Irregular Wave Functions of a Hydrogen Atom in a Uniform Magnetic Field

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We study the irregular wave functions of a highly excited hydrogen atom in a uniform magnetic field. The "scarring" of wave functions by periodic orbits is quantitatively investigated. The shape of unperturbed scars is in good agreement with recent semiclassical predictions.

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In quantum mechanics all information about the system under consideration is contained in its Green's function $G(\mathbf{r}',\mathbf{r},E)$,

$$G(\mathbf{r}',\mathbf{r},E)=\sum_n \frac{\Psi_n^*(\mathbf{r}')\Psi_n(\mathbf{r})}{E-E_n}. \qquad (1)$$

For integrable systems both the wave functions $\{\Psi_n\}$ and the structure of the spectrum $\{E_n\}$ are well understood and conventional semiclassical methods approximate their exact solutions rather well, at least for short de Broglie wavelengths. Unfortunately, the appearance of chaotic motion in nonintegrable systems prevents the applicability of these methods and our general knowledge about quantum systems possessing classically chaotic dynamics is still fragmentary. Most of the progress achieved concerns the structure of the eigenvalue spectra, which have been studied in detail during the last few years (for reviews see, e.g., Refs. 1 and 2, and for the particular problem of a hydrogen atom in a magnetic field, Refs. 3 and 4). Our knowledge of generic properties of the associated wave functions is by far not as well developed. Recently Bogomolny[5] derived an expression for the wave functions using the semiclassical expansion of the Green's function in terms of classical trajectories as derived by Gutzwiller.[6] In this theory the wave function consists of an average, which is given by the projection of the classical microcanonical distribution on the coordinate space (the so-called "semiclassical eigenfunction hypothesis"[7]), and of strongly energy-dependent contributions localized around the closed classical paths (the so-called "scars"[8]). In this way he was able to explain many of the finer details observed in the highly excited eigenfunctions of the quantized stadium billiard.[5,8,9] In a recent paper Berry extended these ideas to a phase-space approach.[10]

So far studies on wave functions of "realistic" ergodic systems (smooth potentials) were only qualitative.[11] In this Letter we report a quantitative approach to wave-function scarring. The physical system under consideration is the hydrogen atom in a uniform magnetic field, which is known to be chaotic around the ionization threshold.[3]

The Hamiltonian of a hydrogen atom in a uniform magnetic field $\mathbf{B}$ is given by (in atomic units)[3]

$$H=\frac{p^2}{2}-\frac{1}{r}+\frac{1}{8}\gamma^2(x^2+y^2). \qquad (2)$$

The z axis is chosen as the direction of the magnetic field $\mathbf{B}$, which is measured in units of $B_0=2.35\times10^5$ T, $B=\gamma B_0$. Because of scaling properties[3] the classical dynamics depend only on the *scaled energy* ϵ, which is a combination of the energy E and the field strength γ, $\epsilon=E\gamma^{-2/3}$. Here we will study the Hamiltonian (2) in semiparabolic coordinates (μ,ν,ϕ), which (after separating the ϕ motion) transform (2) into

$$h=\frac{p_\mu^2+p_\nu^2}{2}-\epsilon(\mu^2+\nu^2)+\tfrac{1}{8}(\mu^4\nu^2+\nu^2\mu^4)\equiv 2. \qquad (3)$$

Analogous transformations can be applied to the Schrödinger equation, which for constant scaled energy ϵ reads[12]

$$[\gamma^{2/3}\Delta-2\epsilon(\mu^2+\nu^2)+\tfrac{1}{4}(\mu^4\nu^2+\mu^2\nu^4)-2]\Psi=0. \qquad (4)$$

In Eq. (4) $\gamma^{1/3}$ replaces the role of $\hbar$. Thus by fixing the scaled energy ϵ we can study the semiclassical limit $\hbar\to0$ by decreasing the field strength γ. We then quantize the field strengths $\gamma^{1/3}$, or equivalently $\hbar$. This situation is also realized in recent experiments.[13]

We will study highly excited wave functions for $\epsilon=-0.2$, where most of the phase space is chaotic ($\sim$90%[4]). Before we discuss the structure of *individual* irregular wave functions we will introduce and discuss a quantitative measure for scarring. For each wave function $\Psi_n(\mathbf{r})$ and for each different periodic orbit r we define a scar strength I_n^r in the following way:

$$I_n^r=\int_\gamma \Psi_n^2(\nu,\mu)(\nu^2+\mu^2)\nu\mu\, ds. \qquad (5)$$

The integrand is chosen such that integration over coordinate space yields unity (wave-function normalization).

