Hydrogen and Helium atoms in strong magnetic fields

Anand Thirumalai and Jeremy S. Heyl
University of British Columbia, Vancouver, British Columbia, V6T 1Z1
(Dated: June 19, 2008)

The energy levels of hydrogen and helium atoms in strong magnetic fields are calculated in this study. The current work contains estimates of the ground and first few excited states of these systems that are improvements upon previous estimates. The methodology involves computing the eigenvalues and eigenvectors of the generalized two-dimensional Hartree-Fock partial differential equations for these one- and two-electron systems in a self-consistent manner. The method described herein is applicable to calculations of atomic structure in magnetic fields of arbitrary strength as it exploits the natural symmetries of the problem without assumptions of any basis functions for expressing the wave functions of the electrons or the commonly employed adiabatic approximation. The method is found to be readily extendable to systems with more than two electrons.

I. INTRODUCTION

The motivation to study atoms in magnetic fields of strength beyond the perturbative regime was in a large part due to the discovery of such fields being present in white dwarf stars [1,2,3] and neutron stars [4,5]. The most commonly observed neutron stars - pulsars, have been observed to have magnetic fields on the order of $10^{11} - 10^{13}$ G [6]. Magnetars [7], which are strongly magnetized neutron stars, can have magnetic field strengths well in excess of $10^{13}$ G. White dwarf stars on the other hand have somewhat less extreme fields, albeit still high, $\sim 10^6 - 10^8$ G [6]. At the high field strengths observed in these compact objects, the electron cyclotron energy of an atom becomes greater than the corresponding Coulomb potential energy, i.e. $\hbar \omega_B > Z e^2/r$. Here, $\omega_B$ is the cyclotron frequency. Thus, a Zeeman-type perturbative treatment of the field is not possible. The structure of atoms in both instances however, is considerably altered from the low field case. At high field strengths, spherical symmetry of the atom is broken and the atom is stretched along the field, however, azimuthal symmetry remains intact and thus it has been observed that it is more convenient to model the atom in cylindrical coordinates [6].

Since the 1970’s this problem has been tackled by various researchers using different methods. Hitherto, the most tractable and accurate approaches have relied upon an assumed basis of functions for expressing the electron wave functions of an atom in a strong magnetic field. Using such an assumption the problem of the hydrogen atom in a strong magnetic field was tackled using either a variational approach [9] or by attempting to solve the Schrödinger equation directly [10, 11, 12, 13, 14, 15, 16]. Initial attempts for estimating the energies and wave functions of different electronic states of the helium atom were based upon a purely variational approach [17, 18, 19, 20, 21, 22, 23, 24, 25] or $Z$-dependent perturbation theory [26]. The majority of these studies however were analytical and were therefore limited in their applicability to a problem that was inherently more tractable numerically. The most accurate and reliable solutions to the helium atom in a strong magnetic field, thus far, involved using the Hartree-Fock (HF) technique [27]. Employing the HF technique researchers in the past have calculated energy levels and wave functions of the ground and first few excited states of the helium atom and helium-like species [28, 29, 30]. These treatises employed Landau orbitals [8] to describe the motion of the electron perpendicular to the field. The electrons were required to reside in the ground Landau state, thereby simplifying calculations somewhat by restricting the wave functions to the so called adiabatic approximation [29]. Ivanov [31] in 1994 obtained similar results for the helium atom in strong magnetic fields using an unrestricted HF technique. Elsewhere, Quantum-Monte-Carlo methods were employed successfully for determining the ground and first few excited states of the helium atom in low to strong magnetic fields [32, 33, 34]. In the treatises described above [28, 29, 30, 31, 32, 33, 34], usually an approximation was employed for calculating both the direct and the exchange interactions between the electrons. Such approximations generally involved finding appropriate expansions that mimicked the behaviour of the inter-electron terms in the Hamiltonian. Necessarily, such an approach is limited by the accuracy of the expansions employed. In addition, this increases the complexity of the computational problem. Heyl & Hernquist [35] in 1998 described both an analytical as well as a numerical approximation for evaluating the effective inter-electronic potentials that was not only intuitive but also computationally less expensive. Their numerical technique extended the idea of adopting a basis of functions for the directions both transverse and parallel to the field. They constructed the wave function in the axial direction with the help of harmonic oscillator Hermite polynomials. This method was seen to yield accurate results for high magnetic fields $\beta_Z \geq 10^3$ for hydrogen and helium. They employed a method of calculating the total energy of the system given an assumed set of wave functions and then proceeded to minimise this energy by varying the free parameters of the wave functions. This was seen to yield accurate results consistent with other work [6]. One of the advantages over other methods [28, 29, 30, 31, 32, 33, 34] was observed to be the significantly lesser amount of computation involved.
More recently, Mori & Hailey [36] and Mori & Ho [37] adopted a perturbative approach to treat the exchange terms and higher Landau states with success for finding upper bounds for the energies for the ground and first few excited states of helium and other mid-Z atoms in high magnetic field strengths.

In the literature there are numerous studies outlining accurate estimates of the energies of different states of the hydrogen atom, however the number of investigations of the helium atom and helium-like species in the strong or intermediate magnetic field regime is rather small. The estimates of the energy levels of these species are only moderately accurate, and the computational expense is rather high. However, for most observable neutron stars and many white dwarf stars one must necessarily have more stringent bounds on the energy levels of atoms in the atmospheres of these compact objects in the intermediate regime of magnetic field strengths. This is the aim of the current work. The work described herein extends previous work [37] and presents a numerical treatment of hydrogen and helium atoms in magnetic fields, yielding accurate results for the eigenvalues and eigenvectors of the first few low-lying states over a wide range of field strengths in the intermediate field regime. The calculated energy eigenvalues are seen to be improvements upon previous estimates. The procedures described herein do not make any assumptions of basis of functions and neither are they restricted to the adiabatic approximation. The direct and exchange interactions of the electrons are computed using a novel method and do not rely upon any approximations. The method is readily extendable to many-electron systems and arbitrary field strengths. The overall method is also computationally straightforward to implement.

II. THE HYDROGEN ATOM

We shall begin with the Hamiltonian for the hydrogen atom in a magnetic field. The Hamiltonian for the single electron of the hydrogen atom in cylindrical coordinates is given by

$$\hat{H} = -\frac{\hbar^2}{2m_e} \left( \frac{1}{\rho} \frac{\partial}{\partial \rho} \left( \rho \frac{\partial}{\partial \rho} \right) + \frac{1}{\rho^2} \frac{\partial^2}{\partial \phi^2} + \frac{\partial^2}{\partial z^2} \right) + \mu_B B (l_z + 2s_z) + \frac{e^2 B^2}{8m_e} \rho^2 - \frac{Z e^2}{4\pi\epsilon_0 |\rho|}$$

(1)

where $m_e$ is the mass of the electron and the $B$ the magnetic field strength; the vector $\vec{B}$ is oriented along the positive z-axis. The remaining symbols have their usual meanings. It is of course implicitly assumed herein that the nucleus is infinitely massive. Let us assume a certain form for the wave function of the single electron

$$\Psi = \psi(\rho, z) e^{im\phi} \chi(s)$$

(2)

It can be seen immediately that such a choice precludes the use of a basis of functions for describing the behaviour of the electron both parallel and perpendicular to the magnetic field. Thus, the time-independent Schrodinger equation in units of Bohr radii can be written

$$\left[ -\left( \frac{1}{\rho} \frac{\partial}{\partial \rho} \left( \rho \frac{\partial}{\partial \rho} \right) + \frac{1}{\rho^2} \frac{\partial^2}{\partial \phi^2} + \frac{\partial^2}{\partial z^2} \right) + \frac{m^2}{\rho^2} + 2\beta(m - 1) + \frac{\beta^2 \rho^2 - \frac{2Z}{\sqrt{\rho^2 + z^2}}}{\rho} \right] \psi(\rho, z) = \epsilon \psi(\rho, z)$$

