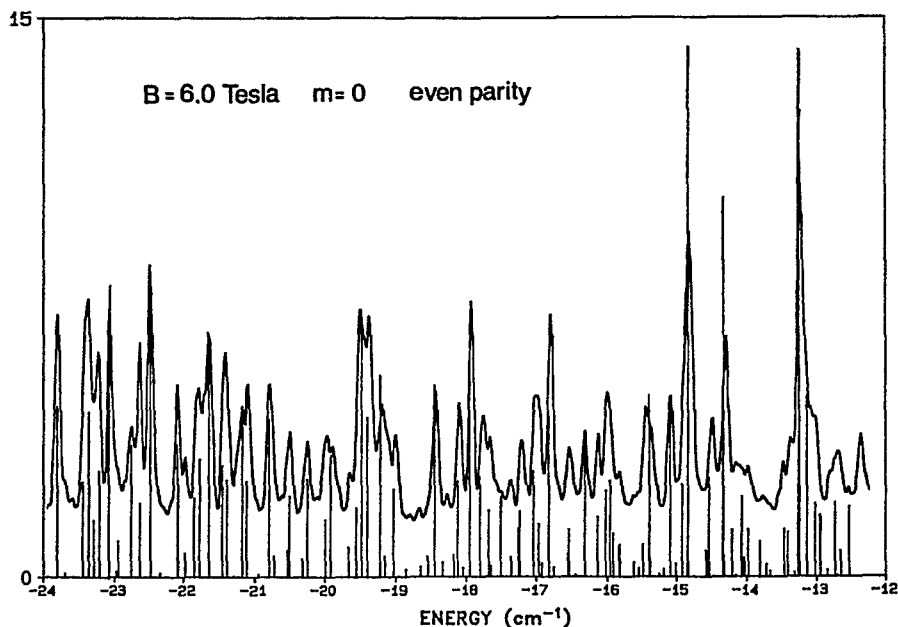


Fig. 3. Comparison between the experimental spectrum and the theoretical photoabsorption spectrum of $\Delta m = 0$ transitions from $2p_0$ to even parity final Rydberg states with energies between -12 cm^{-1} and -24 cm^{-1} in a magnetic field of 6 T. For the theoretical results (straight lines) the ordinate represents the oscillator strength in units of 10^{-6} . The experimental results have kindly been provided by the Bielefeld group [15]. Note that the wealth of theoretical spectral structure can no longer be resolved by the experiment. The range of energy shown lies in the domain of chaotic motion of the corresponding classical system.

5. The Hydrogen Atom in Strong Magnetic Fields – an Object Lesson in "Quantum Chaology"

5.1 Quantum Physics in Classically Chaotic Regions

It has been realized, in recent years, to an increasing extent that in classical Hamiltonian systems the occurrence of "chaotic" behaviour – in the sense of exponential separation of initially infinitesimally neighbouring trajectories in phase space – is the rule rather than the exception. Furthermore, theoretical and experimental techniques have progressed to a point where it is now possible to study in detail quantal systems in the limit of large quantum numbers, in which the laws of quantum theory should reduce to the laws of classical physics. All this has combined in creating a new field of research, for which the term "quantum chaology" has been coined by Berry [16], who defines it as "the study of semiclassical – but still *non-classical* – behaviour characteristic of systems whose classical motion exhibits chaos". It should be emphasized that the term "quantum chaos", which has become rampant in literature, still lacks a rigorous definition. Although finally aiming at such a definition quantum chaology is taking, at present, a more empirical point of view: what one is looking for is archetypal quantum phenomena in a range of parameters where the classical analogs of the systems turn chaotic.

One of the most intriguing features of the spectroscopy of hydrogen atoms in magnetic fields, lies in the fact that magnetized hydrogen atoms are able to play a leading rôle in the search for manifestations of "quantum" chaos. On the one hand, the Kepler problem with Lorentz forces has been shown by a number of authors [17-19] to undergo a transition to chaos once the Lorentz forces acting on the highly excited electron become of the order of, or larger than, the Coulomb forces. On the other hand, high-resolution spectroscopic experiments on "real", quantal, magnetic Rydberg atoms are performed by a number of groups, and, as demonstrated in the foregoing section, large-scale computations have reached a point where it is possible to determine theoretically the energetic positions of, and oscillator strengths of transitions to, Rydberg states in Tesla fields up to almost the field-free ionisation limit. Therefore the hydrogen atom in a strong magnetic field indeed offers itself as a paradigm for studying, both theoretically and experimentally, the basic question of how quantum systems behave in a range of parameters where their classical counterparts exhibit phenomena of chaos.

