Eigenstates of a Chaotic System

Using the hydrogen atom in a magnetic field as an example, we study the behavior of the eigenstates of a quantum chaotic system. We show the extreme importance of the "scarring" phenomenon for understanding the experimental results.

Key Words: *quantum chaos, scars, quadratic Zeeman effect*

A time-independent quantum Hamiltonian system is completely described with its energy spectrum $\{E_i\}$ and its eigenstates $\{|\psi_i\rangle\}$. The properties of the energy spectrum and its connections with the classical dynamics of the system have been widely studied during the last few years.[1,2] There is strong experimental, numerical and theoretical evidence that the local statistical properties of the spectrum belong to different kinds of universality classes, depending on the regular or irregular character of the classical motion and on the existence of an antiunitary symmetry transformation.[2] On the other hand, there exist long-range correlations in the energy spectrum, which have been observed experimentally in regular and chaotic systems. For chaotic systems, they seem to be closely related with the unstable classical periodic orbits.[2]

Our understanding of the eigenstates is less advanced. When the classical motion is regular and takes place on invariant tori in phase space, the quantum eigenstates are known to be localized on those tori satisfying the Einstein, Brillouin, Keller (EBK) quantization condition.[3] In contrast, little is known when the classical

Comments At. Mol. Phys.
1991, Vol. 25, Nos. 4–6, pp. 281–290
Reprints available directly from the publisher

motion is chaotic. In the semiclassical limit ($\hbar \to 0$), the wave-functions are expected to be essentially random Gaussian waves.[3] However, following pioneering work on the stadium billiard,[4] it is clear that many states present some residual localization (that is, enhanced probability density), especially in the vicinity of the classical unstable periodic orbits (the so-called "scars"[4]).

In this paper, we show the importance of the scars for understanding the experimental results and, more generally, the dynamics of complex systems. We will discuss a now well-known chaotic system: the hydrogen atom in a magnetic field, for which the theoretical, numerical and experimental studies are possible.

In atomic units, the Hamiltonian of the hydrogen atom in a magnetic field (along the z-axis) is

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

where γ is the magnetic field strength in units of $B_0 = 2.35\ 10^5$T. L_z, the z-component of the angular momentum, is a constant of motion and can be trivially taken into account. In the following, we discuss the $L_z = 0$ case.

Using the scaled semi-parabolic coordinates,

$$\mu = \gamma^{1/3}\sqrt{r + z},$$

$$\nu = \gamma^{1/3}\sqrt{r - z}, \qquad (2)$$

the Schrödinger equation is

$$\left[\frac{\gamma^{2/3}}{2}\left(\frac{\partial^2}{\partial\mu^2} + \frac{1}{\mu}\frac{\partial}{\partial\mu} + \frac{\partial^2}{\partial\nu^2} + \frac{1}{\nu}\frac{\partial}{\partial\nu}\right) - \epsilon(\mu^2 + \nu^2) + \frac{\mu^2\nu^2(\mu^2 + \nu^2)}{8} - 2\right]\psi(\mu,\nu) = 0 \qquad (3)$$

where ϵ is the scaled energy:

$$\epsilon = E\gamma^{-2/3}. \qquad (4)$$

Equation (3) can be interpreted as the Schrödinger equation for two coupled oscillators where $\gamma^{1/3}$ plays the role of Planck's constant.

The classical dynamics depends only on the scaled energy ϵ. In the low-field limit $\epsilon \to \infty$, the motion is regular (the Coulomb limit), some chaotic motion appears near $\epsilon = -0.5$ and the phase space is nearly fully chaotic above $\epsilon \simeq -0.127$.[5,6,7] Because of the existence of an absolute length scale (the Bohr radius) in the quantum system, the classical scaling property no longer exists in quantum mechanics. However, studying the system at fixed ϵ and varying γ allows a clear understanding of the semi-classical limit, here corresponding to $\gamma \to 0$ (see Eq. (3)).