(3)

where $m$ is the azimuthal quantum number. In defining Eq. (3) it has been assumed that the electron spin is anti-aligned with the magnetic field. Additionally, the energy parameter $\epsilon$, is defined as

$$\epsilon = \frac{2E}{\alpha^2 m_e c^2} = \frac{E}{E_\infty}$$

(4)

$E_\infty$ is the Rydberg energy. The quantity $\alpha \approx 1/137$ is the fine structure constant. The parameter $\beta$ is defined in the usual way as

$$\beta = \frac{B}{B_0}$$

(5)

where $B_0$ is the critical field strength at which point the transition to the intense magnetic field regime occurs [6]. At this field strength the Larmor and the Bohr radii are equal in magnitude.

$$B_0 = \frac{2\alpha^2 m_e c^2}{\epsilon \hbar}$$

(6)

In general, the Larmor radius is related to the Bohr Radius via the equality $a_H = a_B \beta^{-1/2}$. Where $a_H$ and $a_B$ are the Larmor and Bohr radii respectively. Thus, beyond a value of $\beta \approx 1$ the transition to the intense magnetic field regime occurs and the interaction of the electron with the nucleus becomes progressively less dominant as $\beta$ increases. The Larmor radius is given by $a_H = \sqrt{\epsilon \hbar/2m_e}$ while the Bohr radius is given by the expression $a_B = \hbar/\alpha m_e c$. Based upon the above definition of $\beta$ in Eq. (5) it is convenient to classify the field strength [38] as low ($\beta \leq 10^{-3}$), intermediate, also called strong ($10^{-3} \leq \beta \leq 1$), and intense or high ($1 \leq \beta \leq \infty$).

It can be seen that Eq. (3) is a linear second order partial differential equation, and in the present study it was solved numerically on a computer using finite-element techniques. For details on the numerical treatment of Eq. (3) see §4.
III. THE HELIUM ATOM

For calculating the atomic structure of two-electron systems we adopt an iterative method, the so called self-consistent field method [27] which essentially solves the Hartree-Fock equations for the electrons. A short derivation of the key equations are given below assuming a single-configuration form for the atom as described above.

It is to be noted that no restrictions are imposed upon the atomic electrons such as the commonly employed adiabatic approximation [3].

A. Derivation of the generalized Hartree-Fock equations in partial differential form

Let us begin with the Hamiltonian of an $N$-electron atom split into one- and two-body terms

$$\hat{H} = \sum_i h_i + \sum_{j \neq i} w(r_i, r_j)$$  \hspace{1cm} (7)

The first part of the Hamiltonian consisting of one-body interactions is given by the standard prescription (using polar cylindrical coordinates)

$$h_i = -\frac{\hbar^2}{2m_e} \left( \frac{1}{\rho_i} \frac{\partial}{\partial \rho_i} \left( \rho_i \frac{\partial}{\partial \rho_i} \right) + \frac{1}{\rho_i^2} \frac{\partial^2}{\partial \phi_i^2} + \frac{1}{\rho_i^2} \frac{\partial^2}{\partial z_i^2} \right)$$

$$+ \mu_B B \left( \frac{\ell_i^2}{2} + 2s_i^2 \right) + \frac{e^2 B^2}{8m_e \rho_i^8} - \frac{Ze^2}{4\pi\epsilon_0 |\vec{r}_i|}$$ \hspace{1cm} (8)

where $i = 1, 2, ..., N$

And the two-body term in the Hamiltonian is simply the Coulomb interaction between the $i^{th}$ and $j^{th}$ electrons.

$$w(r_i, r_j) = \frac{e^2}{4\pi\epsilon_0 |r_i - r_j|}$$ \hspace{1cm} (9)

Let us assume that the wave function of a given configuration of electrons is given by

$$\Psi = A_N \psi_1 \psi_2 \psi_3 \ldots \psi_{N-1} \psi_N$$ \hspace{1cm} (10)

where, $A_N$ is the anti-symmetrization operator. Thus, it can be seen that a single slater determinant is assumed to represent the atomic configuration of all electrons. The single particle wave functions are assumed to be of the same form as assumed for the case of the hydrogen atom in Eq. (2); explicitly,

$$\Psi_i = \psi_i(\rho_i, z_i)e^{im\phi_i}\chi_i(s_i)$$ \hspace{1cm} (11)

where $i$ labels the electrons for each of the N electrons. The single particle wave functions $\psi_i(\rho_i, z_i)$ are taken to be real functions.

We shall look at only the fully spin-polarised states with each electron’s spin being anti-aligned with the magnetic field. This was considered to be a reasonable assumption as the magnetic fields in white dwarf stars and neutron stars are high enough for such states to be the most tightly bound states [3].

Writing the generalized Hartree-Fock equations for determining the single particle wave functions $\psi_i$ we have

$$h(r_i) \psi_i(r_i) + \sum_{j \neq i} \left[ \langle \psi_j(r_j)|w(r_i, r_j)|\psi_j(r_j)\rangle \psi_i(r_i) \right. - \left. \langle \psi_j(r_j)|w(r_i, r_j)|\psi_i(r_j)\rangle \psi_j(r_j) \right] = E_i \psi_i(r_i)$$ \hspace{1cm} (12)

where $i = 1, 2, 3, ..., N$

Substituting the ansatz given in Eq. (11), the assumed individual electron wave functions, into Eq. (12) we obtain after rearranging some terms

$$\left[ -\frac{1}{\rho_i} \frac{\partial}{\partial \rho_i} \left( \rho_i \frac{\partial}{\partial \rho_i} \right) + \frac{2 \beta Z(m_i - 1) + \beta Z^2 \rho_i^2 - \frac{2}{\sqrt{\beta Z^2 + 2}}}{\sqrt{\beta Z^2 + 2}} \right] \psi_i(\rho_i, z_i) e^{im\phi_i}$$

$$+ \frac{2 \beta Z}{\rho_i^8} \sum_{j \neq i} \left[ \langle \psi_j(\rho_j, z_j)e^{im\phi_j}|\frac{1}{|r_i - r_j|}\psi_j(\rho_j, z_j)e^{im\phi_j}\rangle \psi_i(\rho_i, z_i)e^{im\phi_i} \right. -$$

$$\left. \langle \psi_j(\rho_j, z_j)e^{im\phi_j}|\frac{1}{|r_i - r_j|}\psi_i(\rho_i, z_i)e^{im\phi_i}\rangle \psi_j(\rho_j, z_j)e^{im\phi_j} \right] = \epsilon_i \psi_i(\rho_i, z_i) e^{im\phi_i}$$ \hspace{1cm} (13)

where $i, j = 1, 2, 3, ..., N$

It is to be noted that the contribution due to electron
spin has been averaged out \textit{a priori}. We have chosen to work in units of Bohr radii along with the definitions given below. Additionally, hereafter the exponential factors with $im\phi$ are to be interpreted with the appropriate sign depending upon whether they are written in the bra or in the corresponding ket; a minus sign for the former and a plus sign for the latter. This interpretation should presently be applied to Eq. (13).

The Bohr radius for an atom of nuclear charge $Z$ is given by $a_B/Z$, with $a_B$ as defined earlier. The magnetic field strength parameter is defined as $\beta Z = B/B_Z = \beta/Z^2$. The reference magnetic field strength for nuclear charge $Z$, at which the transition to the intense magnetic field regime occurs is given by $B_Z = Z^2 B_0$ with $B_0$ as defined in Eq. (6). Finally, the energy parameter is defined as $\epsilon_i = E_i/(Z^2 E_\infty)$, with $E_\infty$ as defined in Eq. (4). The above written Eq. (13) represents the $N$-coupled Hartree-Fock equations in partial differential form for an $N$-electron system with nuclear charge $Z$. The system of equations is solved iteratively; see §4 for numerical details.

Of key concern in the computation of the eigenvalues and eigenvectors is the determination of the direct and exchange interactions between the electrons. In the current study these have been dealt with in a manner rather different from earlier treatises. In short, these contributions are essentially extra potentials that add to the existing single particle Hamiltonian, except they are coupled through the wave functions weighting them in a given equation in Eq. (13). The procedure employed for evaluating these potentials is described below.

