Regularity and Irregularity in Spectra of the Magnetized Hydrogen Atom

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On the basis of exact quantum mechanical calculations we study energy-level spectra and photoabsorption cross sections for a hydrogen atom in a uniform magnetic field. In the classically chaotic region near the threshold the level distributions show the irregular pattern predicted by random-matrix theories; on the other hand, the photoabsorption spectra show not only the traditional quasi-Landau modulations but also new and unexpected modulations which may be related to classical periodic orbits embedded in a chaotic system.

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The problem of the quantal manifestation of classical chaos has attracted much attention in recent years.[1–6] In particular, irregularities in level spectra have been proposed as a tool for identifying quantum chaos. Comparisons between the prediction of the random-matrix theory[7] initiated by Wigner and experimental data[1] or spectra of model Hamiltonians[2–5] have been reported in the literature. Although exact conditions have still to be specified,[5] the work up to date supports the idea that, for nonintegrable chaotic classical systems, the overall behavior of the nearest-neighbor spacings (NNS) in the corresponding quantal level spectrum is given by a Wigner distribution while the NNS of an integrable system obey Poisson statistics. However, open questions remain, e.g., the quantal manifestation of isolated periodic orbits embedded in an otherwise chaotic classical system.[6]

In this Letter we study some spectral properties of the nonseparable Schrödinger equation describing a hydrogen atom in a uniform magnetic field.[8] In contrast to the model systems studied in previous investigations[2–6] of quantum chaos, the magnetized hydrogen atom represents a real physical system which can be and has been prepared in the laboratory.[9,10] An interesting feature of this system is the experimentally observed regular modulation of photoabsorption cross sections ("quasi-Landau" phenomenon)[9,11] near the zero-field ionization threshold, where the classical system is known to be chaotic.[12] Our quantum mechanical calculations show that the level spectrum near the zero-field threshold has the irregular behavior expected for a classically chaotic system. On the other hand, calculated photoabsorption cross sections show not only the "traditional" quasi-Landau modulation, but also additional unexpected regular modulations in the irregular and classically chaotic region. Such additional modulations have recently been observed experimentally and have been correlated to a set of classical periodic orbits.[9]

For a very large range of magnetic field strengths the magnetized hydrogen atom is accurately described by the nonrelativistic one-electron Hamiltonian:

$$H = p^2/2\mu - e^2/r + \tfrac{1}{2}\mu\omega^2(x^2+y^2), \qquad (1)$$

where $\omega = eB/2\mu c$ is half the cyclotron frequency, and the trivial normal Zeeman term has been omitted. The azimuthal quantum number m and the z parity π are good quantum numbers, but in each m^π subspace the problem remains nonseparable in the coordinates parallel (z) and perpendicular to the field.

The classical system associated with the Hamiltonian (1) has been studied in detail in the literature.[12] For energies below a critical field-dependent value the motion of the electron is regular for all initial conditions and an approximate third integral of motion has been found.[13] As the energy reaches the escape threshold the system becomes strongly stochastic.

The Schrödinger equation for a given field strength has been shown to be approximately separable[14] for energies not too close to the zero-field threshold.[15] Approximate separability breaks down as we approach the zero-field threshold.[14,16]

The Schrödinger equation was solved as described in Ref. 16 by diagonalization of an equivalent Hamiltonian for fixed values of the parameter $\eta = E/\gamma$, where γ is the magnetic field strength in units of $\mu^2e^3c/\hbar^3 \simeq 2.35\times10^5$ T. The equivalent Hamiltonian corresponds to the radial parts of two two-dimensional harmonic oscillators coupled by a diamagnetic interaction whose strength relative to the oscillator potential is given by the coupling constant $1/\eta^2$.

For negative energies quantum calculations were performed for a dense mesh of coupling strengths η and for various subspaces m^π on a Perkin-Elmer 3210 computer. The diagonalization of ca. 600 banded matrices of dimension 1022 required a few weeks of central processing unit time. Calculations at $E=0$ were performed by diagonalization of matrices with dimensions up to 3721 on a CRAY computer.

