Carbon atom in intense magnetic fields

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(Received 11 September 2014; published 5 November 2014)

The energy levels of the first few low-lying states of carbon in intense magnetic fields upwards of $\approx 10^7$ T are calculated in this study. We extend our previously employed pseudospectral approach for calculating the eigenstates of the carbon atom. We report data for the ground state and a low-lying state that are in good agreement with findings elsewhere, as well as additional data for ten other states of the carbon atom. It is seen that these latter states also become strongly bound with increasing magnetic field strengths. The data presented in this study are relevant for astrophysical applications, such as magnetized white dwarf and neutron star spectral analysis as well as opacity calculations and absorption features, including in the context of material accreting onto the surfaces of these compact objects.

DOI: 10.1103/PhysRevA.90.052501 PACS number(s): 31.15.ac, 31.15.xr

I. INTRODUCTION

The study of atoms in magnetic fields of strength beyond the perturbative regime was largely motivated by the discovery of strong fields present in white dwarf stars [1–3] and neutron stars [4,5]. Pulsars, which are the most commonly observed neutron stars, harbor intense magnetic fields on the order of 10^7–10^9 T [6]. Magnetars [7], which are strongly magnetized neutron stars, can have field strengths well in excess of 10^9 T. White dwarfs possess somewhat weaker but nevertheless still strong magnetic fields, with strengths $\sim 10^2$–10^5 T [6]. Even at these somewhat lower white dwarf field strengths, atomic structure is considerably altered from the low-field case, and a Zeeman-type perturbative treatment of the field [8] is not possible.

The need to calculate atomic structure in high magnetic fields has gained considerable impetus in recent years. It is emerging from x-ray observations that neutron star atmospheres may contain mid-Z neutral atoms, especially carbon [9,10], cosmochemically one of the most important elements. Interpretation of the emergent spectra is hindered by the lack of atomic data pertinent to the extreme environment of neutron star atmospheres. The presence of strong electric as well as magnetic fields has a profound influence on the emergent spectra, altering the energy levels and ionization potentials and affecting ion population distributions at different energy levels. The ubiquitous effects of line broadening further complicate spectral analysis. It is remarkable that even for the simpler case of no electric field, and relatively weak (for a neutron star) magnetic field $B \sim 10^6$ T, photoionization edges and spectral lines differ significantly from those in the field-free case. A considerable amount of atomic data is therefore required for accurately interpreting the spectra of neutron stars.

Similarly, observations of white dwarfs are also motivating study of atoms in intense magnetic fields. A sizable number of white dwarfs are highly magnetized, with magnetic fields around or in excess of 10^5 T (see [11] for a short review). It is also now emerging that about 25% of white dwarfs are contaminated with mid-Z atoms such as carbon, silicon, phosphorus, and sulfur [12,13]. The existence of such contaminants in white dwarf atmospheres has been a surprise, because stellar evolution models predict largely H or He atmospheres (DA or DB white dwarfs, respectively), with heavier species sinking on relatively short time scales $\sim 10^2$ yr [e.g., 13]. The heavier atoms (such as silicon, phosphorus, and sulfur) are predominantly present in hotter white dwarfs where they are still radiatively levitated before submerging, although some observations reveal that even cooler white dwarfs show such contaminants [12]. Carbon meanwhile has been observed in a large variety of white dwarfs, both hot and cooler ones. To reconcile these observations, an exogenous source is therefore argued for, and it is becoming understood that white dwarfs often accrete the remnants of planetary systems. Such observations are being used to determine planetary compositions in these erstwhile systems [13]. Recently, a DQ white dwarf (spectra distinguished by the presence of carbon lines), SDSS J142625.71 + 575218.3, has been observed to harbor a magnetic field of strength $\sim 1.2 \times 10^5$ T [14], further motivating the need for atomic data for carbon in intense magnetic fields, such as energy levels of different orbitals alongside electron densities, with data for oscillator strengths for bound-free and free-free transitions, to facilitate spectral analysis.

An additional need for basic atomic data stems from the realization that in the atmospheres of magnetized white dwarfs and neutron stars, the atomic orbitals of adjacent atoms may bond via a new mechanism, the so-called perpendicular paramagnetic bonding, which can lead to strongly bound H_2, He_2 [15], and possibly other species as well. In these highly magnetized astrophysical objects, even simple atoms behave completely differently from their terrestrial counterparts. It is such considerations that have motivated the current study. We present below a short review of the literature pertaining to this field of study. The reader is referred to a recent article [16] for a more detailed review of this area or research.

Due to the impossibility of achieving such high magnetic field strengths in laboratory settings, atomic data for high-B atoms have traditionally been derived using modeling. A variety of techniques has been used by various researchers since the 1970s, mostly applied to the hydrogen atom [17–26] and many recent studies of helium [27–45] in strong magnetic fields.

