Beryllium in Strong Magnetic Fields

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(Dated: March 31, 2022)

We investigate the electronic structure of the beryllium atom subjected to a strong magnetic field in the regime $0 \leq \gamma \leq 10$ a.u. The ground as well as many excited states of spin singlet, triplet and quintet multiplicity covering the magnetic quantum numbers $|M| = 0, 1, 3, 6$ for both positive and negative $z$-parity are discussed and analyzed. Total and one-particle ionization energies are provided. Transition wavelengths as a function of the field strengths for allowed dipole transitions are provided.

PACS numbers: 32.60+i, 32.30.-r, 32.70.-n

I. INTRODUCTION

The past decades have seen an enormous development with respect our knowledge of the behavior and properties of atoms exposed to strong external fields. This holds equally for time-dependent electric as well as static electric or magnetic fields (for reviews of the subject concerning static fields see Refs. \cite{1, 2, 3, 4, 5}). In case of static homogeneous magnetic fields the hydrogen atom served as a paradigm for the effects due to the combined Coulomb and magnetic interactions \cite{1}. It is one of the most fundamental few-degrees of freedom quantum systems whose classical counterpart shows a transition from regularity to chaos finally exhibiting a (almost) completely chaotic phase space. The investigations on hydrogen in a magnetic field had major impact on a variety of other fields such as nonlinear dynamics, semiclassics of nonintegrable systems as well as magnetized structures in general \cite{1}. On the other hand major advances in high resolution laser spectroscopy allowed a detailed and highly instructive comparison of theoretical results and experimental data.

Turning to astrophysics the success of the investigations on hydrogen in a strong magnetic field is equally impressive. During the eighties comprehensive studies of the spectrum and eigenfunctions for bound states (see Ref.\cite{2} and Refs. therein) were performed with particular emphasis on the regime of field strengths occuring in the atmospheres of magnetic white dwarfs $10^2 \text{T} < B < 10^5 \text{T}$. Among others, the corresponding data have lead to a conclusive interpretation of the observed spectrum of the white dwarf GrW+70\textsuperscript{8247} which was a key to our understanding of the properties of spectra of magnetic white dwarfs in general (see e.g. Refs. \cite{6, 7, 8, 9, 10}). In the nineties detailed investigations of the continuum properties of hydrogen in strong magnetic fields have been accomplished \cite{11, 12}.

More-electron systems are due to the occurence of the electron-electron repulsion that competes with both the electron-nuclear attractions and the magnetic interactions much more complicated. It was only in the late nineties that a sophisticated electronic structure method became available which allows to compute the bound state properties of the helium atom exposed to a strong field \cite{13}. Subsequently \cite{13} hundred excited states and the corresponding oscillator strengths of their transitions have been studied with the necessary accuracy in order to perform a comparison with astrophysical observation. Employing these data strong evidence arose that the mysterious absorption edges of the magnetic white dwarf GD229 \cite{14, 15, 16, 17, 18}, which were for almost 25 years unexplained, are due to helium in a strong magnetic field $B \approx 50 000 \text{T}$ \cite{17, 18}. Also very recently the newly established helium data were used to analyze a number of magnetic and suspected-magnetic southern white dwarfs \cite{17, 20}.

Beyond the one- and two-electron atoms our knowledge on the behavior of multi-electron atoms subjected to strong magnetic fields is very scarce. This is in contrast to the astrophysical necessity for further informations on the spectral properties of multi-electron atoms. The ongoing Sloan Digital Sky Survey already doubled the number of known magnetic white dwarfs \cite{21}. It is believed that heavier atoms are present in the atmospheres of the corresponding stars due to accretion of interstellar matter, and particularly it is expected that these objects are quite common \cite{22}.

To improve the above-mentioned situation of the lack of data for multi-electron atoms we have very recently developed a full configuration interaction approach to more-electron ($N \geq 3$) atoms in strong magnetic fields \cite{23}. As a first investigation the lithium atom has been studied in detail \cite{23}; the ground as well as many excited states

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of different symmetries have been computed for a broad range of field strengths with the astrophysically required accuracy. Thereby our knowledge on the electronic structure of the lithium atom in a strong magnetic field has been advanced significantly (for the state-of-the-art before this work see Refs. 24, 25, 27, 28, 29, 30, 31).

In the present work we investigate the behavior and properties of the Beryllium atom in the complete regime $0 \leq \gamma \leq 10$ a.u. (following the usual convention, the field strengths in atomic units is denoted by $\gamma$, where $\gamma = 1$ corresponds to $2.355 \times 10^5$ T) which covers in particular the field range of the magnetic white dwarfs. Besides the global ground state we present an analysis of many excited states possessing a variety of different symmetries thereby multiplying the up-to-date information on the beryllium atom in the presence of a (strong) magnetic field. Let us comment at this point on the existing literature. Refs. 24, 31 contain for a few field strengths in the high field regime a discussion of the ground state (for that field strengths). In Ref. 32 the field-free ground state has been investigated in the presence of the field and Ref. 28 contains a discussion of the ground state in the high field regime. Both latter investigations deal with a Hartree-Fock approach to the electronic structure. Also within Hartree-Fock Ref. 35 contains an investigation of the global ground state for the weak to the high field regime. The most sophisticated correlated approach up to date is provided in Ref. 34. The regime $0 \leq \gamma \leq 1.0$ is covered and the ground state as well as several excited states are studied with a relatively high accuracy thereby employing a frozen-core correlated approach. When comparing our data with the existing ones in the literature the latter will predominantly be from Ref. 34.

We proceed as follows. Section II contains a discussion of the fixed-nucleus Hamiltonian and its symmetries. Section III describes our computational approach. Section IV presents a discussion and analysis of our results. It starts with a discussion of the global ground state of the beryllium atom with increasing field strength and turns then to a detailed study of the excited states of various symmetries. In section V we report on the transition wavelengths as a function of the field strength. Finally section VI contains the conclusions.

II. HAMILTONIAN AND SYMMETRIES

The electronic Hamiltonian describing the beryllium atom exposed to a strong magnetic field assuming an infinitely heavy nucleus reads as follows

$$H(B) = \sum_{i=1}^{4} H_i(B) + \sum_{i \neq j} H_{ij} \quad \text{with}$$

$$H_i(B) = \frac{p_i^2}{2} + \frac{\mathbf{B} \cdot \mathbf{l}_i}{2} + \frac{(\mathbf{B} \times \mathbf{r}_i)^2}{8} - \frac{4}{|\mathbf{r}_i|} + \frac{g\mathbf{B} \cdot \mathbf{s}_i}{2}$$

$$H_{ij} = \frac{1}{2} \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|}.$$  

where we have adopted the symmetric gauge for the vector potential and we have employed atomic units. $H_i(B)$ represents the field-dependent one-particle operator containing the Zeeman-term $1/2 \mathbf{B} \cdot \mathbf{l}_i$, the diamagnetic term $1/8(\mathbf{B} \times \mathbf{r}_i)^2$, the Coulomb interaction with the nucleus $-4/|\mathbf{r}_i|$ as well as the spin Zeeman contribution $g/2 \mathbf{B} \cdot \mathbf{s}_i$. $H_{ij}$ is a two-particle operator and represents the electron-electron Coulomb repulsion.

