Eur. Phys. J. D **14**, 279–288 (2001)

THE EUROPEAN PHYSICAL JOURNAL D

EDP Sciences
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Springer-Verlag 2001

The beryllium atom and beryllium positive ion in strong magnetic fields

M.V. Ivanov[a] and P. Schmelcher[b]

Theoretische Chemie, Physikalisch–Chemisches Institut, Universität Heidelberg, INF 229, 69120 Heidelberg, Germany

Received 2 October 2000 and Received in final form 8 January 2001

Abstract. The ground and a few excited states of the beryllium atom in external uniform magnetic fields are calculated by means of our 2D mesh Hartree-Fock method for field strengths ranging from zero up to 2.35×10^9 T. With changing field strength the ground state of the Be atom undergoes three transitions involving four different electronic configurations which belong to three groups with different spin projections $S_z = 0, -1, -2$. For weak fields the ground state configuration arises from the $1s^2 2s^2$, $S_z = 0$ configuration. With increasing field strength the ground state evolves into the two $S_z = -1$ configurations $1s^2 2s 2p_{-1}$ and $1s^2 2p_{-1} 3d_{-2}$, followed by the fully spin polarised $S_z = -2$ configuration $1s 2p_{-1} 3d_{-2} 4f_{-3}$. The latter configuration forms the ground state of the beryllium atom in the high field regime $\gamma > 4.567$. The analogous calculations for the Be^+ ion provide the sequence of the three following ground state configurations: $1s^2 2s$ and $1s^2 2p_{-1}$ ($S_z = -1/2$) and $1s 2p_{-1} 3d_{-2}$ ($S_z = -3/2$).

PACS. 32.60.+i Zeeman and Stark effects – 31.15.Fx Finite-difference schemes – 31.15.Ne Self-consistent-field methods

1 Introduction

The behaviour and properties of atoms in strong magnetic fields has become a subject of increasing interest during the past two decades. One motivation for this is certainly the astrophysical discovery of strong fields on white dwarfs and neutron stars [1–3]. On the other hand the competition of the diamagnetic and Coulomb interaction causes a rich variety of complex properties which are of interest on their own.

For a long time the investigations in the literature focused on the hydrogen atom (for a list of references see, for example, [4–7] and references therein). As a result of the corresponding investigations the absorption features of certain magnetic white dwarfs could be understood in detail and a modelling of their atmospheres was possible (see Ref. [8] for a review up to 1994 and [9] for more recent references). Detailed spectroscopic calculations were carried out recently for the helium atom in strong magnetic fields [10]. These calculations allow to identify spectra of other, namely helium-rich objects, including the prominent white dwarf GD229 [11]. On the other hand a number of new magnetic white dwarfs have been found whose spectra are still unexplained (see, *e.g.*, Reimers *et al.* [12] in the course of the Hamburg ESO survey).

Investigations on the electronic structure in the presence of a magnetic field appear to be quite complicated due to the intricate geometry of this quantum problem. For the hydrogen atom the impact of the competing Coulomb and diamagnetic interaction is particularly evident and pronounced in the intermediate regime for which the magnetic and Coulomb forces are comparable. For different electronic degrees of excitation of the atom the intermediate regime is met for different absolute values of the field strength. For the ground state this regime corresponds to field strengths around $\gamma = 1$ (for the magnetic field strength as well as for other physical values we use atomic units and, in particular, $\gamma = B/B_0$, B_0 corresponds to the magnetic field strength $B_0 = \hbar c/e a_0^2 = 2.3505 \times 10^5$ T). Both early [13,14] and more recent works [4,15] on the hydrogen atom have used different approaches for relatively weak fields (the Coulomb force prevails over the magnetic force) and for very strong fields (the Coulomb force can be considered as weak in comparison with the magnetic forces which is the so-called adiabatic regime). A powerful method to obtain comprehensive results on low-lying energy levels of the hydrogen atom in particular in the intermediate regime is provided by mesh methods [5]. For atoms with several electrons there are two decisive factors which enrich the possible changes in the electronic structure with varying field strength compared to the one-electron system. First we have a third competing interaction which is the electron-electron repulsion and second the different electrons feel very different Coulomb forces, *i.e.* possess different one

[a] *Permanent address*: Institute of Precambrian Geology and Geochronology, Russian Academy of Sciences, Nab. Makarova 2, St. Petersburg 199034, Russia.
e-mail: MIvanov@MI1596.spb.edu

[b] e-mail: peter@tc.pci.uni-heidelberg.de

particle energies, and consequently the regime of the intermediate field strengths appears to be the sum of the intermediate regimes for the separate electrons.

Opposite to the hydrogen atom the ground state wavefunctions of the multi-electron atoms change their symmetries with increasing field strength. It is well-known that the singlet zero-field ground state of the helium atom ($1s^2$ in the Hartree-Fock language) is replaced in the high-field regime by the triplet fully spin polarised configuration $1s2p_{-1}$. For atoms with more than two electrons the evolution of the ground state within the whole range of field strengths $0 \leq \gamma < +\infty$ includes multiple intermediate configurations besides the zero-field ground state and the ground state corresponding to the high field limit. In view of the above there is a need for further quantum mechanical investigations and data on atoms with more than two electrons in order to understand their electronic structure in strong magnetic fields. Our approach allowed us to obtain the first conclusive results on the series of ground state configurations for the Li [16] and C [17] atoms. These results go substantially beyond the previously published ones [18]. A previous work on the beryllium atom [19] focused on problems associated with the symmetries of the Hartree-Fock wavefunction of the low-field ground state $1s^22s^2$ of this atom. For strong fields the $1s^22s^2$ state represents a highly excited state. In a very recent investigation [20] the high-field regime has been addressed and the fully spin-polarised ground state configurations for all atoms with nuclear charge numbers $1 \leq Z \leq 10$ have been identified and studied. We therefore know for both very weak and very high fields the ground state configurations of the Be atom and their properties. For the intermediate regime however no investigations have been performed so far. The present work closes this gap and yields the ground state (properties) for arbitrary field strengths $0 \leq \gamma \leq \infty$. As we shall see the zero field ground state configuration $1s^22s^2$ remains the ground state for $0 \leq \gamma \leq 0.0412$ a.u. and the fully spin-polarised configuration $1s2p_{-1}3d_{-2}4f_{-3}$ discussed in reference [20] becomes the ground state for $\gamma \geq 4.567$ a.u. The electronic structure of the Be^+ ion is investigated as well. In order to be self-contained we provide in the following a brief account of our computational method and our conceptual approach to the search for the ground state configurations.

