

Scars of Symmetries in Quantum Chaos

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The hydrogen atom in a magnetic field is a classically chaotic Hamiltonian system. The energy-level fluctuations have been shown recently to obey a random-matrix model. Here we go beyond the statistical analysis by studying the destruction of the low-field dynamical symmetries. We especially establish the existence of scars of symmetries in the chaotic regime. The symmetry properties are no longer associated with one given level, but fractalized onto clusters of levels, generating a long-range order.

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What is the quantum counterpart of classical chaos in a Hamiltonian system? Recently, numerical studies on simple systems¹⁻⁷ have confirmed the conjecture that the statistical properties of the energy levels obey the predictions of the Gaussian orthogonal ensemble (GOE) of random matrices.^{1,2}

But a random-matrix approach cannot describe any property of a Hamiltonian system. This is especially revealed on a simple atomic physics system: the hydrogen atom in a magnetic field. Numerical⁵⁻⁹ and experimental¹⁰ studies have shown that nongeneric features do exist in this system, especially the existence of a long-range order associated with classical periodic orbits. We here establish this point from a quantum point of view by studying the destruction of the dynamical symmetries of the system.

The Hamiltonian of the hydrogen atom in a magnetic field is (in atomic units)¹

$$H = p^2/2 - 1/r + (\gamma/2)L_z + (\gamma^2/8)(x^2 + y^2), \quad (1)$$

where $\gamma = B/B_c$ is the reduced magnetic field along z

axis ($B_c = 2.35 \times 10^5$ T).

L_z and parity are constants of the motion. We shall limit our discussion to $L_z = M = 0$, even-parity states, but similar conclusions can be reached for other series.

This system is equivalent to a pair of coupled harmonic oscillators¹¹ which can be studied with group theoretical techniques. This is conveniently done by introduction of the Coulomb dynamical group (also called noninvariance group) $SO(2,2)$ whose six generators $\mathbf{S}^{(\alpha)} = (S_x^{(\alpha)}, S_y^{(\alpha)}, S_z^{(\alpha)})$ and $\mathbf{T}^{(\alpha)} = (T_x^{(\alpha)}, T_y^{(\alpha)}, T_z^{(\alpha)})$ are defined by (α is a positive adjustable parameter)

$$S_{x,z}^{(\alpha)} = \pm \frac{\alpha}{4} \left[\frac{\partial^2}{\partial \mu^2} + \frac{1}{\mu} \frac{\partial}{\partial \mu} - \frac{M^2}{\mu^2} \right] + \frac{1}{4\alpha} \mu^2,$$

$$S_y^{(\alpha)} = \frac{1}{2} i(1 + \mu \partial/\partial \mu),$$

and the same definition for $\mathbf{T}^{(\alpha)}$ with the interchange $\mu \rightarrow \nu$. (μ, ν) are the semiparabolic coordinates: $\mu, \nu = (r \pm z)^{1/2}$.

Schrödinger's equation $H|\Psi\rangle = E|\Psi\rangle$ expressed as a pure algebraic form as a function of \mathbf{S} and \mathbf{T} is¹¹

$$\{S_z^{(\alpha)} + T_z^{(\alpha)} + \frac{1}{2} \gamma^2 \alpha^4 (S_z^{(\alpha)} + S_x^{(\alpha)})(T_z^{(\alpha)} + T_x^{(\alpha)})(S_z^{(\alpha)} + S_x^{(\alpha)} + T_z^{(\alpha)} + T_x^{(\alpha)}) - \alpha\} |\Psi\rangle = 0, \quad (2)$$

with $\alpha = (-2E)^{-1/2}$. From Eq. (2), the zero-field eigenstates of the hydrogen atom are eigenstates of $S_z^{(\alpha)} + T_z^{(\alpha)}$, with eigenvalue n , the principal quantum number. Several choices of basis are then possible.¹¹ Among them, three are of special interest:

(1) The parabolic basis. The eigenstates are eigenfunctions of both $S_z^{(\alpha)}$ and $T_z^{(\alpha)}$. They separate in semiparabolic coordinates. The eigenstates are labeled with the parabolic quantum numbers n_1 and n_2 (with $n = n_1 + n_2 + |M| + 1$).

(2) The spherical basis associated with the standard coupling of $\mathbf{S}^{(\alpha)}$ and $\mathbf{T}^{(\alpha)}$,

$$\mathbf{U}^{(\alpha)} = \mathbf{S}^{(\alpha)} + \mathbf{T}^{(\alpha)}.$$

The eigenstates are eigenfunctions of $U_z^{(\alpha)}$ and $\mathbf{U}^2 = U_z^{(\alpha)2} - U_x^{(\alpha)2} - U_y^{(\alpha)2} = \mathbf{L}^2$. The wave functions separate in spherical coordinates and are of the usual (n, l, M)

type.