In the above Hamiltonian the direction of the magnetic field coincides with the $z-$axis. Therefore the $z-$projection of the total orbital angular momentum and of the total spin $S_z$ are conserved. These yield the good quantum numbers $M$ and $S_z$, respectively. Furthermore the total spin is conserved and the $z$ parity $\Pi_z$ represents a symmetry. In the following we employ the spectroscopic notation $\nu \Pi_z S_z M^\Pi_z$ for the electronic states, where $\nu$ stands for the degree of excitation of a certain state with given quantum numbers $S, M, \Pi_z$.

III. COMPUTATIONAL METHOD

The energies of the electronic bound states are determined by mapping the Schrödinger equation to an ordinary eigenvalue problem. This is done by applying a direct full configuration interaction (full CI) approach. For the basis set of atomic orbitals we choose anisotropic Gaussian functions, which have been introduced for atomic and molecular calculations in strong magnetic fields by Schmelcher and Cederbaum 32. This basis set has been successfully applied to several atoms, ions and molecules 33, 36, 37, 38, 39. A major advantage of it is the flexibility: The anisotropic Gaussian functions can be adapted to any (zero or non zero) field strength by adjusting the corresponding nonlinear variational parameters. As a result the convergence properties of the electronic structure calculations using the optimized basis sets (see below) are good for any field strengths, although it turns out that for the intrinsically most
complex intermediate field regime our approach converges fastest. The above is in contrast to symmetry adapted basis sets, that have been employed in electronic structure investigations in fields: typically electronic eigenfunctions can be well-described for either low field strengths (approximate spherical symmetry) or for very strong fields (approximate cylindrical symmetry) but lack to converge in the intermediate field regime.

To take full advantage of the flexibility of the basis functions they have to be optimized for each field strength and each symmetry subspace separately. To this end we determine the primitive Gaussian functions by solving different one-particle problems (Be$^{3+}$, He$^+$ and H) for each field strength. In order to converge rapidly thereby using a minimal number of basis functions, the latter have to be selected very carefully.

The four-electron beryllium calculations start with the computation of the overlap matrix $S(m_j, \pi_{z_j})$ of the Gaussian functions. Only those eigenvectors \{v_\nu(m_j, \pi_{z_j})\} of $S$ possessing an eigenvalue above an appropriately chosen threshold $\varepsilon$ are used in the following calculations. As a next step the Schrödinger equation belonging to the one-particle Hamiltonian (2) is represented as an ordinary matrix eigenvalue problem. The numerical solution of this eigenvalue problem yields the eigenvectors \{h_i(m_j, \pi_{z_j})\}, which then serve as the spatial part of the one-particle functions for the four-electron investigations. Spinors $\chi_j$ are constructed as a product of the usual spin eigenfunctions $\alpha$ and $\beta$ and the orthogonal functions \{h_i(m_j, \pi_{z_j})\}. Full CI calculations are performed with four-electron Slater determinants, which are constructed from spinors, thereby obeying the correct symmetries, i.e.

$$\sum_{i=1}^{4} m_i = M \quad (4)$$
$$\prod_{i=1}^{4} \pi_{z_i} = \Pi_z \quad (5)$$
$$\sum_{i=1}^{4} s_{z_i} = S_z \quad (6)$$

In general the core electrons and specifically the 1$s^2$ and 2$p_0$ orbitals, are well described by basis functions that are optimized for the $1^20^+$- and $1^30^-$-states of Be$^{3+}$, respectively. Further basis functions for the full CI calculations of the beryllium atom are obtained by optimizing them for the corresponding one-particle problems of nuclear charge $Z = 1$ and $Z = 2$. For the spin singlet and triplet states of beryllium exclusively only the hydrogen atom has been employed for the optimization. For the quintet states, some of the low-lying orbitals were described by functions optimized for He$^+$. To be more specific, for the $n^10^+$ states functions with one-particle symmetry $m^{s_\pi} = 0^+$, $0^-$, and $\pm 1^+$ have been employed. The same holds for the symmetry subspaces $^1(−1)^+$ and $^3(−1)^+$. In order to achieve convergence also for the excited states, orbitals optimized for the ground states of the $m^{s_\pi} = 0^+$ symmetry in case of $M = 0$ and of the $m^{s_\pi} = (\pm 1)^+$ symmetry in case of $M = −1$ optimized for hydrogen states are important. For the symmetry subspace $^1(−1)^-$ we used more functions of the one-particle symmetry $0^−$ optimized for the ground and excited states of hydrogen. Additionally states for $m^{s_\pi} = (\pm 1)^\pm$ have been used. For the triplet and quintet symmetry subspace with positive $z$-parity and $M = −3$ the orbitals of $m^{s_\pi} = (\pm 2)^+$ replace those with $(\pm 1)^−$ and $0^−$. For the quintet symmetry subspaces $^5(−3)^−$ and $^5(−6)^+$ additionally functions of $m^{s_\pi} = (\pm 3)^+$ symmetry character that have been optimized for hydrogen are included in the calculations. Our calculations have been performed using up to 50 one-particle basis functions resulting in 80 000 Slater determinants.

IV. ENERGIES

A. The global ground state and the properties of total energies

In strong magnetic fields, more precisely in the high field regime, the total energies of bound states of an atomic or molecular system are dominated by the orbital and spin Zeeman-contributions on the one hand side and the increase of the kinetic energy on the other hand side. The kinetic energy depends approximately linear on the field strength (Landau zero point energy of the electrons) and the contributions of the Zeeman terms behave exactly linear with the changing magnetic field strength. The overall effect of these contributions on the total energies are demonstrated in Fig. 1. The latter shows the total energies of all 61 calculated bound states possessing negative magnetic quantum numbers as a function of the field strength $\gamma$. In the high field limit a general pattern can be identified: Energy levels corresponding to fully spin polarized states ($S_z = −2$) decrease monotonically with increasing field strength, energy levels belonging to states with $S_z = −1$ pass through a local minimum, and those belonging to states with a positive total spin projection increase monotonically. This classification of the overall behavior of the energy curves depends exclusively on the spin projection of the states considered.
With increasing field strength the ground state of an atom exposed to a magnetic field changes its symmetry i.e. a crossover of several states individually representing the ground state of the atom for a certain interval of field strengths takes place. The orbital and spin Zeeman-terms are important for the identification of the field-dependent global ground state \[27, 28, 33, 39, 40\]. Beyond this the magnetically tightly bound orbitals \[2, 41\] compared to the non-tightly bound orbitals/states play a central role for the determination of the ground state. Since the ground state is finally obtained by a complicated interplay of the above contributions, the electronic states forming the ground state of the atom depending on the field strength are not predictable \textit{a priori}, but have to be determined by explicit electronic structure calculations. For the beryllium atom investigated here, four electronic states representing the global ground state for different field regimes have been found. This result coincides with an earlier one \[33\] based on Hartree-Fock calculations of the beryllium atom. Having fully correlated results at hand it is now, however, possible to finally conclude on the ground state properties of the atom. The total energies of the states constituting the ground state are presented in Fig. 2. The low field ground state \(0 < \gamma < 0.0612\) is the highly correlated, doubly tightly bound singlet state \(1^1S_{1/2}\). Its total energy increases monotonically as can be observed for all states with a vanishing spin quantum number \(S_z = 0\). In the field regime \(0.0612 < \gamma < 1.0\) the global ground state is represented by the triply tightly bound triplet state \(1^3P_{1/2}\). Concerning the contributions to its total energy the increase of the kinetic energy is now partly compensated by the spin Zeeman-term. Therefore the energy of this state does not monotonically increase with increasing field strength, but passes through a minimum, which is located at \(\gamma \approx 3.22\). For \(1.0 < \gamma < 4.62\) the ground state is given by the triplet state \(1^3P_{3/2}\) which possesses four tightly bound orbitals. Similar to the \(1^1P_{1/2}\) state, the reader should note, that its total energy passes through a minimum, which, for this state, is located at a higher field strength, compared to the state \(1^3P_{1/2}\), namely at \(\gamma \approx 4.23\). In the high field regime \(\gamma > 4.23\) the spin Zeeman-term completely dominates the total energies. The high field ground state is provided by the quadruply tightly bound state \(1^5P_{3/2}\) of spin quintet symmetry. Its energy monotonically decreases as a function of the field strength \(\gamma\). In the field-free case this state is unbound.