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Studies have also been conducted for molecules and chains of both hydrogen and helium atoms relevant to neutron star magnetic fields [46–53]. Recent investigations by Thirumalai and Heyl [54] using single-configuration Hartree-Fock (HF) theory [55] was seen to yield accurate upper bounds for the energies of hydrogen and helium in strong magnetic fields. A follow-up study [56] obtained accurate energy estimates for helium and lithium atoms in strong magnetic fields using a pseudospectral method. This approach was seen to be computationally far more economical than using the earlier finite-element-based approach [54].

In contrast to the somewhat simpler two-electron systems, relatively little work exists in the literature for atoms with more than two electrons in strong magnetic fields. One of the first studies to investigate atoms in intense magnetic fields, in particular the iron atom, was by Flowers *et al.* [57] in 1977. This variational study extended the work due to the authors in Ref. [58] and obtained binding energies of iron atoms and condensed matter in magnetic fields relevant to neutron stars. Errors in this study were later corrected by Mueller [59]. Other methods such as density-functional studies [60,61] and the Thomas-Fermi-Dirac method [62,63] were also employed for estimating binding energies of atoms in intense magnetic fields. Recently, Medin and Lai [49,50] have also studied atoms and molecules and infinite chains of condensed matter in magnetic fields greater than 10^8 T, using density-functional theory. Mori and co-workers [34,35] have studied mid-Z atoms in strong to intense magnetic fields using perturbation theory as well, obtaining results consistent with previous findings.

The first comprehensive HF studies of atoms with more than two electrons were carried out by Neuhauser *et al.* [64,65] for magnetic fields greater than 10^8 T, thus being directly relevant to neutron stars. Elsewhere, HF studies of atoms and molecules in intense magnetic fields were conducted by Demuer *et al.* [66], with results consistent with previous findings. All of the above treatises, Refs. [57–66], concern themselves with magnetic fields in excess of 10^8 T, well into the so-called intense magnetic field regime. At these field strengths, the interaction of the electron with the nucleus of the atom becomes progressively less dominant, in comparison to its interaction with the field itself.

Various fully computational methods have been brought to bear on the case of atoms with more than two electrons in strong fields. One of the first studies to carry out a rigorous HF treatment of atoms with more than two electrons in strong or intermediate field strengths was Ref. [30]. Therein, they obtained estimates of the Hartree-Fock energies of a few low-lying states of lithium and carbon atoms, in low to strong magnetic fields. In recent years, Ivanov [67] and Ivanov and Schmelcher [43,44,68–71] have carried out detailed HF and post-HF studies of multielectron atoms using a numerical mesh method for solving the unrestricted HF equations [43]. The special meshes were constructed so as to facilitate finite-difference calculations in a two-dimensional domain using carefully selected mesh node points [72]. Using this method they were able to ascertain the energy landscape of the first few low-lying states of low-Z atoms such as lithium and beryllium and mid-Z atoms such as boron and carbon, etc. Al-Hujaj and Schmelcher [73,74], adopting a full configuration-interaction method and using a Gaussian basis for the electron wave functions [36–42], obtained accurate estimates of the energies of lithium and beryllium atoms in strong magnetic fields. The sodium atom in a strong magnetic field has also been studied by González-Férez and Schmelcher [75], obtaining estimates for the binding energies. Elsewhere, low-lying states of the lithium atom have also been studied in strong magnetic fields using a configuration-interaction method, employing the so-called freezing full-core method [76,77]. Initially, electron correlation was considered only in the inner k shell [76] with correlation between the core and the outer electron neglected; however in a later study correlation between all the electrons was included to yield an additional contribution to the energy [77]. Using such an approach the beryllium atom and ion have also been investigated in strong magnetic fields, yielding accurate estimates of the energies [78]. In recent years Engel and Wunner and co-workers [79–83] have computed accurate results for several atoms in magnetic fields relevant to neutron stars with a variety of techniques involving finite-element methods with B splines both in the adiabatic approximation and beyond the adiabatic approximation with more than one Landau level. These highly accurate formulations employ a fast parallel Hartree-Fock-Roothan code, in which the electronic wave functions are solved for along the z direction, with Landau orbitals (and combinations of more than one level in the latter studies) describing the remaining parts of the wave functions. Elsewhere, different *ab initio* quantum Monte Carlo approaches [84,85] have also been successfully employed to determine the ground states of atoms and ions in strong magnetic fields. Recently excited states of helium have also been computed quite accurately in intense magnetic fields using a fixed-phase quantum Monte Carlo approach [86].