A very convenient way of visualizing the appearance of chaotic orbits in a classical problem is to look at the Poincaré surfaces of section of the trajectories in phase space. To find the range of energy where, for the parameters used in the Bielefeld experiments, the transition from regularity to chaos occurs in the classical magnetic Kepler problem we computed trajectories as a function of energy for a sufficiently large number of random initial conditions, and determined the area fraction of regular orbits in the Poincaré surfaces of section at $z = 0$. In Fig. 4a the breakdown of regularity in the magnetic Kepler problem is

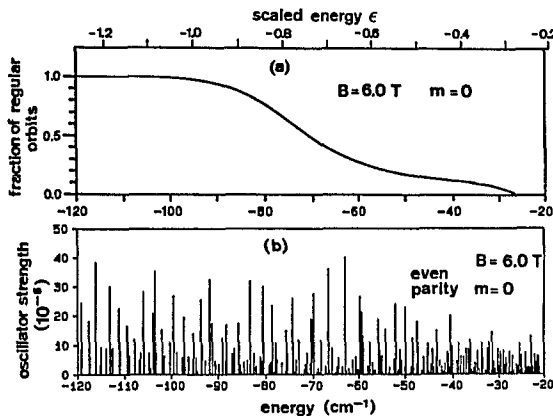


Fig. 4: The area fraction of the Poincaré surfaces of section of classical motion at $z=0$ which are filled by regular orbits as a function of orbital energy (a) compared with the oscillator strengths of $\Delta m = 0$ transitions from $2p_0$ to hydrogen Rydberg states as a function of the quantal energy of the Rydberg states (b). The breakdown of regularity in classical motion is reflected by an increasing complexity of the quantal spectrum.

quantified by plotting the fraction of regular orbits as a function of energy for $\beta = 1.275 \cdot 10^{-5}$ ($B = 6.0$ T) and $m = 0$. Fig. 4a is in fact universal, and not restricted to this set of parameters. The reason for this is a scaling property [18] of the (classical) Hamiltonian (1): by the replacements $r \rightarrow \beta^{2/3}r$, $p \rightarrow \beta^{-1/3}p$ the Hamiltonian is brought into a form where it no longer depends on two parameters, viz. magnetic field strength and energy, but solely on one parameter, the "scaled" energy $\epsilon = E/(2\beta)^{2/3}$ (E in Rydbergs). Converting, in Fig. 4a, absolute to scaled energies we arrive at the ϵ scale shown at the top horizontal axis of Fig. 4a. For $B = 6$ T it is found that irregular orbits become noticeable around $\sim -104 \text{ cm}^{-1}$ ($\epsilon \approx -1.10$), and the regions filled with regular orbits virtually all vanish in the Poincaré surfaces of section at $E_c \approx -24.5 \text{ cm}^{-1}$ ($\epsilon_c \approx -0.25$).

Fig. 4b shows the quantal oscillator strength spectrum of $\Delta m = 0$ transitions from $2p_0$ to even-parity Rydberg states for the same magnetic field strength as in Fig. 4a. The comparison between classical chaos and the oscillator strength spectrum conveys a *qualitative* impression of the increasing complexity of the quantal spectrum as one penetrates into ranges of energy where classical motion becomes more and more chaotic.

To put the notion of increasing complexity of the quantal spectrum in the classically chaotic region on a more *quantitative* footing studies so far concentrated on properties of the energy level spectra, and, in particular, it was demonstrated in a number of systems [20] that nearest-neighbour level spacing distributions exhibit a universal structural change from a Poisson type to a Wigner type as classical motion becomes increasingly chaotic.

Because of space limitations it is impossible to touch on all the lines of research that are currently pursued in the interrelations between classical physics and quantum physics of the hydrogen atom in a strong magnetic field in the chaotic regime. On the classical side, computations of Liapunov exponents, in particular of unstable periodic orbits, in the chaotic regime have been performed to quantify the degree of irregularity of the trajectories [21-23]. On the quantum side, statistical analyses were performed of the distributions of the spacings of adjacent energy levels, and the change from a Poisson to a Wigner distribution was confirmed also in this system [24-26]. Much effort is presently placed on revealing the connection between unstable periodic orbits and long-range modulations in the quantum energy spectra [27, 28].

5.2 Statistical Analysis of Transition Strengths

Here we will report, as a new result, the first analysis of statistical properties of *transition strength spectra* of hydrogen atoms in strong magnetic fields in the chaotic regime, that is we go beyond investigating energy level sequences and look at quantities that are related to wavefunctions in a sensitive way.