The energy spectrum and the eigenstates can be numerically calculated using diagonalization of Eq. (3) in a convenient basis.[5,6,7] It produces hundreds of well converged energy levels and wavefunctions.[8]

At $\epsilon = -0.2$, the main part ($\simeq$90%) of the phase space is chaotic. There is a small stability island surrounding the stable orbit in the $z = 0$ plane (perpendicular to the magnetic field). Therefore, there are some eigenstates localized in this region. Figure 1a shows the wavefunction of such a state (as all the wavefunctions have a cylindrical symmetry around the z-axis, they are plotted in the ρ,z plane). It is possible to assign quantum numbers to these states: a quantum number n labels the number of nodes along the ρ direction and another quantum number K labels the number of nodes in the z direction. These quantum numbers can be interpreted by the EBK quantization procedure. They are in continuity with the exact quantum numbers that exist in the low-field limit (where the problem is separable in momentum coordinates).[6] According to the EBK quantization condition, only states lying on some invariant torus should be localized. However, it is found numerically that some states are still localized in the same way, but out of the last invariant torus (see Fig. 1b). In other words, the EBK quantization procedure extends somewhat in the chaotic part of phase space. Such a phenomenon is not well understood.

Besides these localized states, most of the wavefunctions have substantial values almost everywhere in the classically allowed region.[8,9] Some of them are scarred by periodic orbits. (Fig. 2a: scar

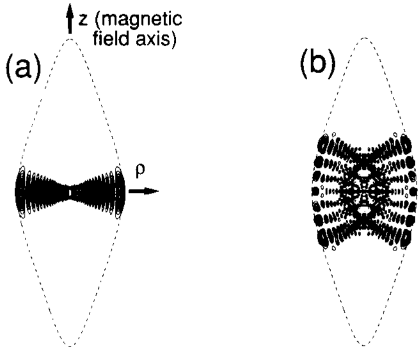

FIGURE 1 Contours of some wavefunctions of the hydrogen atom in a magnetic field. The dotted line in the classically accessible volume. These are "regular" states localized in the vicinity of the $z = 0$ periodic orbit. For the value of the chosen scaled energy ($\epsilon = E\gamma^{-2/3} = -0.2$), this orbit is stable. (a) 244th excited state ($M = 0$, even parity). This state is purely regular. It has no node perpendicular to the $z = 0$ plane. It is in continuity with the ($n = 26$, $K = 0$) state in the low-field limit. (b) 301st excited state ($M = 0$, even parity). Though it is associated with a mostly chaotic phase space region, this wavefunction remains mainly regular, in continuity with the ($n = 31$, $K = 6$) state in the low-field limit.

of the $\rho = 0$ Coulomb orbit; Figs. 2b and 2c: scar of the almost circular orbit; Fig. 2d: scar of the $z = 0$ orbit).

On these wavefunctions, one can notice the role of the focal points of the periodic orbit where the probability density is even more enhanced. These phenomena have been partly explained by Bogomolny,[10] using a semi-classical expansion of the Green's function. Such an analysis explains qualitatively the existence of some of the scars. It also leads us to deduce quantitative information on the *average* behavior of the scars (see below).

However, it suffers from some difficulties. First, similarly to its counterpart for the energy spectrum (Gutzwiller's periodic orbit expansion[2]), its involves a sum over periodic orbits. From a practical point of view, computing the quantum spectrum from this sum is very difficult, even for low excited states, and a direct quantum calculation is more efficient. Secondly, as one given wavefunction involves many scars of different periodic orbits interfering with well-defined phases, this does not lead to reliable predictions on the shapes of individual wavefunctions. Thirdly, it does not explain the existence of very localized wavefunctions, which exist