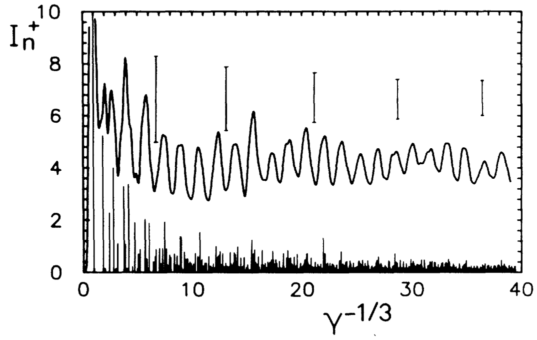

FIG. 1. Distribution of scar strengths as defined by Eq. (5) for the first 600 eigenstates in the $m^\pi = 0^+$ subspace and for the orbit $+$. The smoothed curve is obtained by a Gaussian smoothing and is enhanced by a factor of 2. An $\hbar^{1/2}$ dependence is indicated by the bars.

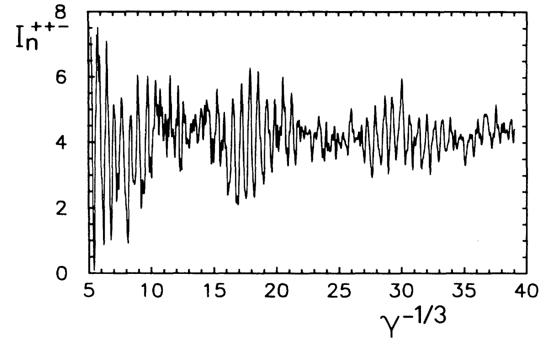

FIG. 2. As Fig. 1, but for the orbit $++-$.

The actual integral (5) is performed along the path γ of the periodic orbit r, where $ds = (dv^2 + d\mu^2)^{1/2}$. Although one may have some objections against the proposed definition (5) (for example, it does not care about the wave function in the vicinity of the periodic orbit), it is obviously a measure of the scarring strength: If the wave function has an accumulation of probability density along the periodic orbit r, the value I_n^r will be large. (Recall that no definition of a scar measure exists so far.)

The distribution of the scar strengths for the first 600 eigenfunctions in the $m^\pi = 0^+$ subspace are shown in Fig. 1 for the orbit which we label with the symbolic code "+."[14] It is the most simple unstable periodic orbit of the system with a (symmetry reduced) stability exponent of $\lambda = 0.8683$. The shape of the orbit will be shown below in connection with individual wave functions. The abscissa of the coordinates in Fig. 1 is inversely proportional to $\hbar$. Apart from the "erratic" pattern of the individual scar strengths, an overall decrease of them is obviously noticeable. In fact, the average scar strength decreases proportionally to $\hbar$, in the same way as the level density increases. This is shown by the smooth curve in the figure, which represents a Gaussian smoothing of the distribution: The average distribution is more or less constant. In addition, however, the smoothed distribution is modulated and these oscillations are caused by the periodic orbit involved. The frequency, e.g., is given by the inverse of the scaled action S_+, which for this orbit is $S_+/2\pi = 0.6173$. The oscillations have a maximum, where the orbit is "quantized," that is $S(\gamma) = \gamma^{-1/3} S_+ = 2\pi\hbar(n + \frac{1}{4}\alpha_+)$. The Morse index α_+ is related to the number of conjugate and focal points of the orbit and is $\alpha_+ = 2$ in this case.

For a more quantitative analysis we compare our results with Bogomolny's semiclassical expression for the wave functions:[5]

$$\langle |\Psi(\mathbf{r})|^2 \rangle = \rho_0 + \hbar^{1/2} \sum_r \mathrm{Im} \langle A_r(x) \exp[iS_r/\hbar + iy^2 W_r(x)/2\hbar] \rangle , \tag{6}$$

where for each periodic trajectory r the x coordinate is chosen along the orbit and the y coordinate is chosen perpendicular to it. $\langle \cdots \rangle$ denotes averaging over small intervals of energy and configuration space. The mean value of the wave function, ρ_0, is modulated by the oscillating terms arising from the periodic orbits r. S_r are the actions of the orbits, and A_r and W_r can be expressed through the elements of the orbit's stability matrix (for details see Ref. 5). Our definition of the scar strength (5) investigates the wave functions on the periodic orbit, that is $y \equiv 0$. From Eq. (6) we see that these contributions and hence the oscillations in the scar strength distribution should vanish in the semiclassical limit as $\hbar^{1/2}$. A closer inspection of the oscillations shown in Fig. 1 indeed gives a decrease of the amplitudes compatible with an $\hbar^{1/2}$ dependence. Thus scarring as the collective effect shown in Fig. 1 *disappears* in the semiclassical limit. This does not exclude, however, that some *individual* wave functions can be strongly scarred. As can be seen in Fig. 1 the scar strengths fluctuate wildly and some particular eigenfunctions have a much larger scar strength than the average. A mechanism for scar enhancement is discussed in connection with Fig. 2.

