Ground State of One Electron Molecular Ions up to Z=3 in a Very Strong Magnetic Field Using Variational Quantum Monte Carlo Method

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Abstract

The variational quantum Monte Carlo method is applied to the ground state of the molecular ions H_2^+, He_2^{3+}, HeH^{2+}, Li_2^{5+}, $LiHe^{4+}$ and LiH^{3+} in the presence of a very strong magnetic field. The molecular axis is assumed to be aligned parallel to the direction of the magnetic field because this configuration is optimal if a magnetic field is sufficiently strong. The Born–Oppenheimer approximation is considered where the positively charged centers are supposed to be infinitely massive. The obtained results are in good agreement with the corresponding previous studies.

Keywords Variational Monte Carlo method; one electron molecular ions; molecules in strong magnetic field.

1. Introduction

Stellar remnants are the end stage of the star life. This end depends on which one prevails the order at the end: the gravitational attraction of matter which attempts to compress the stellar matter to higher and higher densities, or the pressure of the gas which tries to resist this compression. The stars lose energy from their surfaces into the interstellar space due to the nuclear fusion reactions. The star reaches the critical phase in its life when the nuclear fuel is exhausted and stellar evolution reaches the final stages. There are three different possibilities for these end-products: a black hole, a neutron star and white dwarfs, where the pressure is supplied by the degenerate electron gas. A few numbers of white dwarf stars show extremely high magnetic fields of the order of 10^8 G. This is the only possibility to observe the behavior of atoms and molecules in such fields. The surface of the neutron star is characterized by magnetic fields, typically of the magnetic field strength $B \approx 10^{12}$ G and for some neutron stars the magnetic field achieves values up to $B \approx 10^{16}$ G. The neutron star atmosphere composed of mixed hydrogen-helium molecules, new exotic molecular ions are to be found at these extreme magnetic field strengths [1]. Accordingly, many theoretical studies on the molecular ions systems in the presence of a strong magnetic field have been carried on.

U. Kappes and P. Schmelcher [2-4] investigated the electronic bond structure of the H_2^+ ion in a strong magnetic field. They studied many magnetically states of the hydrogen molecular ion for parallel inter-nuclear and magnetic field axes. The numerical calculations of the molecular states and potential-energy curves in the fixed-nuclei approximation are based on an established and optimized atomic orbital basis set. They studied the electronic states within the range $0 \leq |m| \leq 10$ of magnetic quantum numbers and for several field strengths. Also, they investigated many excited states within a subspace for fixed magnetic

quantum number and parity. The results show different possibilities for the topological behavior of the potential-energy surfaces for the lowest electronic states; the global equilibrium configuration for parallel or perpendicular configuration, which are both distinguished by their higher symmetry.

A general method for solving the system of one-electron and two-center Coulomb problem with a uniform strong magnetic field was described by Uwe Wille [5]. For the magnetic field oriented to the line connecting the two centers, Wille solved the Hamiltonian matrix in a basis of Hylleraas functions analytically and the generalized eigenvalue problem for this matrix numerically. A detailed study performed by calculating energies and wave functions for the H_2^+ and HeH^{2+} systems for magnetic field strengths up to 10^{12} G. Molecular-orbital correlation diagrams were presented and discussed, in which energies displayed as a function of inter-nuclear distance R at fixed angle θ between field direction and inter-nuclear axis, and as a function of θ at fixed R. Also, the influence of the magnetic field on molecular binding energies, as well as on the separation behavior of molecular orbitals at large inter-nuclear distances was investigated.