(3) The λ -type basis associated with the nonstandard coupling

$$V_x^{(\alpha)} = -S_x^{(\alpha)} + T_x^{(\alpha)}, \quad V_y^{(\alpha)} = -S_y^{(\alpha)} + T_y^{(\alpha)},$$

$$V_z^{(\alpha)} = S_z^{(\alpha)} + T_z^{(\alpha)}.$$

The eigenstates are eigenfunctions of $V_z^{(\alpha)}$ and $\mathbf{V}^2 = V_z^{(\alpha)2} - V_x^{(\alpha)2} - V_y^{(\alpha)2} = \lambda^2$, where λ in the n shell reduces to a nonstandard angular momentum^{11,12} built from the components of \mathbf{L} and \mathbf{A} (the Runge-Lenz vector), namely $\lambda = (A_x, A_y, L_z)$. The eigenstates are labeled with (n, M) and an integer λ ranging from 0 to $n-1$.

Though they are equivalent descriptions of the Coulomb problem, these three types of bases have very

different symmetry properties. Herrick¹² first showed the usefulness of the λ type and parabolic bases for describing the eigenstates of the hydrogen atom in a magnetic field.

In the low-field limit (inter- l mixing regime when different multiplets are not mixed), the hydrogenic multiplet presents a rovibrational structure as illustrated in Fig. 1. The upper states of the multiplet have an approximate *rotational* symmetry described by the λ -type basis and are localized near the $z=0$ plane perpendicular to the field B . The overlapping between the upper state and the $\lambda=n-1$ state of the λ -type basis is 0.998 (for $n \gg 1$). In turn, the lower states of the multiplet present an approximate *vibrational* symmetry described by the parabolic basis and are localized near the z axis. The overlapping between the lower state and the (conveniently symmetrized) $n_1=0$ state is about 0.85. In between these two limiting cases, there is a crossover in the symmetries¹² leading to some irregularity in the level spacings (see Fig. 1).

The classical dynamics of the system (or its oscillator representation) depends on the coupling parameter $\beta = \gamma^2 / (-2E)^3$ (or on the scaled energy⁵ $E\gamma^{-2/3} = -\frac{1}{2}\beta^{-1/3}$). The motion is regular for $\beta < 0.8$, of mixed regular-chaotic type in the interval (0.8, 60.638), and completely chaotic above.^{6,13} By "completely" we mean that the volume of confining tori in phase space is smaller than 10^{-3} .

The spectrum and eigenfunctions of the Hamiltonian H are efficiently calculated by use of Eq. (2) and numerical diagonalization.⁵⁻⁷

A good indication of how exact the low-field approximate symmetries remain is to plot the squared projections of the computed eigenstates onto a subspace of well-defined symmetry (rotational or vibrational), against the effective principal quantum number $\epsilon = (-2E)^{-1/2}$. This produces a stick spectrum which contains as many lines as the number of eigenstates. In the low-field limit, most of them are vanishingly small as a consequence of the nearly exact character of the symmetries and do not appear in the figures.

Figure 2 refers to projections onto the subspace

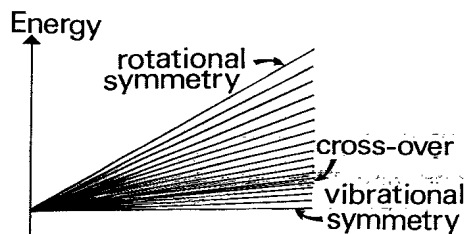


FIG. 1. Diamagnetic multiplet ($n=36$, $M=0$, even parity). The upper states have an approximate rotational symmetry. The lower states have an approximate vibrational symmetry. In between, there is a crossover in the symmetries.

spanned with the $\lambda=n-1$ rotational-type states. At moderate field strengths [Fig. 2(a)],¹⁴ one line with height 0.998 is dominant, associated with the upper state of the diamagnetic multiplet. This clearly indicates that the rotational symmetry remains valid even in the strong-mixing regime, as previously noticed.¹¹

At higher field [$E/\gamma = -2.311$ —see Fig. 2(b)], a new phenomenon is displayed. Many new lines are bursting out in the stick spectrum near $\epsilon=36$ (value $\beta \approx 60$ of the coupling parameter) which indicates that the rotational symmetry breaks down. The value precisely corresponds to the destruction of the last classical invariant tori¹³ with rotational symmetry (located near $Z \approx 0$). However, above $\epsilon=36$, the patterns are still regular. Instead of being concentrated on one level of each multiplet with height nearly unity, the symmetry is redistributed onto clusters of levels, each sharing some part of the initial symmetry.