Recently, in very comprehensive studies, Schimeczek *et al.* [81,82] and Boblest *et al.* [87] obtained accurate estimates of the ground-state energies of atoms and ions up to $Z = 26$, with only a few seconds' worth of computing time for helium and heliumlike atoms. Such speeds are essential for coupling atomic structure codes with atmosphere models and spectral analysis codes for magnetized white dwarfs and neutron stars. While these investigations concerned themselves with the ground state, a recent study by Thirumalai and Heyl [88] employed a fast pseudospectral approach for computing accurately the first few low-lying states of helium and lithium in intense magnetic fields. They obtained data for two additional states of lithium which were observed to become tightly bound with increasing magnetic field strength. By virtue of spectral convergence, the computational times of this approach were seen to be on the order of seconds for heliumlike systems, while maintaining accuracy.

The current study extends the approach due to Thirumalai and Heyl [88] to the carbon atom, investigating the first few low-lying states that become tightly bound in the limit of intense magnetic fields. The reader is referred to Ref. [88] for the two-dimensional HF equations as well as for details regarding their solution employing pseudospectral methods. This article is arranged as follows. In Sec. II we briefly describe the numerical methodology adopted for solving the eigensystem. In Sec. III we present and discuss the results. Finally in Sec. IV we present conclusions and briefly describe avenues for further investigation.

II. NUMERICAL DETAILS

For the carbon atom, the HF equations consist of six coupled equations. The general form for the two-dimensional version of the N-electron problem can be found in Ref. [88]. This represents a coupled eigenvalue problem and its numerical solution proceeds via the so-called self-consistent field (SCF) method due to Hartree [55]. First we find a solution to the hydrogenic problem, without the direct and exchange interactions. This yields ionic single-electron hydrogenic wave functions in the Coulomb potential of charge Ze forming the initial estimates for the HF iterations. Second, using these estimates, the elliptic partial differential equations for the direct and exchange interaction potentials (see Ref. [88]) are solved. With these potentials now obtained, the coupled HF problem including the direct and exchange interactions is solved as an eigensystem. The exchange interactions that couple the equations are expressed using wave functions from the previous iteration to solve the eigenvalue problem for each electron [89]. The eigenvalues obtained are the individual particle energies ϵ_i and the normalized eigenvectors are the wave functions ψ_i. The SCF iterations then proceed with the updated electron wave functions, and the steps from the second step described above are repeated until convergence.

For transforming the partial differential equations into algebraic ones, we follow the domain discretization procedure described in detail in Ref. [88]. The salient points are given below in brief in order to facilitate a later discussion regarding convergence of the method. As a result of the azimuthal symmetry of the problem, and parity with respect to the $z = 0$ plane, it is sufficient to restrict the physical domain of the problem [6,54,88] to $0 \leqslant \rho,z \leqslant \infty$. However, for making the problem numerically tractable, instead of using the above semi-infinite domain, we instead solve the problem in a finite, albeit sufficiently large, domain of size $\rho_{\max} \times z_{\max}$. This finite domain is then mapped using a suitable transformation (see below) to the domain $[-1,1]$, and Chebyshev-Lobatto spectral collocation points are then located on this latter compactified domain [90]. Thereafter, a Chebyshev pseudospectral method can be employed for representing the differential operators and functions in this transformed domain. However, domain truncation can introduce a confinement energy as an artifact of the numerical procedure, artificially increasing the energy of the electron [88]. This is mitigated by using a sequence of domains of increasing sizes, obtaining a converged result in the limit of the computational domain approaching the size of the physical domain of the problem [88].

In our computations, the size of the computational domain given by $\rho_{\max}$ and $z_{\max}$ (in units of the Bohr radius) is given by

$$\rho_{\max},z_{\max} = \frac{100\eta}{1+\log_{10}(\beta_Z)}, \tag{1}$$

where $\eta = \frac{1}{4},\frac{1}{2},1,2$ is a scaling factor used for setting up computations in a sequence of increasing domain sizes. The magnetic field strength parameter is defined as $\beta_Z = B/(Z^2B_0)$, where $B_0 = 4.701\,08 \times 10^5$ T is the critical field strength at which point the transition to the intense magnetic field regime occurs [6]. The effect of the logarithmic term $\log_{10}(\beta_Z)$ in the denominator is that it naturally makes the domain larger or smaller, depending on whether $\beta_Z < 1$ or $\beta_Z > 1$, respectively. With the maximum domain size thus defined, we can then compactify the finite domain $[0,\rho_{\max}] \otimes [0,z_{\max}]$ to $[-1,1] \otimes [-1,1]$ with the transformation

$$x = \log_{10}(1+\rho\alpha_\rho) - 1 \tag{2}$$

and

$$y = \log_{10}(1+z\alpha_z) - 1, \tag{3}$$

where $\alpha_\rho = 99/\rho_{\max}$ and $\alpha_z = 99/z_{\max}$. Note that in our calculations we employed a square domain to achieve the best possible internally consistent convergence. Thus in our work $\rho_{\max} = z_{\max}$ and therefore $\alpha_\rho = \alpha_z \equiv \alpha$, but the possibility remains for using different sizes and scalings in the two orthogonal directions to optimize computational effort, particularly in the intense field regime.

