Evidence of an Approximate Symmetry for Hydrogen in a Uniform Magnetic Field

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From a numerical analysis of the energy-level structure for hydrogen in a uniform magnetic field, evidence is found for an approximate dynamical symmetry which is effectively exact for many highly excited states. Identification of this approximate symmetry is expected to lead to new physical insights and to new calculational methods.

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Studies of the energy-level structure for an electron moving in a Coulombic electric field and a uniform magnetic field of arbitrary strength have been motivated by problems in astrophysics, solid state physics, and atomic physics.[1] For low-lying states various approximation methods, often variational, have been adopted with some success.[2] For higher states standard methods have not been successful and we lack even qualitative understanding of the energy-level structure except in certain limiting cases. The fundamental difficulty is that the Hamiltonian is nonseparable and there is no natural expansion parameter which is valid at both high and low fields. We believe, however, that a heretofore unrecognized "approximate symmetry" exists which may allow accurate approximate solutions at all field strength. Whether or not such an approximate symmetry exists is of intrinsic value and the resulting solutions would be of great practical interest to the interpretation of experiments on highly excited atoms.[3,4] These experiments are now capable of probing the whole range of phenomena with fully resolved levels to the high-field limit.

The existence of an approximate symmetry permits the Hamiltonian to be written as $H=H_s+H_{ns}$, where H_s is separable and reflects the symmetry and H_{ns} is nonseparable. H_{ns} is much less than H_s for excited states and can be treated perturbatively. In fact, we believe that its effect on large classes of highly excited states will be negligible in the sense that the perturbations will be small compared to the natural radiative decay widths. This approach has not been investigated previously because H_{ns} is comparable to H_s for low-lying states, and because the symmetry underlying the separability of H_s is not of a simple geometrical form.

Our conjecture is motivated by earlier studies of atoms in electric fields[5]; it will be helpful to review some of the salient features of that work in order to set the stage for the magnetic field problem. The nonrelativistic electric field Hamiltonian is $H_E=\frac{1}{2}p^2-1/r+Fz$ (atomic units), which is separable in parabolic coordinates. Exact solutions are possible in the sense that the energy can be expressed as an asymptotic power series in the field, and the coefficients can be evaluated exactly for every order.[6] The separation constants for the Stark problem are generally denoted by Z_1 and Z_2, where $Z_1+Z_2=Z$ (Z is the nuclear charge). The constants of motion are the energy, the azimuthal quantum number, m, and Z_1. Degeneracies (level crossings at nonzero fields) can occur between states having the same value of m but different values of the principal quantum number, n, since these states have different values of Z_1. If the Coulomb potential is perturbed, however, Z_1 is destroyed as a constant of motion and levels with the same value of m anticross as required by the "no-crossing" theorem.[7] Numerous examples of this are presented in Ref. 5. The fundamental reason for the anticrossings is that the Stark problem only separates for pure $1/r$ potential.

Determination of whether or not energy levels cross provides a sensitive test of the existence of a constant of motion in the problem. For the hydrogenic Stark problem the constant of motion is a generalized Lenz-Pauli vector, and the symmetry is dynamical in nature.[8] The Hamiltonian is expected to be separable in some coordinate system which reflects that symmetry. In a two-dimensional problem, such as we are discussing here, such a separation is tantamount to an exact solution.

Turning now to the magnetic field problem, the Hamiltonian is $H_M=\frac{1}{2}p^2-1/r+\frac{1}{8}\alpha^2\rho^2B^2$, where $\rho^2=x^2+y^2$, and we have omitted the trivial paramagnetic term. Schrödinger's equation is separable in eleven coordinate systems,[9] but this Hamiltonian does not fit any of the required forms. Lacking a better approach, we have calculated eigen-

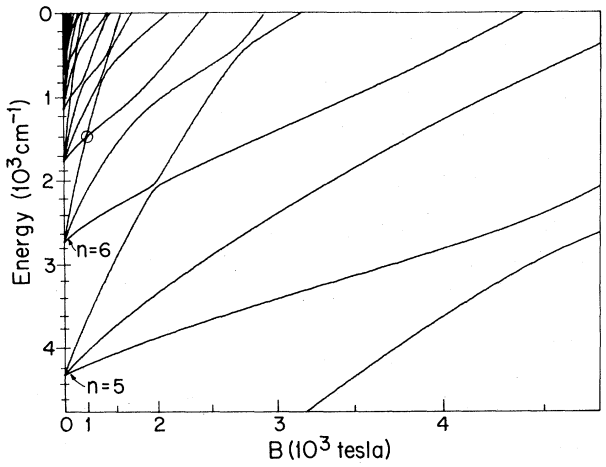

FIG. 1. Energy of hydrogen as a function of magnetic field (plotted on a squared scale) for several low-lying states. The energy is measured from the zero-field ionization limit. The level repulsion of the circled "crossing" is about 8 cm^{-1}.

energies by numerically diagonalizing the magnetic Hamiltonian represented in a truncated spherical basis, treating the B^2 term as the perturbation. The method is expected to be extremely accurate at low fields, but less accurate at high fields. The calculations agree with experiment at low magnetic fields,[3] and the numerical technique has been verified to high precision by applying it to the electric field problem[5] where exact solutions are available. The discussion here is based on the diagonalization of a zero-field spherical basis containing all even-parity, $m=0$ states between $n=1$ and 22. Results for some lower-lying states of hydrogen, shown in Fig. 1, display clear repulsions between numerous energy levels. Certain features, however, such as the one shown circled in the drawing, are suggestive of level crossings, though detailed investigations show that these are actually weak anticrossings.

The situation looks radically different for higher values of n. In Fig. 2, for instance, an energy-level map is presented for the range of $n=10$–16. Here, many levels appear to cross.

