Hydrogen atom in a magnetic field: electromagnetic transitions of the lowest states

J.C. López Vieyra* and H. O. Pilón†

Instituto de Ciencias Nucleares, UNAM, Apartado Postal 70-543, 04510 México

(Dated: September 21, 2007)

Abstract

A detailed study of the lowest states $1s_0, 2p_{-1}, 2p_0$ of the hydrogen atom placed in a magnetic field $B \in (0 - 4.414 \times 10^{13} \text{ G})$ and their electromagnetic transitions ($1s_0 \leftrightarrow 2p_{-1}$ and $1s_0 \leftrightarrow 2p_0$) is carried out in the Born Oppenheimer approximation. The variational method is used with a physically motivated recipe to design simple trial functions applicable to the whole domain of magnetic fields. We show that the proposed functions yield very accurate results for the ionization (binding) energies. Dipole and oscillator strengths are in good agreement with results by Ruder et al. [10] although we observe deviations up to $\sim 30\%$ for the oscillator strength of the (linearly polarized) electromagnetic transition $1s_0 \leftrightarrow 2p_0$ at strong magnetic fields $B \gtrsim 1000 \text{ a.u.}$

PACS numbers: 31.15.Pf,31.10.+z,32.60.+i,97.10.Ld

*Electronic address: vieyra@nucleares.unam.mx
†Electronic address: horop@nucleares.unam.mx
I. INTRODUCTION

Contemporary X-ray space observatories, like Chandra, XMM-Newton and their predecessors, have collected a considerable amount of observational data of the thermal emission coming from surface layers of neutron stars which are characterized by enormous magnetic fields $B \sim 10^{12} - 10^{13}$ G (see [1], [2]). In particular, the observation of absorption features in the X-ray spectrum of some isolated neutron stars (see e.g. [3, 4]) has suggested possible models of atmospheres which allow the presence of Coulomb systems [5, 6, 7, 8]. The hydrogen atom is the simplest and most studied Coulombic system in weak and strong magnetic fields (see for example the early review [9] and references therein, and [10, 11, 12] for more recent studies).

In the present study our goal is to apply a physics recipe (described in full generality in [13]) for choosing variational trial functions to the study the hydrogen atom in a magnetic field and its electromagnetic transitions between the lowest bound states $1s_0$, $2p_{-1}$ and $2p_0$. The study is intended as a test of the methodology developed in [13]. Electromagnetic transitions in the hydrogen atom in the absence of a magnetic field is a widely described subject (see e.g. [14]). In a strong magnetic field such electromagnetic transitions have been studied by a number of authors, specially focusing on the effects of the transverse motion across the magnetic field direction (see e.g. [15, 16, 17, 18]).

Our consideration is non-relativistic, based on a variational solution of the Schroedinger equation. Thus, the magnetic field strength is restricted by the Schwinger limit $B = 4.414 \times 10^{13}$ G. Our study is also based on the Born-Oppenheimer approximation of zero order: the proton is assumed to be infinitely massive. Thus we neglect the effects of the CM motion i.e. the effects of the transverse motion of the atom with respect to the magnetic field orientation.

The study is realized in two steps: (i) a variational calculation of the states $1s_0$, $2p_{-1}$ and $2p_0$ is done with suitable trial functions (selected according to the physics recipe), and (ii) with the variationally obtained approximate wavefunctions we calculate the allowed radiative transitions among these states in the electric dipole approximation (see below).

Atomic units are used throughout ($\hbar=m_e=e=1$), albeit energies are expressed in Rydberg (Ry). The magnetic field $B$ is given in a.u. with $B_0 = 2.35 \times 10^9$ G, although frequently we will also use magnetic fields strengths given in Gauss for convenience.
A. Hamiltonian

The Hamiltonian which describes the Coulomb system formed by an infinitely massive proton and one electron (pe) placed in a homogeneous constant magnetic field directed along the z-axis, \( \mathbf{B} = (0, 0, B) \) is given by

\[
\hat{H} = \left( \mathbf{p} + \mathbf{A} \right)^2 - \frac{2}{r} = \mathbf{p}^2 - \frac{2}{r} + (\mathbf{p} \cdot \mathbf{A} + \mathbf{A} \cdot \mathbf{p}) + \mathbf{A}^2,
\]

(1)

where \( \mathbf{p} = -i\nabla \) is the electron momentum, \( r \) is the distance between the electron and the proton fixed at the origin, and \( \mathbf{A} \) is a vector potential corresponding to the magnetic field \( \mathbf{B} \). A contribution to the energy coming from the coupling between the electron intrinsic magnetic moment and the magnetic field \( \sim \hat{S} \cdot \mathbf{B} \), being constant, has been dropped from (1). Now, if we choose the vector potential in the symmetric gauge

\[
\mathbf{A} = \frac{B}{2}(-y, x, 0),
\]

the Hamiltonian acquires the form

\[
\hat{H} = -\Delta - \frac{2}{r} + \hat{l}_z B + \frac{B^2 r^2}{4},
\]

(2)

where \( \Delta \) is the Laplacian operator, and \( \hat{l}_z \) is the conserved z-component of the electron angular momentum. The Hamiltonian (2) is also invariant with respect to the z-parity \( \pi_z \) (i.e. reflections \( z \to -z \)). Thus the eigenstates can be classified by \( (m, \pi_z) \): the magnetic quantum number \( m \), corresponding to the conservation of \( \hat{l}_z \), and the z-parity quantum number \( \pi_z = \pm 1 \).