In order to obtain a converged solution within any given domain size, we employed six different levels of mesh refinement using $N = 21,31,41,51,61,71$ Chebyshev collocation points in each of the two orthogonal directions.

Utilizing a pseudospectral approach for discretization results in a sparse matrix for the coupled eigenvalue problem [88]. Therefore we employ the widely used sparse matrix generalized eigensystem solver ARPACK, which utilizes the implicitly restarted Arnoldi method (IRAM) [91–94] for solution. The key advantage is that since the Hamiltonian matrix that we are solving has only a few bound-state solutions, employing the IRAM with the shift-invert algorithm [93] for computing only a portion of the spectrum saves considerable computational effort.

It was found that generating a Krylov subspace with about 50 to 250 basis vectors was sufficient for determining around 15 to 100 eigenvalues in the vicinity of a given shift (σ). Runs were carried out for different values of the magnetic field strength parameter β_Z, in the range $0.7 \lesssim \beta_Z \leqslant 250$, for the cylindrical pseudospectral code. A typical tolerance of around 10^{-10} was employed for the internal errors of ARPACK. It was observed during our runs that fast convergence was achieved, within about 3–6 HF iterations. A convergence criterion for the HF iterations was employed wherein the difference between the HF energies for two consecutive iterations was tested. Typically, a tolerance on the order of $10^{-6}E_{Z,\infty}$ was employed. Once the HF iterations attained convergence for a given level of mesh refinement, the total Hartree-Fock energy of the state is obtained according to Eq. (2) in Ref. [88].

III. RESULTS AND DISCUSSION

Using the atomic structure software package developed for an earlier study [88], we carried out computations for several Fully spin-polarized (FSP) states of the neutral carbon atom in intense magnetic fields. After applying the extensive convergence conditions to the computations as described in Ref. [88], we arrived at estimates of the total HF energies for the 12 tightly bound states in the intense field regime. The majority of the data presented herein aims to complement the already available data for two states that have been investigated earlier.

The states that were considered in this study are labeled using both the field-free and strong-field notations for the sake of clarity; these can be found in Table I, which lists the different states of carbon. In the presence of a magnetic field

TABLE I. The different states of carbon considered in this study, listed using both intense field and field-free notation.

Intense field	Field-free
$^7(-15)^+$	$1s_0 2p_{-1} 3d_{-2} 4f_{-3} 5g_{-4} 6h_{-5}$
$^7(-15)^-$	$1s_0 2p_{-1} 3d_{-2} 4f_{-3} 5g_{-4} 7i_{-5}$
$^7(-14)^+$	$1s_0 2s_0 3d_{-2} 4f_{-3} 5g_{-4} 6h_{-5}$
$^7(-14)^-$	$1s_0 2p_{-1} 3d_{-1} 4f_{-3} 5g_{-4} 6h_{-5}$
$^7(-13)^+$	$1s_0 2s_0 2p_{-1} 4f_{-3} 5g_{-4} 6h_{-5}$
$^7(-13)^-$	$1s_0 2p_0 2p_{-1} 4f_{-3} 5g_{-4} 6h_{-5}$
$^7(-12)^+$	$1s_0 2s_0 2p_{-1} 3d_{-2} 5g_{-4} 6h_{-5}$
$^7(-12)^-$	$1s_0 2p_0 2p_{-1} 3d_{-2} 5g_{-4} 6h_{-5}$
$^7(-11)^+$	$1s_0 2s_0 2p_{-1} 3d_{-2} 4f_{-3} 6h_{-5}$
$^7(-11)^-$	$1s_0 2p_0 2p_{-1} 3d_{-2} 4f_{-3} 6h_{-5}$
$^7(-10)^+$	$1s_0 2s_0 2p_{-1} 3d_{-2} 4f_{-3} 5g_{-4}$
$^7(-10)^-$	$1s_0 2p_0 2p_{-1} 3d_{-2} 4f_{-3} 5g_{-4}$

states can be characterized using the notation $^{2S+1}M^{\pi_z}$, where $M = \sum_i m_i$ is the total z component of angular momentum. The summation is over all the electrons in the atom. This then forms a manifold within which different subspaces exist. The spin multiplicity is given in the usual way as $2S + 1$. Finally, the z parity of the state is indicated using $\pi_z = \pm 1$, indicating positive or negative parity. We studied 12 tightly bound states of carbon, 6 in each z-parity subspace, in the intense magnetic field regime ($\beta_Z \gtrsim 1$). Within a given parity subspace, typically there are crossovers that occur as the magnetic field is reduced; the reader is referred to Ivanov and Schmelcher [44,69] for excellent data and discussions regarding ground-state crossovers. A recent study by Boblest *et al.* [87] also represents one of the most comprehensive discussions with regard to transitions concerning the ground states of atoms up to $Z = 26$. The current work adds to the available atomic data by investigating states of the carbon atom not considered in these studies and reports on the Hartree-Fock energies of several low-lying states in the intense field regime.

