ANALYSIS OF HYDROGEN RYDBERG SPECTRA IN A UNIFORM MAGNETIC FIELD: UNCOVERING THE TRANSITION FROM REGULARITY TO IRREGULARITY IN A REAL QUANTUM SYSTEM

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Studies of the behaviour of quantum systems in a range of energy where their classical counterparts undergo transitions from regularity to irregularity, as manifested in phase space by the gradual destruction of invariant tori, to date have largely been confined to model Hamiltonian systems such as harmonic oscillators with cubic, quartic, or higher-degree polynomial corrections, or the stadium problem. We show that phenomena which have turned out characteristic of the onset of "quantum stochasticity" in these model systems can in fact be recovered in the quantal energy spectra of a "real" physical system, viz. spectra of hydrogen Rydberg atoms in strong magnetic fields. This implies that one has a simple prototype system at hand in which to study - not only in theory but also in experiment, quantitatively and in detail, and as a function of a continuously tunable external paramenter - phenomena that are expected to be typical of the quantum properties of nonintegrable systems in general.

With regard to measurements of the Balmer spectra of highly excited hydrogen and deuterium atoms in a magnetic field of 6 Tesla which are in progress in the Bielefeld group (Holle and Welge[1]) we have numerically determined energies and wavefunctions of Rydberg states for this field strength, and have computed, with high accuracy, the oscillator strengths of transitions from 2p to even-parity final states with magnetic quantum numbers $|m| = 0, 1, 2$ up to energies $\sim$-40 cm below the field-free ionization threshold. To solve the (non-separable) Schrödinger equation for an electron moving in a fixed Coulomb potential and a homogeneous magnetic field we expanded the wavefunctions in terms of spherical harmonics, and the radial expansion functions in a complete, orthonormal basis set of Laguerre functions with fixed exponent. In this basis, the Hamiltonian matrix assumes a banded form, and can be diagonalized by use of efficient standard algorithms. Our choice of basis bears some resemblance with the Sturmian basis used previously by Clark and Taylor[2] but avoids the difficulties associated with the non-orthogonality of the Sturmian basis. Furthermore, while calculations using oscillator functions in semi-parabolic coordinates[3] produce eigenstates each of which belongs to a different value of the magnetic field strength, our basis has the advantage that one diagonalization procedure yields the complete spectrum at fixed B.

Taking account of line broadening, in accordance with experimental resolution, and field ionization effects, and summing over the individual lines we arrive at synthetic spectra . As an example, Fig. 1 shows a theoretical spectrum of $\Delta m = 0$ Balmer transitions to $m = 0$ even-parity final states. This opens the way, for the first time, to quantitative comparisons, over a wide range of energy, with experimental spectra of highly excited strongly magnetized hydrogen and deuterium atoms.

The calculations of the level sequences performed by us can now serve as a basis for a thorough investigation of manifestations of "quantum stochasticity" in this system. Fig. 2 gives a comparison between the quantal spectrum and the fraction of regular orbits in the Poincaré surfaces of section at $z = 0$ as a function of energy. We can confirm the conjecture of Hasegawa and Harada[4] that the evanescence of regular orbits in the classical problem is related to erratic increases of oscillator strengths. The statistical analysis of fluctuations of the energy value sequence in the transition region between regularity and irregularity shows a turn-over in the nearest-neigbour spacing distributions from a Poisson to a Wigner distribution (Fig. 3). Calculating the spectra in the tran-