B. Choice of trial functions

The procedure which we use to explore the problem, is the variational method with a well defined recipe for choosing trial functions. This recipe is based on physical arguments, described in full generality in [13]. The basic ingredients are (i) for a given trial function \( \psi_{\text{trial}} \), the potential \( V_{\text{trial}} = \Delta \psi_{\text{trial}}/\psi_{\text{trial}} \), for which such function is an exact eigenfunction, should reproduce as many as possible the basic properties of the original potential, e.g. in the present case it should reproduce the Coulomb singularities and the harmonic oscillator behavior at small and large \( r \) distances respectively, and (ii) the trial function \( \psi_{\text{trial}} \) should
include the symmetries of the problem. For example, if the ground state is studied, the trial function $\psi_{\text{trial}}$ has to be a nodeless function. Adhering to this recipe, in [19] it was proposed the following function for the hydrogen ground state 1s$_0$

$$\Psi_{1s_0} = e^{-\sqrt{\gamma_1 r^2 + (\gamma_2 r^2 + \gamma_3 \rho^2 r + \gamma_4 \rho^3 + \gamma_5 \rho r^2) B^2 + \gamma_6 B^3 \rho^4 + \gamma_7 B^2 \rho^2 r^2}} ,$$

where $\gamma_1, \ldots \gamma_7$ are variational parameters. The potential associated with the function (3) reproduces the Coulomb singularity at $r \to 0$ as well as the harmonic oscillator for $r \to \infty$ of the original Hamiltonian (2). The function (3) has no nodes. In the following we will use the function (3) for the variational study of the ground state 1s$_0$.

For the lowest excited states 2p$_{-1}$, 2p$_0$ the presence of the magnetic field does not modify the nodal structure of the field-free exact eigenfunctions$^1$. A hint for this can be obtained in first order degenerate perturbation theory in $B^2$, where one can see that the states 2p$_{-1}$, 2p$_0$ are not mixed. Thus the following variational functions for the 2p$_{-1}$, 2p$_0$ states are proposed

$$\Psi_{2p_{-1}} = \rho e^{-i \phi} \psi_0 ,$$
$$\Psi_{2p_0} = z \psi_0 ,$$

where the functions $\psi_0$ have the same functional form as (3) but with their own $\gamma$-parameters. Thus, in the functions (4a), (4b) we keep the same polynomial prefactor as in the corresponding field-free wavefunctions and multiply them by a nodeless function. It is easy to check that the functions (3), (4a) and (4b) are orthogonal. These functions describe the lowest energy states, 1s$_0$, 2p$_{-1}$, 2p$_0$, among the states with quantum numbers $(m, \pi_z) = (0, +), (-1, +), (0, -)$ respectively, in all the range of magnetic fields studied.

II. ELECTROMAGNETIC TRANSITIONS

In a magnetic field the $m$-degeneracy of the hydrogen energy levels is fully removed and electromagnetic transitions depend explicitly on the magnetic quantum numbers of the initial and final states in the transition. A consideration of electromagnetic transitions in $^1 i.e. the nodal surfaces defined by the condition $\psi_{\text{trial}}(r, \theta, \phi) = 0.$
the electric dipole approximation is valid even in the case of high magnetic fields as long as transitions occur among states with the same Landau quantum number (in this case the characteristic wave lengths are always much larger than the (longitudinal or transverse) size of the system (see [10])). All the states considered in the present study belong to the same ground Landau-level and thus the electric dipole approximation is justified. Relevant formulas for the electromagnetic transitions in the hydrogen atom in a magnetic field were given in [20]. In the electric dipole approximation we are interested in the square of the matrix element (called dipole strength)

\[ d^{(q)}_{\tau',\tau} = |p^{(q)}_{\tau',\tau}|^2 = |\langle \tau' | r^{(q)} | \tau \rangle|^2, \]  

(5)

where \( \tau', \tau \) label the final and initial states in the transition, and \( r^{(q)} \) are the spherical components \( (q = 0, \pm 1) \) of the electric dipole operator. The oscillator strength of the transition is given by

\[ f^{(q)}_{\tau',\tau} = (E_{\tau'} - E_{\tau}) |p^{(q)}_{\tau',\tau}|^2, \]  

(6)

where \( (E_{\tau'} - E_{\tau}) \) is the (binding) energy difference of the initial and final states. The transition probability is calculated according to the relation

\[ w^{(q)}_{\tau',\tau} = \frac{1}{3\tau_0} (E_{\tau'} - E_{\tau})^3 |p^{(q)}_{\tau',\tau}|^2, \]  

(7)

where \( \frac{1}{\tau_0} = 8.03 \times 10^9 \text{sec}^{-1} \). We have two selection rules implicit in the matrix element \( p^{(q)}_{\tau',\tau} \) (eq. (5)) viz., parity change and

\[ \Delta m = 0, \pm 1, \]  

(8)

which implies \( q = \Delta m \). Thus, the transitions with \( \Delta m = 0 \) are characterized by a linearly polarized radiation along the magnetic field direction with \( q = 0 \), while the transitions with \( \Delta m = 1 \) are characterized by circularly polarized radiation with \( q = +1 \) (for right polarization), or \( q = -1 \) (for left polarization).
III. RESULTS