Since the Zeeman energy and the kinetic energy predominate the total energy of the states and mask the interesting new properties of the atomic states, we will in the following concentrate our discussion on the ionization energies. These will reveal the binding properties of the corresponding states. For each symmetry subspace and each field strength, the corresponding ionization threshold has to be identified. We define here the ionization energy to respect the symmetry properties: The threshold \(E_T(\gamma, M, S_z)\) for total magnetic quantum number \(M\) and \(z\) projection \(S_z\) of the total spin is defined by the equation

\[
E_T(\gamma, M, S_z) = \min_{M_1, S_{z_1}} E^{Be^+}(\gamma, M_1, S_{z_1}) + E^e(\gamma, M_2, S_{z_2}),
\]

where \(E^{Be^+}(\gamma, M_1, S_{z_1})\) and \(E^e(\gamma, M_2, S_{z_2})\) are the total energies of the \(Be^+\) ion and the electron, respectively, depending on their magnetic quantum numbers \(M_i\) and \(S_{z_i}\) \((i = 1, 2)\). Obviously this requires that the electronic quantum numbers \(M_2\) and \(S_{z_2}\) are related to the ionic respectively atomic quantum numbers via

\[
M_2 = M - M_1, \quad S_{z_2} = S_z - S_{z_1}.
\]

In order to determine the ionization thresholds many states of the \(Be^+\) ion have to be computed as a function of the

\[\text{FIG. 1: Total energies } E_{\text{Tot}}\text{ of all 61 calculated bound states with non positive magnetic quantum number } M \text{ in a.u. as a function of the magnetic field strength } \gamma. \text{ It can be seen that the behavior of the total energies can be classified by the spin projection } S_z.\]
FIG. 2: Total energies $E_{\text{Tot}}$ of the states constituting the ground state of the beryllium atom in a.u. as a function of the magnetic field strength $\gamma$. The inset shows a magnification for a certain regime of field strengths.

magnetic field strengths $\gamma$ in detail. Table I presents our results for the total energies of the electronic states of Be$^+$, which are associated to the one-particle ionization thresholds.

| $\gamma$ | $E_{\text{Tot}}$ | $E_{\text{Tot}}$ | $E_{\text{Tot}}$ | $E_{\text{Tot}}$ | $E_{\text{Tot}}$ |
|----------|-----------------|-----------------|-----------------|-----------------|-----------------|
| 0.000    | -14.3247        | -14.1727        | -14.1741        | -10.0650        | -9.4156         |
| 0.001    | -14.3251        | -14.1720        | -14.1751        | -10.0655        | -9.4185         |
| 0.010    | -14.3296        | -14.1765        | -14.1841        | -10.0827        | -9.4452         |
| 0.050    | -14.3482        | -14.1955        | -14.2216        | -10.1067        | -9.6888         |
| 0.100    | -14.3694        | -14.2180        | -14.2672        | -10.2575        | -9.9243         |
| 0.200    | -14.4038        | -14.2572        | -14.3476        | -10.4353        | -10.5188        |
| 0.500    | -14.4606        | -14.3448        | -14.5358        | -10.8918        | -11.3203        |
| 1.000    | -14.4630        | -14.4255        | -14.7520        | -11.4967        | -12.6002        |
| 2.000    | -14.4300        | -14.4558        | -15.0000        | -12.4090        | -15.4367        |
| 5.000    | -13.5971        | -13.9795        | -15.0184        | -14.5106        | -18.8283        |
| 10.000   | -11.6231        | -12.1626        | -13.8087        | -17.2291        | -18.8283        |

TABLE I: Total energies for Be$^+$ in a.u. needed to determine the one-particle ionization thresholds for different field strengths for the beryllium states considered here.

One implication of the above definition of the ionization threshold is the fact, that the ionization energy neither depends on the value of the spin projection $S_z$, nor on the sign of the magnetic quantum number. Therefore, total energies will be provided for one spin projection and the non-positive magnetic quantum number. The maximal negative value of the spin projection onto the magnetic field axis is chosen, i.e $S_z = -S$. By adding the corresponding contributions of the spin Zeeman- and orbital Zeeman-term respectively, the total energies for the states with different quantum numbers $S_z$ and also for the opposite sign of the orbital quantum number $M$ can be obtained.

B. The symmetry subspace $1^20^+$.  

The ionization energies for the $\nu^10^+$ states ($\nu = 1, 2, 3$) are presented in Fig. 3. Numerical values for the total and ionization energies, the symmetries of the ionization threshold, as well as a comparison to previously published data can be found in table II. The state $1^20^+$ represents, as mentioned above, the ground state of the atom in the low field regime. Its ionization energy increases monotonically with increasing field strength. At $\gamma = 0$ it is 0.3158 a.u., whereas for $\gamma = 10$ it has increased to 0.5311 a.u. Comparing the total energies obtained for the $1^20^+$ state within our fully correlated CI approach with the existing data in the literature we arrive at the following conclusions. In the absence of the external field the relative accuracy is $2 \times 10^{-3}$ compared to the more accurate calculations in Ref. (42). This holds equally for the comparison of our data for finite field strengths with the more accurate results in Ref. (44).
which uses a frozen-core correlated approach. The latter statement is correct up to $\gamma \approx 0.5$ whereas for $\gamma > 0.5$ our method yields lower total energies than the one employed in Ref. [34]. For field strengths $\gamma \geq 2$ only Hartree-Fock results are available for comparison [27, 33] and it turns out that these are energetically higher up to one percent for $\gamma = 10$.

For the first excited state $2^10^+$ a different behavior can be observed. Its one-particle ionization energy (OPIE) increases for low fields $0 < \gamma < 0.05$. In the field range $0.05 < \gamma < 0.2$ it passes through a local minimum and increases from 0.0650 a.u. for $\gamma = 0.1$ to 0.2241 at $\gamma = 1$. For $\gamma \leq 1$ the ionization threshold involves the $1^20^+$ electronic state of $\text{Be}^+$ whereas for $\gamma > 1$ it is the $1^20^-$ state. As a consequence, the ionization threshold for the $2^10^+$ state drops to 0.0977 a.u. at $\gamma = 2$. For $\gamma > 2$ the ionization energy decreases as a function of $\gamma$ at a much lower rate. Only for $\gamma = 0$ energies of this state are available for comparison [42] i.e. this state has not been investigated previously in the literature. It turns out that our energies show a relative accuracy of $2 \times 10^{-3}$ similar to the case of the $1^10^+$ state in the absence of the field.