A. The positive-parity ($\pi_z = +1$) subspace

For the states of carbon listed in Table I, eigenvalues were determined using the numerical method described in Sec. II (see Ref. [88] for more details). We began with the lowest value of the domain scaling parameter $\eta = 1/4$. This yielded a domain with dimensions given according to Eq. (1), and this domain size depends on β_Z. HF energies were then calculated using up to six different levels of mesh refinement in the domain. This enabled us to extrapolate the results to the limit of infinitely fine mesh, for a given domain size. We observed exponential convergence, characteristic of spectral methods, wherein the errors diminish exponentially with mesh refinement. We employed an exponential function of the form $ae^{bx} + ce^{dx}$ for extrapolating the total HF energies to the limit of infinitely fine mesh. A Levenberg-Marquardt optimization algorithm [95] was employed for this purpose. The errors associated with the extrapolation procedure were typically on the order of $10^{-4}E_{Z,\infty}$ to $10^{-6}E_{Z,\infty}$ with a normalized R-squared value typically greater than 0.999 for the interpolating function employed. However, at the upper end of the intense magnetic field regime, we noticed slight loss of accuracy as the states become tightly bound, and for $\beta_Z \gtrsim 200$ the extrapolation procedure had an error on the order of a few times $10^{-4}E_{Z,\infty}$ with a normalized R-squared value of $\approx$0.98 on average. For the extrapolation to infinitely fine mesh, the average area per unit grid size in the domain ($A_E \approx \rho_{\max} z_{\max}/N^2$) was taken as the independent variable and the energies extrapolated to the limit of $A_E \to 0$, corresponding to infinitely fine mesh.

This procedure was repeated as the domain was rescaled to larger and larger values, corresponding to $\eta = 1/2,1,2$. Then, using the extrapolated values of the HF energy corresponding to infinitely fine mesh for each of the four domain sizes, a subsequent extrapolated value of the HF energy ($E_{\rm HF}$) was obtained, in the limit of the domain size approaching infinity. These are then the converged $E_{\rm HF}$ values reported in Tables II and III. We employed an extrapolating function of the form $ax^{1/2} + b$, with a Levenberg-Marquardt optimization method [95]. The ordinates in this case were the four different converged HF energies in the limit of infinitely fine mesh in each of the four different domains, and the abscissae were the inverse domain areas, i.e., $(\rho_{\max} z_{\max})^{-1}$. Thus, extrapolating to zero inverse area corresponding to an infinite domain size yields the final converged HF energy, and mitigates errors arising due to domain truncation [88]. The error in the extrapolation to the limit of an infinite domain size was on the order of $10^{-5}E_{Z,\infty}$ to $10^{-6}E_{Z,\infty}$ with a normalized R-squared value of $>$0.999 for the interpolating function employed. Again at the upper end of magnetic field strengths ($\beta_Z \gtrsim 200$) we noticed a slight loss of accuracy, with the extrapolation errors increasing to the level of a few times $10^{-4}E_{Z,\infty}$.

It can be seen upon examining the data in Table II that only one FSP positive-parity state had been investigated in the intense field regime. This is the state $^7(-15)^+$ that becomes tightly bound, and is the ground state of the carbon atom, in the range of magnetic field strengths investigated in this study. It can be seen that the fully converged results obtained in the current study for this state are in good agreement with values obtained elsewhere, given that the current study is a single-configuration calculation. Over the entire range of magnetic field strengths investigated, our estimates of the total Hartree-Fock energies [see Eq. (2) of [88] for definition] agree with estimates elsewhere [44,81] to on average $\Delta \approx 0.75\%$, for the states $^7(-15)^+$. We noticed a slight loss of accuracy of the cylindrical pseudospectral method in the lower magnetic field regime ($\beta_Z \lesssim 1$) wherein the cylindrical code (and the extrapolation method described above) maintained accuracy to within $10^{-5}E_{Z,\infty}$ to $10^{-4}E_{Z,\infty}$. There was also a similar loss of accuracy at the upper end of the intense field regime as well, where the electron orbital geometries become severely anisotropic ($\beta_Z \gtrsim 200$). Energy data for five additional FSP positive-parity states are also provided in Table II. Within a given M-π subspace, we considered only a single state. It is therefore entirely possible that other states within this subspace have crossovers in the intense field and become tightly bound as well. This would require a detailed investigation of all the different states that can comprise a given M-π subspace. Such an investigation is left for a future undertaking, with a cautionary reminder to the reader that other states within a given subspace, apart from the ones

TABLE II. Total Hartree-Fock energies of the positive-parity states of carbon [see Eq. (2) of Ref. [88]]. Energies are in units of Rydberg energies in the Coulomb potential of nuclear charge $Z = 6$ for carbon. Accurate data from other work are also provided for comparison. $\beta_Z = \gamma/2Z^2$. The values given in parentheses are the maximal fitting errors at the fourth decimal place.