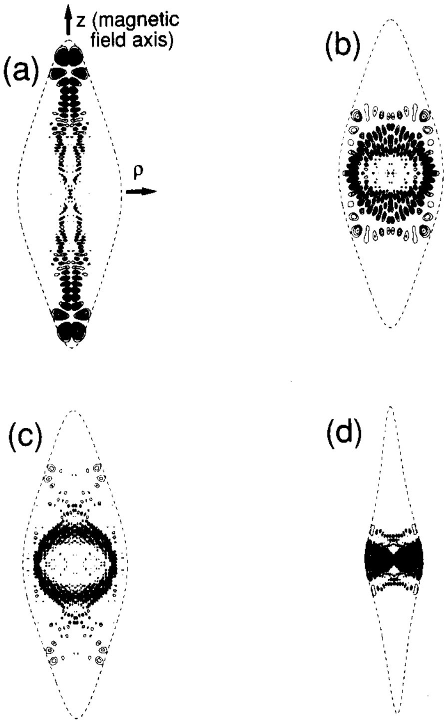

FIGURE 2 Some chaotic wavefunctions of the hydrogen atom in a magnetic field, scarred by some periodic orbits ($\epsilon = E\gamma^{-2/3} = -0.2$, except (d): $\epsilon = -0.1$). (a) 395^{th} excited state ($M = 0$, even parity) scarred by the $\rho = 0$ periodic orbit. (b) 137^{th} excited state ($M = 0$, even parity) scarred by the circular orbit. (c) 474^{th} excited state ($M = 0$, odd parity) scarred by the circular orbit. (d) 201^{st} excited state ($M = 0$, even parity) scarred by the $z = 0$ periodic orbit.

even for very small $\hbar$ (or equivalently, very highly excited states). Figures 2a and 2c are such examples of strongly scarred states.

Despite our global understanding of "scarring," we are lacking a general quantitative measure of the phenomenon. However, for some simple periodic orbits with definite symmetry properties, the projection of the eigenstates on a given subspace having the same symmetry property provides us with such quantitative information on scarring. For instance, the states localized near the $z = 0$ plane can be described with a "rotational" group $(SO(2,1)_\lambda$, subgroup of the SO(2,2) dynamical group of the hydrogen atom.[11] The projection of an eigenstate of the hydrogen atom in a strong magnetic field onto the "rotational" $\lambda = n - 1$ states thus describes the fraction of rotational symmetry of the eigenstate, hence the intensity of the scar of the $z = 0$ periodic orbit. The numerical value of this projection allows us to discriminate among states which are scarred by this orbit. The state shown in Fig. 1a has more than 99% rotational symmetry, while those of Figs. 1b and 2 have of the order of 10^{-3}. One advantage of this quantitative measure of scarring is that it takes into account not only the behavior of the wavefunction along the periodic orbit, but also in its vicinity.

When the classical motion is regular—the $z = 0$ periodic orbit is stable and surrounded by an island—only the states localized near the $z = 0$ plane with no node perpendicular to it (the $K = 0$ states, see Fig. 1a), present a significant part of rotational symmetry. This is illustrated in Fig. 3a where, for each eigenstate, a line is plotted with an intensity equal to the part of rotational symmetry. This is illustrated in Fig. 3a where, for each eigenstate, a line is plotted with an intensity equal to the part of rotational symmetry. The whole spectrum is at fixed $\epsilon = E\gamma^{-2/3} = -0.2$ and the x-axis is the inverse of the effective Planck's constant: $\gamma^{-1/3}$ (see Eq. (3)). It is also proportional to the effective principal quantum $n^* = 1/\sqrt{-2E} = \gamma^{-1/3}(-2\epsilon)^{-1/2}$. Increasing values of $\gamma^{-1/3}$ correspond to more and more "semiclassical" eigenstates.

It is easy to check in Fig. 3a that, though the classical motion is mainly chaotic and the different hydrogenic manifolds are mixed, states strongly localized near the $z = 0$ plane still exist even in the semi-classical limit. The positions of these localized $K = 0$ states are accurately computed using the EBK quantization procedure, giving

$$\gamma^{-1/3} = \frac{(n + \nu/2)2\pi}{S} \tag{5}$$

where S is the action of the periodic orbit (depending only on ϵ), ν is the rotation number around the periodic orbit (i.e., the winding angle divided by 2π), and n a positive integer.