The OPIE of the second excited state $3^10^+$ behaves as a function of the field strength similar to the first excited state. It increases for low fields $0 < \gamma < 0.05$ and passes through a local minimum at $\gamma \approx 0.2$. For $0.2 > \gamma > 2$ it increases. For $\gamma > 2$ we were not able to obtain sufficiently accurate results.

![Graph](image_url)  

**FIG. 3:** One-particle ionization energies for the states $\nu^00^+$ ($\nu = 1, 2, 3$) in a.u. as a function of the magnetic field strength $\gamma$. 

| $\gamma$ | $T_{\text{Sym}}$ | $E_{\text{Tot}}$ | $E_{\text{Ion}}$ | $E_{\text{Lit}}$ | $E_{\text{Tot}}$ | $E_{\text{Ion}}$ | $E_{\text{Lit}}$ | $E_{\text{Tot}}$ | $E_{\text{Ion}}$ | $E_{\text{Lit}}$ |
|---|---|---|---|---|---|---|---|---|---|---|
| 0.000 | $0^+$ | -14.6405 | 0.3158 | -14.66736$^a$ | -14.3908 | 0.0661 | -14.41824$^b$ | -14.3578 | 0.0331 | -14.40793$^c$ |
| 0.010 | $0^+$ | -14.6410 | 0.3168 | -14.66287$^b$ | -14.3733 | 0.0492 | -14.3589 | 0.0347 | -14.3619 | 0.0423 |
| 0.050 | $0^+$ | -14.6393 | 0.3411 | -14.56986$^c$ | -14.3782 | 0.0800 | -14.3625 | 0.0643 | -14.3241 | 0.0548 |
| 0.100 | $0^+$ | -14.6298 | 0.3604 | -14.64955$^d$ | -14.3344 | 0.0650 | -14.3241 | 0.0548 | -14.3241 | 0.0548 |
| 0.200 | $0^+$ | -14.5907 | 0.3868 | -14.61160$^c$ | -14.2858 | 0.0820 | -14.2492 | 0.0454 | -14.2492 | 0.0454 |
| 0.500 | $0^+$ | -14.3882 | 0.4276 | -14.40818$^b$ | -14.1273 | 0.1667 | -14.0136 | 0.0529 | -14.0136 | 0.0529 |
| 1.000 | $0^+$ | -13.9220 | 0.4590 | -13.91717$^b$ | -13.6871 | 0.2241 | -13.5439 | 0.0809 | -13.5439 | 0.0809 |
| 2.000 | $0^-$ | -12.9275 | 0.4717 | -12.88908$^c$ | -12.5353 | 0.0977 | -12.5430 | 0.0873 | -12.5430 | 0.0873 |
| 5.000 | $0^-$ | -9.4907 | 0.5112 | -9.40602$^c$ | -9.0724 | 0.0929 | -9.0724 | 0.0929 | -9.0724 | 0.0929 |
| 10.000 | $0^-$ | -2.6936 | 0.5310 | -2.5988$^d$ | -2.2469 | 0.0843 | -2.2469 | 0.0843 | -2.2469 | 0.0843 |

TABLE II: Total energies $E_{\text{Tot}}$, one-particle ionization energies $E_{\text{Ion}}$, and previously published data for the total energies $E_{\text{Lit}}$ in a. u. for the states $\nu^10^+$ ($\nu = 1, 2, 3$), as well as the symmetry $T_{\text{Sym}}$ of the $\text{Be}^+$ ion belonging to the ionization threshold for different field strengths $\gamma$.

\(a\)Ref. [42].
\(b\)Ref. [34].
\(c\)Ref. [33].
\(d\)Ref. [27].
C. The symmetry subspaces $1/3(-1)^{±}$.

This subsection presents a discussion of our results on the singlet states $\nu^1(-1)^{±}$ for $\nu = 1, 2$ and the triplet states $\nu^3(-1)^{±}$ for $\nu = 1 – 3$. We illustrate the corresponding ionization energies in Fig. 4 and the numerical values for the total energies, OPIEs together with previously published data for the total energies of these states are provided in Table II and in Table IV respectively. The symmetries of the corresponding ground electronic states of the Be$^{±}$ ion in the ionization limit are also provided as a function of the field strength.

Let us first discuss the behavior of the energies of the singlet states. The OPIEs of the energetically lowest state $1^1(-1)^{±}$ which is a triply tightly bound state, does not increase monotonically but passes through a local maximum at $\gamma \approx 0.5$. The increase of the OPIE in the low field regime $0 < \gamma < 0.5$ is more pronounced for the $1^1(-1)^{±}$ state, than for the $1^30^±$. It increases approximately by a factor 3 from 0.1161 a.u. at $\gamma = 0$ to 0.3284 a.u. at $\gamma = 0.5$. For $\gamma > 0.5$ the OPIE decreases. One reason for this is the field-dependent behavior of the ionization threshold. For $\gamma > 0.2$ it involves the triply tightly bound Be$^{±}$ state $1^1(-1)^{±}$. This threshold has in the latter field regime a lower energy than the threshold involving the ionic state $1^30^−$, which represents the high field ionization threshold for the $1^0$ symmetry subspace. Considering the numerical values for the total energies of the $1^1(-1)^{±}$ state compared to the literature we arrive at the following conclusions. For the field-free case the relative accuracy is approximately $2 \times 10^{-3}$ in comparing with the highly accurate values presented in Ref.[42]. In the presence of the field for $\gamma \leq 0.5$ the comparison with Ref.[34] shows that our values are again by a relative factor of $2 \times 10^{-3}$ above the values of this reference. However, for $\gamma > 1$ no data are available up to date in the literature.

![FIG. 4: One-particle ionization energies for the states $\nu^1(-1)^{±}$ ($\nu = 1, 2$) and $\nu^3(-1)^{±}$ ($\nu = 1, 2, 3$) in a.u. as a function of the magnetic field strength $\gamma$.](image)

The OPIE of the first excited state $2^1(-1)^{±}$ shows a similar behavior as that of the ground state. It increases in the low field regime and decreases in the high field regime thereby exhibiting a local maximum at $\gamma \approx 0.2$. Total energies for this state are available only for a vanishing external field and our computed value shows in this case a relative accuracy of $10^{-3}$ compared to the value provided in Ref.[42].