2 Method

The computational method applied in the current work coincides with the method described in our works [5,19, 21,22] and applied afterwards in [16,17,23,20]. We solve the electronic Schrödinger equation for the beryllium atom in a magnetic field under the assumption of an infinitely heavy nucleus in the *unrestricted* Hartree-Fock (UHF) approximation. The solution is established in the cylindrical coordinate system (ρ, ϕ, z) with the z-axis oriented along the magnetic field. We prescribe to each electron a definite value of the magnetic quantum number m_μ. Each one-electron wave function Ψ_μ depends on the variables ϕ and (ρ, z)

$$\Psi_\mu(\rho, \phi, z) = (2\pi)^{-1/2} \mathrm{e}^{-\mathrm{i}m_\mu\phi} \psi_\mu(z, \rho) \tag{1}$$

where μ indicates the numbering of the electrons. The resulting partial differential equations for $\psi_\mu(z, \rho)$ and the formulae for the Coulomb and exchange potentials have been presented in reference [21]. These equations as well as the Poisson equations for inter-electronic Coulomb and exchange potentials are solved by means of the fully numerical mesh method described in references [5,21]. The finite-difference solution of the Poisson equations on sets of nodes coinciding with those of the Hartree-Fock equations turns out to be possible due to a special form of uniform meshes used in the present calculations and in references [16,17,19]. A discussion of these meshes is given in reference [24].

Our mesh approach is flexible enough to yield precise results for arbitrary field strengths. Some minor decrease of the precision appears for electronic configurations with big differences in the spatial distribution of the electronic density for different electrons. This situation is typical for those electronic configurations which do not represent the ground state at the corresponding field strengths (*e.g.* $1s^22s^2$ for very strong fields or $1s2p_{-1}3d_{-2}4f_{-3}$ (see below) in the weak field regime). The precision of our results depends, of course, on the number of mesh nodes and can be always improved in calculations with denser meshes. Most of the present calculations are carried out on sequences of meshes with the maximal number of nodes being 80×80.

Along with the numerical solution of the Schrödinger equation the key element for solving the problem of the ground state electronic configurations is a proper choice of the configurations, which could potentially be the ground state ones. In reference [17] a strategy was developed which enables one to reduce the set of possible ground state configurations subject to a following numerical investigation. This removes the risk of missing some ground state configurations due to the limited possibilities of performing numerical investigations. The above-mentioned strategy is based on a combination of qualitative theoretical arguments and numerical calculations of the energies of electronic configurations. As a first step the set of relevant electronic configurations has to be separated into several groups according to their spin projections S_z. It turns out that it is most appropriate to start with the limit of infinite strong fields and analyse the electronic configurations with decreasing field strengths. Arguments based on the geometry of the spatial part of the wavefunction allow us to determine the ground state for the high-field limit as well as several candidates for the ground state configuration with decreasing field strength. The following numerical calculations allow to decide which of these candidates becomes the actual first intermediate ground state and yield the transition field strength. The knowledge of the first intermediate ground state allows us to repeat the above procedure in order to identify the second intermediate ground state from a list of candidates. Repeating this as many times as necessary the full sequence of the ground

state configurations for each subset S_z is determined and finally the sequence of all ground state configurations of the atomic system is obtained.

3 Ground state electronic configurations for $\gamma = 0$ and $\gamma \to \infty$

In this section we discuss some important properties of ground states of multi-electron atoms in the limits $\gamma = 0$ and $\gamma \to \infty$.

For the case $\gamma = 0$ the ground state configuration of the beryllium atom can be characterised in the framework of the restricted Hartree-Fock approach as $1s^2 2s^2$. The latter is an approximation of limited quality in describing the beryllium atom as it was shown in many fully correlated calculations for the field-free Be atom. For the extensive literature on the electronic structure of the Be atom we refer the reader to reference [25] and the references therein. It was pointed out in these works that the Be atom is a strongly correlated system and that the HF ground state wavefunction (*i.e.* the spherically symmetric $1s^2 2s^2$) is not a very accurate zeroth-order wavefunction, especially for calculations of electric polarisabilities. In a Hartree-Fock language this is due to a significant contribution of the $1s^2 2p^2$ configuration to the ground state wave function (precision calculations require of course a huge number of configurations). The latter configuration is evidently a non-spherical one.

Our Hartree-Fock energy for the ground state of the Be atom in field-free space is -14.57336 a.u. compared to the exact nonrelativistic energy -14.66735 a.u. The missing correlation therefore amounts to 0.09399 a.u. Without doubt effects due to correlation are crucial for the correct description of many physical phenomena. For the present purpose however, *i.e.* a first investigation and clarification of global ground state properties in magnetic fields of arbitrary strength, they are of minor importance. Only in case one would like to obtain more accurate energies or other properties a study including correlation would be indispensable.

It is evident that the field-free ground state of the beryllium atom remains the ground state only for relatively weak fields. The set of one-electron wave functions constituting the HF ground state for the opposite case of extremely strong magnetic fields can be determined as follows. The nuclear attraction energies and HF potentials (which determine the motion along z-axis) are small for large γ in comparison to the interaction energies with the magnetic field (which determines the motion perpendicular to the magnetic field and is responsible for the Landau zonal structure of the spectrum). Thus, all the one-electron wavefunctions must correspond to the lowest Landau zones, *i.e.* the magnetic quantum numbers m_μ for all electrons obey $m_\mu \leq 0$, and the system must be fully spin-polarised, *i.e.* $s_{z\mu} = -1/2$. For the Coulomb central field the one-electron levels form (as $B \to \infty$) quasi 1D Coulomb series with the binding energy $\epsilon_{\rm B} = 1/2n_z^2$ for $n_z > 0$ and $\epsilon_{\rm B} \to \infty$ for $n_z = 0$, where n_z is the number of nodal surfaces of the wave function with respect to the z-axis. The binding energy of a separate electron has the form

$$\epsilon_{\rm B} = (m + |m| + 2s_z + 1)\gamma/2 - \epsilon \tag{2}$$

where ϵ is the energy of the electron.

When considering the case $\gamma \to \infty$ it is evident, that the wave functions with $n_z = 0$ have to be chosen for the ground state configuration. Furthermore starting with the energetically lowest one particle level the electrons occupy according to the above arguments orbitals with increasing absolute value of the magnetic quantum number m_μ. Consequently the ground state of the beryllium atom must be given by the fully spin-polarised configuration $1s2p_{-1}3d_{-2}4f_{-3}$. In our notation of the electronic configurations we assume in the following that all paired electrons, like for example the $1s^2$ part of a configuration, are of course in a spin up and spin down orbital, respectively, whereas all unpaired electrons possess a negative projection of the spin onto the magnetic field direction. On a qualitative level the configuration $1s2p_{-1}3d_{-2}4f_{-3}$ is not very different from similar electronic configurations for other atoms (see Ref. [20]). This is a manifestation of the simplification of the picture of atomic properties in the limit $\gamma \to \infty$ where a linear sequence of electronic configurations replaces the periodic table of elements of the field-free case.