The agreement between this prediction and the actual spectrum in Fig. 3a is excellent.

In Fig. 3b, the same spectrum for $\epsilon = -0.1$ is plotted. The

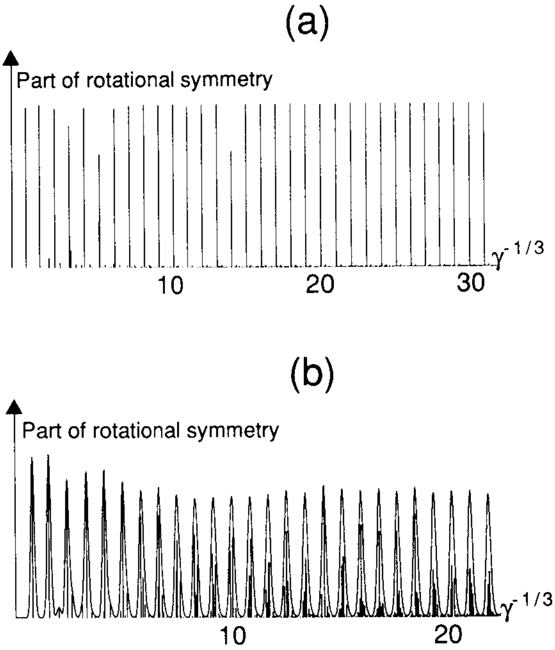

FIGURE 3 Part of the rotational symmetry (see text) of the different eigenstates at constant ϵ. This measures the scar strength of the $z = 0$ periodic orbit. (a) $\epsilon = -0.2$. The $z = 0$ orbit is stable. A set of equally spaced eigenstates are strongly localized near the $z = 0$ plane. (b) $\epsilon = -0.1$. The $z = 0$ orbit is unstable. Instead of being concentrated on one set of states, the scar strength is redistributed onto clusters of states. At low resolution (solid line), a regular behavior is observed and survives in the semi-classical limit (right part of the figure). The positions of the clusters are described by the scar quantization condition (Eq. (6)).

$z = 0$ periodic orbit is unstable and the motion is almost fully chaotic. Under such conditions, it is no longer possible to associate a set of localized states with the periodic orbit. Instead of being concentrated on one state, the scar intensity (part of rotational symmetry) is shared by numerous states, which form a cluster of scarred states. In each cluster, the intensities of the lines have strong fluctuations and look irregular.[11] Figure 3b demonstrates the extreme importance of the scarring phenomenon. Indeed, if the wavefunctions were only random Gaussian waves,[3] the intensity distribution in Fig. 3b should have been random, which is clearly far from being true! For instance, the 201st excited state is strongly scarred (see Fig. 2d). Even in the semi-classical limit (right part of Fig. 3b), the low-resolution spectrum shows very strong modulations. In that sense, scarring survives in the semi-classical limit (though nothing can be said for individual eigenstates).

This has extremely important experimental consequences. Indeed, the *modulation of the density of states*, which arises from the periodic orbit, according to the Gutzwiller's theory [2] is much weaker than the *modulation of intensity* in Fig. 3b. Usually, experimentalists do not measure the density of states, but rather observe a spectrum where the intensity of each line is the square of some transition matrix element. The behavior of the transition operator is thus more important than the energy spectrum itself, especially when the individual states are not resolved.