Let us turn to the discussion of our results for the triplet symmetry shown in Fig. 4. The singlet and triplet symmetry subspaces are closely related. Table IV shows, that the one-particle ionization threshold is represented by the same states of the Be$^{±}$ ion. But the reader should keep in mind, that the ionization thresholds for both subspaces do not possess the same energy, because of the different spin projections, chosen for the total energies. It can be seen in Fig. 4, that the ionization energies of the triplet states are typically larger than those of the corresponding singlet states. However, they follow the same overall behavior: In the low field regime the energies increase, whereas they decrease in the high field regime showing in between a local maximum. Furthermore one observes, that the OPIEs of the $1^1(-1)^{±}$ and $1^3(-1)^{±}$ and the states $2^1(-1)^{±}$ and $2^3(-1)^{±}$ approach each other for the highest field strengths investigated here. Values for total energies for finite $\gamma$ are available in the literature exclusively for the $1^3(-1)^{±}$ state but not for the excitations of this symmetry. We therefore discuss here only the accuracy of the energies of this state. In the absence of the field our relative accuracy compared to the accurate results of Ref.[42] is approximately $5 \times 10^{-4}$. In the presence of a weak field our total energies are above those of Ref.[34] by a relative difference of $2 \times 10^{-4}$. This difference decreases with increasing field strength and for $\gamma > 0.5$ our results are variationally lower compared to those of Ref.[34]. For $\gamma \geq 2$ only Hartree-Fock results are available [35] which are systematically higher in energy by approximately $4 \times 10^{-4}$ relative deviation.
TABLE IV: Total energies $E_{\text{tot}}$.

\[
\begin{array}{cccccccc}
\gamma & T_{\text{Sym}} & E_{\text{tot}} & E_{\text{Ion}} & E_{\text{Lit}} & E_{\text{tot}} & E_{\text{Ion}} & E_{\text{Lit}} \\
0.000 & ^20^+ & -14.4408 & 0.1161 & -14.47344^a & -14.3798 & 0.0551 & -14.39311^a \\
0.001 & ^20^+ & -14.4429 & 0.1188 & -14.46849^b & -14.3820 & 0.0579 & \\
0.010 & ^20^+ & -14.4494 & 0.1298 & -14.47276^b & -14.3729 & 0.0533 & \\
0.050 & ^20^+ & -14.4486 & 0.1504 & & -14.3713 & 0.0731 & \\
0.100 & ^20^+ & -14.4711 & 0.2017 & -14.49663^b & -14.3698 & 0.1004 & \\
0.200 & ^20^+ & -14.4653 & 0.2614 & -14.49334^b & -14.3185 & 0.1147 & \\
0.500 & ^2(−1)^+ & -14.3641 & 0.3284 & -14.39454^b & -14.1517 & 0.1159 & \\
1.000 & ^2(−1)^+ & -14.0674 & 0.3154 & -14.07640^b & -13.8560 & 0.1040 & \\
2.000 & ^2(−1)^+ & -13.2827 & 0.2826 & & -13.092 & 0.0916 & \\
5.000 & ^2(−1)^+ & -10.2740 & 0.2556 & & -10.097 & 0.0787 & \\
10.000 & ^2(−1)^+ & -4.0679 & 0.2593 & & -3.8927 & 0.0840 & \\
\end{array}
\]

TABLE III: Total energies $E_{\text{tot}}$, one-particle ionization energies $E_{\text{Ion}}$, and previously published data $E_{\text{Lit}}$ in a. u. for the states $\nu ^1 \gamma ^0^+ (\nu = 1, 2, 3)$, as well as the symmetries $T_{\text{Sym}}$ of the states at threshold for different field strengths $\gamma$.

\[a\text{Ref. 12}\]
\[b\text{Ref. 34}\]

\[
\begin{array}{cccccccc}
\gamma & T_{\text{Sym}} & E_{\text{tot}} & E_{\text{Ion}} & E_{\text{Lit}} & E_{\text{tot}} & E_{\text{Ion}} & E_{\text{Lit}} \\
0.000 & ^20^+ & -14.5598 & 0.2351 & -14.56724^a & -14.3965 & 0.0718 & -14.39896^a \\
0.001 & ^20^+ & -14.5612 & 0.2361 & -14.56388^b & -14.3980 & 0.0728 & -14.3581 & 0.0329 \\
0.010 & ^20^+ & -14.5744 & 0.2448 & -14.57721^b & -14.4103 & 0.0807 & -14.3642 & 0.0346 \\
0.050 & ^20^+ & -14.6142 & 0.2660 & -14.58281^c & -14.4329 & 0.0847 & -14.3859 & 0.0377 \\
0.100 & ^20^+ & -14.6936 & 0.3242 & -14.69575^b & -14.4787 & 0.1093 & -14.4186 & 0.0493 \\
0.200 & ^20^+ & -14.7979 & 0.3941 & -14.80065^b & -14.5156 & 0.1118 & -14.4631 & 0.0593 \\
0.500 & ^2(−1)^+ & -15.0107 & 0.4749 & -15.01300^b & -14.6616 & 0.1258 & -14.5881 & 0.0523 \\
1.000 & ^2(−1)^+ & -15.1982 & 0.4462 & -15.19348^b & -14.8751 & 0.1231 & -14.8037 & 0.0517 \\
2.000 & ^2(−1)^+ & -15.3551 & 0.3551 & -15.30815^c & -15.1036 & 0.1035 & -15.0438 & 0.0437 \\
5.000 & ^2(−1)^+ & -15.3002 & 0.2818 & -15.25183^e & -15.1011 & 0.0827 & -15.0410 & 0.0226 \\
10.000 & ^2(−1)^+ & -14.0792 & 0.2705 & -14.03046^c & -13.8945 & 0.0858 & -13.8320 & 0.0233 \\
\end{array}
\]

TABLE IV: Total energies $E_{\text{tot}}$, one-particle ionization energies $E_{\text{Ion}}$, and previously published data $E_{\text{Lit}}$ in a. u. for the states $\nu ^2 ^1 (−1)^+ (\nu = 1, 2, 3)$, as well as the symmetry $T_{\text{Sym}}$ of the ionic threshold states at different field strengths $\gamma$.

\[a\text{Ref. 12}\]
\[b\text{Ref. 34}\]
\[c\text{Ref. 35}\]

D. The symmetry subspaces $^3 (−1)^−$

We present in this subsection our results for the triplet states for magnetic quantum number $M = −1$ and negative $\gamma$ parity. The ground and one excited state have been investigated here. Although table IV shows, that the ionization thresholds for this symmetry are the same as for the corresponding subspace with positive $\gamma$ parity, the ionization energies show a completely different behavior. For the $^3(−1)^−$ state it increases monotonically with increasing field strength for the complete regime considered here: from 0.0562 a.u. at $\gamma = 0$ to 0.5215 a.u. at $\gamma = 10$. Comparing our results for the total energies of this state with the literature we arrive at the following conclusions. For $\gamma = 0$ we have a relative accuracy of $10^{-3}$ compared to the values presented in Ref. [12]. In the absence of the field for $\gamma \leq 5$ our variational total energies are larger than those of Ref. [34] by a relative change of $5 \times 10^{-4}$. For $\gamma = 1$ our value is below that of Ref. [34] and for $\gamma > 1$ no data are available in the literature for comparison.

According to our study (and definition of the ionization threshold) the $^2 (−1)^−$ state starts to possess a significant binding energy of the outer electron from $\gamma \approx 0.2$ on. Its ionization energy increases monotonically but the rate of this increase decreases for $\gamma > 0.5$ and seems to approach an asymptotic value at approximately 0.12 a.u. No data are available in the literature on this state in the presence of the field. In the absence of the field the total energy...
given in ref. [42] amounts to -14.38462 a.u.

\[ \gamma \]

\[ E_T - E_{\text{Tot}} \]

\[ \nu_3^{(-1)} \] and \( \nu_3^{(-3)} \) states of spin quintet \( \frac{5}{2} \) (+) symmetry.