A. Binding Energies

The results of the variational calculations of the total \(E_T\) and binding energies for the lowest \(1s_0\), \(2p_{-1}\) and \(2p_0\) states of the hydrogen atom in a magnetic field ranging \(0.235 \times 10^9 \text{ G} \leq B \leq 4.414 \times 10^{13} \text{ G}\) are presented in Tables (I), (II) and (III) respectively. Results for binding energies of these lowest states are also summarized in Fig. (I). In this figure one can immediately see that the binding energy grows steadily as the magnetic field increases for all three states \(1s_0\), \(2p_{-1}\) and \(2p_0\). In particular, the ionization energy reaches \(\sim 0.4\text{keV}\) for a magnetic field at the Schwinger limit where \(B = 4.414 \times 10^{13}\text{ G}\). The increasing in binding energy as the magnetic field grows is faster (and comparable) for the bound states \(1s_0\), and \(2p_{-1}\) (increasing in \(\sim 20\) times for the domain \(B \sim 10^9 - 10^{13}\text{ G}\)) as compared with the rate of increase of the binding energy for the bound state \(2p_0\) (increasing only in \(\sim 2\) times for the domain \(B \sim 10^9 - 10^{13}\text{ G}\)). In fact the binding energy of the state \(2p_0\) approaches asymptotically to the value \(E_b = 1\text{Ry}\) as \(B \to \infty\) (see [21] and Table (III)).

For all states studied the results of the binding energies given by the simple trial functions (3), (4a), (4b) are, in general, in very good agreement with the approaches of Ruder et al. [10] and Kravchenko et al. [11]. For small to moderately high magnetic fields \((B \lesssim 1\text{ a.u.})\) the relative differences between our binding energies and those of [10, 11] are found to be \(\lesssim 10^{-4}\). It is worth to emphasize the remarkable coincidence in 9 digits for the ground state binding energy given by (3) and the today’s most accurate results of [11] in the domain of magnetic fields \(B \lesssim 0.1\text{ a.u.}\). The agreement of the binding energies with the corresponding perturbative results \(E^{1s_0}_b \simeq 1 + B - \frac{1}{7}B^2\), \(E^{2p_{-1}}_b \simeq \frac{1}{4} + 2B - 6B^2\), \(E^{2p_0}_b \simeq \frac{1}{4} + B - 3B^2\), obtained with a logarithmic perturbation theory (see [13, 22, 23] and references therein), is also very good.

However, the results for the binding energies of the three states studied obtained with the variational functions (3), (4a) and (4b) show that the accuracy gradually decreases as

\(^2\) The binding energy is defined as the energy difference between the energy of a free electron in the magnetic field \(B\) and the total energy \(E_T\), i.e. \(E_b = B(1 + |m| + m) - E_T\) (for states in the ground Landau-level).

\(^3\) The case of the ground state \(1s_0\) was analyzed in [19] with the trial function (3). However, in order to have precise numerical information of the variational parameters appearing in the trial function, we repeated the calculations done in [19] for all the magnetic fields quoted there.
the magnetic field increases and the relative differences for such binding energies (when compared with the corresponding results of references [10] and [11]) reach values $\sim 10^{-2}$ for $B \gtrsim 1000$ a.u. (see Tables (I), (II), (III)). It indicates that the adiabatic separation of the transverse and longitudinal degrees of freedom is slightly delayed in the functions (3), (4a) and (4b).

A comparison of the binding energies of the two lowest states $1_{s_0} (m = 0)$ and $2_{p_{-1}} (m = -1)$ with the asymptotic (adiabatic) formulas $E_b^{(m)} \simeq \log^2 \frac{B}{\sqrt{2|m|+1}}$ (see e.g. [11]) shows that, in both cases, the results given by this asymptotic formula are still far from the more accurate variational calculations, being different in about 3 times for the highest magnetic fields studied. For instance, at the magnetic field $B = 10000$ a.u. the adiabatic formula gives $E_b^{1_{s_0}} \simeq 85$ Ry and $E_b^{2_{p_{-1}}} \simeq 75$ Ry, while the present numerical results are $E_b^{1_{s_0}} = 27.96$ Ry and $E_b^{2_{p_{-1}}} = 21.56$ Ry, respectively (see Tables (I), (II)). Even the asymptotic binding energy difference $\Delta E_b^{\text{asympt}} \simeq 9.8$ Ry is about 1.5 times larger than the variational one $\Delta E_b^{\text{var}} \simeq 6.4$ Ry for such a magnetic field.

In practice, a full variational calculation is easily done in a standard desktop computer, it takes few minutes of CPU time.

B. Transitions

With the approximate wavefunctions (3), (4a) and (4b) found in the variational procedure described above, we carried out a study of the electromagnetic transitions between the states $2_{p_{-1}}, 2_{p_0}$ and the ground state $1_{s_0}$, i.e. $1_{s_0} \leftrightarrow 2_{p_{-1}}$ ($\Delta m = 1$), and $1_{s_0} \leftrightarrow 2_{p_0}$ ($\Delta m = 0$). The transition $1_{s_0} \leftrightarrow 2_{p_{-1}}$ occurs by absorption (emission) of circular-right-polarized radiation ($q = +1$), while the transition $1_{s_0} \leftrightarrow 2_{p_0}$ occurs by absorption (emission) of linearly-polarized (along the magnetic field direction) radiation ($q = 0$). Neither $2_{p_{-1}}$, nor $2_{p_0}$ have an excitation (de-excitation) mode to the ground state via left-polarized radiation.