### B. The direct interaction

The treatment of the direct and exchange potentials considered here and in the subsequent section is based upon rigorously determining these potentials by solving their corresponding elliptic partial differential equations. This is carried out in this study by employing the square of the individual electrons’ momentum operators $-i\hbar \nabla_i$. The details of method developed in this study are given below.

Let us first examine the integral representing the direct interaction between the electrons.

$$\Phi_D = \langle \psi_j(\rho_j, z_j)e^{im_j\phi_j} | \frac{1}{|\vec{r}_i - \vec{r}_j|} | \psi_j(\rho_j, z_j)e^{im_j\phi_j}\rangle$$

(14)

Let us act on both sides of Eq. (14) with the operator $\hat{p}_i^2 \equiv -\hbar^2 \nabla_i^2$, we then obtain

$$-\hbar^2 \nabla_i^2 \Phi_D = -\hbar^2 \langle \psi_j(\rho_j, z_j) e^{im_j\phi_j} | -4\pi \delta^3(\vec{r}_i - \vec{r}_j) | \psi_j(\rho_j, z_j)e^{im_j\phi_j}\rangle$$

(15)

Which then immediately yields

$$\nabla_i^2 \Phi_D = -4\pi |\psi_j(\rho_i, z_i)|^2$$

(16)

The RHS of Eq. (16) is the square of the $j^{th}$ electron’s wave function evaluated using the coordinates of the $i^{th}$ electron. Noting that Eq. (16) is simply the Laplace equation, it is observed that it is numerically tractable and solved using the appropriate boundary conditions to yield the potential $\Phi_D$ which is due to the direct interaction between the $i^{th}$ and $j^{th}$ electrons; see §4 for details on the numerical methods employed. It is to be noted however, that in contrast to previous work, the problem in Eq. (16) is somewhat simpler despite having to solve a partial differential equation as one does not have to find approximate expressions for the mixing terms arising from the interaction between different electronic states and the Coulomb potential. The reader is referred to \cite{29} and references therein for the different approximation methods employed in obtaining estimates for Eq. (14).

We now turn our attention to the other two-body term in Eq. (13); the exchange interaction.

### C. The exchange interaction

We shall follow the same methodology as in our treatment of the direct interaction term. Let us re-write the term in Eq. (13) that relates to the exchange interaction between the $i^{th}$ and $j^{th}$ electrons

$$\Phi_E = \langle \psi_j(\rho_j, z_j) e^{im_j\phi_j} | \frac{1}{|\vec{r}_i - \vec{r}_j|} | \psi_i(\rho_j, z_j)e^{im_i\phi_i}\rangle$$

(17)

Again, as in our previous treatment, let us act on both sides of Eq. (17) with the operator $\nabla_i^2$, this time dropping the redundant factor of $-\hbar^2$, to obtain

$$\nabla_i^2 \Phi_E = \langle \psi_j(\rho_j, z_j)e^{im_j\phi_j} | -4\pi \delta^3(\vec{r}_i - \vec{r}_j) | \psi_i(\rho_j, z_j)e^{im_i\phi_i}\rangle$$

(18)
Upon carrying out the integral we get

$$\nabla_i^2 \Phi_E = -4\pi \psi_i^* (\rho_i, z_i) \psi_i (\rho_i, z_i) e^{im_i - m_j} \phi_i,$$

(19)

It is to be noted that by the definition in Eq. (11) $\psi^* = \psi$ for the spatial part of the individual electron wave functions. At this stage, let us make the ansatz that

$$\Phi_E = \alpha_E (\rho_i, z_i) e^{im_i - m_j} \phi_i,$$

(20)

Let us act on both sides of Eq. (20) with the Laplacian operator, $\nabla_i^2$, to obtain

$$\nabla_i^2 \Phi_E = \left[ \frac{1}{\rho_i} \frac{\partial}{\partial \rho_i} \left( \rho_i \frac{\partial}{\partial \rho_i} \right) - \frac{(m_i - m_j)^2}{\rho_i^2} + \frac{\partial^2}{\partial z_i^2} \right] \alpha_E (\rho_i, z_i) e^{im_i - m_j} \phi_i,$$

(21)

It is then a straight-forward matter upon comparing Eq. (19) with Eq. (21) to immediately see that

$$\left[ \frac{1}{\rho_i} \frac{\partial}{\partial \rho_i} \left( \rho_i \frac{\partial}{\partial \rho_i} \right) - \frac{(m_i - m_j)^2}{\rho_i^2} + \frac{\partial^2}{\partial z_i^2} \right] \alpha_E (\rho_i, z_i) = -4\pi \psi_i^* (\rho_i, z_i) \psi_i (\rho_i, z_i)$$

(22)

The elliptical partial differential equation, Eq. (22) is solved numerically and we thus obtain an estimate for the function $\alpha_E (\rho_i, z_i)$ for each of the pair-wise interactions among the $N$ electrons. Knowing $\alpha_E (\rho_i, z_i)$ we can then obtain $\Phi_E$ according to Eq. (20). Once $\Phi_E$ and $\Phi_D$ have been obtained we can substitute them into Eq. (13) for the potentials due to the direct and exchange interactions respectively to obtain

$$\left[ \frac{1}{\rho_i} \frac{\partial}{\partial \rho_i} \left( \rho_i \frac{\partial}{\partial \rho_i} \right) + \frac{2}{\rho_i} \right] \psi_i (\rho_i, z_i) e^{im_i \phi_i} = \frac{m_i^2}{\rho_i^2} + 2 \beta_Z (m_i - 1) + \frac{\beta_Z^2 \rho_i^2}{2} - \frac{2}{\sqrt{\rho_i^2 + z_i^2}} \psi_i (\rho_i, z_i)$$

$$\frac{2}{Z} \sum_{j \neq i} \left[ \Phi_D \psi_i (\rho_i, z_i) e^{im_j \phi_j} - \alpha_E (\rho_i, z_i) e^{im_i - m_j} \phi_i \psi_j (\rho_i, z_i) e^{im_j \phi_j} \right]$$

(23)

Taking the inner product with $\int d\phi_i e^{-im_i \phi_i}$ on both sides of Eq. (23) we obtain; writing in a compact form,

$$\left[ \frac{-\nabla_i^2 (\rho_i, z_i) + \frac{m_i^2}{\rho_i^2} + 2 \beta_Z (m_i - 1) + \frac{\beta_Z^2 \rho_i^2}{2} - \frac{2}{\sqrt{\rho_i^2 + z_i^2}}} \psi_i (\rho_i, z_i)$$

$$\frac{2}{Z} \sum_{j \neq i} \left[ \Phi_D \psi_i (\rho_i, z_i) - \alpha_E \psi_j (\rho_i, z_i) \right] = \epsilon_i \psi_i (\rho_i, z_i)$$

(24)

where $i, j = 1, 2, 3, ..., N$

and $-\nabla_i^2 (\rho_i, z_i) = -\left( \frac{1}{\rho_i} \frac{\partial}{\partial \rho_i} \left( \rho_i \frac{\partial}{\partial \rho_i} \right) + \frac{\partial^2}{\partial z_i^2} \right)$

$$\epsilon_{total} = \sum_i \epsilon_i - \frac{1}{2} \frac{2}{Z} \sum_{j \neq i} \left[ \langle \psi_i (\rho_i, z_i) | \Phi_D \psi_i (\rho_i, z_i) \rangle - \langle \psi_i (\rho_i, z_i) | \alpha_E \psi_j (\rho_i, z_i) \rangle \right]$$

(25)

Eq. (24) is the final form for the generalized Hartree-Fock Equations and for two-electron systems we have two equations, however for arbitrary nuclear charge $Z$. The energy of the Hartree-Fock state is given by Eq. (25).

This completes our derivation of the Hartree-Fock equations for atoms in magnetic fields of arbitrary strength. The following section delineates the numerical procedures employed in the calculation of the energy
eigenvalues and eigenfunctions. Thereafter, results are presented and a discussion follows.