Figure 2 shows the smoothed scar strength distribution for the orbit which we will label "$++-$" and which is shown in Fig. 3(a). Again, the overall amplitudes of the oscillations become smaller with $\hbar$, but more important is the observation of a pronounced beat structure. This beat structure is related to the existence of a further periodic orbit (labeled $++--$), which has a similar scaled action and lies close to the orbit $++-$; see Fig. 3(b). The actual actions are $S_{++-}/2\pi = 1.48647$ and $S_{++--}/2\pi = 1.56462$. The contributions of these orbits can interfere because the orbits scar the wave functions with the finite width $\approx [\hbar/|W(x)|]^{1/2}$ perpendicular to the trajectories;[5] see Eq. (6). Thus there is a spatial overlap of their contributions, which then interfere con-

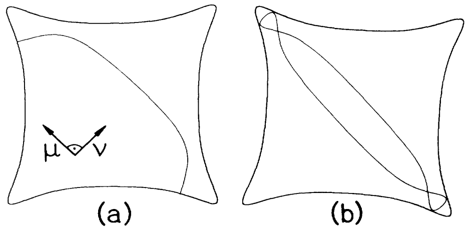

FIG. 3. Shape of the orbits (a) $++-$ and (b) $++--$ together with the boundary of the classical allowed region (thick lines). The Liapunov exponents for the orbits are $\lambda_{++-}=2.4515$ and $\lambda_{++--}=2.3322$.

structively or destructively. This explanation is in agreement with the results shown in Fig. 2. The fundamental frequency is 1/1.49, which agrees with the action of the orbit involved, whereas the beat frequency is 1/0.08 which is consistent with the difference in the actions of the two orbits. A more detailed analysis of the frequencies involved is obtained by the Fourier transform of the scar strength distribution, which reveals only two pronounced peaks located at 1.49 and 1.57.

How much can be seen of these scars in individual wave functions? In Eq. (6) the wave function is averaged over small regions of energy (hence involving an average over several wave functions) and over coordinate space. The energy averaging is necessary to eliminate the contributions of the very long periodic orbits. Because of their exponential proliferation in chaotic systems they would give a divergent contribution.[15] However, it has been shown that energy averaging is unnecessary when the sum over periodic orbits is used as an asymptotic series.[16] Consequently the most simple orbits should show up first in scarring the wave functions. The spatial smoothing is necessary to eliminate the contributions of nonperiodic but recurrent trajectories. A trajectory is recurrent when it starts at some point **r** and comes back to this point with a different momentum. Most of the recurrent orbits live in the neighborhood of a periodic one with a comparable action, and these contributions are included via the harmonic approximation (6). Particularly when the system has discrete symmetries there are, however, recurrent trajectories which do *not* live near such periodic orbits, and which give additional contributions to individual eigenfunctions. Hence we expect a rather complicated pattern for individual wave functions, which, in general, cannot be explained by *one* single contribution of a particular periodic orbit. And in fact, we only found exceptionally wave functions which are dominantly scarred by a single orbit. Most of the wave functions are rather complicated and must be interpreted as a superposition of several contributions. In addition, there is spatial interference between the different contributions, which in most cases makes it very hard to identify them at all.

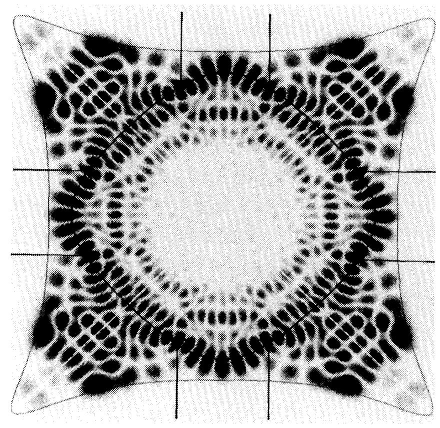

FIG. 4. Wave function of the 116th excited state. The wave function is scarred by the periodic orbit $+$, which is shown as a solid line. The self-focal points of the orbit are indicated.