The first remarkable observation concerning the electromagnetic transitions is the fact that, if for small magnetic fields the transition probabilities for both transitions are comparable in magnitude, for strong magnetic fields the (circularly polarized) transition $1_{s_0} \leftrightarrow 2_{p_{-1}}$ is strongly suppressed in comparison to the corresponding transition probability for the (linearly polarized) transition $1_{s_0} \leftrightarrow 2_{p_0}$ (see Fig. (4)). This phenomenon is a consequence of the strong deformation of the electronic distribution due to the enormous Lorentz force.
FIG. 1: Binding energies $E_b$ for the three lower states $1s_0, 2p_{-1}, 2p_0$ of the hydrogen atom as functions of magnetic field strength $B$. The curves show the calculated values of $E_b$ using the variational function (3) for the ground state $1s_0$ (marked by +), the function (4a) for the state $1p_{-1}$ (marked by ×), and the function (4b) for the state $1p_0$ (marked by *). The points corresponding to the same state are joined by line-segments.

acting on it, being elongated in the direction of the magnetic field, thus, enhancing the longitudinal polarization transition mode $q = 0$ with respect to the transverse transition modes $q = ±1$.

In the other extreme of small magnetic fields, perturbative results for the dipole and oscillator strengths and transition probabilities are given by [23]:

$$d_{1s_0\leftrightarrow 2p_{-1}}^{(+1)} \simeq 0.555 + 29.776 B^2,$$
$$f_{1s_0\leftrightarrow 2p_{-1}}^{(+1)} \simeq 0.416 - 0.555 B + 25.841 B^2,$$
$$w_{1s_0\leftrightarrow 2p_{-1}}^{(+1)} \simeq (6.266 - 25.066 B + 171.280 B^2) \times 10^8 \text{ sec}^{-1},$$

for the $1s_0 \leftrightarrow 2p_{-1}$ transition, and

$$d_{1s_0\leftrightarrow 2p_0}^{(0)} \simeq 0.555 + 9.388 \ B^2,$$
$$f_{1s_0\leftrightarrow 2p_0}^{(0)} \simeq 0.416 + 8.428 B^2,$$
$$w_{1s_0\leftrightarrow 2p_0}^{(0)} \simeq (6.266 + 126.894 B^2) \times 10^8 \text{ sec}^{-1},$$
FIG. 2: Dipole strengths $d^{(q)}_{r'\rightarrow r}$ for the transitions $1s_0 \leftrightarrow 2p_{-1}$, and $1s_0 \leftrightarrow 2p_0$ as functions of magnetic field strength $B$. The curves show the calculated values of the dipole strengths $d^{(+1)}_{1s_0\rightarrow 2p_{-1}}$ (marked by $\times$) and $d^{(0)}_{1s_0\rightarrow 2p_{0}}$ (marked by $+$) joined by line-segments.

for the $1s_0 \leftrightarrow 2p_0$ transition, where the magnetic field strength $B$ is in a.u. These results show different behaviors for both transitions. While for the $1s_0 \leftrightarrow 2p_0$ transition all quantities $d^{(0)}_{1s_0\rightarrow 2p_{0}}$, $f^{(0)}_{1s_0\rightarrow 2p_{0}}$ and $w^{(0)}_{1s_0\rightarrow 2p_{0}}$ are growing functions of $B^2$, in the case of the $1s_0 \leftrightarrow 2p_{-1}$ transition the oscillator strength $f^{(+1)}_{1s_0\rightarrow 2p_{-1}}$ and the transition probability $w^{(+1)}_{1s_0\rightarrow 2p_{-1}}$ slightly decrease for small increasing magnetic fields reaching a minimum for $B \simeq 10^{-2}$ a.u., and $B \simeq 10^{-1}$ a.u. respectively. For larger magnetic fields $B \sim 10^{-1}$ a.u. all quantities $d^{(0)}_{1s_0\rightarrow 2p_{0}}$, $f^{(0)}_{1s_0\rightarrow 2p_{0}}$, $w^{(0)}_{1s_0\rightarrow 2p_{0}}$ and $d^{(+1)}_{1s_0\rightarrow 2p_{-1}}$, $f^{(+1)}_{1s_0\rightarrow 2p_{-1}}$, $w^{(+1)}_{1s_0\rightarrow 2p_{-1}}$ are growing functions of $B^2$. As we go to higher (non-perturbative) magnetic fields the results obtained with the variational functions (3), (4a) and (4b) show that the dipole strengths and the oscillator strengths of both transitions eventually reach a maximum as the magnetic field grows after which they start to decrease monotonously in the region of high magnetic fields $B \gtrsim 1$ a.u. For the $1s_0 \leftrightarrow 2p_{-1}$ transition the maximum in the dipole strength $d^{(+1)}_{1s_0\rightarrow 2p_{-1}}(B)$ and the maximum in the oscillator strength $f^{(+1)}_{1s_0\rightarrow 2p_{-1}}(B)$ approximately coincide at $B \simeq 0.3$ a.u. The transition probability also shows a maximum for the same value magnetic field. In contrast, in the $1s_0 \leftrightarrow 2p_0$ transition the maximum in the dipole
FIG. 3: Oscillator strengths $f_{\tau'\tau}^{(q)}$ for the transitions $1s_0 \leftrightarrow 2p_{-1}$, and $1s_0 \leftrightarrow 2p_0$ as functions of magnetic field strength $B$. The curves show the calculated values of the oscillator strengths $f_{1s_0\rightarrow 2p_{-1}}^{(+1)}$ (marked with the symbol ×) and $f_{1s_0\rightarrow 2p_0}^{(0)}$ (marked with the symbol +) joined by line-segments.

strength $d_{1s_0\rightarrow 2p_0}^{(0)}(B)$ occurs for $B \simeq 0.3$ a.u. but the maximum in the oscillator strength $f_{1s_0\rightarrow 2p_0}^{(0)}(B)$ occurs for $B \simeq 2$ a.u. However, the transition probability $w_{1s_0\rightarrow 2p_0}^{(0)}(B)$ is an increasing function of the magnetic field (Fig. (I)).

