One-electron atomic–molecular ions containing lithium in a strong magnetic field

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Abstract

The one-electron lithium-containing Coulomb systems of atomic type Li2+ and molecular type Li5+, LiHe4+ and LiH3+ are studied in the presence of a strong magnetic field \( B \leq 10^7 \) au in a non-relativistic framework. They are considered at the Born–Oppenheimer approximation of zero order (infinitely massive centres) within the parallel configuration (molecular axis parallel to the magnetic field). The variational and Lagrange-mesh methods are employed, complementing each other. It is demonstrated that the molecular systems LiH3+, LiHe4+ and Li5+ can exist for sufficiently strong magnetic fields \( B \gtrsim 10^4 \) au and that Li5+ can even be stable at magnetic fields typical of magnetars.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

The existence of very strong magnetic fields in the atmospheres of neutron stars \( B \sim 10^{12} \) G (\( \sim 10^3 \) au)\(^3\) and magnetars \( B \sim 10^{16} \) G (\( \sim 10^7 \) au) has posed various questions about the structure of matter under the influence of such extreme magnetic fields (see for a review e.g. [1]). In particular, it has raised the question about the possible atomic and molecular systems which can exist in a strong magnetic field: can molecular chains be formed? The interest in getting answers to these questions dramatically increased after the long-awaited discoveries made by the Chandra and XMM-Newton X-ray observatories of absorption features in the soft X-ray spectra of several magnetic stars. The first of those was the celebrated 2002 findings in the radiation coming from the isolated neutron star 1E1207.4-5209 of two wide absorption features at \( \sim 0.7 \) keV and \( \sim 1.4 \) keV [2]. One of the possible explanations of these features is the presence of the traditional \( H_2^+ \) and the exotic \( H_2^{11} \) [3] molecular ions in the atmosphere of this neutron star [4]. It is one of the reasons to assume that other traditional and exotic systems—atomic and/or molecular, containing one or more electrons—might be present in the atmosphere of the neutron stars and magnetars. It has recently been predicted that a variety of hydrogenic, helium and mixed hydrogen/helium molecular ions of one and two electrons can be formed when a sufficiently strong magnetic field is imposed [5, 6].

It is already known that the simplest molecular ion \( H_2^+ \) exists for all magnetic fields, while two more one-electron exotic ions, \( \text{He}_3^+ \) and \( \text{HeH}_2^+ \), might begin to exist for magnetic fields \( B \approx 10^2 \) au and \( B \approx 10^4 \) au, respectively (see [7]). Furthermore, for magnetic fields \( B \gtrsim 10^4 \) au the exotic compound \( \text{He}_3^{11} \) becomes the most bound one-electron system among the one-electron hydrogenic-helium ions. Then, a natural question arises: can other one-electron two-centre systems \( (Z_1, Z_2, e) \) exist in a strong magnetic field? A simple electrostatic analysis indicates that this is indeed possible for \( Z_{1,2} < 4 \) (see [5]).

The goal of the present work is to study the existence of lithium-containing ions \( \text{Li}_2^{2+}, \text{LiH}_3^+, \text{LiHe}_4^+ \) and \( \text{Li}_5^{2+} \) in the presence of a strong magnetic field. The relativistic corrections are assumed to be of small importance for \( B \leq 10^7 \) au following the analysis by Duncan [8] that the longitudinal electronic motion is still deeply non-relativistic. The molecular axis is assumed to be aligned parallel to the magnetic field line since it is rather evident that this configuration is
optimal if a magnetic field is sufficiently strong $[5, 9]$. The positively charged centres are considered to be infinitely heavy (zero-order Born–Oppenheimer approximation).

Since the first attempts to study the simplest two-centre, one-electron molecular ion $H_2^+$ in a magnetic field, various methods were employed: the variational $[10]$, the continuous-fraction $[11]$, the finite-element $[12]$ methods among others (for an overview see $[5]$). Two methods proved to be the most efficient leading to highly accurate results: the variational method with physically motivated trial functions and the Lagrange-mesh method. In particular, the Lagrange-mesh method $[13]$ nowadays provides the most accurate results for the total energy of the $H_2^+$ ion when it could be used. In practice, the implementation of the Lagrange-mesh method is made easier with an a priori knowledge of the equilibrium distance and the corresponding total energy. Our strategy is the following: as a first step, we use the variational method to obtain preliminary but already sufficiently accurate results for the equilibrium distance and the total energy, and then the Lagrange-mesh method is used to check and possibly improve the variational results.

Atomic units $\hbar = e = 1$ are used throughout although the energy is given in Rydbergs.