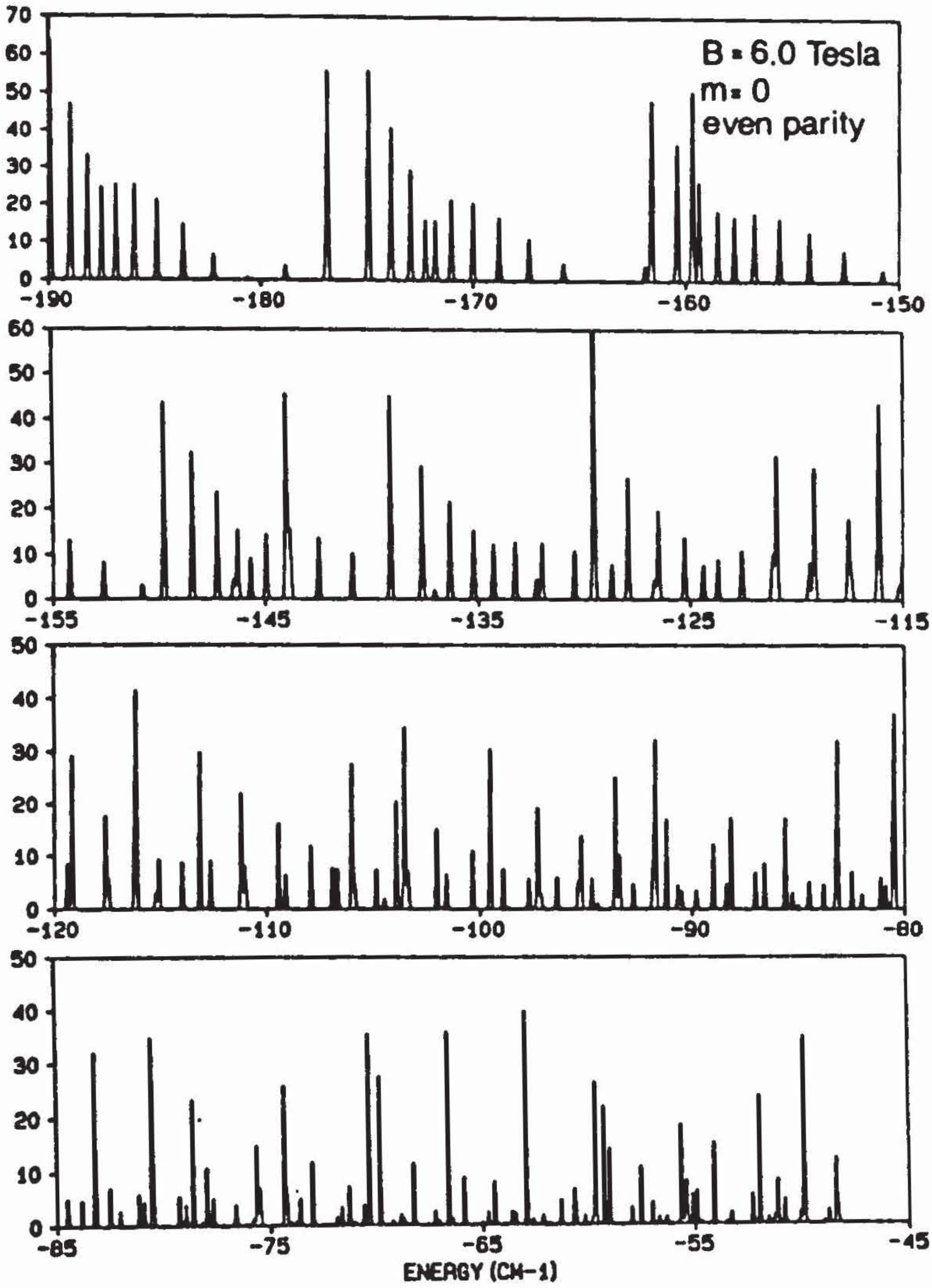

Fig. 1. Theoretical spectrum for $\Delta m=0$ Balmer transitions to $m=0$, even-parity final states. A total of 255 lines contribute to the spectrum in the range of energy shown. The intensity scale is in arbitrary units.

sition region as a function of the magnetic field, we find an increase of multiple avoided crossings of levels, and, related to this, a strong sensitivity of eigenvalues and transition rates to small changes in the perturbation, viz. the magnetic field. All these are manifestations of "quantum stochasticity" which had been present in the investigations of model systems[5]. Our investigations reinforce the universality of these characterizations of "chaotic" quantum spectra in a "real" physical system.