Our results for $d^{(+1)}, f^{(+1)}, w^{(+1)}$ corresponding to the $1s_0 \leftrightarrow 2p_{-1}$ transition are in good agreement with the results in [10] in the whole domain of magnetic fields. The relative differences between our results for the dipole and oscillator strengths and the corresponding results in [10] are $\sim 10^{-5}$ for magnetic fields $B \sim 0.1$ a.u. increasing rather monotonously when the magnetic field grows being $\sim 10^{-3}$ at $B \sim 1000$ a.u. Our result for the transition probability are also in good agreement with the results in [10], the relative differences being $\sim 10^{-4} - 10^{-3}$ for magnetic fields $B \sim 0.1 - 100$ a.u. The largest relative difference $\sim 10^{-2}$ is observed at $B = 1000$ a.u. (see Table (II)).

Major differences occur in the case of the $1s_0 \leftrightarrow 2p_0$ transition. For instance, the relative differences between present results for the oscillator strengths and the corresponding results
FIG. 4: Transition probabilities $w^{(q)}_{\tau'\tau}$ for the transitions $1s_0 \leftrightarrow 2p_{-1}$, and $1s_0 \leftrightarrow 2p_0$. The curves show the calculated values of the transition probabilities $w^{(+1)}_{1s_0\rightarrow 2p_{-1}}$ (marked with the symbol ×) and $w^{(0)}_{1s_0\rightarrow 2p_0}$ (marked with the symbol +) joined by line-segments.

In [10] are $\sim 10^{-4}$ for magnetic fields $B \sim 0.1$ a.u. increasing with a magnetic field increase being $\sim 10^{-1}$ at $B \sim 1000$ a.u. The corresponding relative differences for the dipole strength are $\sim 10^{-4}$ for magnetic fields $B \sim 0.1$ a.u. increasing up to $\sim 0.3$ at $B = 1000$ a.u. A similar deviation is observed in the results for the transition probability for $1s_0 \leftrightarrow 2p_0$ where the relative difference is $\sim 10^{-4}$ for magnetic fields $B \sim 0.1$ a.u. and increasing up to $\sim 0.3$ at $B = 1000$ a.u. It is important to emphasize here that there exist no criterion for other observables, but the case of the total (or binding) energy, to decide about which values are more accurate.

In the domain of very strong magnetic fields ($B \gtrsim 10^{12}$ G) our results for dipole strengths of both transitions show the approximate scalings $d^{(0)}_{1s_0\rightarrow 2p_0} \sim \left(\frac{B}{B_0}\right)^{-2/3}$, and $d^{(+1)}_{1s_0\rightarrow 2p_{-1}} \sim \left(\frac{B}{B_0}\right)^{-1}$, accurate in $\lesssim 10\%$ and $\lesssim 1\%$ respectively. Likewise, the results for the oscillator strengths scale approximately as $f^{(0)}_{1s_0\rightarrow 2p_0} \sim \frac{3}{2} \left(\frac{B}{B_0}\right)^{-1/3}$, and $f^{(+1)}_{1s_0\rightarrow 2p_{-1}} \sim \left(\frac{B}{B_0}\right)^{-4/5}$, both accurate in $\lesssim 5\%$. 

11
Finally, in Fig. (5) we show the wavelengths \( \lambda = 2\pi/\alpha (E^f\prime_b - E^i_b) \) (\( \alpha \approx 1/137 \) is the fine structure constant and \( E^f\prime_b - E^i_b \) is the (variational) energy difference between the initial and final states) of the electromagnetic radiation associated with each transition as function of the magnetic field strength \( B \). From Fig. (5), we can see that the wavelength of the longitudinal polarized radiation in the transition \( 1s_0 \leftrightarrow 2p_0 \) is a monotonously decreasing function of the magnetic field, reaching the domain of X-rays for \( B \sim 10^{12} \) G, while the wavelength of the right polarized radiation corresponding to the transition \( 1s_0 \leftrightarrow 2p_{-1} \) increases for small to weak magnetic fields reaching a maximum\(^4\) for \( B \sim 0.2 \) a.u. (with \( \lambda_{\text{max}} \sim 1340.7 \) Å), and decreasing for larger magnetic fields. Yet, this transition remains always visible in the UV-region even for the stronger magnetic fields considered in the present study \( B \sim 10000 \) a.u.

Figures (2), (3) and (4) show the results of the calculations for the dipole strengths, oscillator strengths and transition probabilities (formulas (5), (6) and (7) respectively) for

\(^4\) Hydrogen transitions whose wavelengths go through maxima or minima as functions of the magnetic field are called stationary lines.
the transitions $1s_0 \leftrightarrow 2p_{-1}$, and $1s_0 \leftrightarrow 2p_0$ in the domain of magnetic fields $B \sim 0.1 - 10000$ a.u. Tables (IV) and (V) also show the results of those quantities for magnetic fields $B = 0 - 10000$ a.u.