2. One-electron molecular ion at the Born–Oppenheimer approximation

The Hamiltonian which describes two infinitely heavy centres 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, $B = (0, 0, B)$, is given by

$$\hat{H} = -\Delta - \frac{2Z_1}{r_1} - \frac{2Z_2}{r_2} + \frac{2Z_1Z_2}{R} \hat{\rho} A + A \hat{\rho} + A^2$$  \hspace{1cm} (1)

(for geometrical setting see figure 1; the origin of the coordinate system is the middle point between the nuclei for all molecular ions considered here). The vector potential corresponding to a constant magnetic field $B = (0, 0, B)$ is chosen in the symmetric gauge

$$A = \frac{B}{2}(-y, x, 0)$$  \hspace{1cm} (2)

Then the Hamiltonian takes the form

$$\hat{H} = -\Delta - \frac{2Z_1}{r_1} - \frac{2Z_2}{r_2} + \frac{2Z_1Z_2}{R} + B\hat{L}_z + \frac{B^2}{4}\rho^2,$$  \hspace{1cm} (3)

where $\rho^2 = x^2 + y^2$ and $\hat{L}_z$ is the $z$-component of the electron orbital momentum, which is a constant of motion. In practice, we consider the charges $Z_1 = 3$ and $Z_2 = 1, 2, 3$ for lithium-containing ions.

For the case of unequally charged centres, the only integral of motion apart from the energy is the angular momentum projection $\hat{L}_z$ on the magnetic field direction, and the eigenstates are labelled by a quantum number corresponding to the excitation, and a Greek letter $\sigma, \pi, \delta$ corresponding to the magnetic quantum number $m = 0, -1, -2$, respectively. In the equilibrium configuration, the eigenstates of the Hamiltonian (3) with equal charges ($Z_1 = Z_2$) are characterized by two integrals of motion: $\hat{L}_z$ and the spatial parity operator $\hat{P}$ ($\sigma \rightarrow -\sigma$) with eigenvalues $p = \pm 1$. The parallel symmetric configuration is also characterized by the $z$-parity, $\hat{P}_z (z \rightarrow -z)$ with eigenvalues $\sigma = \pm 1$. The magnetic quantum number $m$, spatial parity $p$ and $z$-parity $\sigma$ are related by

$$p = \sigma(-1)^m.$$  \hspace{1cm} (4)

Thus, any eigenstate has two definite quantum numbers: $m$ and $p$. Therefore, the space of eigenstates is split into subspaces (sectors), each of them characterized by definite $m$ and $\sigma$, or $m$ and $p$. Notation involves the subscript $g/u$ (gerade/ungerade) corresponding to positive/negative eigenvalues of the spatial parity operator $\hat{P}$.

3. Methods

3.1. The variational method

We first study the ground state of the Hamiltonian (3) by means of the variational method. We follow the general recipe for the choice of physically relevant trial functions presented in $[14]$. For the case of unequal charged centres, we use a trial function of a similar form to the one used to study the HeH$^{2+}$ molecular ion in a strong magnetic field (see $[7]$):

$$\Psi_{\text{trial}} = \psi_1 + \psi_2 + \psi_3,$$  \hspace{1cm} (4)

with

$$\psi_1 = A_1 e^{-\alpha r_1 - \alpha r_2} e^{-\beta_0 \frac{2}{\Delta} \rho^2},$$  \hspace{1cm} (5a)

$$\psi_2 = A_2 e^{-\alpha r_1} e^{-\beta_0 \frac{5}{2} \rho^2} + A_3 e^{-\alpha r_2} e^{-\beta_0 \frac{5}{2} \rho^2},$$  \hspace{1cm} (5b)

$$\psi_3 = A_4 e^{-\alpha r_1 - \alpha r_2} e^{-\beta_0 \frac{2}{\Delta} \rho^2} + A_5 e^{-\alpha r_1 - \alpha r_2} e^{-\beta_0 \frac{2}{\Delta} \rho^2},$$  \hspace{1cm} (5c)

where $A_{1, 5}$, $\alpha_{1, 5}$ and $\beta_{1, 5}$ are variational parameters. Considering the internuclear distance $R$ as a variational parameter, we have in total 19 variational parameters (a free normalization of the trial function (4) allows us to keep one of the parameters $A_{1, 5}$ fixed).

For the case of symmetric systems with equal charges $Z_1 = Z_2 = Z$, we use a ground state trial function which was successfully used to explore the $H_2^+$ and HeH$^{2+}$ molecular ions in a strong magnetic field $[5]$. It has the same form (4) with permutationally symmetric functions $\Psi_{\text{trial}} (5a)\sim(5c)$.
where $A_{1,2,3, \alpha_{1,4}}$ and $\beta_{1,3}$ are variational parameters. Here we end up with ten variational parameters. The functions $\psi_1, \psi_2$ describe the coherent and incoherent interactions of the electron with the charged centres, respectively. Obviously, they are suitable modifications of the celebrated Heitler–London and Hund–Mulliken $\mathrm{H}^2$ trial functions by multiplication with the lowest Landau orbital. In turn, the function $\psi_3$ is a modified Guillemin–Zener function. It can also be considered as a nonlinear superposition of the functions $\psi_{1,2}$.