A. V. Turbiner et al. [6-8] developed wave functions that described the one-electron molecular ions in a strong magnetic field. The system of two protons and one electron placed in a magnetic field ranging from 10^9 G to 4.414×10^{13} G was investigated. The study focused on the existence of the molecular ion H_2^+ in a magnetic field. They showed that between the two stable one-electron systems in the absence of a magnetic field, the H atom and H_2^+, the molecular ion H_2^+ is more stable. The H_2^+ ion has been widely studied for both with and without the presence of a magnetic field, due to its importance in many branches in physics. Their study was focused on the case of the parallel configuration, where the angle between the molecular axis and the magnetic field direction is zero, $\theta = 0^\circ$. As a rule, in their study, the nuclear motion was separated from the electronic motion using the Born-Oppenheimer approximation. The important feature of the hydrogen molecular ion was that if the magnetic field increases, the total and binding energies increase, as well as a smaller equilibrium distance, were observed. They demonstrated a theoretical existence of the exotic ion HeH^{2+} for $B \geq 5\times10^{12}$ G. Also, they showed that the exotic ion, He_2^{3+} can also exist for $B \geq 2.35\times10^{11}$ G. They demonstrated that the molecular systems LiH^{3+}, $LiHe^{4+}$ and Li_2^{5+} can exist for strong magnetic fields ($B \geq 2.35\times10^{13}$ G) and that Li_2^{5+} can even be stable at magnetic fields typical of magnetars (neutron star that has an extremely powerful magnetic field).

More accurate methods are used to calculate the one-electron molecular systems in the presence of a very strong magnetic field. Zhang Yue-Xia et.al [9,10] improved an accurate method combining the spheroidal coordinates and B-spline basis to study the ground state $1\sigma_g$ and low excited states of the H_2^+ in magnetic fields from the range of 10^9 G to 4.414×10^{13} G. While Yuexia Zhang et al. [11] used the one-center method to calculate the equilibrium distances and the energies for the hydrogen molecular ion in magnetic fields for ranges from 10^9 G to 4.414×10^{13} G. Both the radial and angular wave functions were expanded in terms of optimized B-splines. For the ground state of the H_2^+ in the free field, accuracy of 7×10^{-8} was obtained. The nuclear distances and the total energies of the $1\sigma_{g,u}$, $1\pi_u$, $1\delta_{g,u}$ and $2\sigma_g$ states of the H_2^+ for the magnetic field strength 2.35×10^9 G were also obtained. Furthermore, Horacio Olivares Pilón [12] performed accurate calculations for the ground state of the molecular ions He_2^{3+} and HeH^{2+} placed in a strong magnetic field using the Lagrange-mesh method.

Moreover, by using the variational Monte Carlo (VMC) method S. B. Doma et al. [13] calculated the $1\sigma_g$ state energies, the dissociation energies, and the binding energies of the hydrogen molecule and its molecular ion in the presence of an aligned magnetic field regime between 0 and 2.35×10^{10} G. The calculations were based on a type of wave function proposed by Ishikawa et al. [14] to calculate the ground state of H_2^+ in the presence of magnetic field. They have obtained accurate results compared to the corresponding exact values.

Accordingly, we focused our attention in the present paper to the structure of the molecular ions H_2^+, He_2^{3+}, HeH^{2+}, Li_2^{5+}, $LiHe^{4+}$ and LiH^{3+} in the presence of a very strong magnetic field. In general, these molecular ions may be dissociated into two components: an atomic ion and charged particle (such as proton or α-particle). If the binding energy of the molecular ion is slightly smaller than its atomic ion, the molecular ion begins to exist. However, it will decay fast to its components. When the binding energy of the molecular ion is larger than its atomic ion, the molecular ion will be stable at certain strength of the magnetic field, and this will be a part of our investigation. Hence, we applied the VMC technique to the molecular ions H_2^+, He_2^{3+}, HeH^{2+}, Li_2^{5+}, $LiHe^{4+}$ and LiH^{3+} in the presence of a very strong magnetic field, by neglecting the relativistic corrections. The molecular axis is assumed to be aligned parallel to the magnetic field line because this configuration is optimal if a magnetic field is sufficiently strong. The Born–Oppenheimer approximation is considered where the positively charged centers are supposed to be infinitely massive. For more details concerning the VMC method, see Refs [15,16].

