Diamagnetic informational exchange in hydrogenic avoided crossings

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Abstract

The irregular behavior of the hydrogen atom in the presence of strong magnetic fields is examined by means of the ionization energy and the Shannon information entropy of the excited states involved in some high-lying avoided crossings. In addition to the energy level repulsion, which is known to occur for a certain field strength in going through a chaotic region of this type, it is found that the two states: (i) show up maximal entropies for just around this critical field and (ii) exchange their informational character in that region.
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1. Introduction

In the same manner as the field-free Coulomb problem is the basis to analyze the structure of normal matter, the hydrogen atom under strong magnetic fields has been shown to be the key to open the new atomic physics which studies the structure of matter under these extreme conditions [1–3]. This abnormal matter has been encountered in the atmosphere of some white dwarfs and on the surface of neutron stars where magnetic field strengths up to $10^3$ a.u. or even larger have been observed [2–4]. Moreover, the excitons and shallow impurities in semiconductors behave at laboratory-strength magnetic fields (i.e., less that $10^{-4}$, a.u.) in a very similar way as hydrogen atoms in magnetic fields of astronomical strengths, due to its reduced effective mass and the high dielectric constant, respectively [2,3].

The structure of matter in the presence of magnetic fields drastically changes according to the field strength, leading to a rich variety of complicated, often highly irregular and narrow, spectral features called avoided crossings. This is mainly due to the interplay between the Coulomb and diamagnetic contributions to the Hamiltonian of the system which requires the coexistence of spherical and cylindrical symmetries to govern the dynamics. In the case of the hydrogen atom, the presence of the diamagnetic term completely destroys the spherical symmetry of the system, so
that the associated Schrödinger equation is not separable. This makes the theoretical description of the problem quite difficult, which has obliged to the development of a large number of computational methods to solve it for all field regimes [1–3,5,6]. Especially complicated is the intermediate regime where the strength of the Coulomb and magnetic fields are comparable, so that the Lorentz force acting on the electron equals or exceeds the Coulomb binding force. In such a case sufficiently accurate numerical methods of non-perturbative character are necessarily required, see e.g. [5,6].

In this work we analyze some avoided crossings between high-lying excited states of the hydrogen atom in the presence of strong magnetic fields from both dynamics and information theory standpoints. This is done by studying in detail the ionization energy and the Shannon’s entropy of the involved states by means of a hybrid non-perturbative computational approach [6].

The extent or spreading of the hydrogenic wavefunctions $\psi(\vec{r})$ is best described by the Shannon’s entropy [7] which is defined by

$$S_\rho = - \int \rho(\vec{r}) \ln \rho(\vec{r}) \, d\vec{r},$$

where $\rho(\vec{r}) = |\psi(\vec{r})|^2$ is the quantum mechanical probability density distribution. This quantity which is closely related to the concept of thermodynamical entropy and other fundamental and/or experimentally measurable quantities (kinetic and exchange energies, magnetic susceptibility...) of the system [8–10], is a quantitative measure of the electron uncertainty of much better quality than the Heisenberg’s standard deviation [11]. For a given state the higher is this quantity, the more extended is the wavefunction, the more delocalized is the charge of the electron, the larger is the uncertainty and the smaller is the accuracy in predicting the localization of the electron.

Our results show that in going through the irregular region when the magnetic field strength is varied, the system behaves so that the involved energy levels: (i) do not cross each other, but rather they come close and then they repel yielding an avoided crossing (see e.g. [12]) and (ii) present maximal entropies and exchange their informational character in that region. We believe that the latter is a general effect induced by strong magnetic fields not yet known up until now, to the best of our information.

The Letter is organized as follows. In Section 2 we give the Hamiltonian of the system in a non-relativistic framework, and briefly describe the computational approach used. Later on, in Section 3 we use this approach to obtain and discuss the ionization energies, the wavefunctions and the information entropies of the excited states with azimuthal quantum number $m = 0$ and positive–parity involved in some avoided crossings when the magnetic field strength is varied. Finally, in Section 4 some concluding remarks are given.