Figure 4 shows an intensity plot of the 116th excited state in the $m^{\pi}=0^{+}$ subspace, which is dominantly scarred by the single periodic orbit $+$ drawn as a solid line. The quantized field strength divided by the scaled action of the orbit gives 10.576, which is close to the "quantization" condition 10.5 obtained by counting in the fundamental domain the nodal excitations along the orbit. Because the scar is nearly unperturbed we can study some of its finer details: Depending on the relative signs of the terms occurring in the exponential, Eq. (6) predicts different structures of the scar perpendicular to the orbit ($y\neq 0$). The maxima of the scar are either on the orbit or symmetrically next to it ("bridge" structure).[5] The relative signs of the terms change at the self-focal points, where a certain stability matrix element vanishes. The self-focal points of the periodic orbit are indicated in the figure. Indeed, the structure of the scar changes from localization on the orbit to a bridge structure nearby (and vice versa) after passing a self-conjugate point.

Other examples of scarred wave functions are shown

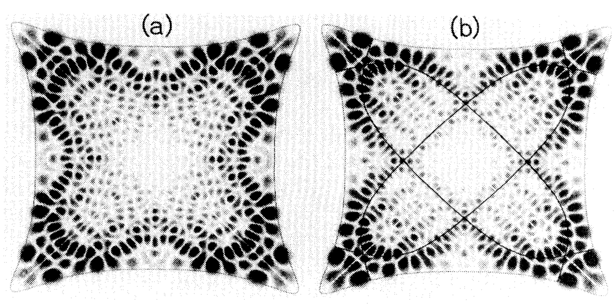

FIG. 5. Wave functions of the (a) 107th and (b) 115th excited states. The scarring periodic orbit $++-$ is drawn in (b).

in Fig. 5, where we plotted the 107th and 115th excited states. Both wave functions are very similar and are scarred by the same orbit $++-$. Again the bridge structure between the self-focal points is visible. The quantized actions of the periodic orbit for both wave functions differ by one unit or one nodal excitation (the exact difference is 1.0006). However, the wave functions also have significant contributions from the orbit $++--$, which may explain some details near the end-caps of the potential. The additional contributions from the orbit $++--$ become obvious in connection with Fig. 2: The eigenvalue of the 115th state is $\gamma^{-1/3}=7.1201$, which corresponds to a maximum in the interference beat structure as discussed above.

In summary, we have studied the highly excited irregular wave functions of a hydrogen atom in a uniform magnetic field. Our results confirm that the contributions of closed classical orbits to the spatial wave functions vanish in the semiclassical limit. However, the disappearance is rather slow. A numerical example illustrates this: To decrease the scarring strength of an orbit at the nth eigenfunction by 1 order in magnitude one has to investigate the $10^4 \times n$ excited level in a two-dimensional system. In addition, interference between contributions arising from different orbits can lead to an enhancement (or disappearance) of particular scars. For (unperturbed) scars fine structures in the wave functions are in good agreement with a recent theory of Bogomolny.

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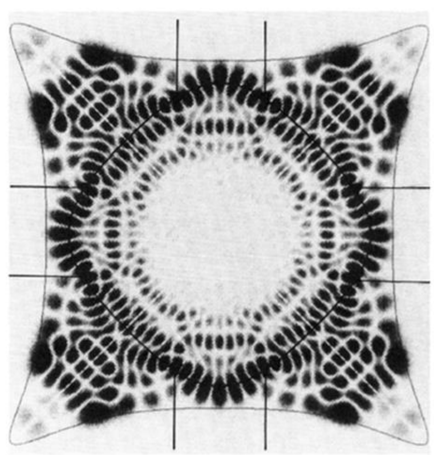

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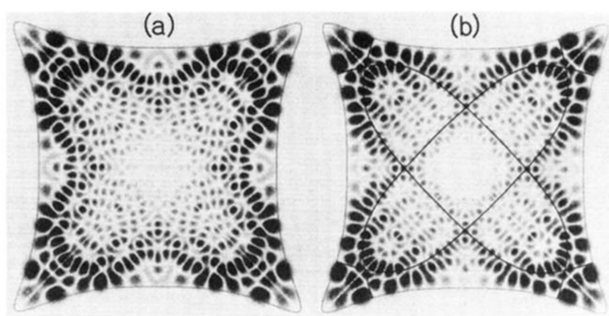

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