2. Hamiltonian of One Electron Molecular Ion in a Magnetic Field

We choose the vector potential corresponding to a constant magnetic field $\boldsymbol{B} = (0, 0, B)$ in the symmetric gauge as $\boldsymbol{A} = \frac{B}{2}(-y, x, 0)$, as usual. Figure-1 represents the geometrical setting of the one electron molecular ion, with two nuclei of charges Z_1 and Z_2, placed in a magnetic field directed along the z-axis.

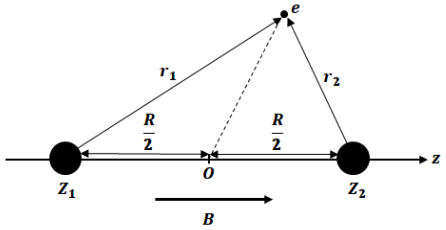

Figure-1 Geometrical setting of the ground state for the molecular system of one electron placed in a magnetic field directed along the z-axis. The protons are situated at a distance R from each other.

The Hamiltonian which describes two infinitely heavy centers of charges Z_1 and Z_2 situated along the z-axis and one electron placed in a uniform constant magnetic field directed along the z-axis is given by

$$H = -\frac{1}{2}\nabla^2 - \frac{Z_1}{r_1} - \frac{Z_2}{r_2} + \frac{Z_1 Z_2}{R} + \frac{BL_z}{2} + \frac{B^2\rho^2}{8} \qquad (2.1)$$

where R is the inter-nuclear distance and r_1, r_2 are the distances between the electron and the charged centers. In equation (2.1) $\rho^2 = (x^2 + y^2)$ and L_Z is the z-component of the orbital angular momentum $\boldsymbol{L}$.

3. Wave Functions

In the following we study the solution of the Schrodinger wave equation for the Hamiltonian given by (2.1) by means of the VMC method using Turbiner wave functions [7, 8]. Our calculations are based on using the following trial wave function presented in the case of symmetric systems with equal charges $Z_1 = Z_2 = Z$, to explore the H_2^+, He_2^{2+} and Li_2^{5+} molecular ions in a strong magnetic field, namely;

$$\Psi_{trial} = \psi_1 + \psi_2 + \psi_3 \tag{3.1}$$

$$\psi_1 = A_1 e^{-Z\alpha_1(r_1+r_2)} e^{-\beta_1 \frac{B}{4}\rho^2} \tag{3.2}$$

$$\psi_2 = A_2 (e^{-Z\alpha_2 r_1} + e^{-Z\alpha_2 r_2}) e^{-\beta_2 \frac{B}{4}\rho^2} \tag{3.3}$$

$$\psi_3 = A_3 (e^{-Z\alpha_3 r_1 - Z\alpha_4 r_2} + e^{-Z\alpha_4 r_1 - Z\alpha_3 r_2}) e^{-\beta_3 \frac{B}{4}\rho^2} \tag{3.4}$$

where $A_1, A_2, A_3, \alpha_1, \alpha_2, \alpha_3, \alpha_4, \beta_1, \beta_2$ and β_3 are variational parameters. Considering the inter-nuclear distance R as a variational parameter, we have in total 11 variational parameters.

For the case of unequal charged centers $Z_1 \neq Z_2$ we use another trial wave function to study the HeH^{2+}, $LiHe^{4+}$ and LiH^{3+} molecular ions in a strong magnetic field. This function has the form

$$\Psi_{trial} = \psi_4 + \psi_5 \tag{3.5}$$

$$\psi_4 = A_1 e^{-Z_1\alpha_1 r_1 - \beta_1 \frac{B\rho^2}{4}} + A_2 e^{-Z_2\alpha_2 r_2 - \beta_2 \frac{B\rho^2}{4}} \tag{3.6}$$

$$\psi_5 = A_3 e^{-Z_1\alpha_3 r_1 - Z_2\alpha_4 r_2 \beta_3 \frac{B\rho^2}{4}} + A_4 e^{-Z_1\alpha_5 r_1 - Z_2\alpha_6 r_2 \beta_4 \frac{B\rho^2}{4}} \tag{3.7}$$

where $A_{1\ldots4}$, $\alpha_{1\ldots6}$ and $\beta_{1\ldots4}$ are variational parameters. Considering the inter-nuclear distance R as a variational parameter, we have in total 15 variational parameters.