IV. NUMERICAL DETAILS

The eigenvalue problem for the hydrogen atom in Eq. (3) is solved by discretising the equation and solving the resultant algebraic eigenvalue problem. The discretisation is done using the finite-element method (FEM) \[39\]. The generalized eigenvalue problem is then solved using a sparse matrix generalized eigensystem solver \[40\]. This method was found to yield accurate results for the energy eigenvalues for the first few eigenstates with different azimuthal quantum number, \( m_l \). Runs were carried out for different values of the magnetic field strength parameter \( \beta \) in the range \( 10^{-2} \leq \beta \leq 10 \). For testing additional convergence for every run we employed six different levels of mesh refinement, ranging from coarse to sufficiently fine mesh. The fine mesh calculations took up to two days of computing time on AMD Opteron\(^\text{®} 844\) 1.8 GHz processors.

For solutions to the helium atom in strong magnetic fields an atomic structure software was developed as a part of this study for the purpose of calculating the energies of different states of multi-electron atoms. The program takes as its input, the number of electrons in the atom \( n_e \), the nuclear charge \( Z \), and the magnetic field strength parameter \( \beta \) and then proceeds to compute systematically the eigenvalues and eigenfunctions of the coupled system of equations in Eq (24) according to the iterative procedures described below in brief.

The Eqs. (16), (22) and (24) are solved in a three step process. First an initial estimate is obtained for the eigenvectors by solving Eq. (24) without the contributions due to the interaction between the electrons. The wave functions are then used as starting points for further improvements. The second step involves obtaining estimates for the potentials due to the direct and exchange interactions amongst the electrons, vis-a-vis, the elliptical partial differential Eqs. (16) and (22) are solved using the estimates for the wave functions obtained in the previous step. These estimates are then used to solve for better estimates of the eigenfunctions along with the relevant eigenvalues in Eq. (24). The last two steps are iterated in the order described above to obtain progressively better estimates for the eigenvalues and eigenvectors with each iteration. It was observed during our runs that fast convergence was achieved; within the first few iterations. A convergence criterion was employed wherein the difference between the solutions for two consecutive iterations was tested. If the difference was smaller than the desired tolerance for convergence then it was considered to be a solution of the iterative scheme. Typically, a tolerance on the order of \( 10^{-6} \) was employed. Thereafter, the total energy of the Hartree-Fock state under consideration is reported according to Eq. (25). Again as in the case of the hydrogen atom runs were carried out for different values of \( \beta \) with five different levels of mesh refinement in each case for additional convergence testing.

Once again, the generalized system of eigenvalue equations were solved using appropriate FEM discretisation yielding accurate results for the eigenvalues and eigenvectors for the first few low-lying states of helium. For details on the finite-element method the reader is referred to Ref. \[39\]. It was found that domain compactification was computationally expensive in terms of memory and computation time for obtaining sufficiently accurate results. On the other hand, limiting the domain size in the two orthogonal directions (parallel and perpendicular to the magnetic field) to several Bohr radii (\( \approx 20 \)) was observed to give accurate results for the range of magnetic field strengths considered in this study. Concordantly the computational expense was many times less in comparison to the former case. Numerical errors arising from truncating the domain were not significant (i.e. they were smaller than the discretization errors).

V. RESULTS & DISCUSSION

The results from the calculations carried out for hydrogen and helium atoms in strong magnetic fields are presented below. Only the results pertaining to the ground and first two excited states of these atoms in strong magnetic fields are given. It is to be mentioned that the present study focuses on calculations for magnetic field strength within the so called strong or intermediate regime \( (10^{-2} \leq \beta \leq 10) \).

A. The Hydrogen Atom

For magnetic fields in the range \( 10^{-2} \leq \beta \leq 10 \) the time-independent Schrödinger equation given in Eq.(3) was solved for different values of the magnetic field strength parameter. However only the results obtained for the most tightly bound states with azimuthal quantum number, \( m = 0, -1 \) and \(-2 \) are presented here. The binding energies are reported in Rydberg units. (The states with \( m > 0 \) become unbound with increasing magnetic field strength \[6\].)

The variation in the binding energy for the state corresponding to \( m = 0, \pi = +1 \) is shown in Figure [1]. The quantity \( \pi \) indicates parity with respect to the \( z \)-axis. The data points are eigenvalues obtained from the numerical solution of Eq. (3). The energy eigenvalues are reported as the values corresponding to infinitely fine mesh sizes, or in other words when the average area of the finite elements approaches zero. A short discussion of this estimation procedure is given later. As can be seen in the figure, the electron becomes more and more bound as the magnetic field strength increases. The line through the data represents a fit to the data. A rational function was used to model the data in this regime using a robust Levenberg-Marquardt method \[41\]. The values for
A range of magnetic fields from Table I. The maximum fractional error of the eigenvalue relative to the fit from $\beta = 10^{-4}$ to $\beta = 10^3$ follows the the list of coefficients.  

| State     | Coefficients | State     | Coefficients |
|-----------|--------------|-----------|--------------|
| $1s_0$    | $a_0 = 3.0849526$ | $a_0 = 3416640.9$ |
|           | $a_1 = 6.6571666$ | $a_1 = 12197155$ |
|           | $a_2 = -0.1404947$ | $a_2 = 4879198.1$ |
|           | $a_3 = 0.43176735$ | $a_3 = 425959.45$ |
|           | $b_0 = 3.0792681$ | $b_0 = 119957.96$ |
|           | $9 \times 10^{-3}$ | $b_1 = 5216732.1$ |
| $2p_{-1}$ | $a_0 = 0.58201924$ | $a_0 = 0.038324719$ |
|           | $a_1 = 13.769289$  | $a_1 = 2.7226023$  |
|           | $a_2 = 17.780336$  | $a_2 = 6.9791245$  |
|           | $a_3 = -0.52325377$| $a_3 = -0.5568026$ |
|           | $a_4 = 0.74135964$ | $a_4 = 0.4177192$  |
|           | $b_0 = 2.3266637$  | $b_0 = 0.34444067$ |
|           | $b_0 = 3.424245$   | $b_1 = 6.7184551$  |
|           | $3 \times 10^{-3}$ | $1 \times 10^{-2}$ |

The coefficients of the interpolating function are given in Table I. These rational functions accurately model the data in a range of magnetic fields from $\beta = 10^{-4}$ to $\beta = 10^3$ (twice the range indicated in Figure 1) and could potentially be used directly in atmospheric models for neutron stars and white dwarf stars. Having such accurate analytical forms for the energies of atoms in strong magnetic fields obviates the need for performing laborious calculations for the energy estimates making atmospheric models computationally less intensive. In addition, it becomes possible to analyze observed spectra of neutron and white dwarf stars with relative ease at arbitrary field strengths within the intermediate field regime. The fits to the data are rational functions obtained as described above. The functions have the form

$$f(x) = \frac{\sum_{i=0}^{n} a_i x^i}{x^{n-2} + \sum_{i=0}^{n-3} b_i x^i}$$

where $x = \ln(1+ \beta)$. The coefficients and the maximal fitting errors over the entire range $\beta = 10^{-4}$ to $\beta = 10^3$ are given in Table I. The data in the range $\beta = 10^{-2}$ to $\beta = 10$ are results from calculations of the present study while, to construct the fits for larger and smaller values of $\beta$ than the indicated range we used the results of Ref. [6].

As can be clearly seen in the figure the binding energy of the state of hydrogen with quantum numbers $m = 0, \pi = +1$ increases monotonically with increasing magnetic field strength. The dashed line in the graph represents a first order perturbation theory calculation. The purpose being to illustrate the fact that perturbation theory breaks down with increasing the magnetic field strength. It is evident upon inspection that the breakdown of perturbation theory occurs within the so called intermediate field regime. Thus arises the need for accurate data for the structure of atoms in this regime of magnetic field strength $10^{-2} \leq \beta \leq 10$.