### 3.2. The Lagrange-mesh method

With the aim to confirm and improve the variational results, we apply the Lagrange-mesh method [13, 15, 16] which is an approximate variational calculation performed with the Lagrange basis and simplified by the use of the corresponding Gauss quadrature. So far, this method gives the most accurate total energy of the $\mathrm{H}^2$ ion in a magnetic field. The implementation of this method is made easier with an $a$ priori knowledge of the equilibrium configuration and the total energy of the system. Thus, the variational results obtained for all studied systems $\mathrm{Li}^2+$, $\mathrm{Li}^2+$, $\mathrm{LiHe}^{4+}$, and $\mathrm{LiH}^3+$ can serve as input information for the Lagrange-mesh method.

In order to study a two-centre molecular system of charges $Z_1$ and $Z_2$, it is adequate to use the spheroidal coordinates $(\xi, \eta, \varphi)$ defined as

$$
\xi = \frac{r_1 + r_2}{R} - 1, \quad \eta = \frac{r_1 - r_2}{R},
$$

(7)

(see figure 1) with $\xi \in (0, \infty)$, $\eta \in (-1, 1)$ and the azimuthal angle $\varphi \in (0, 2\pi)$. Since the $z$-projection of the orbital angular momentum $\mathbf{L}$ commutes with the Hamiltonian (3), it is replaced by its eigenvalue $m$ (magnetic quantum number). Because we are interested in the ground state, the wavefunction should be nodeless; hence, $m = 0$ and it can be written as [13]

$$
\Psi_{m=0}(\mathbf{r}) = \frac{2}{(\pi R^3)^{1/2}} \psi_0(\xi, \eta).
$$

(8)

Substituting (8) into the Schrödinger equation for the Hamiltonian (3), we arrive at the differential equation for the ground state function $\psi_0(\xi, \eta)$,

$$
\frac{4}{R^2 J(\xi, \eta)} (T_\xi + T_\eta + V(\xi, \eta)) \psi_0(\xi, \eta) = E \psi_0(\xi, \eta),
$$

(9)

with the effective potential

$$
V(\xi, \eta) = \frac{2}{R^2} \left( Z_1 Z_2 - \frac{2(Z_1 + Z_2)(\xi + 1) - 2\eta(Z_1 - Z_2)}{(\xi + 1)^2 - \eta^2} \right)
$$

$$
+ \frac{R^2 B^2}{16} \xi(\xi + 2)(1 - \eta^2),
$$

(10)

where

$$
J(\xi, \eta) = (\xi + 1)^2 - \eta^2.
$$

(11)

Here

$$
T_\xi = -\frac{d}{d\xi} (\xi(\xi + 2) \frac{d}{d\xi}) T_\eta = -\frac{d}{d\eta} (1 - \eta^2) \frac{d}{d\eta}.
$$

(12)

We consider $\psi_0(\xi, \eta)$ spanned in some finite basis

$$
\psi_0(\xi, \eta) = \sum_{i=1}^{N_i} \sum_{j=1}^{N_i} c_{ij} F_{ij}(\xi, \eta),
$$

(13)

where $N_i$ is the size in the $\xi$-direction and $N_\xi$ is in the $\eta$-direction. Explicitly, a basis function is given by (see [13])

$$
F_{ij}(\xi, \eta) = J_{ij}^{-1/2} f_i(\xi) g_j(\eta),
$$

(14)

where

$$
f_i(\xi) = (-1)^i (h x_i)^{1/2} L_{N_\xi}(\xi/h) e^{-x_i^2/2h},
$$

(15)

$$
g_j(\eta) = (-1)^{N_\xi-j} \frac{1 - \eta_j^2}{\eta - \eta_j} \frac{P_{N_\xi}(\eta)}{2},
$$

(16)

and $J_{ij} = J(h x_i, \eta_j)$ (see (11)), where $x_i$ and $\eta_j$ are the $i$th zero of the Laguerre polynomial $L_{N_\xi}(x)$ and the $j$th zero of the Legendre polynomial $P_{N_\xi}(\eta)$, respectively. The dimensionless parameter $h$ is introduced for convenience. Making its variation, it allows us to adapt the Lagrange mesh to the actual size of the molecular ion. Taking the wavefunction (13) and using the Gaussian quadratures associated with each coordinate, equation (9) gets the form of mesh equations (see [13]),

$$
\sum_{i=1}^{N_i} \sum_{j=1}^{N_\xi} [T_{ij} c_{ij} + V(h x_i, \eta_j) \delta_{ij} \delta_{jj} - E \delta_{ij} \delta_{jj}] c_{ij} = 0.
$$

(17)

The kinetic energy matrix elements $T_{ij} c_{ij}$ are calculated in [13]. The potential $V(\xi, \eta)$ is evaluated at the zeros of the Laguerre (scaled by the dimensionless parameter $h$) and Legendre polynomials. Finally, the problem of solving the Schrödinger equation is reduced to searching eigenvalues of the matrix equation (17).