4 Ground state electronic configurations for arbitrary field strengths

In order to determine the ground state electronic configurations of the beryllium atom we employ the strategy introduced in reference [17] and summarized in Section 2. First of all, we divide the possible ground state configurations into three groups according to their total spin projection S_z: the $S_z = 0$ group (low-field ground state configurations), the intermediate group $S_z = -1$ and the $S_z = -2$ group (the high-field ground state configurations). For the following investigation it is expedient to introduce *local* ground states for each S_z subset which are the energetically lowest states with a certain S_z value along with the *global* ground state of the atom. Of course, for each value of the field strength one of the local ground states represents the global ground state of the atom.

From Section 3 we know that the ground state configuration of the beryllium atom in the high field limit must be the fully spin-polarised state $1s2p_{-1}3d_{-2}4f_{-3}$. The optimal strategy to determine the sequence of ground state configurations of the atom with decreasing field strength is a repeating procedure starting from the high field ground state. It consists of both qualitative arguments based on the geometry of the orbitals which yield a preliminary list of relevant configurations as well as subsequent calculations on these configurations. The total energies for the considered states and particularly of those states which become the global ground state of the atom for some regime of the field strength are illustrated in Figure 1.

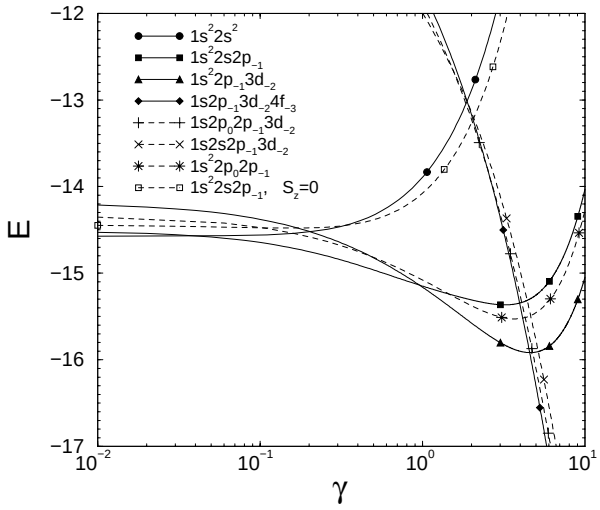

Fig. 1. The total energies (in atomic units) of the states of the beryllium atom as functions of the magnetic field strength considered for the determination of the ground state electronic configurations. The field strength is given in units of $\gamma = (B/B_0)$, $B_0 = \hbar c/ea_0^2 = 2.3505 \times 10^5$ T.

Following the above procedure let us consider other possible candidates in question for the electronic ground state for $S_z = -2$ (see Fig. 1) *with decreasing field strength*. A study of the high-field regime was carried out in reference [20]. In particular, we have found in reference [20] that the beryllium atom, opposite to the carbon atom and other heavier elements has only one fully spin-polarised ground state configuration. Let us describe the arguments leading to this conclusion here in more detail.

All the one electron wave functions of the high-field ground state $1s2p_{-1}3d_{-2}4f_{-3}$ possess no nodal surfaces crossing the z-axis and occupy the energetically lowest orbitals with magnetic quantum numbers ranging from $m = 0$ down to $m = -3$. The $4f_{-3}$ orbital possesses the smallest binding energy of all orbitals constituting the high-field ground state. Its binding energy decreases rapidly with decreasing field strength. Thus, we can expect that the first crossover of ground state configurations happens due to a change of the $4f_{-3}$ orbital into one possessing a higher binding energy at the corresponding lowered field strength. One may think that the first transition while decreasing the magnetic field strength will involve a transition from an orbital possessing $n_z = 0$ to one for $n_z = 1$. The energetically lowest available one particle state with $n_z = 1$ is the $2p_0$ orbital. Another possible orbital into which the $4f_{-3}$ wave function could evolve is the $2s$ state. For the hydrogen atom or hydrogen-like ions in a magnetic field the $2p_0$ is stronger bound than the $2s$ orbital. On the other hand, owing to the electron screening in multi-electron atoms in field-free space the $2s$ orbital tends to be more tightly bound than the $2p_0$ orbital. Thus, two states *i.e.* $1s2p_02p_{-1}3d_{-2}$ and $1s2s2p_{-1}3d_{-2}$ are candidates for becoming the ground state in the $S_z = -2$ set when we lower the field strength coming from the high field situation. The numerical calculations show that the first crossover of the $S_z = -2$ subset takes place between the $1s2p_{-1}3d_{-2}4f_{-3}$ and $1s2p_02p_{-1}3d_{-2}$ configurations (Fig. 1). On the other hand, the calculations show that even earlier (*i.e.* at higher magnetic field strengths) the global ground state acquires the total spin $S_z = -1$ due to a crossover of the energy curve of the $1s2p_{-1}3d_{-2}4f_{-3}$ configuration with that of the configuration $1s^22p_{-1}3d_{-2}$ (which is the local ground state for the $S_z = -1$ subset in the high-field limit). For the fields below this point $\gamma = 4.567$ the ground state electronic configurations of the beryllium atom belong to the subset $S_z = -1$. This means that, as mentioned above, the beryllium atom has only one fully spin polarised ground state configuration.

The electronic configurations $1s^22p_{-1}3d_{-2}$ and $1s2p_{-1}3d_{-2}4f_{-3}$ differ by the replacement of the spin down $4f_{-3}$ orbital through the spin up $1s$ orbital and according to the arguments presented in the previous sections the $1s^22p_{-1}3d_{-2}$ represents the *local* ground state configuration for the subset $S_z = -1$ in the limit $\gamma \to \infty$. Analogous arguments to that presented in the previous paragraph provide the conclusion, that with decreasing field strength the $1s^22p_{-1}3d_{-2}$ ground state electronic configuration can be replaced either by the $1s^22s2p_{-1}$ or by the $1s^22p_02p_{-1}$ configuration. The numerical calculations show, that the curve $E_{1s^22s2p_{-1}}(\gamma)$ intersects the curve $E_{1s^22p_{-1}3d_{-2}}(\gamma)$ at a higher magnetic field ($\gamma = 0.957$) than $E_{1s^22p_02p_{-1}}(\gamma)$ crosses $E_{1s^22p_{-1}3d_{-2}}(\gamma)$. The difference with respect to the order of the local ground state configurations in the subsets $S_z = -2$ and $S_z = -1$ stems from the difference in the magnetic field strengths characteristic for the crossovers in these subsets. At moderate field strengths ($S_z = -1$) the influence of the Coulomb fields of the nucleus and electrons prevails over the influence of the magnetic field and make the energy of the $2s$ orbital lower than that of the $2p_0$ orbital. On the other hand, at stronger fields characteristic for the subset $S_z = -2$ the energies of these orbitals are governed mostly by the magnetic field and, in result, the energy of the $2p_0$ orbital becomes lower than the energy of the $2s$ orbital.