The level spectra at fixed η can be represented by the set of field strengths $\{\gamma_i\}$ or (for $\eta\neq0$) by the corresponding set of energies $E_i = \eta\gamma_i$. To study NNS distributions it is necessary to unfold each spectrum in order to obtain a constant mean spacing D. This is achieved by mapping $\{\gamma_i\}$ to $\{N(\gamma_i)\}$, where $N(\gamma)$ is the average number of levels up to γ. For each spectrum we have fitted $N(\gamma)$ by the form $N(\gamma) = |m|$

$+a\gamma^b$, which describes the average level density excellently. To increase the statistical significance, 21 different spectra in the approximately separable region and eight different spectra for $E=0$ are analyzed as corresponding to single strings.

We now turn to the results. Figure 1(a) shows the NNS distribution $P(x)$, $x=(\text{spacing})/D$, of the level spectra in the approximately separable region, together with the Poisson and Wigner distributions. Except for very small values of x the NNS distribution in Fig. 1(a) is very close to the Poisson distribution that we would expect for an exactly separable system.

The situation changes completely as we approach the zero-field threshold. The NNS distribution of levels at

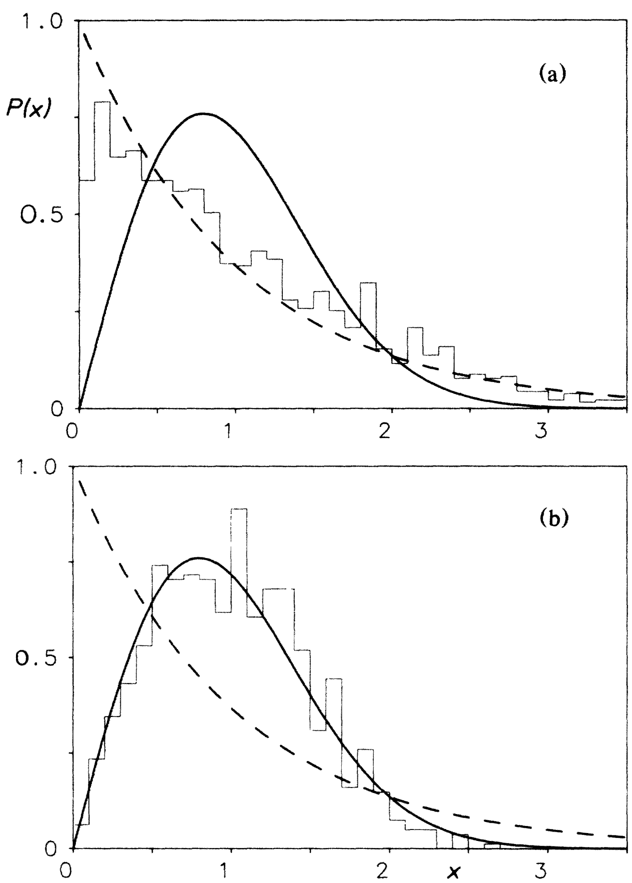

FIG. 1. NNS histograms for level spectra (a) in the approximately separable region, and (b) at the zero-field threshold $E=0$, together with the Wigner (smooth solid lines) and Poisson distributions (dashed lines). In (a) a total of 1823 spacings belonging to 21 different spectra for $m^\pi=1^-$ are analyzed. The spectra cover the energy range between -65 and -95 cm^{-1} and field strength parameters η between -26 and -61 (Rydberg units). For the histogram in (b) a total of 938 converged eigenvalues at $E=0$ in eight different subspaces ($0\leq m\leq 3$, both parities) were calculated. The lowest fifteen levels in each subspace were omitted, so that the number of level spacings analyzed is 810.

$E=0$ is shown in Fig. 1(b) and is seen to be very close to a Wigner distribution. The suppression of small level spacings as a consequence of strong level repulsions is obvious. This irregular behavior of the quantum mechanical level spectrum fits well with the fact that the corresponding classical system is chaotic.[12] The present calculation further underlines our previous observation[16] made on the basis of fewer states at very high fields, namely that approximate separability definitely breaks down at the zero-field threshold. This observation contradicts an earlier assumption[17] that approximate separability should become better with increasing energy (see also Robnik[12]).