### 4. Results

The results of the variational and mesh calculations for the $m = 0$ ground state of the lithium-containing one-electron Coulomb systems $\mathrm{Li}^2+$ as well as $\mathrm{Li}^2+$, $\mathrm{LiHe}^{4+}$, and $\mathrm{LiH}^3+$ in magnetic fields $B \lesssim 10^4$ au in parallel configuration are presented in tables 1–4, respectively. The results for the molecular systems show that the corresponding potential energy curve starts to display a well-pronounced minimum at finite internuclear distance at the threshold magnetic fields $B_{\text{th}} \sim 2 \times 10^4$, $\sim 10^5$ and $\sim 10^6$ au. It provides a theoretical indication of the possible existence of the bound exotic diatomic molecular ions $\mathrm{Li}^2+$, $\mathrm{LiHe}^{4+}$ and $\mathrm{LiH}^3+$. For each molecular system, the potential energy curve as a function of the internuclear distance $R$ is characterized by the presence of a potential barrier. At large internuclear distances, the interaction of the two charged centres becomes repulsive; the total energy curve approaches from above to the total energy of the atomic ion $\mathrm{Li}^2+$ (see figures 2, 4 and 7).
If the energy of Li$_2^+$ is lower than the minimum on the potential curve, the system is metastable towards the decay to Li$^2+$. All studied systems display two general properties of the Coulomb systems in a magnetic field: as the strength of the magnetic field increases, they become more bound (the binding energy grows) and more compact (the equilibrium internuclear distance decreases).

In tables 2–4 we present the equilibrium internuclear distance $R_{eq}$, the corresponding total $E_{t}^{min}$ and binding $E_{b}=E_{t}^{min}−E_{vib}$ energies, the dissociation energy $E_{diss}=E_{t}^{min}−E_{t}^{Li^2+}$ (corresponding to the decay to Li$^2+$), as well as the position $R_{max}$ of the maximum $E_{t}^{max}$ of the barrier and its height, i.e. the difference $ΔE=E_{t}^{max}−E_{t}^{min}$ for the molecular ions Li$_2^+$, LiHe$^{4+}$ and LiH$^{3+}$, respectively.

For each molecular system, we calculated the lowest vibrational energy $E_{vib}^{0}$ by using the harmonic oscillator approximation around the equilibrium position. It defines the zero point energy and is presented in tables 2–4. Finally, $R_{cross}$ indicates the value of the internuclear distance $R$ beyond the cross.

![Figure 2. Total energy for the 1$\sigma_g$ state of the Li$_2^+$ ion in parallel configuration at a magnetic field $B=10^4$ au as a function of the internuclear distance $R$. The Li$_2^+$ energy (dotted line) and the lowest vibrational energy (dashed line) are displayed. At the minimum $R_{eq}≈0.06$ au.](image)

### Table 1. Results for the total ($E_{t}$) and binding ($E_{b}$) energies (in Ry) of the 1$s_0$ ground state of the atomic ion Li$^{2+}$ in a magnetic field using the variational method (upper lines) and the Lagrange-mesh method (lower lines) when available.

| $B$  | $E_{t}$ | $E_{b}$ |
|------|---------|---------|
| $2.1 \times 10^4$ | 20 825.331 | 174.6695 |
| $5 \times 10^4$ | 20 825.3232 | 174.6768 |
| $10^5$ | 49 780.425 | 219.5746 |
| $5 \times 10^5$ | 99 738.828 | 261.1273 |
| $10^6$ | 99 738.7958 | 261.2042 |
| $5 \times 10^6$ | 499 620.917 | 379.083 |
| $10^7$ | 999 560.377 | 439.623 |
| $10^8$ | 999 560.340 | 439.660 |
| $10^9$ | 4 999 395.71 | 604.29 |

### Table 2. Molecular ion Li$_2^+$ in a magnetic field $B$: equilibrium internuclear distance $R_{eq}$, total $E_{t}^{min}$ and binding $E_{b}=E_{t}^{min}−E_{vib}$ energies in the variational method (upper lines) and the Lagrange-mesh method (lower lines); dissociation energy $E_{diss}=E_{t}^{min}−E_{t}^{Li^2+}$ (corresponding to the decay to Li$^2+$), as well as the position $R_{max}$ of the maximum $E_{t}^{max}$ of the barrier and its height, i.e. the difference $ΔE=E_{t}^{max}−E_{t}^{min}$.