From our simple qualitative considerations we can conclude, that the configuration $1s^22s2p_{-1}$ is the *local* ground state configuration of the subset $S_z = -1$ for the weak field case, *i.e.* for $\gamma \to 0$. Indeed, when we construct such a configuration, the first three electrons go to orbitals $1s$ and $2s$ forming the $1s^22s$ configuration with $S_z = -1/2$. The fourth electron must then have the same spin as the $2s$ orbital electron to obtain the total spin value $S_z = -1$. Thus, the lowest orbital which it can occupy is the $2p_{-1}$. Therefore, there are two local ground state configurations in the subset $S_z = -1$ and they both represent the global ground state for some ranges of the magnetic field strengths.

The necessary considerations for the subset $S_z = 0$ are quite simple. At $\gamma = 0$ and, evidently, for very weak fields the ground state of the beryllium atom has the configuration $1s^22s^2$. We can expect, that when increasing the magnetic field strength, the next lowest state with $S_z = 0$ will be the $1s^22s2p_{-1}$ configuration with opposite directions of the spins of the $2s$ and $2p_{-1}$ electrons.

Table 1. The Hartree-Fock ground state configurations of the beryllium atom in external magnetic fields. The configurations presented in the table are the ground state configurations for $\gamma_{\min} \leq \gamma \leq \gamma_{\max}$. Atomic units are used.

no.	$\gamma_{\min}$	$\gamma_{\max}$	The ground state configuration	M	S_z	$E(\gamma_{\min})$
1	0	0.0412	$1s^2 2s^2$	0	0	−14.57336
2	0.0412	0.957	$1s^2 2s 2p_{-1}$	−1	−1	−14.57098
3	0.957	4.567	$1s^2 2p_{-1} 3d_{-2}$	−3	−1	−15.13756
4	4.567	∞	$1s 2p_{-1} 3d_{-2} 4f_{-3}$	−6	−2	−15.91660

But both contributions, the Zeeman spin term and the electronic exchange make the energy of this state higher than the energy of the state $1s^2 2s 2p_{-1}$ with the parallel orientation of the spins of the $2s$ and $2p_{-1}$ electrons (*i.e.* $S_z = -1$) considered above. The calculated energies for these states are presented in Figure 1. Thus, the beryllium atom has one ground state electronic configuration $1s^2 2s^2$ with the total spin z-projection $S_z = 0$. This state is the global ground state for the magnetic field strengths between $\gamma = 0$ and $\gamma = 0.0412$. Above this point the ground state configuration is $1s^2 2s 2p_{-1}$ with $S_z = -1$. Therefore the beryllium atom has four different electronic ground state configurations in the complete regime $0 < \gamma < \infty$ which are summarized in Table 1. We remark that correlation effects will change the values of the field strengths of the crossovers to some limited extent but certainly not the (qualitative) conclusions drawn above.

The next aim of this section is the corresponding investigation of the ground state configurations of the ion Be^+. The field-free ground state of this ion corresponds to the $1s^2 2s$ configuration ($S_z = -1/2$ and $M = 0$). In the opposite case $\gamma \to \infty$ the ground state is obviously given by the $1s 2p_{-1} 3d_{-2}$ configuration ($S_z = -3/2$ and $M = -3$). Thus, we need to investigate only two different subsets of electronic ground state configurations: $S_z = -1/2$ and $S_z = -3/2$. The energy curves which are necessary for this investigation are presented in Figure 2. The subset $S_z = -1/2$ contains only two possible ground state configurations $1s^2 2s$ and $1s^2 2p_{-1}$. The latter is the *local* ground state configuration for this subset in the limit $\gamma \to \infty$. The curves $E_{1s^2 2s}(\gamma)$ and $E_{1s^2 2p_{-1}}(\gamma)$ intersect at $\gamma = 0.3185$ and above this point $E_{1s^2 2p_{-1}} < E_{1s^2 2s}$. In the subset $S_z = -3/2$ we have to consider the configurations $1s 2p_0 2p_{-1}$ and $1s 2s 2p_{-1}$ along with the high-field ground state configuration $1s 2p_{-1} 3d_{-2}$. But the numerical calculations show that the energies of both $1s 2p_0 2p_{-1}$ and $1s 2s 2p_{-1}$ lie above the energy of the $1s 2p_{-1} 3d_{-2}$ configuration at the intersection point ($\gamma = 4.501$) between $E_{1s 2p_{-1} 3d_{-2}}(\gamma)$ and $E_{1s^2 2p_{-1}}(\gamma)$. Thus, the ion Be^+ possesses three different electronic ground state configurations in external magnetic fields which are summarised in Table 2. The set of the electronic ground state configurations for the Be^+ ion appears to be qualitatively the same as for the lithium atom [16]. The field strengths for the corresponding transition points are roughly two times higher for the Be^+ ion compared to the Li atom.

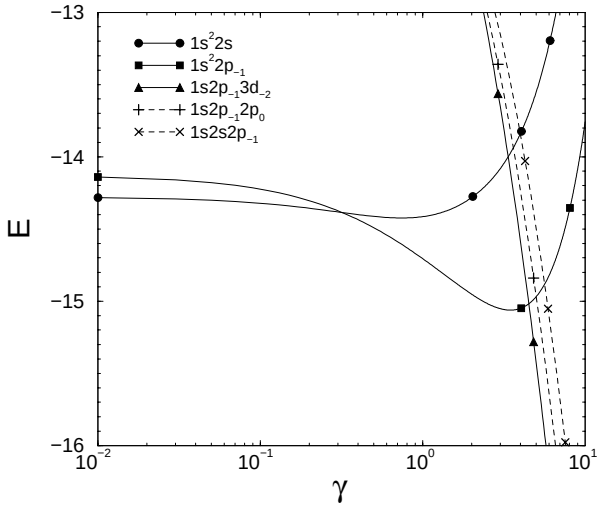

Fig. 2. The total energies (in atomic units) of the states of the beryllium positive ion as functions of the magnetic field strength considered for the determination of the ground state electronic configurations. The field strength is given in units of $\gamma = (B/B_0)$, $B_0 = \hbar c/e a_0^2 = 2.3505 \times 10^5$ T.