	$^7(-15)^+$		$^7(-14)^+$	$^7(-13)^+$	$^7(-12)^+$	$^7(-11)^+$	$^7(-10)^+$
β_Z	Present work	Other work	Present work	Present work	Present work	Present work	Present work
0.5909	−3.7898(0)	−3.7586[a]					
0.6944	−4.0165(1)	−3.9794[b]	−3.5545(1)	−3.7294(1)	−3.8084(0)	−3.8592(2)	−3.9078(1)
1.0000	−4.5889(1)		−4.0546(1)	−4.2520(0)	−4.3432(1)	−4.4020(2)	−4.4583(1)
1.3889	−5.1824(3)	−5.1364[b]	−4.5754(2)	−4.7957(1)	−4.8991(1)	−4.9659(1)	−5.0301(1)
2.0000	−5.9372(1)		−5.2398(4)	−5.4887(2)	−5.6071(1)	−5.6840(1)	−5.7576(1)
2.7778	−6.7127(1)	−6.6563[b]	−5.9245(2)	−6.2018(2)	−6.3355(3)	−6.4223(2)	−6.5057(1)
2.9544	−6.8692(1)	−6.8213[a]					
5.0000	−8.3560(2)		−7.3771(2)	−7.7130(2)	−7.8780(1)	−7.9859(1)	−8.0890(0)
5.9088	−8.8894(1)	−8.8339[a]					
6.9444	−9.4354(1)	−9.3625[b]					
7.0000	−9.4632(1)		−8.3590(7)	−8.7331(1)	−8.9184(1)	−9.0399(2)	−9.1561(0)
10.0000	−10.7851(2)		−9.5322(1)	−9.9517(0)	−10.1609(0)	−10.2987(0)	−10.4307(4)
13.8889	−12.1511(1)	−12.0634[b]	−10.7462(4)	−11.2112(0)	−11.4450(1)	−11.5989(0)	−11.7461(0)
20.0000	−13.8493(1)		−12.2583(1)	−12.7780(2)	−13.0411(2)	−13.2152(0)	−13.3813(1)
25.0000	−14.9905(1)		−13.2754(1)	−13.8306(8)	−14.1140(1)	−14.3011(0)	−14.4798(1)
27.7778	−15.5577(1)	−15.4534[b]	−13.7813(3)	−14.3551(4)	−14.6471(2)	−14.8409(0)	−15.0259(0)
29.5440	−15.8984(0)	−15.8263[a]					
50.0000	−19.0832(1)		−16.9279(1)	−17.6089(9)	−17.9602(0)	−18.1937(2)	−18.4170(4)
69.4444	−21.3415(2)	−21.2117[b]	−18.9470(2)	−19.6950(3)	−20.0822(1)	−20.3405(2)	−20.5867(2)
100.0000	−24.1131(4)		−21.4272(4)	−22.2547(4)	−22.6856(2)	−22.9737(4)	−23.2492(1)
138.8889	−26.8673(3)	−26.7153[a]					
200.0000	−30.2271(6)		−26.9070(22)	−27.9012(33)	−28.4255(25)	−28.7783(20)	−29.1161(1)
250.0000	−32.4533(16)		−28.9040(15)	−29.9575(16)	−30.5141(15)	−30.8902(6)	−31.2499(20)

[a]Reference [81].
[b]Reference [44].

TABLE III. Total Hartree-Fock energies of the negative-parity states of carbon [see Eq. (2) of Ref. [88]]. Energies are in units of Rydberg energies in the Coulomb potential of nuclear charge $Z = 6$ for carbon. Accurate data from other work are also provided for comparison. $\beta_Z = \gamma/2Z^2$. The values given in parentheses are the maximal fitting errors at the fourth decimal place.