With the wave functions at $E=0$ we have calculated oscillator strengths of the Lyman and Balmer series. As examples, Fig. 2(a) shows results for the $\Delta m=-1$ Balmer transitions into the $m^\pi=-2^+$ subspace and Fig. 2(b) shows the $\Delta m=0$ transitions into the $m^\pi=-1^-$ subspace. We plot the renormalized oscillator strengths $f\nu^3$, where ν is the effective quantum number of the final states with respect to the real ionization threshold. The abscissas in Figs. 2(a) and 2(b) are linear in $\gamma^{-1/3}$, so that the traditional quasi-Landau peaks, whose position at $E=0$ is given by[18–20] $\gamma n^3 \simeq 1.6$, become equidistantly spaced. (At fixed field strength these quasi-Landau peaks have an energy spacing of roughly 1.5 times the normal Landau spacing.) The quasi-Landau modulation in Fig. 2(a) becomes evident when we smear the calculated spectrum with a Gaussian with FWHM of 0.2 (thick solid line). An important result is that the Gaussian smearing of the oscillator strengths in Fig. 2(b) also reveals regular modulations. This shows the regular modulations of photoabsorption cross sections occur not only in σ-polarized spectra, as has been known for a long time,[11] but also in π-polarized spectra. Such a modulation has been discovered in recent experiments by Holle *et al.*[9]

A more precise account of modulations in the photoabsorption spectra of Figs. 2(a) and 2(b) can be obtained by a study of their Fourier transforms which are plotted in Figs. 2(c) and 2(d), respectively. The strong peak at $\gamma^{1/3}=1.16$ in Fig. 2(c) corresponds to the traditional quasi-Landau photoabsorption peaks whose spacing at threshold is $\Delta(\gamma^{-1/3})=(1.16)^{-1}=0.86$, in agreement with the $\gamma n^3\simeq 1.6$ rule referred to above. The strong peak at $\gamma^{1/3}=1.72$ in Fig. 2(d) corresponds to the more closely spaced photoabsorption peaks in Fig. 2(b) with $\Delta(\gamma^{-1/3})=0.58$. Note that the peak at $\gamma^{1/3}=1.72$ is also (weakly) present in the Fourier transform of the σ-polarized spectrum of Fig. 2(a), while the traditional quasi-Landau modulation expressed by the peak at $\gamma^{1/3}=1.16$ is absent in Figs. 2(b) and 2(d). This observation is consistent with the interpretation that the traditional quasi-Landau modulation is related to an oscillation of the

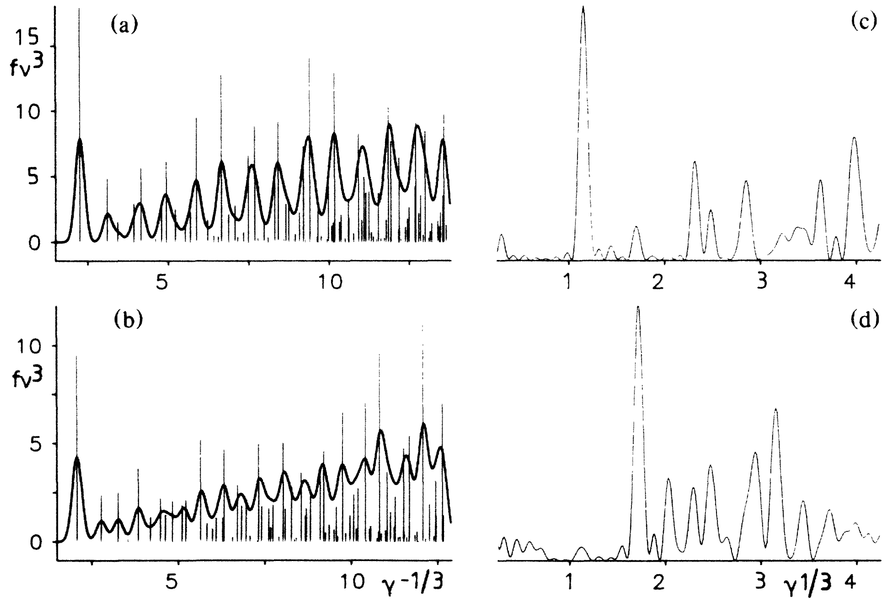

FIG. 2. (a),(b) Renormalized Balmer-oscillator strengths $f\nu^3$ (Rydberg units) for the states at $E=0$, and (c),(d) the corresponding Fourier transforms of the spectra. $\Delta m=-1$ transitions to $m^\pi=-2^+$ final states are shown in (a) and $\Delta m=0$ transitions into the $m^\pi=-1^-$ subspace are shown in (b).