Let us begin our analysis with the spin triplet states. Results for this symmetry subspace are presented in Fig. 6 and table V. The ground state of the spin triplet symmetry with magnetic quantum number \(-3\) and positive \( z \) parity is a quadruply tightly bound state, being predominantly described by the orbitals \( 1s^22p_{-1}3d_{-2} \). These orbitals are the energetically lowest tightly bound orbitals. As a consequence the \( 1\frac{3}{2}^{(-3)} \) state becomes for sufficiently high field strengths the state with the largest OPIE among the states considered here (the most tightly bound state of the beryllium atom in the high field limit is the \( 1s^22p_{-1}^2 \) state which however is a spin singlet state and is not investigated here). This holds particularly in the high field limit, although in this field regime the total energy of the quintet states is much lower. For \( \gamma = 0 \) the ionization energy amounts to 0.0388 a.u. and at \( \gamma = 10 \) to 0.2789 a.u. The corresponding monotonous increase of the OPIE can clearly be seen in Fig. 6. For field strengths \( \gamma < 0.2 \) we could not detect the existence of this bound state in the presence of the magnetic field. For \( \gamma \geq 0.5 \) the only available

\[ \begin{array}{ccccccccccc}
\gamma & T_{\text{Sym}} & E_{\text{Tot}} & E_{\text{Ion}} & E_{\text{Lit}} & E_{\text{Tot}} & E_{\text{Ion}} & E_{\text{Lit}} & E_{\text{Tot}} & E_{\text{Ion}} \\
0.000 & ^00^+ & -14.3809 & 0.0562 & -14.3954^a & -14.3809 & 0.0562 & -14.3954^a & -14.3809 & 0.0562 & -14.3954^a \\
0.001 & ^00^+ & -14.3810 & 0.0559 & -14.3906^b & -14.3810 & 0.0559 & -14.3906^b & -14.3810 & 0.0559 & -14.3906^b \\
0.010 & ^00^+ & -14.3944 & 0.0648 & -14.4039^b & -14.3944 & 0.0648 & -14.4039^b & -14.3944 & 0.0648 & -14.4039^b \\
0.050 & ^00^+ & -14.4504 & 0.1022 & -14.4504 & 0.1022 & -14.4504 & 0.1022 & -14.4504 & 0.1022 & -14.4504 \\
0.100 & ^00^+ & -14.5136 & 0.1442 & -14.5136 & 0.1442 & -14.5136 & 0.1442 & -14.5136 & 0.1442 & -14.5136 \\
0.200 & ^00^+ & -14.6223 & 0.2184 & -14.6223 & 0.2184 & -14.6223 & 0.2184 & -14.6223 & 0.2184 & -14.6223 \\
0.500 & ^2(-1)^+ & -14.8600 & 0.3243 & -14.8600 & 0.3243 & -14.8600 & 0.3243 & -14.8600 & 0.3243 & -14.8600 \\
1.000 & ^2(-1)^+ & -15.1210 & 0.3690 & -15.1210 & 0.3690 & -15.1210 & 0.3690 & -15.1210 & 0.3690 & -15.1210 \\
2.000 & ^2(-1)^+ & -15.4183 & 0.4183 & -15.4183 & 0.4183 & -15.4183 & 0.4183 & -15.4183 & 0.4183 & -15.4183 \\
5.000 & ^2(-1)^+ & -15.4990 & 0.4805 & -15.4990 & 0.4805 & -15.4990 & 0.4805 & -15.4990 & 0.4805 & -15.4990 \\
10.000 & ^2(-1)^+ & -14.3302 & 0.5215 & -14.3302 & 0.5215 & -14.3302 & 0.5215 & -14.3302 & 0.5215 & -14.3302 \\
\end{array} \]

\[ \text{TABLE V: Total energies } E_{\text{Tot}}, \text{ one-particle ionization energies } E_{\text{Ion}}, \text{ and previously published data } E_{\text{Lit}} \text{ in a.u. for the states } \nu_3^{(-1)} \text{ and } \nu_3^{(-3)} \text{ as well as the threshold symmetry } T_{\text{Sym}} \text{ at different field strengths } \gamma. \]

\[ ^a\text{Ref. [12]} \]
\[ ^b\text{Ref. [34]} \]
\[ ^c\text{Ref. [28]} \]

E. The \( \frac{3}{2} \) symmetry subspaces

Here we discuss the ground and a single excited state of spin triplet \( \frac{3}{2} \) symmetry and the ground as well as two excited states of spin quintet \( \frac{5}{2} \) symmetry.

FIG. 5: One-particle ionization energies for the states \( \nu_3^{(-1)} \) (\( \nu = 1, 2 \)) in a.u. as a function of the magnetic field strength \( \gamma \).
values for the total energies in the literature are due to the Hartree-Fock approach employed in Ref.\[28\]. Our values are systematically lower than the Hartree-Fock values showing a typical relative deviation of $3 \times 10^{-3}$.

The ionization energy of the first excited state $2^3(-3)^+$ increases monotonically for $\gamma < 5$ but shows a decrease when doubling the field strength to $\gamma = 10$. We obtain an ionization energy 0.0872 a.u. at $\gamma = 0.5$ and 0.1490 a.u. for $\gamma = 5$. This state has up to date not been investigated in the literature.

Let us now discuss the states of the quintet spin symmetry. The ground state $1^5(-3)^+$ of this symmetry is a triply tightly bound state, which is predominantly described by the configuration 1s2s2p$^+$3d$^-$2. A monotonically increasing OPIE for $\gamma < 2$ can be observed for this state (see Fig. [10]). For $\gamma \geq 2$ the ionization energy decreases, which is a consequence of the change with respect to the ionization threshold: For lower fields the ionization threshold involves the doubly tightly bound $1^4(-1)^+$ state of Be$^+$ and for $\gamma \geq 2$ it involves the triply tightly bound state $1^4(-3)^+$. Similar statements hold for the first and second excited states of this symmetry. Table [VI] shows, that the increase of the OPIE for the ground state $1^5(-3)^+$ as well as the first and second excited state $2^3(-3)^+$ and $3^3(-3)^+$ are very strong for $\gamma < 2$. For the ground state the ionization energy increases from 0.0547 a.u. at $\gamma = 0$ to 0.5558 a.u. at $\gamma = 2$, i.e. by approximately one order of magnitude. For the first and second excited state we encounter 0.0293 a.u. and 0.0172 a.u. at $\gamma = 0$ and 0.1297 a.u. and 0.0521 a.u., respectively, at $\gamma = 2$, i.e. increase by approximately a factor of 4 respectively 3. In the regime $\gamma \geq 2$ the relative decrease of the ionization energy of the ground state is stronger than those for the first and the second excited states. Data from the literature to compare with are only available for the ground state $1^5(-3)^+$ of this symmetry and only Hartree-Fock results in the strong field regime. Comparing with the latter data \[28\] our total energies are systematically lower by a relative change of $5 \times 10^{-4}$.