This is well known from the experimental results obtained on the hydrogen atom in a magnetic field: depending on the choice of polarization of the laser used in the optical excitation process, different modulations corresponding to various periodic orbits appear.[12,13]

The positions of the clusters in Fig. 3b are predicted in Bogomolny's paper.[10] It is

$$\gamma^{-1/3} = \frac{(n - 1/2)2\pi}{S}. \tag{6}$$

When the $z = 0$ periodic orbit turns from stable to unstable at $\epsilon \simeq -0.127$, the winding angle is exactly $-\pi$. (Actually, the 1:2 resonance between the two eigenfrequencies of the system leads to the $-\pi$ winding angle; this leads to destabilization of the periodic orbit and to chaos). Hence, there is a continuity between the EBK quantization condition (Eq. (5)) valid when the orbit is stable and the scar quantization condition (Eq. (6)) for unstable orbits. However, one should stress a key difference: the first formula refers to the quantization of individual eigenstates while the second one refers to the maxima of scarring. This is the reason for which, when observed at low-resolution, the experimental spectra look continuous even when the classical motion turns from regular to chaotic.[11]

The periodic character of scarring, as seen in Fig. 3b, allows us to perform an averaging over many different scarred eigenstates and to extract quantitative information about the scars visible in the wavefunctions. This procedure has been shown in Ref. 9 to be equivalent to considering the Green's function of the system. The numerical results then obtained[9] show that the average strength of a scar (i.e., maximum enhancement compared to the background) scales as $\hbar^{1/2}$, while its width perpendicular to the orbit scales as $\hbar^{1/2}$, too. In the semi-classical limit, the average scar is more and more localized near the periodic orbit, but its intensity vanishes.

The increasing number of states cooperating to form a cluster makes them visible even for very high quantum numbers (for instance, the quasi-Landau resonances in Ref. 14.)

In conclusion, we want to stress the importance of scars for the interpretation of experimental results. In complex systems where the classical motion is expected to be chaotic (nuclei, molecules, clusters, etc.), the individual eigenstates are usually not resolved and the question of energy level fluctuations is mainly academic. The important physical properties are expressed in the long-range correlations, for instance, modulations in the matrix elements of some transition operator, closely related to the existence of scars.

DOMINIQUE DELANDE
Laboratoire de Spectroscopie Hertzienne de l'ENS
Université Pierre et Marie Curie,
Tour 12-01, 4, Place Jussieu,
75252 Paris Cedex 05,
France

References

1. O. Bohigas and M. J. Giannoni, *Chaotic Motion and Random Matrix Theories, Lecture Notes in Physics*, Vol. 209 (Springer-Verlag, Berlin, 1984).
2. NATO Les Houches Lecture Notes 1989, *Chaos and Quantum Physics*, eds. A. Voros and M. J. Giannoni (North-Holland, Amsterdam, 1990).
3. NATO Les Houches Lecture Notes 1981, *Chaotic Behaviour of Deterministic Systems*, eds. G. Iooss, R. Helleman andd R. Stora (North-Holland, Amsterdam, 1983).
4. E. J. Heller, Phys. Rev. Lett. **53**, 1515 (1984).
5. D. Delande and J. C. Gay, Phys. Rev. Lett. **57**, 2006 (1986).
6. D. Delande, in Ref. 2.
7. A. Hönig and D. Wintgen, Phys. Rev. A. **39**, 5642 (1989).
8. D. Wintgen and A. Hönig, Phys. Rev. Lett. **63**, 1467 (1989).

9. D. Delande and J. C. Gay, to be published (1990).
10. E. B. Bogomolny, Physica D **31**, 169 (1988).
11. D. Delande and J. C. Gay, Phys. Rev. Lett. **59**, 1809 (1987).
12. W. R. S. Garton and G. S. Tomkins, Astrophys. J. **158**, 839 (1969).
13. J. Main, G. Weibusch, A. Holle and K. H. Welge, Phys. Rev. Lett. **57**, 2789 (1986).
14. J. Neukammer, H. Rinneberg, K. Vietzke, A. Hönig, H. Hieronymus, M. Khol, H. J. Grabka and G. Wunner, Phys. Rev. Lett. **59**, 2947 (1987).