electron confined to the $z=0$ plane perpendicular to the magnetic field,[18,19] whereas the dominant modulation in π polarization, where the final-state wave functions vanish at $z=0$, is related to a classical periodic orbit moving outside the $z=0$ plane.[9]

If the interpretation relating modulations of the photoabsorption cross sections to isolated classical periodic orbits in the two dimensions parallel and perpendicular to the field is correct, then the dominant modulation frequencies should appear for various transitions into different m^π subspaces unless they are suppressed by symmetry properties of the initial or final states as in Figs. 2(b) and 2(d) above. Indeed, this is apparently the case as illustrated in Fig. 3, which displays the Fourier transforms of the photoabsorption cross sections for various transitions. The Fourier spectra for the $\Delta m=-1$ Lyman and Balmer series [Figs. 3(b) and 3(a)] are very similar with regard to both the positions and the heights of the peaks, although the details of the underlying level spectra are completely different. In addition to the peaks at $\gamma^{1/3}=1.16$ and $\gamma^{1/3}=1.72$ discussed above, other peaks appear to persist for several transitions.

In conclusion, our calculations have shown that the NNS distribution of the level spectra follow the predictions of random-matrix theory well, both in the region of approximate separability and in the region of strong nonseparability and classical chaoticity. In the latter region the calculated photo cross sections show the traditional quasi-Landau modulations as well as new and unexpected regular modulations which appear for various transitions into different subspaces of final

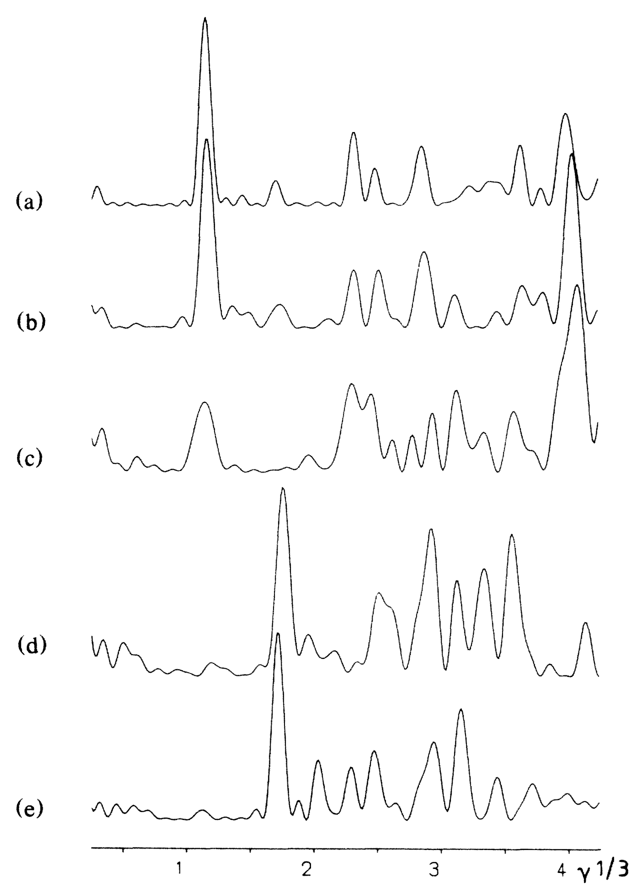

FIG. 3. Fourier transforms as in Figs. 2(c) and 2(d). Transitions and quantum numbers of final states are (a) $\Delta m=-1$, Balmer, $m^\pi=-2^+$; (b) $\Delta m=-1$, Lyman, $m^\pi=-1^+$; (c) $\Delta m=0$, Balmer, $m^\pi=0^+$; (d) $\Delta m=0$, Lyman, $m^\pi=0^-$; (e) $\Delta m=0$, Balmer, $m^\pi=-1^-$.

states. These new modulations may be related to isolated periodic orbits embedded in the classically chaotic system and they should also be observable in highly resolved photoabsorption spectra of other magnetized atoms. Experimental investigations along these lines are highly desirable and may help to give us new insights into the dynamics of strongly nonseparable quantum systems.

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