The functions ψ_4 and ψ_5 describe the coherent and incoherent interactions of the electron with the charged centers, respectively. Obviously, they are suitable modifications of the celebrated Heitler-London and Hund-Mulliken H_2^+ trial functions by multiplication with the lowest Landau orbital. In turn, the function ψ_3 is a modified Guillemin-Zener function.

4. Results and Discussions

4.1 Ground state of H_2^+ in a Strong Magnetic Field

In Table-1 we present the results of calculating the total energy (E_T) and the binding energy (E_b) for the molecular ion H_2^+ in a uniform constant magnetic field directed along the z-axis where the two protons are situated on the z-axis at a distance R from each other. Selected values for the intensity of the magnetic field, B, are given in a.u. in the first column, representing the cases of weak, intermediate and strong field. Values of the equilibrium inter-nuclear distances parameter R_{eq} are given in the second column.

Table-1 Molecular ion H_2^+ in a magnetic field B with equilibrium inter-nuclear distance R_{eq}, total energy E_T, binding energy $E_b = \frac{B}{2} - E_T$ (all energies are in atomic units).

B (a.u.)	R_{eq}	E_T	E_b	Ref
0	1.997	−0.602625	0.602625	[6]
	1.997	−0.602635	0.602635	[5]
	1.997193	−0.602501104	0.602501104	[13]
	1.9971	−0.602354	0.602354	This Work
0.425532	1.923 ± 0.003	−0.57535	0.788116	[17]
	1.924	−0.57536	0.788126	[5]
	1.9234	−0.57536	0.788126	[18]
	1.9234	−0.575358949	0.788124949	[10]
	1.9234	−0.575358615	0.788124615	[11]
	1.9234	−0.5748408001	0.7876068	[13]
	1.923	−0.573789	0.786555	This Work
1	1.752 ± 0.003	−0.47496	0.97496	[17]
	1.76	−0.47321	0.97321	[2-4]
	1.752	−0.47499	0.97499	[18]
	1.7520828	−0.474988245	0.974988245	[10]
	1.752	−0.47498822	0.97498822	[11]
	1.7520838	−0.474988245	0.974988245	[19]
	1.752	−0.474020	0.97402	This Work
4.25532	1.246 ± 0.002	0.54522	1.58244	[17]
	1.246	0.545155	1.582505	[5]
	1.2464	0.54515	1.58251	[18]
	1.2464	0.545151062	1.582508938	[10]
	1.2465	0.5451514	1.5825086	[11]
	1.2465	0.53040741	1.59725259	[13]
	1.246	0.551119	1.576541	This Work
10	0.957 ± 0.002	2.82511	2.17489	[17]
	0.957	2.825015	2.174985	[18]
	0.9570223	2.825013964	2.174986036	[10]
	0.957	2.8250141	2.1749859	[11]
	0.9570236	2.825013964	2.174986036	[19]
	0.958	2.825	2.175	[20]
	0.957	2.82210305	2.17789695	[13]
	0.9571	2.827527	2.172473	This Work
42.5532	0.593 ± 0.001	17.5216	3.755	[17]
	0.593	17.5214	3.7552	[5]
	0.5933	17.521287	3.755313	[10]
	0.5917	17.521335	3.755265	[11]
	0.593	17.533108	3.743492	This Work
100	0.448 ± 0.001	44.8545	5.1455	[17]
	0.447793	44.853918538	5.146081462	[10]
	0.4472	44.8539015	5.1460985	[11]
	0.447794	44.853918538	5.146081462	[19]
	0.448	44.86	5.14	[20]
	0.448	44.927055	5.072945	This Work
425.532	0.283 ± 0.001	204.1948	8.5712	[17]
	0.278	204.283	8.483	[5]
	0.2834	204.193649	8.572351	[10]
	0.2832	204.193595	8.572405	[11]
	0.28	204.23655	8.52945	[21]
	0.283	204.396957	8.369043	This Work