Figure 2 shows variation in the binding energy the three most tightly bound states of the hydrogen atom with magnetic field strength, $\beta$. Explicitly, in order of decreasing binding energy, the three states $m = 0; \pi = +1$, $m = -1; \pi = +1$ and $m = -2; \pi = +1$, are plotted in Figure 2. Again the lines through the data points represent fits to the data. Every data point in these figures was obtained as an estimate corresponding to limit of the finite element size going to zero; see later. It can be seen in Figure 2 that the binding energy of the different states increases dramatically after $\beta \approx 1$. Thereafter, the binding energy increases at an increasing rate with increasing magnetic field strength.

It is to be noted that, in all cases, the rational functions were so chosen as to reflect the fact that eventually at large values of the magnetic field strength parameter $\beta$ the energy would be proportional to $\ln^2 \beta$ [8]. For the sake of comparison with previously determined accurate results, the fit to the calculated data for the ground state of hydrogen corresponding to $m = 0, \pi = +1$ is plotted against the calculated data of the researchers in Ref [8] in Figure 3. The line through their data is a spline fit. As can be seen in the figure, the two lines are nearly com-

![FIG. 1: Figure showing the variation in the binding energy of the ground state of hydrogen $m = 0, \pi = +1$ with the magnetic field strength parameter in the range $10^{-2} \leq \beta \leq 10$.

The energy is reported in units of Rydberg energy. The data points are results of the numerical calculation while the line represents a fit to the data. The dashed line represents the results from first order perturbation theory.](image-url)
FIG. 2: Figure showing the variation in the binding energies of three lowest \( m \)-states of hydrogen corresponding to \( m = 0, -1, -2 \), with \( \pi = +1 \) with the magnetic field strength parameter in the range \( 10^{-2} \leq \beta \leq 10 \). The energy is reported in units of Rydberg energy. The data points are results of the numerical calculation while the lines represent fits to the data.

FIG. 3: Figure showing the variation in the binding energies of the state of hydrogen corresponding to \( m = 0 \) with \( \pi = +1 \) with the magnetic field strength parameter in the range \( 10^{-2} \leq \beta \leq 10 \). Results from both the present study as well as those from Ref. [6] are plotted herein. The energy is reported in units of Rydberg energy. The line through the data from Ref. [6] is a spline fit. With regard to the current study, the data points are results of the numerical calculation while the line represents a fit to the data.

The differences were seen to be in the fifth or sixth decimal place between the results of the present study and those of Ruder et al [6]; or in other words the results were considered to be of comparable accuracy. For details of the energy eigenvalues obtained in this study the reader is referred to Table III in the appendix to this paper.

Figure 4 shows how the eigenvalues obtained from the solution of Eq. (3) depend upon the mesh size. As was mentioned earlier, the calculations were carried out on a finite domain of several Bohr radii in each of the two directions both parallel and perpendicular to the field. While keeping the domain fixed, the number of finite elements constituting the mesh was varied. Runs were performed on each mesh size for every value of magnetic field strength considered in the study for each of the three states of hydrogen, \( m = 0, -1 \) and \(-2 \). The eigenvalues thus obtained were plotted against the average area per finite element in the mesh corresponding to each value of the magnetic field strength parameter \( \beta \). Extrapolation of the data to the limit of zero mesh size in each case yielded the values that would correspond to an infinitely fine mesh. These values were reported as the calculated data points in the preceding figures. The reader is referred to Ref. [41] for details regarding the method employed. The average accuracy of the estimate of the asymptotic value was determined to be on the order of \( 3 \times 10^{-6} \) Rydbergs. Such estimation errors were too small to be shown on the plots. The line through the data points is merely a guide to the eye.

The wave functions for the most tightly bound state of hydrogen \( m = 0, \pi = +1 \) are plotted in Figure 5 for four different values of the magnetic field strength \( \beta \). The plots represent a slice through the three dimensional atom in the upper half of the \( r-z \)-plane. The complete representation in three dimensions is the figure of revolution about the \( z \)-axis and simultaneously reflected about the \( xy \)-plane. The length units are Bohr radii of the hydrogen atom and the \( x \)-axis represents the direction perpendicular to the magnetic field direction while the \( y \)-axis represents the direction parallel to the magnetic field, i.e. the \( z \)-direction in three dimensional cylindrical polar coordinates. The purpose here is to illustrate the dramatic change that occurs near \( \beta \approx 1 \) when the electron becomes tightly bound and the binding energy increases dramatically with increasing \( \beta \). It is immediately evident upon inspection that the spherical symmetry of the atom is clearly broken as we approach higher and higher magnetic field strengths.
FIG. 4: Figure showing a plot of the eigenvalues calculated as a function of the area per finite element in the mesh for a calculation for the ground state of hydrogen at $\beta = 10^{-2}$. With increasingly finer meshes for a sufficient domain size the eigenvalue obtained approaches an asymptote corresponding to the limit of infinitely fine mesh. The parameter describing the mesh size is the average area per finite element in the mesh.

**B. The Helium Atom**

For magnetic fields in the range $10^{-2} \leq \beta \leq 10$ we solved the set of coupled Hartree-Fock equations given in Eq. (24) for different values of the magnetic field strength parameter. We shall however be showing the results obtained for the states corresponding to $M = 0, -1$ and $-2$ corresponding to the three most tightly bound states of helium. The two electrons are taken to possess azimuthal quantum numbers given by $m_1$ and $m_2$ respectively with $M = m_1 + m_2$. We consider here in the study only the fully spin-polarised states, thus each of the electrons has its spin anti-aligned with the magnetic field as assumed in the derivation of Eq. (24). These states have been seen to be the most tightly bound states of helium in strong magnetic fields [2]. It is to be noted that the binding energies are reported in units of Rydberg energy in the Coulomb potential of nuclear charge $Ze$ (alternatively called atomic units or simply a.u.)

At the very outset, as a preliminary test of the Hartree-Fock atomic structure software developed as part of this study, we carried out calculations for the binding energy of the $^1S_0$ singlet state of neutral helium without any magnetic field ($B = 0$ case). However, in this case the wave function of the configuration of electrons is completely symmetrized with respect to the spatial part of the total wave function while the spins of the two electrons are anti-parallel to each other. With these changes Eq. (24) was solved using the numerical procedures outlined in §4 and the energy reported according to Eq. (25). The runs were carried out for different mesh sizes over the domain and the final eigenvalue is reported after extrapolating to the limit of infinitely fine mesh as described above. The eigenvalue obtained using this procedure was 1.4499 a.u., while the most accurately determined result via numerical techniques thus far is 1.4519 a.u [42]. The difference is about $2 \times 10^{-3}$ a.u. This was considered to be sufficiently accurate given the fact the calculations carried out as part of this study were single-configuration calculations while the result from Ref. [42] is essentially a multi-configuration calculation which is a computationally more intensive method. Thus, the atomic structure software developed for this study was considered to be sufficiently accurate for the purposes of the current study.

The variations in the binding energies for the most tightly bound states corresponding to $M = -1, -2$ and 0 with $S_z = -1$ are shown in Figure 6. The data points are eigenvalues obtained from the numerical solution of Eq. (24) according to the numerical procedures described.

**FIG. 5:** Figure showing a plot of the change in the real part of the wave functions, i.e. $\psi(\rho, z)$, of the ground state of the hydrogen atom with varying magnetic field strength. The wave functions show the ground state of hydrogen with quantum numbers $m = 0, s_z = -1/2$ and $\pi = 1$ in magnetic fields of strength corresponding to (a) $\beta = 10^{-2}$, (b) $\beta = 10^{-1}$, (c) $\beta = 1$ and (d) $\beta = 10$. It can be clearly seen that as the magnetic field strength increases so does the binding energy as indicated by the clear shrinking of the wave function with increasing $\beta$. These plots are not to be confused with electron density.
The energy eigenvalues are once again reported as the values corresponding to infinitely fine mesh sizes, estimated according to the discussion above; see Figure 10 and discussion thereof. As in the case of hydrogen, runs were performed on each mesh size for every value of magnetic field strength considered in the study for each of the three states of helium, \( M = 0, -1 \) and \(-2\). These eigenvalues were extrapolated using rational functions \([11]\) to the limit of zero mesh size. Eigenvalues obtained by this extrapolation procedure are reported as the calculated data points in Figure 6. The average accuracy of the estimate of the asymptotic value was determined to be on the order of \(2 \times 10^{-5}\) Rydbergs. Again, for details regarding the extrapolation method, the reader is referred to Ref. [11]. As can be seen in Figure 6, the binding energy of the state increases with increasing magnetic field strength \(\beta_Z\). The line through the data represents a fit to the data. In addition, a good measure of the discretization error was considered to be the difference between the computed eigenvalues for the most finely refined mesh size employed and the extrapolated result for the mesh size tending to zero. This error associated with the discretization of the problem is reported in the number appearing in the parentheses in Tables IV, V and VI in the appendix to this paper; the number therein corresponds to the absolute error in the fifth decimal place. Concordantly, the error bars were too small to be shown on the plots.