Table 2. The Hartree-Fock ground state configurations of the Be^+ ion in external magnetic fields. The configurations presented in the table are the ground state configurations for $\gamma_{\min} \leq \gamma \leq \gamma_{\max}$. Atomic units are used.

no.	$\gamma_{\min}$	$\gamma_{\max}$	The ground state configuration	M	S_z	$E(\gamma_{\min})$
1	0	0.3185	$1s^2 2s$	0	−1/2	−14.27747
2	0.3185	4.501	$1s^2 2p_{-1}$	−1	−1/2	−14.38602
3	4.501	∞	$1s 2p_{-1} 3d_{-2}$	−3	−3/2	−15.01775

5 Selected quantitative aspects

In Tables 3 and 4 we present the total energies of the four ground state electronic configurations of the beryllium atom and the three ground state electronic configurations of the ion Be^+, respectively. These data cover a very broad range of the field strengths from $\gamma = 0$ and very weak magnetic fields starting with $\gamma = 0.001$ up to extremely strong fields $\gamma = 10000$. The latter value of the field strength can be considered as a rough limit of applicability of the non-relativistic quantum equations to the problem (see below).

So far there exist three works which should be mentioned in the context of the problem of the beryllium atom in strong magnetic fields. Reference [19] deals with the $1s^2 2s^2$ state of this atom in fields $0 \leq \gamma \leq 1000$ and reference [20] investigates the ground state energies of atoms with nuclear charge number $Z \leq 10$ in the high-field, *i.e.* fully spin polarised regime. Both these works contain calculations carried out by the method used in the current work and do not represent a basis for comparison. The comparison of our results with an adiabatic Hartree-Fock calculation of atoms with $Z \leq 10$ [26] is presented in [20] and we can briefly summarise this comparison for two values of the magnetic field strengths: for $B_{12} = 0.1$

Table 3. The total energies of the ground state configurations of the beryllium atom depending on the magnetic field strength. Atomic units are used.

γ	$E(1s^2 2s^2)$	$E(1s^2 2s 2p_{-1})$	$E(1s^2 2p_{-1} 3d_{-2})$	$E(1s 2p_{-1} 3d_{-2} 4f_{-3})$
0.000	−14.57336	−14.51206	−14.19023	−9.44321
0.001	−14.57336	−14.51357	−14.1928	−9.4483
0.002	−14.57335	−14.51507	−14.1952	−9.4532
0.005	−14.57332	−14.51953	−14.2025	−9.4675
0.01	−14.57322	−14.52690	−14.2142	−9.4903
0.02	−14.57279	−14.54138	−14.2361	−9.5331
0.05	−14.56986	−14.58281	−14.29437	−9.6493
0.07	−14.56657	−14.60879	−14.32933	−9.7198
0.15	−14.54367	−14.70108	−14.45145	−9.9692
0.3	−14.46861	−14.83520	−14.63369	−10.36220
0.3185		−14.84905		
0.5	−14.32860	−14.96264	−14.82272	−10.80901
1.0	−13.89120	−15.14899	−15.16178	−11.72880
2.0	−12.88908	−15.30815	−15.57496	−13.16961
4.501			−15.91626	
5.0	−9.40602	−15.25183	−15.91027	−16.30690
10.0	−2.5988	−14.03046	−15.04644	−20.01753
20.0	+12.8201	−9.49118	−10.97100	−25.23250
40.0	+46.5935	+3.04026	+0.95677	−32.28415
50.0	+64.186	+10.1472	+7.83395	−35.00768
100.0	+155.286	+49.4177	+46.25962	−45.10519
200.0	+343.899	+135.659	+131.4188	−58.08264
500.0	+924.20	+411.830	+405.7027	−80.67357
1000.0	+1905.14	+888.70	+880.706	−102.75480
2000.0	+3881.5	+1860.40	+1850.052	−129.9790
5000.0		+4813.56	+4799.35	−175.2704
10000.0		+9770.37	+9752.24	−217.695

(*i.e.* $B = 0.1 \times 10^{12}$ G) our result is $E = -0.89833$ keV whereas reference [26] yields $E = -0.846$ keV; for $B_{12} = 5$ (*i.e.* $B = 5 \times 10^{12}$ G) our result is $E = -3.61033$ keV, whereas reference [26] yields $E = -3.5840$ keV. This comparison allows us to draw the conclusion of a relatively low precision of the adiabatic approximation for multi-electron atoms even for relatively high magnetic fields.

In Figure 3 we present the ionisation energy $E_{\rm ion}$ of the beryllium atom depending on the magnetic field strength. This continuous dependence is divided into six parts corresponding to different pairs of the ground state configurations of the Be atom and Be^+ ion involved into the ionisation energy. The five vertical dotted lines in Figure 3 mark the boundaries of these sections. The alteration of the sections of growing and decreasing ionisation energy originates from different dependencies of the total energies of the Be and Be^+ on the magnetic field strength for different pairs of the ground state configurations of these two systems. One can see the sharp decrease of the ionisation energy between the crossovers (4) and (5). This behaviour is due to the fact that $E_{\rm ion}$ is determined in this section by the rapidly decreasing total energy of the state $1s2p_{-1}3d_{-2}$ of the Be^+ ion (Fig. 2) and by the energy of the Be atom in the state $1s^2 2p_{-1} 3d_{-2}$ which is very weakly dependent on the field strength (Fig. 1). Another remarkable feature of the curve $E_{\rm ion}(\gamma)$ is its behaviour in the range of field strengths between the transitions (2) and (3). The ionisation energy in this region contains a very shallow maximum and in the whole section it is almost independent of the field. Thus, the ionisation energy is stationary in this regime of field strengths $\gamma = 0.3$–0.5 a.u.

The above-discussed properties are based on the behaviour of the total energy of the Be atom and Be^+ ion. On the other hand, the behaviour of the wavefunctions and many intrinsic characteristics of atoms in external magnetic fields are associated not with the total energy, but with the binding energies of separate electrons (2) and the total binding energy of the system

$$E_{\rm B} = \sum_{\mu=1}^{N} (m_\mu + |m_\mu| + 2s_{z\mu} + 1)\gamma/2 - E \qquad (3)$$

where N is the number of electrons. The binding energies of the ground state electronic configurations of Be and Be^+ depending on the magnetic field strength are

Table 4. The total energies of the ground state configurations of the Be^+ ion depending on the magnetic field strength. Atomic units are used.