IV. CONCLUSIONS

Along the present study we have used a variational approach with a physics recipe for choosing simple trial functions, as a test for an alternative method to study electromagnetic transitions in the hydrogen atom placed in a constant magnetic field. We assume that the proton is infinitely massive (Born-Oppenheimer approximation of zero order). It was found that the method yields very accurate results for the binding energies, in particular, for the lowest states studied $1s_0, 2p_{-1}, 2p_0$, in all the range of magnetic fields $B = 0 - 4.414 \times 10^{13}$ G. The results for binding energies show that the accuracy given by the simple 7-parametric trial functions (3), (4a) and (4b) is excellent for small magnetic fields $B \lesssim 0.1$ a.u., however it decreases monotonously as the magnetic field grows: the relative differences between the results given by the proposed trial functions (3), (4a) and (4b) and the today’s most accurate results [10] and [11] reach about $\sim 1\%$ for $B = 1000$ a.u. A possible explanation for this reduction in accuracy is the fact that transverse and longitudinal degrees of freedom ($\rho$ and $z$ respectively) in the trial functions (3), (4a) and (4b) appear ‘isotropically’ in the electron-proton distance $r$, preventing their adiabatic separation at $B \to \infty$.

Dipole $d^{(q)}(B)$, and oscillator strengths $f^{(q)}(B)$, of the electromagnetic transitions ($1s_0 \leftrightarrow 2p_{-1}$ and $1s_0 \leftrightarrow 2p_0$) were computed with the approximate wave functions (3), (4a), (4b) as functions of the magnetic field strength $B$. Our results for the $1s_0 \leftrightarrow 2p_{-1}$ transition are in very good agreement with the results of [10], with small deviations varying rather monotonously in $0.001 - 0.1\%$ for the interval of magnetic fields $B = 0.1 - 1000$ a.u. Major deviations between the present results and the results in [10] for the dipole and oscillator strengths were observed in the case of the $1s_0 \leftrightarrow 2p_0$ transition, where we have differences up to $\sim 30\%$ in the oscillator strength $f^{(0)}_{1s_0 \rightarrow 2p_0}(B)$ at $B = 1000$ a.u. A similar difference $\sim 30\%$ is obtained for the corresponding transition probability $w^{(0)}_{1s_0 \rightarrow 2p_0}(B)$. It is worth to emphasize that for a strong magnetic field $B \simeq 1000$ a.u. the transition probability $w^{(0)}_{1s_0 \rightarrow 2p_0}(B)$ is 3 orders of magnitude larger than the transition probability $w^{(+1)}_{1s_0 \rightarrow 2p_{-1}}(B)$ corresponding to the $1s_0 \leftrightarrow 2p_{-1}$ transition, so the difference in results for the transition probability $w^{(+1)}_{1s_0 \rightarrow 2p_{-1}}(B)$
might be of relevance for the analysis of the X-ray spectra of neutron stars.

It is important to mention that if for the variational binding energies there exists a criterion to decide which results given by different approximate wavefunctions are better (since variational binding energies approach from below to the true binding energies), there exists no similar criterion for other expectation values or matrix elements. Thus, it is not clear so far which results for dipole strengths are better. Therefore, more investigations on the electromagnetic transitions in the hydrogen atom in a magnetic field, specially in the domain of strong magnetic fields, would be desirable in order to answer this question.

Acknowledgments

This work was supported in part by DGAPA grant PAPIIT IN121106 (Mexico). The authors are heartily grateful to A. Turbiner for his valuable and numerous discussions, and for his careful readings of the manuscript.

[1] W. Becker and G. Pavlov, *Pulsars and isolated neutron stars*, Edited by Johan A. M. Bleeker, Johannes Geiss and Martin C.E. Huber, *The century of Space Science* Volume 1, Kluwer Academic Publishers, 721-758, (2001), astro-ph/208356
[2] V. E: Zavlin, *Thermal emission from isolated neutron stars: theoretical and observational aspects*, (2007); [astro-ph/0702426v1](#)
[3] D. Sanwal, G.G. Pavlov, V.E. Zavlin and M.A. Teter, “Discovery of absorption features in the X-ray spectrum of an isolated neutron star”, *ApJL*, 574, L61, (2002); [astro-ph/0206195](#)
[4] M.H. van Kerkwijk et al., *A strong, broad absorption feature in the X-ray spectrum of the nearby neutron star RX J1605.3+3249*, *ApJ*, 608, 432-443, (2004); [astro-ph/0311195](#)
[5] A.V. Turbiner and J.-C. Lopez Vieyra, *A hydrogenic molecular atmosphere of a neutron star*, *Mod.Phys.Lett.* A19, 1919-1923, (2004); [astro-ph/0404290](#)
[6] A. V. Turbiner, *A helium-hydrogenic molecular atmosphere of neutron star 1E1207.4-5209*, Contribution to *Physics Of Neutron Stars* - 2005, June 27 - 29, Ioffe Physico-Technical Institute, Saint-Petersburg, Russia (2005); [astro-ph/0506677](#)
[7] K. Mori and W.C.G. Ho, *Modelling mid-Z element atmospheres for strongly-magnetized neutron stars*, Mon. Not. R. Astron. Soc. **377**, 905-919, (2007); [astro-ph/0611145]

[8] K. Mori and J. S. Heyl, *Ionization and dissociation equilibrium in strongly magnetized helium atmosphere*, Mon. Not. R. Astron. Soc. **376**, 895-906, (2007); [astro-ph/0610253v2]