1000	0.2197	488.61065	11.38935	[17]
	0.219783	488.60916511	11.39083489	[10]
	0.2198	488.609175	11.390825	[11]
	0.219783	488.60916511	11.39083489	[19]
	0.2197	488.802490	11.19751	This Work
4255.32	0.1472 ± 0.0002	2109.7815	17.8785	[17]
	0.125	2115.91	11.75	[5]
	0.1472	2109.7794	17.8806	[10]
	0.1472	2109.7795	17.8805	[11]
	0.15	2109.79	17.87	[21]
	0.14719	2110.027344	17.632656	This Work
10000	0.1183 ± 0.0002	4977.1005	22.8995	[17]
	0.1183	4977.0974	22.9026	[10]
	0.1183	4977.0975	22.9025	[11]
	0.1183	4977.262207	22.737793	This Work
18782.9787	0.1016 ± 0.0002	9364.2375	27.25185	[17]
	0.1016	9364.23375	27.2556	[10]
	0.1016	9364.234	27.25535	[11]
	0.10154	9364.241211	27.248139	This Work

The results in Table-1 show the existence of the H_2^+ molecular ion for magnetic fields $B = 0 - 18782.9787$ a. u.

3.2 Ground State of HeH^{2+} in a Strong Magnetic Field

The hybrid system HeH^{2+}, made from α-particle, proton and electron, was attempted to explore for field-free case [22] and for the case of a magnetic field of moderate strength B = 1 a. u. [6]. In both studies no indication to appearance of a bound state was observed. In Table-2 we present the obtained results for the molecular ion HeH^{2+} in a magnetic field B. The equilibrium inter-nuclear distance R_{eq}, total energy E_T, and binding energy $E_b = \frac{B}{2} - E_T$ are given in this table. All energies are given in atomic units. It is seen from Table-2 that for larger magnetic fields $B \geq 425.523$ a. u. the binding energy of HeH^{2+} is always larger than the binding energy of the hydrogen atom. This implies that ion HeH^{2+} does not decay to H + α, so the exotic hybrid ion HeH^{2+} can exist and it decays to He^+ + p. For all magnetic fields, the binding energy of HeH^{2+} is slightly smaller than the binding energy of the atomic ion He^+ and their difference decreases as the magnetic field grows.

In Table-3 we present the binding energies of He^+ in strong magnetic field. In general, the binding energy of HeH^{2+} grows very fast with the increase in the magnetic field, being smaller than the binding energy of the He^+ atomic ion (see Table-3). The ion HeH^{2+} is unstable towards decay to He^+ + p. However, at very high magnetic field, this decay is forbidden and the exotic molecular ion HeH^{2+} becomes stable.

Table-2 Molecular ion HeH^{2+} in a magnetic field B with equilibrium inter-nuclear distance R_{eq}, total energy E_T, binding energy $E_b = \frac{B}{2} - E_T$ (all energies in atomic units).

B (a.u.)	R_{eq}	E_T	E_b	Ref
1000	0.32	481.347	18.653	[7]
	0.316	481.3175	18.6825	[23]
	0.3161	481.30175995	18.69824005	[12]
	0.32	481.413861	18.586139	This Work
2000	0.24	976.586	23.414	[7]
	0.239	976.541	23.459	[23]
	0.239	976.610107	23.389893	This Work
4255.32	0.186	2097.915	29.745	[7]
	0.185	2097.8465	29.8135	[23]
	0.1846	2097.8256515	29.8343485	[12]
	0.185	2097.857812	29.802188	This Work
8000	0.153	3963.8825	36.1175	[7]
	0.152	3963.8825	36.1175	[23]
	0.152	3963.904834	36.095166	This Work
10000	0.143	4961.453	38.547	[7]
	0.142	4961.3485	38.6515	[23]
	0.14073	4961.3197925	38.6802075	[12]
	0.142	4961.935547	38.064453	This Work
14000	0.13	6957.4595	42.5405	[7]
	0.129	6957.3375	42.6625	[23]
	0.129	6957.359766	42.640234	This Work
18782.9787	0.12	9345.199	46.29035	[7]
	0.119	9345.0605	46.42885	[23]
	0.119	9345.038345	46.451005	[12]
	0.119	9345.160938	46.328412	This Work