| $B$  | $R_{eq}$ | $E_{t}^{min}$ | $E_{b}$ | $E_{diss}$ | $R_{max}$ | $ΔE$ | $E_{vib}^{0}$ | $R_{cross}$ |
|------|---------|--------------|--------|-----------|-----------|-----|-------------|---------|
| $2.1 \times 10^4$ | 0.211 | 20 854.933 | 145.067 | 29.603 | 0.234 | 0.014 | 0.11 | 0.247 |
| $5 \times 10^4$ | 0.2118 | 20 854.8373 | 145.1627 | 29.5141 | 0.232 | 0.0096 | 0.11 | 0.218 |
| $10^5$ | 0.139 | 49 809.483 | 190.517 | 29.058 | 0.252 | 2.9 | 0.48 | 0.37 |
| $10^6$ | 0.1394 | 49 809.3904 | 190.6906 | 28.9820 | 0.252 | 2.8843 | 0.48 | 0.3655 |
| $5 \times 10^7$ | 0.110 | 99 764.908 | 235.092 | 26.080 | 0.245 | 7.99 | 0.76 | 0.45 |
| $10^8$ | 0.1107 | 99 764.8113 | 235.1887 | 26.0155 | 0.246 | 7.98 | 0.76 | 0.4451 |
| $10^9$ | 0.071 | 499 628.776 | 371.224 | 7.859 | 0.225 | 31.51 | 1.69 | 1.56 |
| $10^10$ | 0.0707 | 499 628.631 | 371.369 | 7.748 | 0.2246 | 31.6 | 1.69 | – |
| $10^11$ | 0.0597 | 999 554.225 | 445.775 | – | 6.15 | 0.215 | 48.06 | 2.33 |
| $10^12$ | 0.037 | 999 225.689 | 774.311 | – | 88.35 | 0.186 | 138.59 | 5.98 |

### Table 3. Same as in table 2 for the molecular ion LiHe$^{4+}$ in a magnetic field $B$.

| $B$  | $R_{eq}$ | $E_{t}^{min}$ | $E_{b}$ | $E_{diss}$ | $R_{max}$ | $ΔE$ | $E_{vib}^{0}$ | $R_{cross}$ |
|------|---------|--------------|--------|-----------|-----------|-----|-------------|---------|
| $10^3$ | 0.110 | 99 775.455 | 224.545 | 36.628 | 0.144 | 0.4 | 0.56 | 0.1663 |
| $10^4$ | 0.1101 | 99 775.3783 | 224.6217 | 36.5825 | 0.144 | 0.3917 | 0.55 | 0.1661 |
| $5 \times 10^4$ | 0.067 | 499 654.950 | 345.050 | 34.033 | 0.136 | 9.229 | 1.72 | 0.2268 |
| $10^5$ | 0.067 | 499 654.857 | 345.142 | 33.974 | 0.136 | 9.213 | 1.57 | 0.2267 |
| $5 \times 10^5$ | 0.057 | 999 589.934 | 410.066 | 29.557 | 0.130 | 16.630 | 2.31 | 0.2679 |
| $10^6$ | 0.0568 | 999 589.810 | 410.190 | 29.470 | 0.130 | 16.610 | 2.30 | – |
| $10^7$ | 0.040 | 999 404.74 | 595.26 | 9.02 | 0.117 | 44.40 | 4.26 | 0.940 |
| $10^8$ | 0.035 | 999 390.05 | 690.95 | – | 4.99 | 0.111 | 61.42 | 5.35 |
maximum for which the total energy is equal to the energy value at the minimum. \( R_{0i}, R_{max}, R_{cross} \) and \( \Delta E \) give a qualitative description of the barrier.

Variational calculations were performed in MacBook with an Intel Core 2 Duo CPU at 2.4 GHz. The minimization package MINUIT from CERN-LIB and an adaptive multidimensional numerical integration routine D01FCF from NAG-LIB were used in the variational calculations. For the lowest eigenvalue search in the mesh calculations, the software code JADAMILU [17] was used.

### 4.1. The atomic ion Li\(^{2+}\)

The hydrogenic ion Li\(^{2+}\) exists for all magnetic fields and is stable. In table 1 we present the results obtained for the ground state total energy of Li\(^{2+}\) in a magnetic field in the range \( 2.1 \times 10^4 \leq B \leq 10^7 \) au using both the variational method and the Lagrange-mesh method. In the variational approach, the trial function is taken as a linear combination of the products of the lowest Coulomb orbital and the lowest Landau orbital:

\[
\Psi_{\text{trial}} = \sum_{i=1}^{4} A_i e^{-\alpha_i r - \beta_i \frac{R}{Z}} \rho^i,
\]

where \( A_{1,4}, \alpha_{1,4} \) and \( \beta_{1,4} \) are variational parameters. This few parametric trial function provides highly accurate results for the total energy in comparison to the more accurate Lagrange mesh calculations (when converged) for the whole domain of magnetic fields studied (see table 1). They are systematically higher than those obtained with the Lagrange mesh method. Their absolute accuracies increase from about \( \sim 0.1 \) Ry at \( B = 2.1 \times 10^4 \) au to \( \sim 0.4 \) Ry at \( B = 10^6 \) au. In turn, the relative accuracy on the binding energies varies from 0.005% to 0.1%. A feature that arises here (and which is also found in other systems, see below) is the fact that when we increase the magnetic field, the number of points that are necessary in the Lagrange-mesh method for a reliable (converged) calculation gradually increase as the magnetic field increases. Eventually, it limits the domain of application of the Lagrange-mesh method. For example, with available computer resources it was impossible to get a number of mesh points at \( B = 5 \times 10^6 \) au and higher magnetic fields in order to reach convergence.