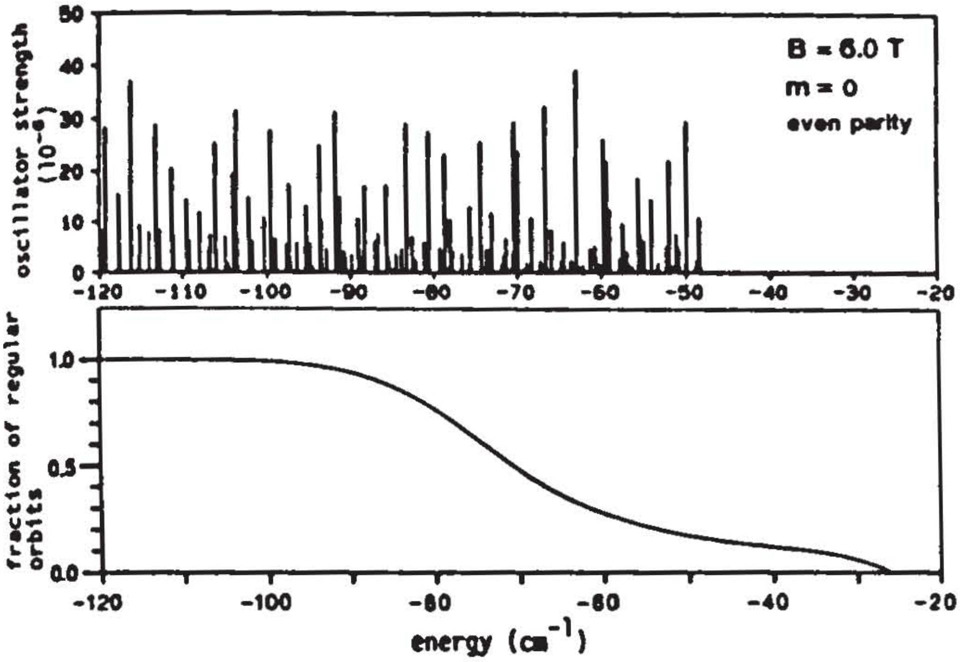

Fig. 2. Oscillator strengths of $\Delta m=0$ transitions from 2p0 to Rydberg states as a function of the energy of the Rydberg state in comparison with the ratio of the area of the regular parts of the Hill region to the total area of the Hill region in the phase space of the classical motion.

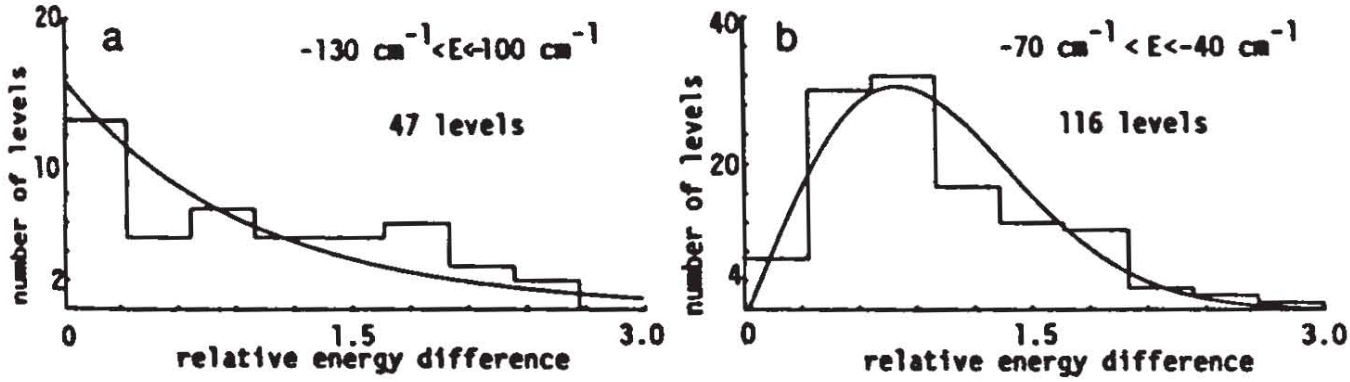

Fig. 3. Nearest-neigbour spacing histograms for the energy levels of the hydrogen atom in a magnetic field of 6 T. In the energy interval where the corresponding classical motion is regular (a) we obtain a Poisson-like distribution, in the interval where the classical motion becomes increasingly irregular (b) we arrive at a Wigner-type distribution.

References

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