![Graph](image)

**FIG. 6:** One-particle ionization energies for the states $\nu^3(-3)^+$ ($\nu = 1, 2$) and $\nu^3(-3)^+$ ($\nu = 1, 2, 3$) in a.u. as a function of the magnetic field strength $\gamma$.

| $\gamma$ | $T_{Sym}$ | $E_{tot}$ | $E_{Ion}$ | $E_{Lit}$ | $E_{tot}$ | $E_{Ion}$ | $E_{tot}$ | $E_{Ion}$ |
|----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|
| 0.000    | 4(-1)$^+$ | -10.1197  | 0.0547    | -10.0943  | 0.0293    | -10.0822  | 0.0172    |
| 0.010    | 4(-1)$^+$ | -10.1245  | 0.0590    | -10.0991  | 0.0336    | -10.0870  | 0.0215    |
| 0.010    | 4(-1)$^+$ | -10.1549  | 0.0722    | -10.1265  | 0.0437    | -10.1111  | 0.0283    |
| 0.050    | 4(-1)$^+$ | -10.2736  | 0.1129    | -10.2173  | 0.0566    | -10.1930  | 0.0324    |
| 0.100    | 4(-1)$^+$ | -10.4070  | 0.1495    | -10.3243  | 0.0667    | -10.2948  | 0.0373    |
| 0.200    | 4(-1)$^+$ | -10.6438  | 0.2685    | -10.5146  | 0.0793    | -10.4726  | 0.0373    |
| 0.500    | 4(-1)$^+$ | -11.2406  | 0.3487    | -11.2326$^a$ | -10.9975  | 0.1057    | -10.9342  | 0.0521    |
| 1.000    | 4(-1)$^+$ | -12.0042  | 0.5076    | -11.9964$^a$ | -11.6186  | 0.1219    | -11.5363  | 0.0396    |
| 2.000    | 4(-3)$^+$ | -13.1560  | 0.5558    | -13.1423$^a$ | -12.7300  | 0.1297    | -12.6523  | 0.0521    |
| 5.000    | 4(-3)$^+$ | -15.7897  | 0.3529    | -15.7829$^a$ | -15.5375  | 0.1008    | -15.4826  | 0.0458    |
| 10.000   | 4(-3)$^+$ | -19.1314  | 0.3090    | -19.1247$^a$ | -18.9211  | 0.0927    | -18.8712  | 0.0429    |

**TABLE VI:** Total energies $E_{Tot}$, one-particle ionization energies $E_{Ion}$, and previously published data $E_{Lit}$ in a. u. for the states $\nu^3(-3)^+$ ($\nu = 1, 2, 3$) as well as the threshold symmetry $T_{Sym}$ at different field strengths $\gamma$.

$^a$Ref. \[28\].
In this subsection we discuss the spin quintet states with magnetic quantum numbers $-3$ and $-6$ possessing negative and positive $z$-parity, respectively. For the states of $^5(-3)^-\text{ symmetry}$ a particular behavior of their ionization energies can be observed in Fig. 7. The corresponding numerical results are given in Table VII. For the ground state the OPIE increases in the field regime $0 < \gamma < 0.05$: we encounter 0.0172 a.u. at $\gamma = 0.001$ and 0.0572 a.u. at $\gamma = 0.05$. In the regime $0.05 < \gamma < 0.2$ it passes through a local minimum and for $0.2 < \gamma < 2$ a rapid increase of the ionization energy with increasing field strength takes place. At $\gamma = 0.2$ it amounts to 0.0578 a.u. whereas at $\gamma = 2$ it is one order of magnitude larger and amounts to 0.6364 a.u. Thereafter for even larger field strengths the increase is slowing down significantly. The reason for the latter is a change with respect to the ionization threshold. For $\gamma \leq 1$ the ionization threshold involves the Be$^+$ state $^4(-1)^+$ where as for $\gamma > 1$ the triply tightly bound Be$^+$ state $^1(3)^+$ defines the threshold. It represents the high field global ground state of the beryllium positive ion.

![FIG. 7: One-particle ionization energies for the states $\nu^7$($-3)^-$ ($\nu = 1, 2$) in a.u. as a function of the magnetic field strength $\gamma$.](image)

The OPIE of the first excited state $2^5(-3)^-$ shows a similar behavior as that of the ground state. However, in contrast to the ground state its ionization energy decreases for $\gamma \geq 2$ significantly. Again only for the ground state $1^5(-3)^-$ and in the strong field regime there are data of Hartree-Fock calculations [28] available to compare with. Equally our total energies are variationally lower than those of the Hartree-Fock calculations by a relative deviation of $10^{-3}$.

| $\gamma$ | $T_{\text{Sym}}$ | $E_{\text{tot}}$ | $E_{\text{Ion}}$ | $E_{\text{Lit}}$ | $E_{\text{tot}}$ | $E_{\text{Ion}}$ | $E_{\text{tot}}$ | $E_{\text{Ion}}$ | $E_{\text{tot}}$ | $E_{\text{Ion}}$ |
|---------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|
| 0.001   | $^4(-1)^+$      | -10.0826        | 0.0172          | -10.0712        | 0.0057          |                  |                  |                  |                  |                  |
| 0.010   | $^4(-1)^+$      | -10.1107        | 0.0279          | -10.0939        | 0.0112          |                  |                  |                  |                  |                  |
| 0.050   | $^4(-1)^+$      | -10.2179        | 0.0572          | -10.1773        | 0.0166          |                  |                  |                  |                  |                  |
| 0.100   | $^4(-1)^+$      | -10.3079        | 0.0503          |                  |                  |                  |                  |                  |                  |                  |
| 0.200   | $^4(-1)^+$      | -10.4931        | 0.0578          | -10.4431        | 0.0078          |                  |                  |                  |                  |                  |
| 0.500   | $^4(-1)^+$      | -11.0818        | 0.1899          | -11.06254$^a$   | -10.9058        | 0.0139          |                  |                  |                  |                  |
| 1.000   | $^4(-1)^+$      | -11.9151        | 0.4184          | -11.89891$^a$   | -11.5260        | 0.0294          | -11.7358        | 0.2389          | -11.72880$^a$   |                  |
| 2.000   | $^4(-3)^+$      | -13.2366        | 0.6364          | -13.22133$^a$   | -12.6992        | 0.0989          | -13.1762        | 0.5759          | -13.16961$^a$   | -12.7321 0.1319 |
| 5.000   | $^4(-3)^+$      | -16.1233        | 0.6866          | -16.10812$^a$   | -15.5101        | 0.0734          | -16.3139        | 0.8772          | -16.30690$^a$   | -15.5887 0.1520 |
| 10.000  | $^4(-3)^+$      | -19.5270        | 0.6987          | -19.51207$^a$   | -18.8781        | 0.0498          | -20.0242        | 1.1959          | -20.01753$^a$   | -18.9887 0.1604 |