### 4.2. The molecular ion Li\(^{5+}\)

The results of the variational and the Lagrange mesh calculations for the 1\(\sigma_g^0\) state of the one-electron system containing two lithium nuclei, Li\(^{5+}\), for magnetic fields \( B \leq 10^7 \) au in parallel configuration are presented in table 2. It is worth mentioning that for one-electron symmetric systems with two nuclei with charge \( Z \) at distance \( R \), the total energy is related to the total energy of H\(^+\) by a relation similar to a scaling relation for the single nucleus case presented in [18],

\[
E_i(Z, B, R) = Z^2 E_i(1, B/Z^2, ZR) + \frac{2Z(Z-1)}{R}.
\]

Though it is known that H\(^+\) is stable at all studied magnetic fields \( 0 < B < 10^7 \) au (see [6]), the presence in the rhs of the repulsive term \( 2Z(Z-1)/R \) (which is absent in the single nucleus case) indicates that other one-electron molecular ions may not exist. For example, for \( Z = 2 \), the He\(^{6+}\) ion does not exist at \( B < 10^2 \) au but it starts to exist for \( B \geq 10^2 \) au at first as a metastable state and then for \( B \geq 10^4 \) au as a stable one. For \( Z = 3 \), the Li\(^{6+}\) ion does not exist for \( B \lesssim 2 \times 10^4 \) au (see the discussion below).

A trial function of the form (4) is used in the variational calculations. For each value of the magnetic field shown in table 2, the upper line corresponds to the variational results while the lower line (when displayed) corresponds to the Lagrange-mesh results. For \( B = 10^7 \) au, it was impossible to get a sufficiently large number of mesh points with our available computer resources in order to obtain a converged result. The converged Lagrange-mesh energies when available are better than the corresponding variational results. The absolute accuracies of the variational energies increase from about \( \sim 0.1 \) Ry at \( B \leq 10^5 \) au to \( \sim 0.2 \) Ry at \( B = 10^6 \) au. For the binding energy, the relative accuracy is \( \sim 0.07\% \) at \( B = 2.1 \times 10^4 \) au, while it is \( \sim 0.05\% \) at \( B = 10^6 \) au.

For a magnetic field \( B \sim 2.1 \times 10^4 \) au, the potential energy curve starts to display a minimum for \( R = 0.21 \) au indicating the existence of a metastable state of the molecular ion Li\(^{5+}\), unstable towards the decay to Li\(^{3+}\) + Li\(^{3+}\). Further calculations of the energy curve show that the potential barrier is not high enough to keep a vibrational level, \( E_{0vib} > \Delta E \). Hence, the system is unstable against vibrations. For magnetic fields \( B \gtrsim 5 \times 10^4 \) au, the potential energy well becomes sufficiently deep to keep at least one vibrational state. The height of the barrier increases when the magnetic field is increased and the system becomes more stable against vibrations, i.e. while both \( \Delta E \) and \( E_{0vib} \) increase monotonically with the magnetic field, their ratio \( \Delta E / E_{0vib} \) increases from \( \sim 6 \) for \( B = 5 \times 10^4 \) au up to \( \sim 23 \) for \( B = 10^7 \) au. At the same time, the dissociation energy \( E_{diss} = E_{min} - E_{0vib} \) decreases and eventually, for magnetic fields \( B \sim 10^6 \) au, the total energy becomes smaller than the total energy of the Li\(^{3+}\) atomic ion. The system becomes stable towards the decay Li\(^{5+}\) → Li\(^{3+}\) + Li\(^{3+}\), a situation depicted in figure 2 for

| \( B \)  | \( R_{eq} \) | \( E_{1\sigma g}^{min} \) | \( E_0 \) | \( E_{diss} \) | \( R_{max} \) | \( \Delta E \) | \( E_{vib}^{0_{vib}} \) | \( R_{cross} \) |
|---|---|---|---|---|---|---|---|---|
| \( 10^6 \) | 0.0621 | 999 587.579 | 412.421 | 27.20 | 0.092 | 0.95 | 1.741 | 0.1173 |
| \( 0.0622 \) | 999 587.42 | 412.57 | 27.08 | 0.0928 | 0.96 | 1.745 |
| \( 5 \times 10^6 \) | 0.0415 | 4999 419.11 | 580.89 | 23.39 | 0.089 | 8.4 | 4.403 | 0.1668 |
| \( 0.0415 \) | <4999 419.3 | >580.7 | >23.39 | >0.089 | >8.4 | >4.403 |
| \( 10^7 \) | 0.0360 | 9999 333.65 | 666.35 | 19.61 | 0.087 | 14.2 | 5.385 | 0.2048 |
B = 10^6 au. The qualitative behaviour of this molecular system is typical: when we increase the magnetic field strength, the molecular ion LiHe^4+ becomes more compact (the equilibrium distance decreases) and more bound (the binding energy increases).