Table-3 He^+ binding energies in magnetic field (in atomic units).

B (a. u.)	E_b	Ref
100	9.555	[7]
	9.560546525	[12]
	9.547386	This Work
200	12.055	[7]
	12.053389	This Work
300	13.78	[7]
	13.784426	This Work
425.532	15.435	[7]
	15.465744545	[12]
	15.435744	This Work
1000	20.2	[7]
	20.2706953	[12]
	20.21731	This Work
4255.32	30.995	[7]
	31.1963695	[12]
	30.998755	This Work
8000	36.92	[7]
	36.908482	This Work
10000	39.215	[7]
	39.5489875	[12]
	39.209713	This Work
14000	42.87	[7]
	42.863056	This Work
18782.9787	46.265	[7]
	46.728775	[12]
	46.257596	This Work

3.3 Ground State of He_2^{3+} in a Strong Magnetic Field

The molecular ion He_2^{3+} can exist at B ≥ 100 a.u. [23]. This system consists of two infinitely heavy α-particles situated along the line forming the angle, $\theta = 0^{\circ}$ with the z-axis, and one electron placed in a uniform constant magnetic field directed along the z-axis. As a method to explore the problem we use the VMC procedure. The ground state trial function is the same as the function which was successfully used to explore the H_2^+ molecular ion in a strong magnetic field. In Table-4 we present the magnetic field strength B, the equilibrium inter-nuclear distance R_{eq}, the total energy E_T, and the binding energy $E_b = \frac{B}{2} - E_T$ (all energies are given in atomic units).

Table-4 Molecular ion He_2^{3+} in a magnetic field B with equilibrium inter-nuclear distance R_{eq}, total energy E_T, and binding energy $E_b = \frac{B}{2} - E_T$ (all energies in atomic units).

B (a.u.)	R_{eq}	E_T	E_b	Ref
100	0.78	41.742	8.258	[7]
	0.77926	41.73796913	8.26203087	[12]
	0.78	41.820322	8.179678	This Work
150	0.64	65.351	9.649	[7]
	0.64	65.441714	9.558286	This Work
200	0.565	89.2275	10.7725	[7]
	0.565	89.370023	10.629977	This Work
300	0.48	137.433	12.567	[7]
	0.48	137.547229	12.452771	This Work
425.532	0.42	198.432	14.334	[7]
	0.42004	198.4245096	14.3414904	[12]
	0.42	198.446548	14.319452	This Work
1000	0.309	480.366	19.634	[7]
	0.30923	480.3569958	19.6430042	[12]
	0.309	480.437714	19.562286	This Work
4255.32	0.193	2095.091	32.569	[7]
	0.19314	2095.081337	32.578663	[12]
	0.193	2095.093818	32.566182	This Work
10000	0.15	4956.8835	43.1165	[7]
	0.14955	4956.8701205	43.1298795	[12]
	0.15	4956.892578	43.107422	This Work
18782.9787	0.126	9338.9285	52.56085	[7]
	0.1256	9338.91703	52.57232	[12]
	0.126	9338.929883	52.559467	This Work

The obtained results in Table-4 indicate that for a magnetic field B ≥ 100 a.u., the binding energies display clearly the existence of the exotic molecular ion He_2^{3+}. The equilibrium distance decreases as the magnetic field increases making the system more and more compact. The total and binding energies grow as the magnetic field increases. For magnetic fields B < 1000 a.u., the binding energy of the atomic ion He^+ is larger than one of the molecular ions He_2^{3+} (see Table-3). Therefore, He_2^{3+} is unstable towards the decay $He_2^{3+} \rightarrow He^+ + \alpha$. However, for B ≥ 1000 a.u., the situation is inverted; the binding energy of the atomic ion He^+ is systematically smaller than one for the molecular ion He_2^{3+}. Thus, the above mentioned decay becomes forbidden and the exotic ion He_2^{3+} becomes stable.