Again a rational function was used to model the data in this regime using a robust Levenberg-Marquardt method \([11]\). The values of the coefficients of the interpolating functions are given in Table \([\11]\). It is to be noted at this juncture that the rational functions were so chosen as to reflect the fact that eventually, for large values of the magnetic field strength parameter \(\beta_Z\), the binding energies are proportional to \(\ln^2 \beta_Z\). With this in mind, the aim was to find an accurate analytical function that described the variation in binding energy over a wide range of \(\beta_Z\) such that it employed the least number of parameters. Inspection of Table \([\11]\) reveals that this was accomplished with five free parameters for modeling the data in the range of magnetic field strength \(10^{-2} \leq \beta_Z \leq 10\). Potentially, as was noted earlier, these analytical functions can be employed with relative ease in atmospheric models directly, thus circumventing the need for both laborious calculations of the energies via HF methods and simultaneously avoiding the need for spline interpolations of tabulated data of binding energies. The maximum errors in the fits are also provided in Table \([\11]\).

As can be clearly seen Figure 6, the binding energies increase monotonically with increasing magnetic field strength. Beyond \(\beta_Z \approx 2.5 \times 10^{-1}\) which corresponds to \(\beta \approx 1\) the departure from spherical symmetry of the atom becomes more pronounced as the magnetic field strength increases; see Figure 10. This is indicated by the steep rise in the curves signifying the increasing rate at which the binding energies increase with increasing magnetic field strength.

For the sake of comparison with previously determined results, the fits to the calculated data for the three most tightly bound states of helium corresponding to \(M = -1, -2\) and 0 with \(S_Z = -1\) are plotted against the calculated data of the researchers in Refs. [6] and Refs. 32, 33 in Figures 7, 8 and 9. The lines through the data of the other researchers are spline fits. It can be seen that the rational functions used to fit the calculated eigenvalues for the binding energies of the three states of the helium atom are consistent with previous work. In particular they are seen here to be improvements upon the estimates of Ruder et al [6] over the entire range of \(\beta_Z\) considered in this study. Jones et al on the other hand had employed a Monte-Carlo approach [32] for solving the HF equations. They assumed a large number of basis functions with variable parameters that could be fine tuned within the framework of Monte-Carlo simulations to arrive at upper bounds for the energies. Though this method is effective, as can be seen from their estimates shown in Figures 7, 8 and 9 it is computationally demanding and it restricts the wave functions of the electrons to be expressed using a finite number of basis functions. The method described in the current study does not impose such a condition and thus the wave functions that are determined are in effect superpositions of a very large number of such basis functions and arise naturally from the solution itself. However, it is to be mentioned...
that for high magnetic field strength parameter $\beta_z \approx 10$ for the state $M = -1$ and $\beta_z \approx 20$ for the states $M = -2$ and 0, the eigenvalues were seen to drop below those of Jones et al’s estimates; see Figures 7,8 and 9. It is to be noted that this effect was due to insufficient computer memory to carry out calculations with the desired mesh refinement at high magnetic field strengths where the electrons are tightly bound to the nucleus and their wave functions shrink closer to the nucleus; see Figure 10. With sufficient computer memory it is expected that the results presented here can be extended to higher magnetic field strengths.

In Figure 7, it can be seen that the estimates of the present study are improvements upon the estimates of Ruder et al [6]. The long-dashed line representing the data of the researchers in Ref. 6 has a kink at about $\beta_z = 1$, this is because they used cylindrical rather than spherical coordinates at this stage for solving the eigenvalue problem. The eigenvalues obtained are seen to be better estimates than those of Jones et al [32, 34] in the range $10^{-2} \leq \beta_z \leq 2 \times 10^{-1}$ by about 7% maximum and 4% minimum. However above that field strength, the estimates of the current study fall below those of Refs. 32, 34 by about 2% maximum. Since the present study is a numerically less complicated technique, thus it was expected that the Monte-Carlo simulations of Jones et al [32, 34] would arrive at a result slightly better than those of the current study given the limitations of computing memory at higher magnetic field strengths. However, one of the aims of the current work to was facilitate a numerically straightforward and computationally less intensive method for computing the energies of atoms in strong magnetic fields and in that regard the results obtained herein were considered to be good.

In Figures 8 and 9, it can be seen that estimates of the binding energies of the first and second excited states of the helium atom in strong magnetic fields are consistent with the findings of other researchers [6, 32, 34]. The range of improvements were between 11% maximum to about 1% minimum over the entire range $10^{-2} \leq \beta_z \leq 10$ relative to the eigenvalues obtained by the the researchers in Refs. 32, 34. Towards higher magnetic field strengths it was observed that the improvements in the estimates tended to drop; this is due to the fact that at such high magnetic field strengths for obtaining more accurate estimates of the energies, greater computer memory was required to accommodate for finer meshes and this was not possible within the framework of the current project. On the other hand, it can be seen that the results of the current work presented in Figures 7, 8 and 9 are seen to be on average 8% improvements relative to the results obtained by Ruder et al [6]; the reader is referred to Tables IV, V and VI, provided in the appendix to this paper, for exact eigenvalues of the three most tightly bound states of helium calculated in this study. A comparison with the results of other researchers can also be found therein. Once again the kinks in the curves in Figures 8 and 9 of the results of Ruder et al [6] at around $\beta_z \approx 1$ are due to the fact that they changed from a spherical to a cylindrical representation of the wave functions.

Finally, the wave functions for one of the electrons in the most tightly bound state determined from the calculations are plotted in Figure 10 for four different values of the magnetic field strength $\beta_z$. For the purpose of illustrating the dramatic change in the structure of the atom with increasing magnetic field strength we chose to show the electron in the state with quantum numbers $m = -1, s_z = -1/2, \pi_z = +1$, which is equivalent to $2p_{-1}$ orbital in the low field limit. The length units are Bohr radii of the helium atom, i.e. $a_0/Z$ and the $x$-axis represents the direction perpendicular to the magnetic field direction while the $y$-axis represents the direction parallel to the magnetic field, i.e. the $z-$ direction in three dimensional cylindrical coordinates. It can be seen that the electron becomes more and more tightly bound and the binding energy consequently increases dramatically with increasing $\beta_z$. It can be seen that comparing Figure 10(d) with Figures 10(a-c) that the electron wave function shrinks considerably over the range of magnetic field strengths considered in the current study.
FIG. 8: Figure showing the variation in the binding energies of the state of helium corresponding to $M = -2$ with $\pi_z = +1$ with the magnetic field strength parameter in the range $10^{-2} \leq \beta_Z \leq 10$. Results from both the present study as well as those from Ref [6] and Jones et al [32, 34] are plotted herein. The energy is reported in units of Rydberg energy for nuclear charge $Z_e$. The data points are results of the numerical calculation while the lines represent fits to the data.