The average positions of the clusters are regularly distributed in continuity with the individual dominant lines of the regular regime and are approximately obeying the semiclassical predictions for $z=0$ ¹³ (quasi-Landau resonances). This finally justifies the diabatic picture of the building of the quasi-Landau spectrum previously used in the interpretation of the experimental spectra. In each cluster, the individual positions and heights of the lines are irregular: The rotational symmetry may be concentrated on one dominant line (e.g., near $\epsilon=62.2$) or equally redistributed over several lines (near ϵ

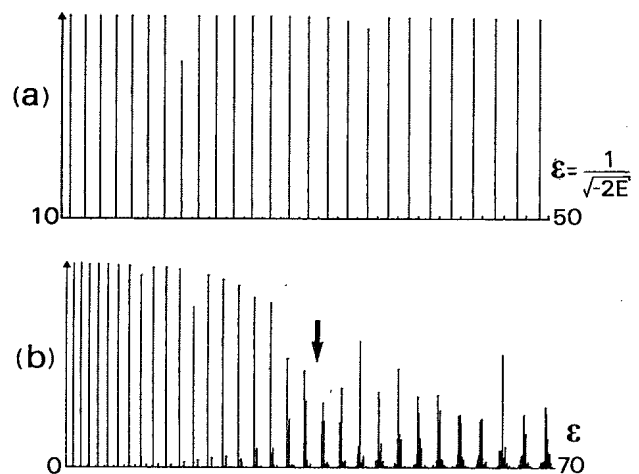


FIG. 2. Squared projections of the eigenstates of the hydrogen atom in magnetic field onto the *rotational* subspace $\lambda=n-1$. The heights of the lines measure the fraction of rotational symmetry carried by the eigenstates. (a) Calculated spectrum for $E/\gamma = -8.678$ (moderate field strength). The irregularity near $\epsilon=20$ is due to *accidental* quasidegeneracy. (b) Calculated spectrum for $E/\gamma = -2.311$ (high field strength). The arrow indicates the *classical* transition to chaos. The clustering of levels above $\epsilon=36$ indicates the scar of the rotational symmetry.

=59.1).

The same phenomenon occurs for the vibrational symmetry (Fig. 3). Here, the eigenstates are projected onto the subspace with parabolic quantum number $n_1=0$. At moderate field strengths [$E/\gamma=-8.768$, same as in Fig. 2(a)], there is one dominant line associated with the lower state of each multiplet. The symmetry remains valid to better than 85% up to $\epsilon=30$ where it breaks down. This corresponds to the destruction of the classical invariant tori with vibrational symmetry (essentially localized near the z axis) near $\beta=3$.¹³ Above $\epsilon=30$, the fractalization and clustering of the vibrational symmetry onto several states is exhibited. This phenomenon extends far into the chaotic regime as can be seen on Fig. 3(b) obtained at higher field ($E/\gamma=-2.311$). The average positions of the clusters are approximately given by the semiclassical quantization along the z axis. The spacings between vibrational and rotational clusters are very different [compare Figs. 2(b) and 3(b)].

The region $\epsilon > 36$ in Figs. 2(b) and 3(b) corresponds to a *completely chaotic* classical motion. The energy-level fluctuations are then described by a random-matrix theory (Wigner distribution of the energy-level spacings⁵⁻⁷). In spite of this, there exist *scars of the Coulomb symmetries* extending far into the chaotic regime. Moreover, one given spectrum contains scars of *both limiting symmetries*.

These features have experimental consequences. As optical excitation is a process which does not comply with the internal symmetries of the system¹²; both rotational- and vibrational-type states are excited. Experimental spectra will then exhibit the two types of clusters though entangled, and their Fourier transforms will be peaked at the various cluster spacings. For

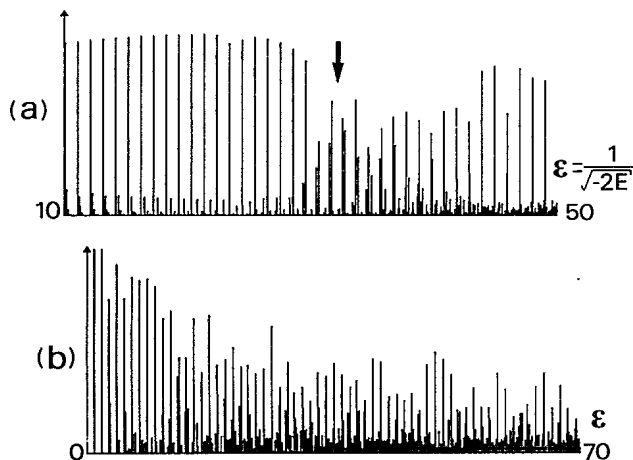


FIG. 3. Squared projections of the eigenstates onto the vibrational subspace $n_1=0$. (a) $E/\gamma=-8.678$. The arrow indicates the *classical* transition to chaos for the *vibrational* symmetry. The clustering of levels above $\epsilon=30$ indicates the scar of the vibrational symmetry. (b) $E/\gamma=-2.311$.