| $E_{\text{Lit}}$ | $E_{\text{tot}}$ | $E_{\text{Ion}}$ | $E_{\text{total}}$ | $E_{\text{Ion}}$ | $E_{\text{total}}$ | $E_{\text{Ion}}$ | $E_{\text{total}}$ | $E_{\text{Ion}}$ |
|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|
| 0.001           | -10.0826        | 0.0172          | -10.0712        | 0.0057          |                  |                  |                  |                  |
| 0.010           | -10.1107        | 0.0279          | -10.0939        | 0.0112          |                  |                  |                  |                  |
| 0.050           | -10.2179        | 0.0572          | -10.1773        | 0.0166          |                  |                  |                  |                  |
| 0.100           | -10.3079        | 0.0503          |                  |                  |                  |                  |                  |                  |
| 0.200           | -10.4931        | 0.0578          | -10.4431        | 0.0078          |                  |                  |                  |                  |
| 0.500           | -11.0818        | 0.1899          | -11.06254$^a$   | -10.9058        | 0.0139          |                  |                  |                  |
| 1.000           | -11.9151        | 0.4184          | -11.89891$^a$   | -11.5260        | 0.0294          | -11.7358        | 0.2389          | -11.72880$^a$   |                  |
| 2.000           | -13.2366        | 0.6364          | -13.22133$^a$   | -12.6992        | 0.0989          | -13.1762        | 0.5759          | -13.16961$^a$   | -12.7321 0.1319 |
| 5.000           | -16.1233        | 0.6866          | -16.10812$^a$   | -15.5101        | 0.0734          | -16.3139        | 0.8772          | -16.30690$^a$   | -15.5887 0.1520 |
| 10.000          | -19.5270        | 0.6987          | -19.51207$^a$   | -18.8781        | 0.0498          | -20.0242        | 1.1959          | -20.01753$^a$   | -18.9887 0.1604 |

TABLE VII: Total energies $E_{\text{tot}}$, one-particle ionization energies $E_{\text{Ion}}$, and previously published data $E_{\text{Lit}}$ in a.u. for the states $\nu^7$($-3)^-$ ($\nu = 1, 2$) and $\nu^7$($-6)^+$ ($\nu = 1, 2$) as well as the threshold symmetry $T_{\text{Sym}}$ at different field strengths $\gamma$.

$^a$Ref. 28.

Let us now turn to the states of $^5(-6)^+$ symmetry. The ground state $^1(3)^+$ represents the global ground state of the beryllium atom in the high field limit. It is the energetically lowest (we are referring, of course, to the total energy) quadruply tightly bound quintet state and is predominately described by the configuration $1s2p_{-1}3d_{-2}4f_{-3}$. 

F. The $^5(-3)^-$ and $^5(-6)^+$ symmetry subspaces
However, this configuration does not represent the most tightly bound state with four occupied tightly bound orbitals for any field strength. The OPIEs of the ground and the first excited state increase monotonically in the strong field regime $\gamma \geq 1$. In the low field regime these states represent highly excited states in the continuum which are not bound. Similar to the previously discussed cases also for this symmetry there are only Hartree-Fock data [28] available for the ground state. Comparing with the latter our total energies are variationally lower by typically $4 \times 10^{-4}$.

![Graph](attachment:image.png)

**FIG. 8:** One-particle ionization energies for the states $\nu^3(−6)^− (\nu = 1, 2)$ in a.u. as a function of the magnetic field strength $\gamma$.

V. ELECTROMAGNETIC TRANSITIONS

In the present section we discuss the behavior of the wavelengths $\lambda$ of the allowed electric dipole transitions as a function of the magnetic field strength. The regime of wavelengths to be considered is $\lambda < 10^5$ Å. We will focus on the circular polarized transitions $\nu^00^+ \rightarrow \mu^3(−1)^+ (\nu = 1, 2, 3, \mu = 1, 2)$ shown in Fig. 7 and the linear polarized transitions $\nu^3(−1)^+ \rightarrow \mu^3(−1)^− (\nu = 1, 2, 3, \mu = 1, 2)$ presented in Fig. 10.

For the circular polarized transitions $\nu^10^+ \rightarrow \mu^1(−1)^+ (\nu = 1, 2, 3, \mu = 1, 2)$ presented in Fig. 9 one observes, that in the field range $0 < \gamma < 0.05$ the transition wavelengths are approximately constant. In this field regime the influence of the magnetic field is weak. However, in the intermediate and high field regime the transition wavelengths show a pronounced field-dependence. For $\gamma > 1$ an overall decrease of the transition wavelengths is observable. In the regime $0.05 < \gamma < 1$ some lines increase, others do not. To be more specific: The transitions $(\nu, \mu) = (1, 1), (1, 2),$ and $(2, 2)$ show an increase of the wavelengths, whereas the transitions $(\nu, \mu) = (2, 1), (3, 1),$ and $(3, 2)$ show a monotonous decrease. The origin of this behavior is the less rapid increase of the total energies of the $\mu^1(−1)^+$ states compared to the $\nu^10^+$ states. Therefore crossovers of the corresponding energy levels occur, which lead to divergent transition wavelengths (these are, due to the crude grid of field strengths employed here, visible as peaks in the figure).

For the linear polarized transitions $\nu^3(−1)^+ \rightarrow \mu^3(−1)^− (\nu = 1, 2, 3, \mu = 1, 2)$ depicted in Fig. 11 the behavior in the low field regime $\gamma < 0.05$ is very similar to the one of the circular polarized transitions discussed above, i.e. two of the three wavelengths in this regime are almost independent of the field strength. This does not hold for the transition $3^3(−1)^+ \rightarrow 1^3(−1)^−$ (shown with dotted line and black circles). The latter is due to the fact, that the OPIE of the state $3^3(−1)^+$ is nearly field independent and is at $\gamma = 0$ only a factor of two smaller than the OPIE of the state $1^3(−1)^−$. The ionization energy of the latter state increases for weak fields ($\gamma < 0.05$) about a factor of two and as a result the corresponding transition wavelengths decrease.

VI. CONCLUSIONS

We have investigated the electronic structure of the beryllium atom exposed to a strong magnetic field in the regime $0 \leq \gamma \leq 10$ a.u. Our approach is based on a recently developed full configuration interaction method for multi-electron systems that employs anisotropic Gaussian orbitals which are optimized for each field strength separately. Our results comprise the global ground state and its crossovers as a function of the field strengths. Earlier results on the Hartree-Fock level have been confirmed and refined. Beyond this we have studied many excited states of various symmetries thereby covering spin singlet, triplet and quintet states with magnetic quantum numbers $|M| = 0, 1, 3, 6$. 

and for both positive and negative $z$–parity. A total of 18 excited states (not counting the spin multiplicity) have been studied and analyzed i.e. their total and one-particle ionization energies as well as the corresponding transition wavelengths for allowed dipole transitions have been discussed. The one-particle ionization energies show a rich variability as a function of the field strength depending in particular on the number and type of tightly bound orbitals that are contained in the configurations dominating the individual electronic states. Many excited states have been investigated for the first time for finite field strengths. For the states that have already been studied in the literature a comparison of our data shows that our total energies are variationally higher by a relative change of typically $10^{-3}$ or less for the regime of field strengths $0 \leq \gamma \leq 0.5$. This discrepancy is however not due to limitations of our basis set, which possesses a very high flexibility, but more an effect of the large number of configurations emerging for a four-electron system within a full configuration interaction approach for a given (moderately sized) basis set. Going to larger atomic systems it is therefore desirable to choose another configuration interaction approach instead of the full one which allows to treat larger basis sets. For $\gamma \geq 0.5$ our results are almost exclusively variationally lower than the existing ones in the literature by typical relative deviations of several times $10^{-3}$. This confirms the already known feature that our approach performs best in the intermediate regime of field strengths.
VII. ACKNOWLEDGMENTS

P.S. acknowledges fruitful discussions with J. Liebert.

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