γ	$E(1s^2 2s)$	$E(1s^2 2p_{-1})$	$E(1s2p_{-1}3d_{-2})$
0.000	−14.27747	−14.13093	−9.41056
0.001	−14.27797	−14.13195	−9.41358
0.002	−14.27846	−14.13294	−9.41657
0.005	−14.27995	−14.13593	−9.42551
0.01	−14.28241	−14.14087	−9.44028
0.02	−14.28725	−14.15066	−9.46939
0.0412	−14.29714		
0.05	−14.30111	−14.17916	−9.55332
0.1	−14.32207	−14.22390	−9.68356
0.2	−14.35648	−14.30406	−9.91878
0.4	−14.40046	−14.43599	−10.32817
0.5	−14.41282	−14.49163	−10.51259
0.957		−14.69069	
1.0	−14.41478	−14.70591	−11.31312
2.0	−14.28225	−14.95181	−12.59206
4.567			−15.07310
5.0	−13.55019	−14.96820	−15.42817
10.0	−11.57652	−13.75773	−18.820184
20.0	−6.03364	−9.217910	−23.612005
50.0	+15.4261	+10.42836	−32.61959
100.0	+56.5516	+49.70820	−41.93414
200.0	+145.1649	+135.95916	−53.90638
500.0	+425.471	+412.14745	−74.73619
1000.0	+906.37	+889.0264	−95.07513
2000.0	+1883.08	+1860.7100	−120.11947
5000.0	+4844.6	+4814.005	−161.7052
10000.0	+9809.3	+9770.643	−200.5709

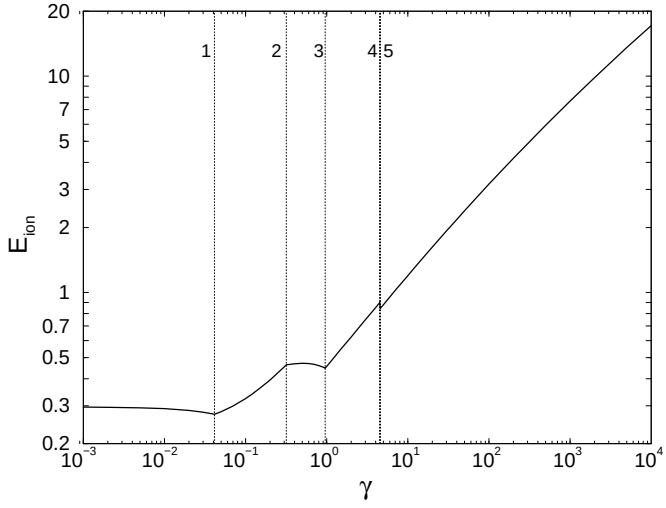

Fig. 3. Be atom ground state ionisation energy $E_{\rm I}$. Transition points are marked by broken vertical lines. The sequence of the transitions are (from left to right): 1 – Be: $1s^2 2s^2 \longrightarrow 1s^2 2s2p_{-1}$; 2 – Be^+: $1s^2 2s \longrightarrow 1s^2 2p_{-1}$; 3 – Be: $1s^2 2s2p_{-1} \longrightarrow 1s^2 2p_{-1}3d_{-2}$; 4 – Be^+: $1s^2 2p_{-1} \longrightarrow 1s2p_{-1}3d_{-2}$; 5 – Be: $1s^2 2p_{-1}3d_{-2} \longrightarrow 1s2p_{-1}3d_{-2}4f_{-3}$. Crossovers (4) and (5) take place at relatively close values of γ and are not resolved in the figure.

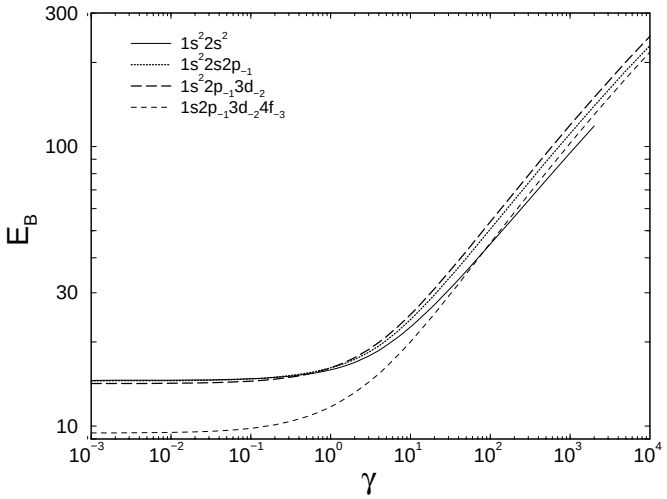

Fig. 4. The binding energies (in atomic units) of the ground state electronic configurations of the Be atom depending on the magnetic field strength. The field strength is given in units of $\gamma = (B/B_0)$, $B_0 = \hbar c/ea_0^2 = 2.3505 \times 10^5$ T.

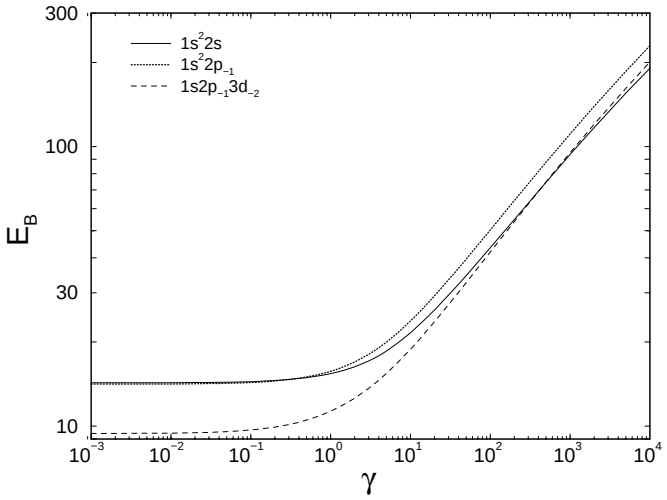

Fig. 5. The binding energies (in atomic units) of the ground state electronic configurations of the Be^+ ion depending on the magnetic field strength. The field strength is given in units of $\gamma = (B/B_0)$, $B_0 = \hbar c/ea_0^2 = 2.3505 \times 10^5$ T.

presented in Figures 4 and 5. These dependencies at very strong magnetic fields may illustrate our considerations of the previous sections. One can see in Figure 4 that the high-field ground state $1s2p_{-1}3d_{-2}4f_{-3}$ is not the most tightly bound state of the beryllium atom. For all the values of the magnetic fields considered in this paper its binding energy is lower than that of the states $1s^2 2s2p_{-1}$ and $1s^2 2p_{-1}3d_{-2}$ and for $\gamma < 100$ it is lower than $E_{\mathrm{B}1s^2 2s^2}$. The latter circumstance can be easily explained by the fact that the $1s^2 2s^2$ configuration contains two tightly bound orbitals $1s$ whereas the $1s2p_{-1}3d_{-2}4f_{-3}$ configuration possesses only one such orbital. However, with increasing magnetic field strengths the contribution of the group of orbitals $2p_{-1}3d_{-2}4f_{-3}$ to the binding energy turns out to be larger than that of the $1s2s^2$ group. Analogously