checking this point, we calculate the $M=0$, even-parity spectrum of hydrogen in a field of 8 T ($\gamma=3.4\times 10^{-5}$), in the energy range $(-132+44\text{ cm}^{-1})$.¹⁵ The classical dynamics is completely chaotic above -29 cm^{-1} . The squared projections of the eigenstates onto the $\lambda=n-1$ rotational subspace, displayed in Fig. 4(a), clearly show the partial breaking of the symmetry and its clustering in the chaotic region. The cluster spacing is $\frac{3}{2}\gamma=\frac{3}{2}\hbar\omega_c$ at $E=0$, indicating that they correspond to the usual quasi-Landau features of the spectrum. Figure 4(b) shows the simulated experimental spectrum as it will look under *optical excitation* from the $(2p, M=-1)$ state in experimental conditions.¹⁰ Clustering is still present, but weakened. The $1.5\hbar\omega_c$ spacing can be rediscovered if we make a Fourier transform. With the assumption of a finite resolution (modeled through convolution with a Gaussian curve), the short-range irregular behavior is smoothed out and the spectrum looks regular [see Fig. 4(c)].

The character of the modulations thus actually reflects the global properties of the eigenstates which do exhibit scars of the symmetries. In particular, this leads to a remnant of localization near the origin which character compares with the scars earlier found by Heller in bil-

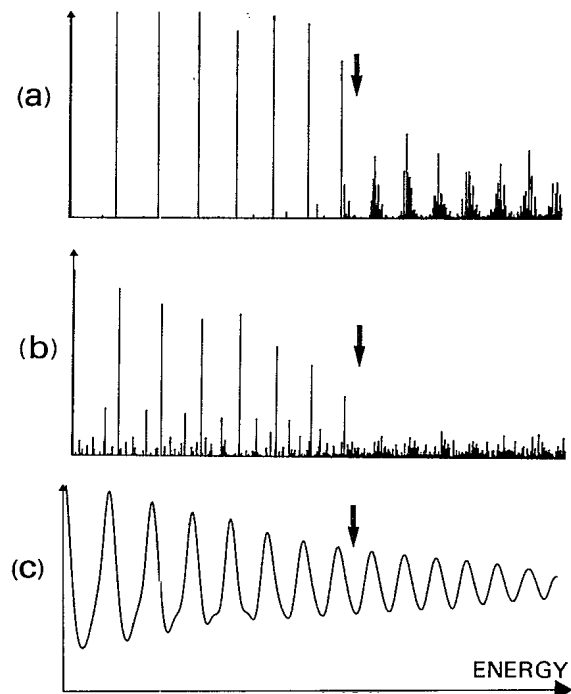


FIG. 4. Simulation of the $M=0$, even-parity spectrum of the hydrogen atom in a field of 8 T ($\gamma=3.4\times 10^{-5}$) between -132 and 44 cm^{-1} . The arrow indicates the transition to complete chaos (-29 cm^{-1}). (a) Squared projections onto the $\lambda=n-1$ subspace. (b) Oscillator strength from the $(2p, M=-1)$ state (infinite resolution). (c) Same than (b), with a resolution 2×10^{-5} a.u. (4 cm^{-1}). The spectrum looks regular and the chaotic behavior is smoothed out.

liards.¹⁶ But our present approach aims at a more general understanding of the phenomenon, not relying on spatial properties of eigenfunctions or classical periodic orbits.

This can be exemplified as follows: For odd z -parity states, the scar of the rotational symmetry is responsible for the usual quasi-Landau modulation of the spectrum at $\frac{3}{2}\hbar\omega_c$ (more clearly seen on the even z -parity spectrum). This is actually seen on theoretical simulations but surprising if considered from the periodic orbit analysis as the wave function identically vanishes on the $z=0$ orbit.⁹

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¹⁴The spectrum is not calculated at a fixed magnetic field γ , but for a fixed ratio $E/\gamma = -8.768$ which makes calculations easier (Refs. 5 and 6). Strictly similar conclusions are reached at fixed γ ; see Fig. 4.

¹⁵The calculations converge for negative energy. Above $\epsilon = \frac{1}{2}\gamma = 3.7 \text{ cm}^{-1}$, the spectrum is composed of resonances, so that individual positions and intensities have not fully converged. However, the global behavior is correct.

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