3.4 Ground State of Li_2^{5+} in a Strong Magnetic Field

The energies of the $1\sigma_g$ state of the one-electron system containing two Lithium nuclei, for magnetic fields $B \leq 10^7$ a. u. in parallel configuration are presented in Table-5.

Table-5 Molecular ion Li_2^{5+} in a magnetic field B with equilibrium inter-nuclear distance R_{eq}, total energy E_T, and binding energy $E_b = \frac{B}{2} - E_T$ (all energies in atomic units).

B (a. u.)	R_{eq}	E_T	E_b	Ref
2.1×10^4	0.211	10427.4665	72.5335	[8]
	0.2118	10427.41865	72.58135	[8]
	0.211	10427.715199	72.284801	This Work
5×10^4	0.139	24904.7415	95.2585	[8]
	0.1394	24904.6952	95.3048	[8]
	0.139	24904.833830	95.16617	This Work
10^5	0.111	49882.454	117.546	[8]
	0.1107	49882.40565	117.59435	[8]
	0.111	49882.500505	117.499495	This Work
5×10^5.	0.071	249814.388	185.612	[8]
	0.0707	249814.3155	185.6845	[8]
	0.071	249814.425150	185.57485	This Work
10^6	0.06	499777.1125	222.8875	[8]
	0.0597	499777.01	222.99	[8]
	0.06	499777.164670	222.83533	This Work
10^7	0.037	4999612.8445	387.1555	[8]
	0.037	4999612.867496	387.132504	This Work

The binding energy of the Li_2^{5+} molecular ion in the $1\sigma_g$ state for $B = 10^6$ a. u. is displayed in Table-6 for the inter-nuclear distance $R_{eq} \approx 0.06$ a. u. For a magnetic field $B \approx 2.1\times10^4$ a. u., the energy displays a minimum for $R = 0.21$ a. u., indicating the existence of a metastable state of the Li_2^{5+} molecular ion $Li_2^{5+} \rightarrow Li_2^{+} + Li$. For magnetic fields $B \approx 10^6$ a. u., the binding energy becomes larger than the binding energy of the Li^{2+} atomic ion (see Table-6). The system becomes stable towards this decay. When we increase the magnetic field strength, the molecular ion Li_2^{5+} becomes more compact (the equilibrium distance decreases) and more bound (the binding energy increases).

Table-6 Li^{2+} binding energies in atomic units.

B (a. u.)	E_b	Ref
2.1×10^4	87.33475	[8]
	87.344476	This Work
5×10^4	109.7873	[8]
	109.790179	This Work
10^5	130.58615	[8]
	130.594324	This Work
5×10^5.	189.5415	[8]
	189.555474	This Work
10^6	219.8115	[8]
	219.812467	This Work
5×10^6	302.145	[8]
	302.154066	This Work
10^7	342.98	[8]
	342.980047	This Work

3.5 Ground State of $LiHe^{4+}$ in a Strong Magnetic Field

Table-7 contains the results of the VMC calculations for the $1\sigma_g$ state of the one-electron system containing Lithium-Helium nuclei for magnetic fields $B \leq 10^7$ a. u.

Table-7 Molecular ion $LiHe^{4+}$ in a magnetic field B with equilibrium inter-nuclear distance R_{eq}, total energy E_T, and binding energy $E_b = \frac{B}{2} - E_T$ (all energies in atomic units).