The electronic distribution of the LiHe^4+ molecular ion in the 1σ_g state for B = 10^6 au is displayed in figure 3 for the internuclear distances R_eq ≈ 0.06, R_max ≈ 0.21 and R = 1.0 au. At equilibrium, the electronic distribution is characterized by two overlapping peaks centred at the positions of the charged centres. Eventually, at large internuclear distances, the electronic distribution consists of two symmetric electronic distributions each of them corresponding to the atomic ion Li^2+. Eventually, at large internuclear distances, the electronic distribution consists of two symmetric electronic distributions each of them corresponding to the atomic ion Li^2+. The schematic picture shown in figure 3 for the ground state electronic distribution of LiHe^4+ is typical for all the magnetic fields where this molecular ion exists.

4.3. The molecular ion LiHe^4+

Table 3 contains the results of the variational and the Lagrange-mesh calculations for the 1σ state of the one-electron system LiHe^4+, for magnetic fields B ≤ 10^7 au in parallel configuration. For this asymmetric system, a trial function of the form (4) is used in the variational calculations. For each value of the magnetic field shown in table 3, the upper line corresponds to the variational results while the lower line (when displayed) corresponds to the Lagrange-mesh results. For the binding energy, the relative improvement of the mesh calculations is ≈ 0.03%, almost uniformly for magnetic fields B = 10^5–10^6 au. For B = 5 x 10^6 au, the Lagrange-mesh energy is worse than the variational one.

For a magnetic field B ~ 10^5 au, the potential energy curve starts to display a minimum for R ≈ 0.11 au indicating the formation of a metastable state, unstable for the decay to LiHe^4+ → LiHe^2+ + α. Also, the potential barrier is small and it does not allow us to keep a vibrational level, E^vb → ΔE. For magnetic fields B ≥ 5 x 10^5 au, the potential energy well is sufficiently deep to keep more than one vibrational state. Also, the height of the barrier increases when the magnetic field is increased, and the system becomes more stable against vibrations, i.e. the ratio ΔE/E^vb increases from ~5 for B = 5 x 10^5 au up to ~12 for B = 10^7 au. At the same time, the dissociation energy E_{diss} = E_r - E_{L^2+} decreases and, eventually, for magnetic fields B ~ 10^7 au, the total energy becomes smaller than the total energy of the atomic ion LiL^2+, indicating that the system can become stable towards the decay LiHe^2+ → Li^2+ + α. However, even at B = 10^7 au, the system is still probably metastable with respect to vibrations since E^vb > E_{diss}. The total energy E_t as a function of the internuclear distance R, for B = 10^6 au, is shown in figure 4.

The electronic distribution of the molecular ion LiHe^4+ in its 1σ ground state for B = 10^6 au is displayed in figure 5 for three different internuclear distances: R_eq ≈ 0.06, R_max ≈ 0.13 and R_cross ≈ 0.27 au. The profile of the electronic distribution is asymmetric. At equilibrium, the electronic distribution for LiHe^4+ is characterized by one pronounced peak at the position of the Li nucleus and a shoulder due to

![Figure 3](image-url)  
**Figure 3.** Evolution of the electronic distribution \( \int |\psi_0(x, y, z)|^2 \, dy \) for the ground state 1σ_x of LiHe^4+ in a magnetic field B = 10^6 au for internuclear distances: (a) R_eq ≈ 0.06, (b) R_max ≈ 0.21 and (c) R = 1.0 au.

![Figure 4](image-url)  
**Figure 4.** Total energy for the ground state 1σ of the molecular ion LiHe^4+ placed in a magnetic field B = 10^6 au in parallel configuration. The LiHe^4+ energy (dotted line) and the lowest vibrational energy (dashed line) are displayed. The equilibrium distance R_eq ≈ 0.057 au.

![Figure 5](image-url)  
**Figure 5.** Total energy for the ground state 1σ of the molecular ion LiHe^4+ placed in a magnetic field B = 10^6 au in parallel configuration. The LiHe^4+ energy (dotted line) and the lowest vibrational energy (dashed line) are displayed. The equilibrium distance R_eq ≈ 0.057 au.
the presence of the $\alpha$ particle. The electronic distribution evolves in such a way that eventually the shoulder disappears and the distribution becomes centred at the position of the Li nucleus and less asymmetrical. This ionic-bonding behaviour is typical for all the magnetic fields studied.

In order to have a better picture of this evolution, figure 6 presents the $z$-profile of the electronic distribution as a function of the internuclear distance for two values of the magnetic field $B = 10^6$ au and $B = 5 \times 10^6$ au. The electronic cloud becomes narrower in the $z$-direction when the magnetic field increases.

4.4. The molecular ion LiH$^3^+$

In table 4 we present the results of the variational and mesh calculations for the $1\sigma$ state of the system LiH$^3^+$ for magnetic fields $B \leq 10^7$ au. The trial functions (4) are used for this asymmetric system. For a magnetic field $B \sim 10^6$ au, the potential energy curve starts to display a minimum for $R \approx 0.06$ au. The potential barrier does not keep a vibrational level, $E_{vib}^0 > \Delta E$. For $B \gtrsim 5 \times 10^6$ au, the potential energy well is sufficiently deep to keep at least one vibrational state. However, this system remains unstable towards the decay $\text{LiH}^3^+ \rightarrow \text{Li}^2^+ + p$ for all magnetic fields studied.