2. Hamiltonian and computational method

The motion of a hydrogen atom in an uniform magnetic field $\vec{B}$ is appropriately well described by the non-relativistic Hamiltonian [2] in spherical coordinates

$$H(\vec{r}) = -\frac{1}{2r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial}{\partial r} \right) + \frac{1}{2r^2} \vec{L}^2(\theta, \phi) - \frac{1}{r} - iB \frac{\partial}{\partial \phi}$$

$$+ \frac{B^2}{2} r^2 \sin^2 \theta,$$

where the field has been chosen to be oriented along the $z$-axis of a coordinate system centered at the proton (assumed to have an infinite mass). Moreover, the atomic system of units is chosen so that the strength $B$ is measured in units of $B_0 = 2\pi^3 \hbar^2 c^2 / \hbar \approx 4.701 \times 10^5 \text{ T}$, and the operator $\vec{L}^2(\theta, \phi)$ denotes the squared angular momentum. It is well known that relativistic corrections and the spin–orbit coupling can be neglected [2] for the magnetic fields $B < 10^3 \text{ a.u.}$ and for excited states satisfying $n > 0.126B^{-1/3}$. The only exact integrals of motion of our system are the $z$-component of the electronic angular momentum $L_z$ and the parity $P_{z}$, corresponding to the reflection $z \to -z$. Then, the states can only be described by means of the azimuthal quantum number $m$ and the $z$-parity. Without loose of generality, we can restrict our considerations to the subspace of states with $m = 0$ and positive $z$-parity.
To solve the non-integrable two-dimensional Schrödinger equation associated to the previous Hamiltonian we have used a hybrid non-perturbative computational approach, which combines the discrete variable method in the angular coordinate $\theta$ and the finite element method in the radial variable. With the help of these two numerical algorithms and employing the variational principle, the initial differential equation is reduced to a generalized symmetric eigenvalue problem solved by a Krylov type technique. It has been shown that this approach is an accurate and efficient tool to describe non-integrable quantum systems [6].

3. Results and discussion

To begin with, we have checked our computational approach by evaluating the wavefunctions and the Shannon's information entropies of various low-lying and high-lying states of field-free hydrogen atom already available in the literature [8,10]. Contrary to previous authors, the nonspherical part of the entropy for states with orbital quantum number $l \neq 0$ was included in our calculations. Let us also mention that the radial and angular integrals involved in the entropy (1) are computed by means of a Gauss–Legendre quadrature in the corresponding variables. In our computations, we give six converged digits for energies and entropies. Moreover, to simplify the discussion the principal quantum number $n$ of the field-free states is frequently used to refer to the states in the field, although it is not any longer a good quantum number.

Heretoforth we center our attention in the chaotic region of the spectrum of the hydrogen atom in a magnetic field, where numerous avoided crossings have been encountered providing a mechanism for the system to order the states as the field is increased [5]. First of all we have investigated the avoided crossing which is produced between the two energetically adjacent states evolving from field-free states with principal quantum numbers $n = 6$ and $n = 7$ when the field strength is varied on the range $0.002 \text{ a.u.} < B < 0.00214 \text{ a.u.}$ The computed results for the ionization energies are shown in Fig. 1a, where we observe how the irregular phenomenon appears. The neighboring states monotonically approach each other when $B$ is enhanced up to a critical value $B_c$ (in this case $B_c \approx 2.079 \times 10^{-3}$ a.u.), then being very close one to another ($\Delta E \approx 3.3 \times 10^{-5}$ a.u.); however, they cannot cross over because both have the same symmetry and the Wigner–von Neumann non-crossing rule [13] operates, and they repel yielding an avoided crossing, so that for $B > B_c$ the states monotonically separate out more and more.