TABLE II: Table listing the coefficients of the different rational functions for fitting the three states of helium discussed. The maximum fractional error of the eigenvalue relative to the fit from $\beta_Z = 10^{-2}$ to $\beta_Z = 10^1$ follows the list of coefficients in each case.

| State     | Coefficients State | Coefficients |
|-----------|--------------------|--------------|
| $M = -1$  | $a_0 = 0.19161951$ | $a_0 = 0.56302392$ |
|           | $a_1 = 1.8523924$  | $a_1 = 2.5417308$  |
| $1s_0; 2p_{-1}$ | $a_2 = 1.5767066$ | $a_2 = 1.2729779$ |
|           | $a_3 = 0.10192465$ | $a_3 = 0.1570292$  |
|           | $b_0 = 0.1655611$  | $b_0 = 0.4756007$  |
|           | $1 \times 10^{-2}$ | $6 \times 10^{-3}$  |

VI. CONCLUSIONS

The work described here was motivated by the need to have accurately determined values for the upper bounds for the energy levels of atoms in strong magnetic fields. As was discussed earlier, this need has arisen due to the presence of strong magnetic fields in neutron stars and white dwarf stars. The most commonly present atoms in the atmospheres of these compact objects, hydrogen and helium were studied here with the intention of obtaining accurate estimates of the energy levels of the first few low lying states in strong magnetic fields. We described a method adopting a physically motivated approach governed by the inherent symmetries of the problem. We simultaneously circumvented the need for adopting a definite basis of functions to describe the wave functions of the electrons in either of the directions, parallel and perpendicular to the magnetic field. The approach is unrestrictive with regard to the wave function; it has the distinct advantage over methods that require a basis of functions to describe the wave functions because in numerical solutions one can only have a finite number of such functions. The wave functions determined in the present study came about naturally from the symmetries of the problem and are thus in effect superpositions of a large number of basis functions.

Such an approach however resulted in elliptical partial differential equations for the electrons that were subsequently solved using finite element techniques. It is to be noted that the novel method adopted for determining the direct and exchange interactions between the electrons in
corresponding to (a) the most tightly bound state of helium with quantum numbers \( m_1 = 1, n_2 = 1/2, \pi = +1 \) in magnetic fields of strength corresponding to (a) \( \beta Z = 10^{-2} \), (b) \( \beta Z = 10^{-1} \), (c) \( \beta Z = 1 \) and (d) \( \beta Z = 10 \). It can be clearly seen that as the magnetic field strength increases so does the binding energy as indicated by the clear shrinking of the wave function with increasing \( \beta Z \). These plots are not to be confused with electron density.

the helium atom is also exact in the sense that it does not rely upon any ab initio assumptions to approximate the integrals. These interaction potentials are solved in a natural manner by solving the elliptical partial differential equations, Eqs. (16) and (22). The eigenvalues found in the range of the magnetic field strength parameter \( 10^{-2} \leq \beta Z \leq 10 \) considered in this study were seen to be consistent with previous findings \([3, 32, 34]\). Rational functions were also used to find sufficiently accurate interpolating functions for the binding energies of various states of both the hydrogen and helium atoms in the range of magnetic fields considered herein. These were seen to be accurate to (an average for all six fits) within 0.8%. Potentially such interpolating functions could be used in atmosphere models of neutron stars and white dwarf stars thus obviating the need for involved and laborious calculations of the same.

Thus, the current work describes an unrestricted and computationally less intensive method for calculating the energy levels of atoms in strong magnetic fields. There are in essence three directions in which the current work could be extended. First, the current work can be readily extended to higher magnetic field strengths by changing the domain of calculations appropriately to incorporate the fact that the electrons become more and more bound. Simultaneously, the calculations and the software developed as a part of this study are readily extendable to systems with more than two electrons, i.e., Li, Be, B, C, O etc. Finally, the procedures implemented herein can also be extended towards a multi-configuration framework \([43]\). In essence, the calculations employed herein are for a single configuration of the electrons. Thus having found the energies of the different configurations, it is possible to extend the theory to incorporate a multi-configuration approach which is likely to improve the results already obtained here.

FIG. 10: Figure showing a plot of the real part of the wave functions, i.e. \( \psi(\rho, z) \), of one of the electrons comprising the ground state of the helium atom with changing magnetic field strength. The wave functions show the outer electron in the most tightly bound state of helium with quantum numbers \( m_1 = -1, n_2 = 1/2, \pi = +1 \) in magnetic fields of strength corresponding to (a) \( \beta Z = 10^{-2} \), (b) \( \beta Z = 10^{-1} \), (c) \( \beta Z = 1 \) and (d) \( \beta Z = 10 \). It can be clearly seen that as the magnetic field strength increases so does the binding energy as indicated by the clear shrinking of the wave function with increasing \( \beta Z \). These plots are not to be confused with electron density.

[1] J. C. Kemp, J. B. Swedlund, J. D. Landstreet, and J. R. P. Angel, ApJ 161, L77+ (1970).
[2] J. R. P. Angel, ARA&A 16, 487 (1978).
[3] J. R. P. Angel, E. F. Borra, and J. D. Landstreet, ApJ 45, 457 (1981).
[4] J. Trümper, W. Pietsch, C. Reppin, and B. Sacco, in Eighth Texas Symposium on Relativistic Astrophysics, edited by M. D. Papagiannis (1977), vol. 302 of New York Academy Sciences Annals, pp. 538+.
[5] J. Truemper, W. Pietsch, C. Reppin, W. Voges, R. Staubert, and E. Kendziorra, ApJ 219, L105 (1978).
[6] H. R. et al, Atoms in Strong Magnetic Fields: Quantum Mechanical Treatment and Applications in Astrophysics and Quantum Chaos, Astronomy and Astrophysics Library (Springer-Verlag, New York, 1994).
[7] R. C. Duncan and C. Thompson, ApJ 392, L9 (1992).
[8] L. Landau and E. Lifshitz, Quantum Mechanics (Non-relativistic Theory), Third Edition (Butterworth Heinemann, MA, 2003).
[9] V. Camuto and D. C. Kelly, ApSS 17, 277 (1972).
[10] H. C. Praddaude, Phys. Rev. A 6, 1321 (1972).
[11] J. Simola and J. Virtamo, Journal of Physics B Atomic Molecular Physics 11, 3309 (1978).
[12] H. Friedrich, Phys. Rev. A 26, 1827 (1982).
[13] G. Wunner and H. Ruder, Astron. & Astroph. 89, 241 (1980).
[14] W. Roesner, H. Herold, H. Ruder, and G. Wunner, Phys. Rev. A 28, 2071 (1983).
[15] W. Roesner, G. Wunner, H. Herold, and H. Ruder, Journal of Physics B Atomic Molecular Physics 17, 29 (1984).
[16] M. V. Ivanov, Journal of Physics B Atomic Molecular Physics 21, 447 (1988).
[17] R. Cohen, J. Lodenquai, and M. Ruderman, Physical Review Letters 25, 467 (1970).
[18] R. J. Henry, R. F. O’Connell, E. R. Smith, G. Chanmugam, and A. K. Rajagopal, Phys. Rev. D 9, 329 (1974).
[19] R. O. Mueller, A. R. P. Rau, and L. Spruch, Phys. Rev. A 11, 789 (1975).
[20] B. Banerjee, D. H. Constantinescu, and P. Rehák, Phys.
### APPENDIX A: TABLES OF BINDING ENERGIES

TABLE III: Table listing the binding energies of the three most tightly bound states of hydrogen. Energies are in units of Rydbergs. The states are labeled according to their counterparts in the low-field limit. Results from Ref. [6] are also provided for comparison. The number in the parentheses is the absolute error at the fifth decimal place; this is determined as the difference between the computed eigenvalues for the most finely refined mesh size employed and the extrapolated result for the mesh size tending to zero.