[9] R. H. Garstang, *Atoms in high magnetic fields*, Rep. Prog. Phys. **40**, 105, (1976)

[10] H. Ruder, G. Wunner, H. Herold and F. Geyer, Atoms in strong magnetic fields, Springer-Verlag, (1994)

[11] Yu. P. Kravchenko, M. A. Liberman and B. Johansson, *Exact Solution for a Hydrogen atom in a magnetic field of arbitrary strength*, Phys. Rev. **A54**, 287-305, (1996)

[12] B. M. Karnakov, and V. S. Popov, *A hydrogen atom in a superstrong magnetic field and the Zeldovich effect*, ZhETF **124**, 996-1022, (2003), JETP **97**, 890-914, (2003) (English Translation)

[13] A.V. Turbiner, *On Perturbation Theory and Variational Methods in Quantum Mechanics*, ZhETF **79**, 1719 (1980); Soviet Phys.-JETP **52**, 868, (1980) (English Translation); Usp. Fiz. Nauk. **144**, 35, (1984); Sov. Phys. – Uspekhi **27**, 668, (1984) (English Translation); Yad. Fiz. **46**, 204 (1987); Sov. Journ. of Nucl. Phys. **46**, 125, (1987) (English Translation); Doctor of Sciences Thesis, ITEP, Moscow, 1989 (unpublished), *Analytic Methods in Strong Coupling Regime (large perturbation) in Quantum Mechanics*

[14] I. I. Sobel’man, *Introduction To The Theory Of Atomic Spectra*, Pergamon Press Oxford - New York - Toronto - Sydney - Paris - Braunschweig, (1972)

[15] Cuvelliez, C. and Baye, D. and Vincke, M., *Center-of-mass corrections to the electromagnetic transitions of hydrogen atoms in strong magnetic fields*, Phys. Rev. A, **46**, 4055–4059, (1992)

[16] G.G. Pavlov and A.Y. Potekhin, *Bound-bound transitions in strongly magnetized hydrogen plasma*, ApJ. **450**, 883-895, (1995)

[17] A.Y. Potekhin, *Structure and radiative transitions of the hydrogen atom moving in a strong magnetic field*, J. Phys. **B27**, 1073-1090, (1994)

[18] A.Y. Potekhin, *Hydrogen atom moving across a strong magnetic field: analytical approximations*, J. Phys. **B31**, 49-63, (1998)

[19] A.Y. Potekhin and A.V. Turbiner, *Hydrogen atom in a magnetic field: the quadrupole moment*, Phys. Rev. **A63**, 065402, (2001)

[20] G. Wunner and H. Ruder, *Electromagnetic transitions for the hydrogen atom in strong mag-
TABLE I: Total $E_T$ and binding $E_b$ energies for the ground state $1s_0$ of the hydrogen atom in a magnetic field calculated with the variational function \( E_b \) compared with the results obtained by Ruder et al. \cite{10} and Kravchenko et al. \cite{11}. The values of the energies have been rounded to the first two non-coinciding digits respect to the values of \cite{11}.

| $B \times 10^9 G$ | $E_T$ (Ry)   | $E_b$ (Ry)   |
|-------------------|--------------|--------------|
| 0.235             | -0.99505296  | 1.09505296\(^a\) | 1.095053 | 1.09505296 |
| 1.0               | -0.9208225   | 1.3463544\(^a\) | -        | -        |
| 2.35              | -0.662332    | 1.662332\(^a\) | 1.662338 | 1.66233779 |
| 10.0              | 1.640362     | 2.614957\(^a\) | -        | -        |
| 23.5              | 6.50522      | 3.4948\(^a\) | 3.495594 | 3.49559433 |
| 100.0             | 36.8398      | 5.7134\(^a\) | -        | -        |
| 235.0             | 92.4356      | 7.564\(^a\) | 7.5781   | 7.57960847 |
| 1000.0            | 413.662      | 11.870\(^a\) | -        | -        |
| 2350.0            | 984.773      | 15.23\(^a\) | 15.3241  | 15.32484649 |
| 10000.0           | 4232.77      | 22.55\(^a\) | -        | -        |
| 23500.0           | 9972.0       | 27.96        | -        | -        |
| 44140.0           | 18750.5      | 32.5\(^a\)  | -        | -        |

\(^a\)Results of Ref. \cite{19}.
| $B \times 10^9 G$ | $E_T$ (Ry) | $E_b$ (Ry) |
|----------------|----------|----------|
| 0.235         | -0.3016912 | 0.40169120  |
| 1.0           | -0.232205  | 0.657737   |
| 2.35          | 0.08684    | 0.913163   |
| 10.0          | 2.64128    | 1.6140     |
| 23.5          | 7.75028    | 2.2497     |
| 100.0         | 38.6802    | 3.873      |
| 235.0         | 94.744     | 5.256      |
| 1000.0        | 416.975    | 8.557      |
| 2350.0        | 998.80     | 11.20      |
| 10000.0       | 4238.22    | 17.10      |
| 23500.0       | 9978.44    | 21.56      |
| 44140.0       | 18757.6    | 25.4       |

TABLE II: Total $E_T$ and binding $E_b$ energies for the state $2p_{-1}$ of the hydrogen atom in a magnetic field as given by the trial function (4a) compared with the results obtained by Ruder et al. [10] and Kravchenko et al. [11]. The values of the energies have been rounded to the first two non-coinciding digits respect to the values of [11].