Because the anticrossings in a pure Coulomb potential are so pronounced for low n states, it is important to understand their behavior with increasing n. Calculated anticrossing energy separations between the n and $n+1$ manifolds of $m=0$ states are shown in Fig. 3. As n increases, the separation decreases so rapidly that we cannot distinguish between an exponential or a factorial dependence. In either case the level repulsions (or anticrossings) quickly become small compared to the radiative width of the levels, which has a power law dependence in the range n^{-3} to n^{-5}.

Our conjecture that magnetic energy levels approximately cross in a Coulomb field is not, how-

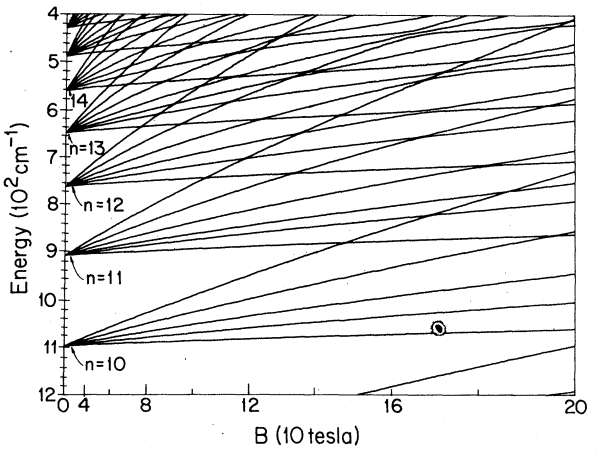

FIG. 2. Energy of hydrogen as a function of magnetic field (plotted on a squared scale) for several higher excited states.

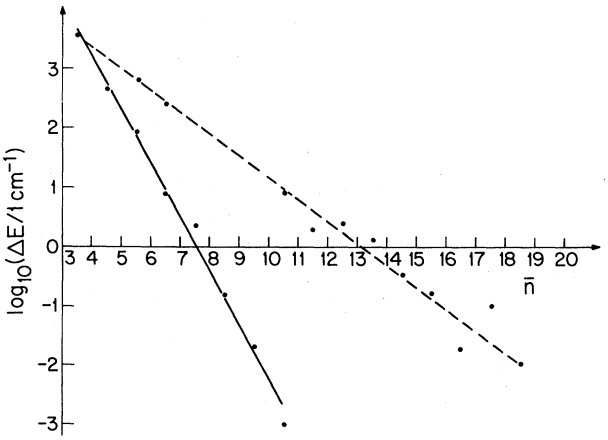

FIG. 3. Anticrossing size as a function of $\bar{n}$, the geometric mean of the principal quantum numbers of the adjacent manifolds. The solid line depicts the anticrossing size between the lowest-energy state of the $n+1$ manifold and the highest-energy state of the n manifold. The dashed line shows the anticrossing size between the lowest-energy state of the $n+1$ manifold and the "middle" energy state of the n manifold. (The fluctuation of the points about the lower end of this line reflects the logarithmic ordinate and the problem of defining the "middle" of a manifold.)

ever, based entirely on the evidence of the calculated energy levels. The conjecture is also motivated by observing effects of small perturbations to the Coulomb potential on level crossings. A simple perturbation can be produced by introducing a quantum defect δ into the zero-field energy of the $l=0$ state: $E=-\frac{1}{2}(n-\delta)^{-2}$. Such a perturbation arises from any short-range interaction which creates a phase shift $\phi=\pi\delta$ in the s-state wave function. This perturbation causes the energy levels to anticross, in close analogy to the behavior of anticrossings for the Stark problem in Ref. 5. In particular, the anticrossings obey an n^{-4} scaling law for a constant quantum defect. H_{ns} has a much stronger n dependence, suggesting that the Coulomb potential in a magnetic field is special. Figure 4 shows the calculated sizes of a number of anticrossings as a function of the quantum defect.

Because H_{ns} is presently unknown it is in general not possible to predict the size of repulsions between states for which the numerical diagonalization has not been done. However, there is a trend that states from adjacent n manifolds possessing the most dissimilar slopes (the derivative of energy with respect to field squared) have the smallest anticrossings or $\langle H_{ns}\rangle$. This is expected from the following consideration: States with the largest slope lie completely in the plane perpendicular to the magnetic field, while states with smaller slopes are increasingly "tipped" out of this plane. Thus, states with the most dissimilar slopes have the least spatial overlap.

Identifying the approximate symmetry or the constant of motion and finding the separable form for the Hamiltonian has proven to be an elusive task for us, undoubtedly made more difficult by the fact that it cannot be accomplished for low-lying states. Nevertheless, we are optimistic that the goal is achievable. This would represent an important theoretical advance and a most useful development in view of the experiments currently in progress.

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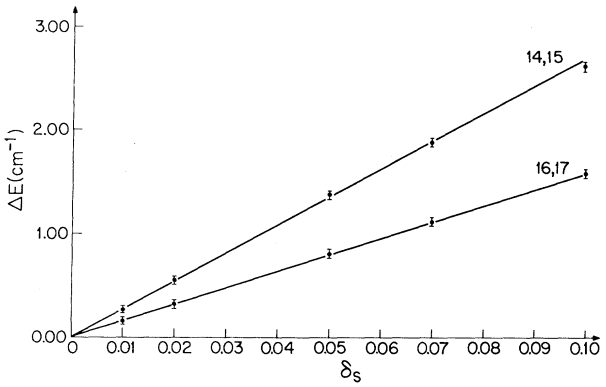

FIG. 4. Anticrossing size as a function of the $l=0$ quantum defect. These values are taken from the first "crossing" between $n=14, 15$ and $n=16, 17$ manifolds. The error bars represent the estimated numerical error, $\pm 5\times 10^{-3}$ cm^{-1}.

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