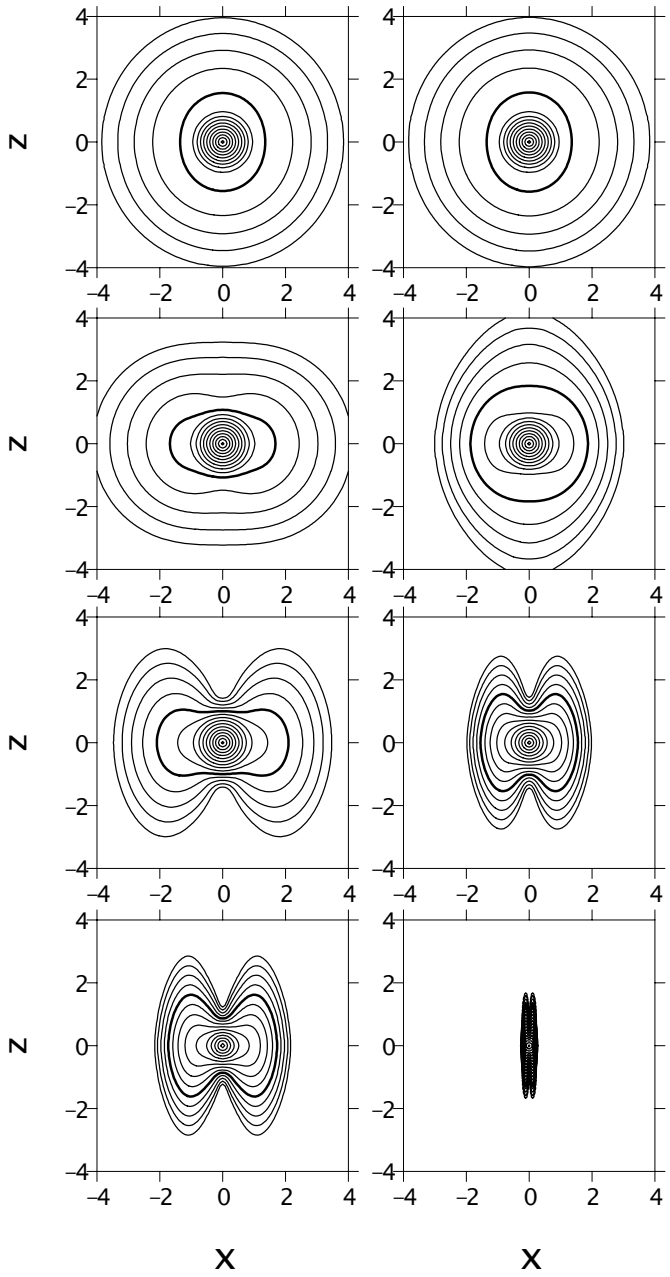

Fig. 6. Contour plots of the total electronic densities for the ground state of the beryllium atom. For neighbouring lines the densities are different by a factor of 2. The coordinates z, x as well as the corresponding field strengths are given in atomic units. Each row presents plots for a ground state configuration at its lower (left) and upper (right) intersection points. Rows: 1 – $1s^2 2s^2$: $\gamma = 0$ and $\gamma = 0.0412$; 2 – $1s^2 2s 2p_{-1}$: $\gamma = 0.0412$ and $\gamma = 0.957$; 3 – $1s^2 2p_{-1} 3d_{-2}$: $\gamma = 0.957$ and $\gamma = 4.567$; 4 – $1s 2p_{-1} 3d_{-2} 4f_{-3}$: $\gamma = 4.567$ and $\gamma = 500$.

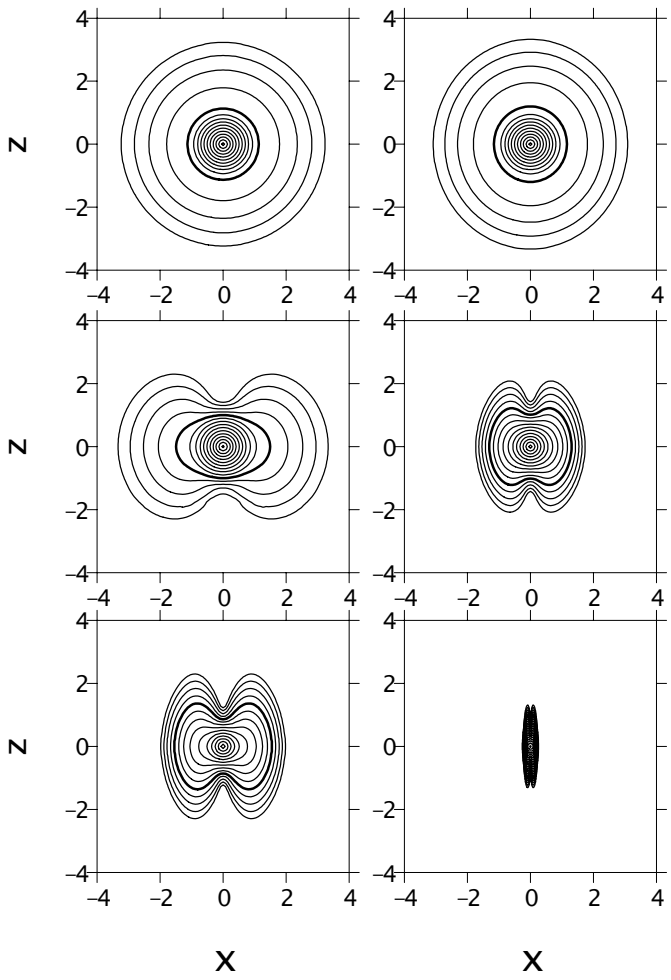

Fig. 7. Contour plots of the total electronic densities for the ground state of the beryllium positive ion. For neighbouring lines the densities are different by a factor of 2. The coordinates z, x as well as the corresponding field strengths are given in atomic units. Each row presents plots for a ground state configuration at its lower (left) and upper (right) intersection points. Rows: 1 – $1s^2 2s$: $\gamma = 0$ and $\gamma = 0.3185$; 2 – $1s^2 2p_{-1}$: $\gamma = 0.3185$ and $\gamma = 4.501$; 3 – $1s 2p_{-1} 3d_{-2}$: $\gamma = 4.501$ and $\gamma = 500$.

we can expect $E_{\mathrm{B}1s2p_{-1}3d_{-2}4f_{-3}} > E_{\mathrm{B}1s^2 2s 2p_{-1}}$ at some very large fields $\gamma > 10000$. On the other hand, it is evident that the state $1s 2p_{-1} 3d_{-2} 4f_{-3}$ must be less bound than $1s^2 2p_{-1} 3d_{-2}$ because both these configurations are constructed from orbitals with binding energies, logarithmically increasing as $\gamma \to \infty$, but the $1s^2 2p_{-1} 3d_{-2}$ contains an additional $1s$ orbital, which is more tightly bound than $4f_{-3}$ for arbitrary field strengths. The plot for the Be^+ ion (Fig. 5) illustrates the same features and one can see in this figure almost parallel curves $E_{\mathrm{B}1s^2 2p_{-1}}(\gamma)$ and $E_{\mathrm{B}1s2p_{-1}3d_{-2}}(\gamma)$ in the strong field regime.