We could obtain converged results with the mesh method only for the magnetic field $B = 10^6$ au. For the binding energy, the relative improvement was $\sim 0.04\%$. For $B = 5 \times 10^6$ au, we also present the best Lagrange-mesh results obtained, although they are less accurate than the variational ones.
distances of magnetic fields considered, one-electron lithium-containing ions Li\(^{2+}\), Li\(^{3+}\), Li\(^{4+}\), Li\(^{5+}\).

We presented a non-relativistic study of the ground state of the molecular ion LiH\(^{3+}\) for internuclear distances: \(R_{\text{eq}}, R_{\text{max}} = 0.2 \au\) and magnetic fields: (a) \(B = 10^6 \au\) and (b) \(B = 5 \times 10^6 \au\).

A plot of the total energy \(E_b\) as a function of the internuclear distance \(R\) for \(B = 5 \times 10^6 \au\) is shown in figure 7. The ground state electronic distribution for a magnetic field \(B = 10^6 \au\) for three values of the internuclear distances: \(R_{\text{eq}} \approx 0.06, R_{\max} \approx 0.09\) and \(R_{\text{cor}} \approx 0.12 \au\) is very much similar to the one obtained for LiHe\(^{4+}\) (see figure 5).

At equilibrium, the electronic distribution displays one peak which follows the position of the Li nucleus. Another view is presented in figure 8 where the integrated electronic distribution along the \(z\)-axis is displayed for three different values of the internuclear distance and for \(B = 10^6 \au\) and \(B = 5 \times 10^6 \au\). In the latter case, the electronic distribution is almost symmetric around the position of the Li nucleus with a small asymmetry due to the presence of the proton. When we compare the distribution for both fields, we can see how it shrinks along the \(z\)-axis as the magnetic field increases.

5. Conclusions

We presented a non-relativistic study of the ground state of the one-electron lithium-containing ions Li\(^{2+}\), LiH\(^{3+}\), LiHe\(^{4+}\), Li\(^{5+}\) in the presence of a strong magnetic field \(B \leq 10^7 \au\) in parallel configuration within the Born–Oppenheimer approximation of zero order. Two methods were employed, complementing each other: the variational method and the Lagrange-mesh method.

The obtained results give clear indications that the exotic molecular ions Li\(^{2+}\), LiHe\(^{4+}\), LiH\(^{3+}\) begin to exist as metastable states starting at the threshold magnetic fields \(B_\text{th} \approx 2 \times 10^4, \sim 10^5\) and \(\sim 10^6\) \au\), respectively. As the magnetic field increases, the potential wells of all three systems become sufficiently deep to keep more than one (longitudinal) vibrational state. Eventually, the ions Li\(^{2+}\), LiHe\(^{4+}\) become stable or almost stable at magnetic fields \(B \approx 10^6\) and \(B \approx 10^7\) \au\), respectively, whereas the ion LiH\(^{3+}\) remains unstable towards the decay LiH\(^{3+}\) \(\rightarrow\) Li\(^{2+}\) + p in the whole domain of magnetic fields considered, \(B \leq 10^7\) \au\). The energies obtained with the variational method were improved with the Lagrange-mesh calculations for magnetic fields \(B \lesssim 10^6\) \au\) for all three molecular ions studied (see tables ). For magnetic fields \(B > 10^6\) \au\), we were unable to reach converged results in the Lagrange-mesh calculations.

The accuracy of the variational energy can be tested using the converged Lagrange-mesh results. For \(B \approx 10^6\) \au\), the relative accuracies on the binding energy are very close: \(\sim 0.05\%\), \(\sim 0.03\%\), \(\sim 0.04\%\) for Li\(^{2+}\), LiHe\(^{4+}\), LiH\(^{3+}\), respectively.

All these molecular ions have a similar behaviour: when the magnetic field increases, each molecular ion becomes more compact (the equilibrium distance decreases) and more bound (the binding energy increases). For a given magnetic field where all three molecular ions display a minimum in the corresponding potential curves that support at least one vibrational level, we find a hierarchy of the binding energies,

\[
E_{b_{\text{Li}^{2+}}} > E_{b_{\text{LiHe}^{4+}}} > E_{b_{\text{LiH}^{3+}}},
\]

i.e. the most bound lithium-containing molecular system is Li\(^{5+}\). If we consider other ions with two centres and one electron [6], He\(^{2+}\), HeH\(^{2+}\) and H\(^{2+}\), in a magnetic field \(10^6 \leq B \leq 10^7\) \au\), there is a hierarchy of ionization energies,

\[
E_{b_{\text{He}^{2+}}} > E_{b_{\text{HeH}^{2+}}} > E_{b_{\text{H}^{2+}}}. \]

The ionization energy grows with an increase in the total charge of the nuclei. In the case of the same charge, the higher binding energy corresponds to the presence of the nuclei with the higher charge.

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