Fig. 5 shows, for a magnetic field strength of 5.96 T, our computed oscillator strength spectrum of the $\Delta m = 0$ dipole transitions from $2p_o$ to even-parity Rydberg states with energies from -20 cm^{-1} up to the field-free ionization limit. Remember that at this field strength, classical motion becomes irregular around -25 cm^{-1} .

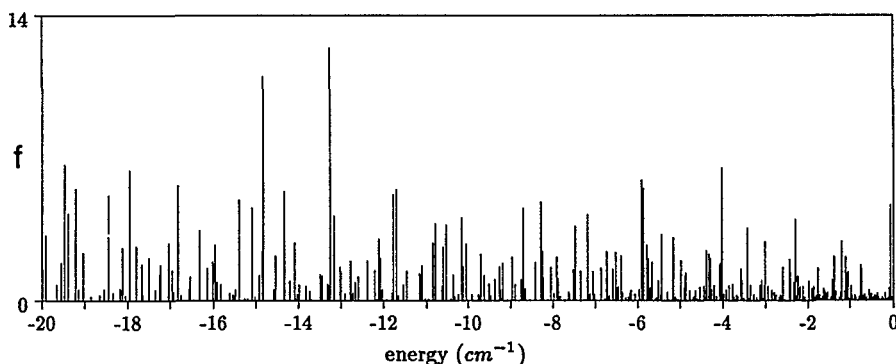


Fig. 5. Oscillator strength spectrum of $\Delta m = 0$ Balmer transition from $2p_o$ to even-parity Rydberg states with energies between -20 cm^{-1} and the field-free ionization limit at a field strength of 5.96 T (oscillator strengths in units of 10^{-6}). In our computations convergence of the f values is obtained to within a few percent. The range of energy shown lies in the domain of chaotic motion of the classical hydrogen atom.

In quest of further manifestations of chaos in quantal spectra we have analyzed the fluctuations of oscillator strengths of Balmer transitions to Rydberg states in the near-regular, near-irregular, and irregular regime. Following Alhassid and Levine [29] we consider the probability $P(y)dy$ of finding a value y of the strength of an allowed transition from a given to an arbitrary final state between y and $y+dy$. For a structureless spectrum the maximum-entropy principle, together with the completeness relation of the states and the normalization condition, implies the Porter-Thomas form for $P(y)$, viz. $P(y) \propto \exp(-y/2\bar{y})/\sqrt{y}$. For situations where structures in the spectrum impose additional constraints we adopt the form

$P(y) \propto y^{(\nu-1)/2} \exp(-\nu y/2\bar{y})/\sqrt{\bar{y}}$. Here ν denotes a parameter characterizing the deviance of y from its averaged value \bar{y} (see [29] for details). Fig. 6 shows three histograms of computed

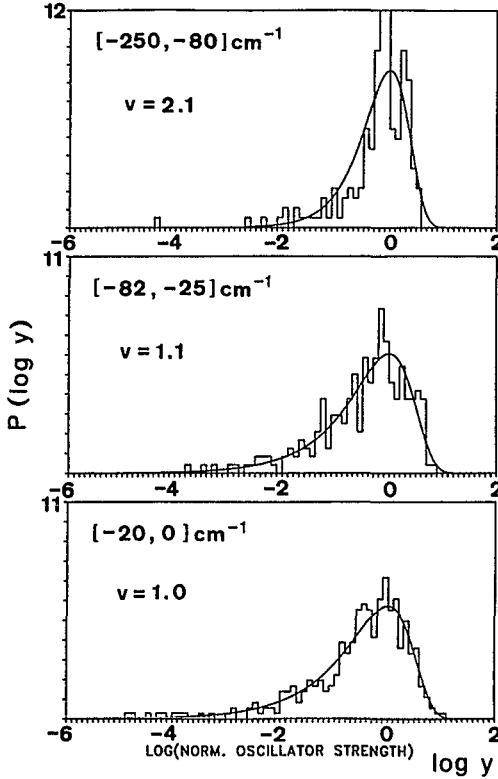


Fig. 6: Three histograms of computed Balmer transition strengths at 5.96 T and their fits (continuous curves) by the Alhassid-Levine form of $P(y)$. Each panel gives the energy range of the final Rydberg states. In the classical system, motion changes from near-regular over near-irregular to irregular, as one passes through these intervals. In the quantum system we find a decrease of ν towards 1 (the Porter-Thomas limit). Oscillator strengths have been scaled by the secular variation prior to binning and normalized in such a way that $\bar{y} = 1$. On the vertical axis, $P(\log y)$ is given in units of 10^{-2} .

oscillator strengths of Balmer transitions to Rydberg states in a magnetic field of 5.96 T and their fits by this functional form. In the three energy ranges of the final states covered in Fig. 6 classical motion changes from almost completely regular to irregular. The results presented in Fig. 6 reveal an increase in the spreading of the fluctuations of the quantal oscillator strengths as this change takes place in the classical system. Correspondingly ν decreases from top to bottom in Fig. 6, and, in particular, we find that the fluctuations in the spectrum shown in Fig. 5 are best fitted by a value of $\nu = 1.0$, that is the Porter-Thomas limit for "chaotic" spectra. The characteristic differences in the distributions of transition strength fluctuations between classically regular and chaotic parameter ranges evident from Fig. 6 confirm findings [29] for transition strengths in a Hénon-Heiles-type model system. Our results thus point to another universal signature of classical chaos in the spectra of quantal systems.