Figures 6 and 7 allow us to add some details to the considerations of the previous section. These figures present spatial distributions of the total electronic densities for the ground state configurations of the beryllium atom and its positive ion, respectively. These pictures allow us to gain insights into the geometry of the distribution of the electronic density in space and in particular its dependence on the magnetic quantum number and the total spin. The first pictures in these figures present the distribution of the electronic density for the ground state for $\gamma = 0$. The following pictures show the distributions of the electronic densities for values of the field strength which mark the boundaries of the regimes of field strengths belonging to

the different ground state configurations. For the high-field ground states we present the distribution of the electronic density at the crossover field strength and for $\gamma = 500$. For each configuration the effect of the increasing field strength consists in compressing the electronic distribution towards the z-axis. However the crossovers of ground state configurations involve the opposite effect due to the fact that these crossovers are associated with an increase of the total magnetic quantum number M.

In the first rows of Figures 6 and 7 one can see a dense core of $1s^2$ electrons inside the bold solid line contour and a diffuse distribution of $2s$ electrons outside this core. This contour roughly corresponds to a maximum of the electron density formed by the $2s$ electrons at $\gamma = 0$. The prolate shape of the bold solid line contour in the first plot of Figure 6 ($1s^2 2s^2$, $\gamma = 0$) reflects the non-spherical distribution of the $2s$ electrons in our unrestricted HF calculations or the admixture of the $1s^2 2p_0^2$ configuration to the $1s^2 2s^2$ one from the point of view of the multi-configurational approach [25].

Some additional comments concerning the results presented above are in order. First, our HF results do not include the effects of correlation. To take into account the latter would require a multi-configurational approach which goes beyond the scope of the present paper. We, however, do not expect that the correlation energy changes our main conclusions like, for example, the fact of the crossovers with respect to the different ground states configurations. With increasing field strength the effective one particle picture should be an increasingly better description of the wave function and the percentage of the correlation energy should therefore decrease (see Ref. [23] for an investigation on this subject). Two other important issues are relativistic effects and effects due to the finite nuclear mass. Both these points are basically important for very high magnetic field strengths and they have been discussed in reference [20]. Even for $\gamma = 10^4$ a.u. the relative change of the total energy ($E \propto \gamma$) due to relativistic corrections is of the order of 10^{-4}. Since the ionisation energy of the Be atom for this field strength is approximately 20 a.u. we can suspect that for $\gamma \geq 10^3$–10^4 a.u. relativistic corrections become significant. However, for a definite clarification fully relativistic many-body calculations would have to be performed in the high field regime.

6 Summary and conclusions

We have applied our 2D mesh Hartree-Fock method to the magnetised neutral beryllium atom and beryllium positive ion. The method is flexible enough to yield precise results for arbitrary field strengths and our calculations for the ground and several excited states are performed for magnetic field strengths ranging from zero up to 2.3505×10^9 T ($\gamma = 10000$). Our considerations focused on the ground states and their crossovers with increasing field strength. The ground state of the beryllium atom undergoes three transitions involving four different electronic configurations. For weak fields up to $\gamma = 0.0412$ the ground state arises from the field-free ground state configuration $1s^2 2s^2$ with the total spin z-projection $S_z = 0$. With increasing strength of the field two different electronic configurations with $S_z = -1$ consequently become the ground state: $1s^2 2s 2p_{-1}$ and $1s^2 2p_{-1} 3d_{-2}$. At $\gamma = 4.567$ the last crossover of the ground state configurations takes place and for $\gamma > 4.567$ the ground state wavefunction is represented by the high-field-limit fully spin polarised configuration $1s 2p_{-1} 3d_{-2} 4f_{-3}$, $S_z = -2$.

For the ion Be^+ we obtain three different ground state configurations possessing two values of the spin projection. For fields below $\gamma = 0.3185$ the ground state electronic configuration has the spin projection $S_z = -1/2$, magnetic quantum number $M = 0$ and qualitatively coincides with the zero-field ground state configuration $1s^2 2s$. Between $\gamma = 0.3185$ and $\gamma = 4.501$ the ground state is represented by another configuration with $S_z = -1/2$, *i.e.* $1s^2 2p_{-1}$ ($M = -1$). Above the point $\gamma = 4.501$ the fully spin polarised high-field-limit configuration $1s 2p_{-1} 3d_{-2}$ ($S_z = -3/2$) is the actual ground state of the Be^+ ion. Thus, the sequence of electronic ground state configurations for the Be^+ ion is similar to the sequence for the Li atom [16]. We present detailed tables of energies of the ground state configurations for Be and Be^+.

For Be and Be^+ we have presented also the binding energies of the ground state configurations dependent on the magnetic field strength and maps of electronic densities for these configurations. For the Be atom we present its ionisation energy dependent on the field strength.

Our investigation represents the first conclusive study of the ground state of the beryllium atom and Be^+ ion for arbitrary field strengths. For the Be atom we have obtained a new sequence of electronic configurations with increasing field strength. This sequence does not coincide with any such sequences obtained previously for other atoms and ions and could not be predicted even qualitatively without detailed calculations. Putting together what we currently know about ground states of atomic systems in strong magnetic fields we can conclude that the H, He, Li, Be, C, He^+, Li^+ and Be^+ ground states have been identified. For other atoms and multiple series of ions the question about the ground state configurations is still open.

Finally we remark that the present approach (UHF) also yields certain excited states but only on a qualitative level. To meet astrophysical requirements, however, a high precision is required for many excited states. In principal it is possible to extend our method in order to include correlation effects and the complete excitation spectrum by superimposing many (excited) determinants and performing a so-called configuration interaction calculation. This means however a substantial conceptual and programming effort and goes beyond the scope of the present investigation.

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