	$^7(-15)^-$	$^7(-14)^-$	$^7(-13)^-$	$^7(-12)^-$	$^7(-11)^-$	$^7(-10)^-$	
β_Z	Present work	Present work	Present work	Present work	Present work	Present work	Other work
0.6944	−3.9117(1)	−3.7567(2)	−3.7907(2)	-3.8658(3)	−3.9123(2)	−3.9568(4)	−3.9177[a]
1.0000	−4.4630(0)	−4.2766(6)	−4.3028(2)	−4.3903(3)	−4.4451(2)	−4.4979(4)	
1.3889	−5.0346(1)	−4.8156(2)	−4.8354(3)	−4.9355(3)	−4.9991(2)	−5.0601(3)	−5.0153[a]
2.0000	−5.7617(1)	−5.5036(2)	−5.5161(3)	−5.6320(2)	−5.7063(2)	−5.7778(4)	
2.7778	−6.5090(0)	−6.2122(1)	−6.2194(4)	−6.3511(1)	−6.4366(4)	−6.5184(2)	−6.4671[a]
5.0000	−8.0927(0)	−7.7195(1)	−7.7209(1)	−7.8854(3)	−7.9926(2)	−8.0954(2)	
6.9444						−9.1338(2)	−9.0672[a]
7.0000	−9.1593(2)	−8.7376(1)	−8.7379(1)	−8.9229(2)	−9.0444(1)	−9.1605(2)	
10.0000	−10.4312(1)	−9.9535(2)	−9.9534(1)	−10.1625(1)	−10.3001(2)	−10.4316(2)	
13.8889	−11.7465(2)	−11.2121(1)	−11.2117(1)	−11.4452(1)	−11.5994(1)	−11.7465(3)	−11.6656[a]
20.0000	−13.3811(1)	−12.7781(2)	−12.7776(2)	−13.0406(1)	−13.2148(1)	−13.3810(2)	
25.0000	−14.4793(2)	−13.8314(7)	−13.8305(1)	−14.1132(2)	−14.3004(2)	−14.4793(1)	
27.7778	−15.0252(1)	−14.3548(6)	−14.3539(0)	−14.6461(1)	−14.8400(1)	−15.0250(1)	−14.9284[a]
50.0000	−18.4151(1)	−17.6087(5)	−17.6026(1)	−17.9526(7)	−18.1867(4)	−18.4154(1)	
69.4444	−20.5850(0)	−19.6006(16)	−19.6872(2)	−20.0743(2)	−20.3328(3)	−20.5790(4)	−20.4500[a]
100.0000	−23.2470(5)	−22.2553(11)	−22.2523(3)	−22.6831(3)	−22.9713(4)	−23.2522(5)	
138.8889						−25.8961(8)	−25.7611[a]
200.0000	−29.1191(8)	−27.9131(15)	−27.8991(22)	−28.4235(25)	−28.8014(13)	−29.1198(8)	
250.0000	−31.2522(9)	−29.9686(54)	−29.9602(68)	−30.5110(15)	−30.8871(6)	−31.2537(9)	

[a]Reference [44].

listed here, may be important as well from a spectroscopic viewpoint.

B. The negative-parity ($\pi_z = -1$) subspace

We investigated six FSP negative-parity states of the carbon atom in intense magnetic fields. We have provided data for the total Hartree-Fock energies [see Eq. (2) of [88] for definition] of these states in Table III. Of these, there appears to be a lack of information except for the state $^7(-10)^-$ [44]. The data of the current computation are seen to be in agreement with those results to on average $\approx$0.74%. It can also be seen that the state $^7(-15)^-$ is also a tightly bound state, with the energies of this state being nearly equal to those of $^7(-10)^-$, making them the two most tightly bound states of the negative-parity subspace. We noticed that at both the low and the high ends of the intense field regime considered here, there was a slight loss of accuracy; this can be seen in the slightly larger errors reported in the parentheses. Once more however, we would like to remind the reader that in any given M-π subspace, we have only investigated a single state; other configurations in the subspace would need to be investigated before determining the ordering of states according to their energies in a given M-π subspace, as well as answering the important question regarding crossovers. We again note that such an undertaking is beyond the scope of the current investigation, whose aim is merely to complement the data in the literature for the carbon atom in intense magnetic fields, by providing data for additional states that also become tightly bound with increasing magnetic fields.

It can also be seen that the energies of the different states shown in Tables II and III are fairly close together, particularly at the higher end of the intense field regime, even with the handful of states considered here. This would have an impact on transition probabilities wherein many transition probabilities between states may be nearly equally likely. This would also affect the emergent spectra wherein several lines may be rather close together. This effect may become more pronounced should other states in the different M-π subspaces be investigated as well.

IV. CONCLUSIONS AND OUTLOOK

In the current study we have investigated the carbon atom in intense magnetic fields employing a two-dimensional single-configuration Hartree-Fock approach with a pseudospectral method of solution. We employed an atomic structure software package that was developed earlier [88] for this purpose.

We presented data for 12 tightly bound FSP states of carbon, six in each parity subspace. Data were lacking for ten of these states. Where available, the data of the current computation for certain states were seen to be in good agreement with findings elsewhere.