5.3 What Do Hydrogen Atoms in Strong Magnetic Fields Look Like?

"Blessed are they that have not seen, and yet have believed" [30]. In the light of this word physicists can be reckoned among the group of blessed people since they believe in the reality of atoms, although no one has ever "seen" an atom. It is, however, a very human desire to really *see* the objects of one's occupation, and we have therefore represented pictorially hydrogen atoms in strong magnetic fields using the graphics display media available today. Starting point is of course the quantum mechanical interpretation of the squared modulus of the wavefunction as the spatial probability of presence of the electron. Imagining the equivalence of this scalar field to an optically thin self-radiating gaseous nebula, that is, assuming

that the scalar field emits "light" with an intensity proportional to the local numerical value of the scalar field, and which propagates without absorption, the intensity a distant observer receives from such an object out of a specific direction is simply the integral along the line-of-sight of the intensities emitted towards the observer. By scanning the whole object with the line-of-sight moving across it in a fine grid, a raster image can be computed which is a good approximation to what the observer actually sees. The raster image is mapped onto the bit planes of a raster graphics display using an intensity or a colour-coding scheme to yield a true picture of the self-radiating object. In our computations we employed a raster of 575×575 lines-of-sight and 256 intensity levels.

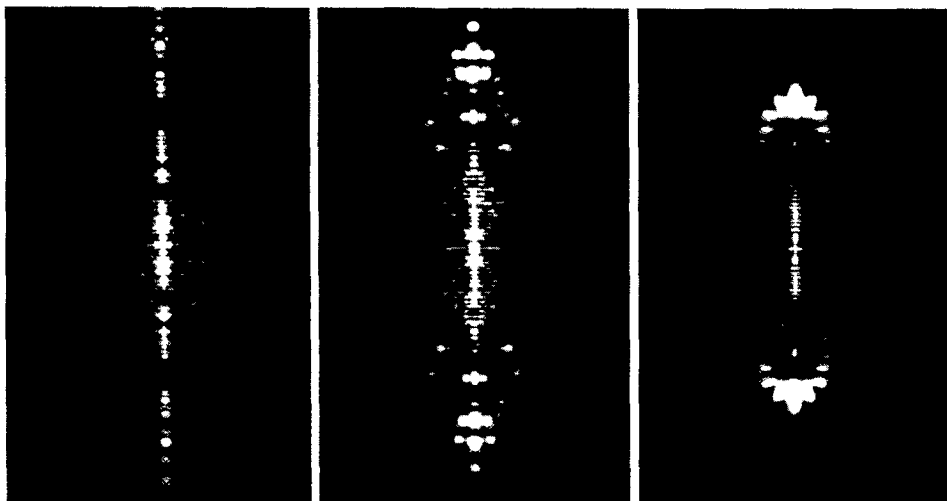


Fig. 7 Pictures of the probabilities of presence of the electron in different highly excited $m = 0$ states, with energies in the classically chaotic regime, of the hydrogen atom in a magnetic field of 5.96 T. The spatial extent of the bizarre atomic structures shown is on the order of 10^{-3} mm.

In Fig. 7 we present first examples of pictures of hydrogen Rydberg states with $m = 0$ in a magnetic field of 5.96 T. The energies of the states lie in the range between -30 and -10 cm^{-1} , and thus in the classically chaotic regime. The pictures demonstrate that the atoms have become extended objects along the direction of the magnetic field (linear dimensions ~ 10000 Bohr radii), and are more or less delocalized, in the sense that they fill most of the configuration space available on account of the remaining conservation laws. Patterns in the shape of the atoms are caused by the nodal structures of the wavefunctions. We have not yet analyzed the pictures with respect to the presence or absence of "scars" [31] along classical periodic orbits, but evidently an analysis of this type is an obvious application of the optical visualization of the states.

The objective of this paper was to show that hydrogen atoms in strong magnetic fields exhibit features of both chaos and order in many respects. Fig. 7 illustrates that, in addition, they also contain a high element of beauty.

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