| \( \beta \) | Present Study | Ref. [6] | Present Study | Ref. [6] | Present Study | Ref. [6] | Present Study | Ref. [6] |
|-----|---------------|----------|---------------|----------|---------------|----------|---------------|----------|
|     | 1s_0          | 1s_0     | 2p_{-1}       | 2p_{-1}  | 3d_{-2}       | 3d_{-2}  |
| \( 1 \times 10^{-2} \) | 1.0198(1) 0.10198 | 0.2876(1) 0.2876 | 0.1614(0) 0.1614 | \( 2 \times 10^{-2} \) | 1.0392(1) 0.10392 | 0.3209(1) 0.3209 | 0.1982(0) 0.1982 | \( 5 \times 10^{-2} \) | 1.0951(1) 0.10951 | 0.4017(2) 0.4017 | 0.2757(0) 0.2757 | \( 7 \times 10^{-2} \) | 1.1304(1) 0.11304 | 0.4452(2) 0.4452 | 0.3144(1) 0.3144 | \( 1 \times 10^{-1} \) | 1.1808(1) 0.11808 | 0.5010(3) 0.5011 | 0.3626(1) 0.3626 | \( 2 \times 10^{-1} \) | 1.3293(1) 0.13292 | 0.6427(5) 0.6427 | 0.4820(2) 0.4820 | \( 5 \times 10^{-1} \) | 1.6624(1) 0.16623 | 0.9132(20) 0.9132 | 0.7061(9) 0.7061 | \( 7 \times 10^{-1} \) | 1.8324(0) 1.8323 | 1.0420(34) 1.0420 | 0.8125(18) 0.8125 | \( 1 \times 10 \)   | 2.0445(2) 2.0444 | 1.1992(60) 1.1992 | 0.9423(36) 0.9423 | \( 2 \times 10 \)   | 2.5616(3) 2.5616 | 1.5756(37) 1.5757 | 1.2540(21) 1.2540 | \( 5 \times 10 \)   | 3.4956(5) 3.4956 | 2.2507(188) 2.2508 | 1.8164(122) 1.8164 | \( 7 \times 10 \)   | 3.9225(6) 3.9224 | 2.5604(353) 2.5605 | 2.0758(230) 2.0758 | \( 10 \times \)     | 4.4308(14) 4.4308 | 2.9303(630) 2.9310 | 2.3872(451) 2.3873 |
TABLE IV: Table listing the binding energies of the most tightly bound state of helium in moderate to large magnetic fields; $M = -1, S_z = -1, \pi_z = +1$. Energies are in units of Rydberg energies in the Coulomb potential of nuclear charge $Z_e$, where $Z = 2$ for helium. The results from the current work can be compared readily with previous work by the researchers in Refs. [6, 31, 32, 34]. The number in the parentheses is the absolute error at the fifth decimal place; this is determined as the difference between the computed eigenvalues for the most finely refined mesh size employed and the extrapolated result for the mesh size tending to zero.

| $\beta Z$ | Present Study | Ref. [6] | Ref. [31] | Ref. [32] | Ref. [34] |
|-----------|---------------|----------|-----------|-----------|-----------|
| $1 \times 10^{-2}$ | 1.1993(6)     | 1.1182   | 1.1183    | 1.1177    |
| $2 \times 10^{-2}$ | 1.2335(8)     | 1.1609   | 1.1183    |           |
| $5 \times 10^{-2}$ | 1.3303(19)    | 1.2658   | 1.2683    | 1.2683    | 1.1810    |
| $7 \times 10^{-2}$ | 1.3912(20)    | 1.3258   | 1.3303    |           |
| $1 \times 10^{-1}$ | 1.4684(24)    | 1.4069   | 1.4150    | 1.4151    |
| $2 \times 10^{-1}$ | 1.6754(34)    | 1.6270   | 1.6509    | 1.6508    | 1.4151    |
| $5 \times 10^{-1}$ | 2.1191(84)    | 2.0508   | 2.1475    | 2.1490    | 1.7511    |
| $7 \times 10^{-1}$ | 2.3425(135)   | 2.2329   | 2.3927    | 2.5039    |
| $1$          | 2.6204(233)   | 2.4675   | 2.6897    | 2.7000    | 2.1492    |
| $2$          | 3.4246(117)   | 3.2394   | 3.4333    | 3.7003    |
| $5$          | 4.6439(435)   | 4.5899   | 4.7441    | 3.7139    |
| $7$          | 5.2071(803)   | 5.3408   |           |           |
| $10$         | 5.9402(865)   | 5.9206   | 6.0506    |           |

TABLE V: Table listing the binding energies of the low-lying state of helium; $M = -2, S_z = -1, \pi_z = +1$. Energies are in units of Rydberg energies in the Coulomb potential of nuclear charge $Z_e$, where $Z = 2$ for helium. The results from the current work can be compared readily with previous work by the researchers in Refs. [6, 32, 34]. The number in the parentheses is the absolute error at the fifth decimal place; this is determined as the difference between the computed eigenvalues for the most finely refined mesh size employed and the extrapolated result for the mesh size tending to zero.

| $\beta Z$ | Present Study | Ref. [6] | Ref. [31] | Ref. [32] | Ref. [34] |
|-----------|---------------|----------|-----------|-----------|-----------|
| $1 \times 10^{-2}$ | 1.2078(8)     | 1.0828   | 1.0832    | 1.0830    |
| $2 \times 10^{-2}$ | 1.2424(8)     | 1.1207   |           |           |
| $5 \times 10^{-2}$ | 1.3225(11)    | 1.2097   | 1.2155    | 1.2160    |
| $7 \times 10^{-2}$ | 1.3616(12)    | 1.2596   | 1.2690    |           |
| $1 \times 10^{-1}$ | 1.4249(20)    | 1.3266   | 1.3412    | 1.3436    |
| $2 \times 10^{-1}$ | 1.6293(27)    | 1.5073   | 1.5401    | 1.5503    |
| $5 \times 10^{-1}$ | 2.0607(64)    | 1.8508   | 1.9806    | 1.9945    |
| $7 \times 10^{-1}$ | 2.2774(102)   | 1.9935   | 2.1800    | 2.2171    |
| $1$          | 2.5469(195)   | 2.2572   | 2.4362    | 2.4933    |
| $2$          | 3.2599(89)    | 2.9683   | 3.1634    |           |
| $5$          | 4.4344(536)   | 4.2161   | 4.3693    |           |
| $7$          | 4.9853(1023)  | 4.9203   |           |           |
| $10$         | 5.6321(2077)  | 5.4492   | 5.5770    |           |
TABLE VI: Table listing the binding energies of the low-lying state of helium; $M = 0, S_z = -1, \pi_z = -1$. Energies are in units of Rydberg energies in the Coulomb potential of nuclear charge $Z_e$, where $Z = 2$ for helium. The results from the current work can be compared readily with previous work by the researchers in Refs. [6, 31, 32, 34]. The number in the parentheses is the absolute error at the fifth decimal place; this is determined as the difference between the computed eigenvalues for the most finely refined mesh size employed and the extrapolated result for the mesh size tending to zero.

| $\beta Z$   | Present Study | Ref. [6] | Ref. [32] | Ref. [31] | Ref. [31] |
|-------------|---------------|----------|-----------|-----------|-----------|
| $1 \times 10^{-2}$ | 1.2014(22)    | 1.1016   | 1.1018    | 1.1016    |
| $2 \times 10^{-2}$ | 1.2338(22)    | 1.1314   |           |           |
| $5 \times 10^{-2}$ | 1.3068(23)    | 1.2028   | 1.2098    | 1.2099    | 1.1465    |
| $7 \times 10^{-2}$ | 1.3436(24)    | 1.2421   | 1.2551    |           |
| $1 \times 10^{-1}$ | 1.3944(28)    | 1.2933   | 1.3174    | 1.3174    |
| $2 \times 10^{-1}$ | 1.5497(33)    | 1.4197   | 1.4914    | 1.4914    |
| $5 \times 10^{-1}$ | 1.8968(49)    | 1.5864   | 1.8571    | 1.8593    | 1.5654    |
| $7 \times 10^{-1}$ | 2.0713(63)    | 1.7833   | 2.0349    | 2.0404    |
| 1            | 2.2875(85)    | 2.0304   | 2.2431    | 2.2641    |
| 2            | 2.8989(83)    | 2.6037   | 2.7989    |           |
| 5            | 3.8400(488)   | 3.5916   | 3.7466    | 3.0024    |
| 7            | 4.2688(857)   |          |           | 4.1762    |
| 10           | 4.7805(1655)  | 4.5560   | 4.6862    |           |