| $B \times 10^9 G$ | $E_T$ (Ry) | $E_b$ (Ry) |
|----------------|----------|----------|
| 0.235         | -0.2248199 | 0.3248199 |
| 1.0           | -0.008703  | 0.434235  |
| 2.35          | 0.48008    | 0.5199    |
| 10.0          | 3.5779     | 0.6774    |
| 23.5          | 9.2359     | 0.7641    |
| 100.0         | 41.674     | 0.8796    |
| 235.0         | 99.074     | 0.9255    |
| 1000.0        | 424.561    | 0.9710    |
| 2350.0        | 999.016    | 0.9844    |
| 10000.0       | 4254.33    | 0.9938    |

TABLE III: Total $E_T$ and binding $E_b$ energies for the state $2p_0$ of the hydrogen atom in a magnetic field as given by the trial function (4b) compared with the results obtained by Ruder et al. [10] and Kravchenko et al. [11]. The values of the energies have been rounded to the first two non-coinciding digits respect to the values of [11].
| $B \times 10^9$G | Dipole Strength $d_{\text{1s0} \rightarrow \text{2p}_{-1}}^{(1)}$ | Ref. [10] | Oscillator Strength $f_{\text{1s0} \rightarrow \text{2p}_{-1}}^{(1)}$ | Ref. [10] | Transition Probability $w_{\text{1s0} \rightarrow \text{2p}_{-1}}^{(1)}$ | Ref. [10] |
|--------------|---------------------------------|----------|---------------------------------|----------|---------------------------------|----------|
| 0.0          | 0.55493                         |          | 0.41620                         |          | 6.2664                          |          |
| 0.235        | 0.64837 0.6484                  |          | 0.44955 0.4496                 |          | 5.7849 5.7852                   |          |
| 1.0          | 0.68681 -                        |          | 0.47295 -                       |          | 6.0030 -                        |          |
| 2.35         | 0.50133 0.5015                  |          | 0.37558 0.3757                 |          | 5.6423 5.6437                   |          |
| 10.0         | 0.18073 -                        |          | 0.18089 -                       |          | 4.8509 -                        |          |
| 23.5         | 0.08576 0.08584                 |          | 0.10678 0.1069                 |          | 4.4305 4.4313                   |          |
| 100.0        | 0.021987 -                       |          | 0.04046 -                       |          | 3.6683 -                        |          |
| 235.0        | 0.009581 0.009591               |          | 0.02212 0.02214                |          | 3.1552 3.1587                   |          |
| 1000.0       | 0.002296 -                       |          | 0.00761 -                       |          | 2.2355 -                        |          |
| 2350.0       | 0.0009837 0.0009847             |          | 0.00396 0.003985               |          | 1.7231 1.7474                   |          |
| 10000.0      | 0.0002325 -                      |          | 0.00127 -                       |          | 1.0068 -                        |          |
| 23500.0      | 0.0000992 -                      |          | 0.00063 -                       |          | 0.6950 -                        |          |
| 44140.0      | 0.0000529 -                      |          | 0.00038 -                       |          | 0.5165 -                        |          |

TABLE IV: Results for the electromagnetic transition $1s_0 \leftrightarrow 2p_{-1}$ in the hydrogen atom in a magnetic field $B$ obtained with the variational functions (3) and (4a) compared with the results of Ruder et al. [10] for the case of infinite nuclear mass. The units for the transition probability are $10^8$ sec$^{-1}$.

| $B \times 10^9$G | Dipole Strength $d_{\text{1s0} \rightarrow \text{2p}_{0}}^{(0)}$ | Ref. [10] | Oscillator Strength $f_{\text{1s0} \rightarrow \text{2p}_{0}}^{(0)}$ | Ref. [10] | Transition Probability $w_{\text{1s0} \rightarrow \text{2p}_{0}}^{(0)}$ | Ref. [10] |
|--------------|---------------------------------|----------|---------------------------------|----------|---------------------------------|----------|
| 0.0          | 0.55493                         |          | 0.41620                         |          | 6.2664                          |          |
| 0.235        | 0.60843 0.6083                  |          | 0.46864 0.4685                 |          | 7.4417 7.4401                   |          |
| 1.0          | 0.67290 -                        |          | 0.61377 -                       |          | 13.668 -                        |          |
| 2.35         | 0.58565 0.5902                  |          | 0.66905 0.6742                 |          | 23.372 23.549                   |          |
| 10.0         | 0.33129 -                        |          | 0.64189 -                       |          | 64.499 -                        |          |
| 23.5         | 0.21101 0.2252                  |          | 0.57621 0.6149                 |          | 115.01 122.69                   |          |
| 100.0        | 0.088027 -                       |          | 0.42551 -                       |          | 266.12 -                        |          |
| 235.0        | 0.050464 0.06217                |          | 0.33502 0.4135                 |          | 395.24 489.56                   |          |
| 1000.0       | 0.019169 -                       |          | 0.20893 -                       |          | 664.29 -                        |          |
| 2350.0       | 0.010898 0.01585                |          | 0.15522 0.2273                 |          | 842.82 1250.81                  |          |
| 10000.0      | 0.0043462 -                      |          | 0.093697 -                      |          | 1165.6 -                        |          |

TABLE V: Results for the electromagnetic transition $1s_0 \leftrightarrow 2p_{0}$ in the hydrogen atom in a magnetic field $B$ obtained with the variational functions (3) and (4b) compared with the results of Ruder et al. [10] for the case of infinite nuclear mass. The units for the transition probability are $10^8$ sec$^{-1}$.