The pseudospectral atomic structure software employed in this investigation also has certain limitations. First, computations are currently required to be carried out in a sequence of increasing finite domain sizes, so that a converged result for the total Hartree-Fock energy may be obtained in the limit of the domain size becoming infinite. This adds a layer of computational complexity. We have discussed in Ref. [88] a possible way to circumvent this, in essence by monitoring the wave functions at the outer edges of the domain and requiring their values to fall below a certain threshold, while varying the domain size. While this may not be straightforward to implement within the framework of a pseudospectral approach, it would nevertheless make the computation more streamlined if implemented. Second, the current work does not include relativistic corrections to the energies. For the magnetic field strengths considered herein, the relativistic corrections to the energies were estimated using the scaling formula in Ref [96]. Their results for the hydrogen atom were used for this purpose and the corrections were estimated to be on the order of $10^{-6}E_{Z,\infty}$. This was seen to be smaller than the numerical errors arising from convergence of the entire numerical method including the extrapolation to the limit of a semi-infinite domain. Thus, relativistic corrections are important; however, it was not possible to account for them accurately in the current study. Moreover, as the magnetic field strength increases in the intense magnetic field regime, effects due to finite nuclear mass become relevant. In the current study, the mass of the nucleus is assumed to be infinite, and as such we have not carried out a suitable correction. One way to account for the finite nuclear mass is to employ a scaling relationship wherein the energies determined at a certain magnetic field strength β_Z for an infinite nuclear mass would be related to the corresponding energies for a finite nuclear mass at a different value of the magnetic field strength $\tilde{\beta}_Z$ [41].

Finally, and perhaps the most important, is the fact that the current study is only a single-configuration calculation for a system that has six electrons. Therefore, the effects of electron correlation are of great importance and, if included, would yield much more accurate results than those given here. The current two-dimensional (2D) wave functions computed in this study could form the initial estimates for 2D configuration-interaction or multiconfiguration calculations. We leave this much larger undertaking for a future endeavor.

The amount of data that is required for careful analysis of the emergent spectra from a white dwarf (or neutron star) is staggering. Foremost, multiwavelength observations are required over the entire spectral energy distribution of the compact object, e.g., spectroscopic data, photometry, and polarimetric data (see, e.g., [97]). Observations are often complicated by rotation of the compact object, and thus it becomes necessary to have phase-resolved spectra to identify spectral lines accurately. This entails long-period observations using multiple high-sensitivity and high-spectral-resolution instruments from various physical locations around the globe. Thus, obtaining such data for the sizable number of magnetized compact objects known is a formidable task, since dedicated and prolonged instrument time for each object would be required. Even from the perspective of theoretical atomic data there are many challenges ahead. Foremost, for identifying spectral features and lines one requires a wealth of data regarding transition rates. In the presence of a strong magnetic field many zero-field transitions forbidden due to dipole selection rules now become permissible [97]. This situation is further complicated by the ubiquitously present strong electric fields in the atmospheres of these objects, which not only lead to further violations of the zero-field selection rules, but also significantly affect oscillator strengths and transition rates.

It is also important to have data for stationary components of the spectra. These lines are typically between 300 and 1000 nm for hydrogen, and these transitions go through either a maximum or a minimum as a function of the magnetic field strength. Such transitions produce sharp absorption features, in contrast to fast-moving wavelengths which get smeared out due to variations in the magnetic field structure on the surface of the compact object [6]. The majority of such data currently available are for atoms such as hydrogen and helium. However, with the discovery of several mid-Z atmospheric contaminants such as carbon, sulfur, phosphorus, and silicon, it becomes necessary to have such extended atomic data for interpreting spectral features of these objects. In addition to atomic data for bound-bound transitions, data are also needed for bound-free transitions, in particular photoionization cross sections of various states of different low- to mid-Z atoms, as a function of magnetic field strength. Such transitions contribute significantly to continuum opacity as well as to polarization effects in the atmospheres of compact objects. However, data here are even more scarce and limited to hydrogen bound-free photoionization cross sections [98–100]. Such data for helium and mid-Z elements such as carbon would also be required for accurately modeling the spectra of DB and DQ white dwarfs.

In summary, apart from extensive multiwavelength observations, a great wealth of atomic data are required for spectral analysis of magnetized compact objects. The first step in that direction is to obtain data for the energy levels and wave functions of various low-lying states of mid-Z atoms. This investigation considerably extends the currently available data in the literature for the energy levels of the carbon atom in intense magnetic fields. We would however like to remind the reader that, at a minimum, several more states would need to be computed within the different M-π subspaces for delineating the full energy landscape of the carbon atom.

ACKNOWLEDGMENTS

Calculations and the majority of the code development were performed on computing equipment purchased with funds from NSF Grant No. 1148502. A part of the code development was also carried out on computing infrastructure purchased with funds from the Canadian Foundation for Innovation and the British Columbia Knowledge Development Fund. A.T. gratefully acknowledges support from an Arizona State University School of Earth and Space Exploration Postdoctoral Fellowship.

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