This phenomenon is examined in Fig. 1b by means of the Shannon’s entropy, what is novelty. The entropies of the two involved states have the same global behavior within the range of variation of the field strength, both presenting a maximum. The two entropies increase regularly when $B$ is enhanced so that their difference decreases. However, contrary to the ionization energies, the entropies do cross over for the critical field $B_c$. Moreover, the entropy of the state emerging from a field-free state with $n = 6$ reaches the maximum for $B = 2.076 \times 10^{-3}$ a.u., just before the avoided crossing, while the entropy maximum of the $n = 7$
state occurs for \( B = 2.085 \times 10^{-3} \) a.u. (i.e., just over the critical value \( B_c \)). Most interesting is the fact that the entropy difference \( \Delta S_p = S_{p=6}^n - S_{p=7}^n \) changes its sign when the system goes through the avoided crossing region. Indeed, for \( B < B_c \) the entropy difference is positive and for \( B > B_c \) it has the opposite sign. This means that the informational character of the two involved states has been adiabatically exchanged because the corresponding wavefunctions strongly mix up in that region. Once the system has left it, the entropy of both states behave again in a smooth manner when \( B \) is enhanced, although now the state with higher energy (\( n = 6 \) in our case) has not any more the largest entropy. These two figures provide a nice illustration of this phenomenon: the states do not exchange their relative positions in the spectrum, but they do exchange the informational character of their wavefunctions adiabatically.

Secondly, we have also studied the first avoided crossing between states with \( m = 0 \) and positive \( z \)-parity evolving from field-free states with \( n = 7 \) and \( n = 8 \), when the field strength is varied on the range \( 0.00116 \) a.u. \( \leq B \leq 0.00117 \) a.u. The computed results for their ionization energies and information entropies are shown in Figs. 2a, b, respectively. It is observed that both quantities have a behavior similar to the previous case when the field strength is enhanced. Now, the phenomenon of repulsion between the two states takes place for the critical field \( B_c \approx 1.1653 \times 10^{-3} \) a.u., at which moment the difference between the corresponding energy levels is \( \Delta E \approx 4.5 \times 10^{-6} \) a.u., as shown in Fig. 2a. Furthermore, again here the entropies of the two states cross over and adiabatically exchange their informational character when the system goes through the irregular region, as shown in Fig. 2b. Indeed, the entropy difference \( \Delta S_p = S_{p=7}^n - S_{p=8}^n \) has opposite sign at both sides of this region, what means that the states have exchanged their delocalization properties: the state of the pair initially (i.e., for \( B < B_c \)) more spread, becomes more concentrated for \( B > B_c \) in spite of its higher ionization energy.

4. Concluding remarks

The highly non-linear and narrow spectral feature known as avoided crossing, which occurs between two energetically adjacent states of a hydrogen atom in strong magnetic fields, has been investigated from both dynamical and informational points of view. We have analyzed the variation of the ionization energy and the Shannon’s entropy of the states involved in these phenomena when the field strength is increased. We have used a highly efficient and accurate non-perturbative computational approach which combine three numerical algorithms: the discrete variable representation, the finite element method and a Krylov-type technique of matrix diagonalization.

From our computed results two main concluding remarks can be done. First, the avoided crossing phenomenon is a mechanism for state reordering with energy as the field strength is adiabatically changed, as shown by the known repulsion of the associated levels. Second, the involved states: (i) present maximal Shannon’s entropies for just around the critical field strength \( B_c \) of the irregular feature and (ii) exchange their...
informational characters as the system is taken through the avoided crossing region by varying the magnetic field. Then, the two states involved in the phenomenon keep their spectral relative positions but they do exchange their respective degrees of spatial delocalization across the irregular region. Moreover, the state with higher (smaller) values of ionization energy and entropy gets more localized (delocalized) in going through that region. So, the avoided crossing phenomenon is also a mechanism for state spatial localization exchanging as the field strength is adiabatically varied. We conjecture that the informational exchange, here quantitatively shown by means of the Shannon’s entropy, does not only occur between diamagnetic states with \( m = 0 \) and positive \( z \)-parity, but it is a general effect which takes places in the avoided crossing phenomena between atomic states under external electromagnetic fields when its strength is varied. Further related work is in progress [14].

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References