B (a. u.)	R_{eq}	E_T	E_b	Ref
10^5.	0.11	49887.7275	112.2725	[8]
	0.1101	49887.68915	112.31085	[8]
	0.11	49887.742705	112.257295	This Work
5×10^5	0.067	249827.475	172.525	[8]
	0.067	249827.520010	172.47999	This Work
10^6	0.057	499794.967	205.033	[8]
	0.0568	499794.905	205.095	[8]
	0.057	499794.95086	205.04914	This Work
5×10^6	0.04	2499702.37	297.63	[8]
	0.04	2499702.381660	297.61834	This Work
10^7	0.035	4999654.525	345.475	[8]
	0.035	4999654.676678	345.323322	This Work

For a magnetic field $B \approx 10^5$ a. u., the energy starts to display a minimum for $R \approx 0.11$ a. u. indicating the formation of a metastable state, unstable for the decay to $LiHe^{4+} \rightarrow Li^{2+} + \alpha$. For magnetic fields $B \approx 10^7$ a. u., the binding energy becomes larger than the binding energy of the atomic ion Li^{2+} (see Table-6), indicating that the system can become stable towards this decay. The molecular ion $LiHe^{4+}$ in its $1\sigma_g$ ground state for $B = 10^6$ a. u. is displayed for inter-nuclear distance $R_{eq} \approx 0.06$.

3.6 Ground State of LiH^{3+} in a Strong Magnetic Field

In Table-8 we present the results of the $1\sigma_g$ state for the one-electron system containing Lithium-Hydrogen nuclei for magnetic fields $B \leq 10^7$ a. u. by using the VMC method.

Table-8 Molecular ion LiH^{3+} in a magnetic field B with equilibrium inter-nuclear distance R_{eq}, total energy E_T and binding energy $E_b = \frac{B}{2} - E_T$.

B (a. u.)	R_{eq}	E_T	E_b	Ref
10^6	0.0622	499793.71	206.29	[8]
	0.0622	499793.720031	206.279969	This Work
5×10^6	0.0415	2499709.555	290.445	[8]
	0.0415	2499709.876988	290.123012	This Work
10^7	0.036	4999666.825	333.175	[8]
	0.036	4999666.836843	333.163157	This Work

For a magnetic field $B \approx 10^6$ a. u., the energy displays a minimum for $R \approx 0.06$ a. u. However, this system remains unstable towards the decay $LiH^{3+} \rightarrow Li^{2+}$ + p for all considered magnetic field strengths (see Table-6).

Conclusion

In this paper, We presented a non-relativistic study of the ground state of the one-electron molecular ions up to $Z = 3$; H_2^+, He_2^{2+}, HeH^{2+}, Li_2^{5+}, $LiHe^{4+}$ and LiH^{3+} in the presence of a very strong magnetic field in parallel configuration within the Born-Oppenheimer approximation. By using the VMC technique, we presented a theoretical study about a possible existence of exotic ions He_2^{2+} at $B \geq 100$ a. u. and for HeH^{2+} at $B \geq 1000$ a. u. The ions Li_2^{5+} and $LiHe^{4+}$ become stable or almost stable at magnetic fields $B \simeq 10^6$ and $B \simeq 10^7$ a. u., respectively. While the ion LiH^{3+} remains unstable towards the decay $LiH^{3+} \rightarrow Li^{2+} + p$ in the whole domain of the considered magnetic fields up to $B \leq 10^7$ a. u. So that, there is a hierarchy of ionization energies

$$E_b^{Li_2^{5+}} > E_b^{LiHe^{4+}} > E_b^{LiH^{3+}} > E_b^{He_2^{3+}} > E_b^{HeH^{2+}} > E_b^{H_2^+}$$

The ionization energy grows with an increase of the total charge of the nuclei. In the case of the same charge, the higher binding energy corresponds to the presence of the nucleus with the higher charge. The obtained results by using the VMC method are in good agreement with the corresponding previous studies.

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