The $\text{H}_3^+$ molecular ion in a magnetic field: linear parallel configuration

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(Dated: December 5, 2021)

Abstract

A first detailed study of the ground state of the $\text{H}_3^+$ molecular ion in linear configuration, parallel to a magnetic field direction, and its low-lying $\Sigma, \Pi, \Delta$ states is carried out for magnetic fields $B = 0 - 4.414 \times 10^{13}$ G in the Born-Oppenheimer approximation. The variational method is employed with a single trial function which includes electronic correlation in the form $\exp(\gamma r_{12})$, where $\gamma$ is a variational parameter. It is shown that the quantum numbers of the state of the lowest total energy (ground state) depend on the magnetic field strength. The ground state evolves from the spin-singlet $^1\Sigma_g$ state for weak magnetic fields $B \lesssim 5 \times 10^8$ G to a weakly-bound spin-triplet $^3\Sigma_u$ state for intermediate fields and, eventually, to a spin-triplet $^3\Pi_u$ state for $5 \times 10^{10} \lesssim B \lesssim 4.414 \times 10^{13}$ G. Local stability of the linear parallel configuration with respect to possible small deviations is checked.

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I. INTRODUCTION

The behavior of atoms, molecules and ions placed in a strong magnetic field has attracted a significant attention during the last two decades (see, in particular, review papers [1, 2, 3]). It is motivated by both pure theoretical interest and by possible practical applications in astrophysics and solid state physics. In particular, the knowledge of the energy levels can be important for interpretation of the spectra of white dwarfs (where a surface magnetic field ranges in \( B \approx 10^6 - 10^9 \, \text{G} \)) and neutron stars where a surface magnetic field varies in \( B \approx 10^{12} - 10^{13} \, \text{G} \), and even can be \( B \approx 10^{14} - 10^{16} \, \text{G} \) for the case of magnetars.

Recently, it was announced that in a sufficiently strong magnetic field \( B \gtrsim 10^{11} \, \text{G} \) the exotic molecular ion \( \text{H}_3^+ \) can exist in linear configuration with protons situated along the magnetic line [4] (for discussion see a review [3]). In general, it is a metastable long-living system which decays to \( \text{H}_2^+ + p \). However, at \( B \gtrsim 10^{13} \, \text{G} \) the ion \( \text{H}_3^+ \) becomes stable. This system does not exist without or for weak magnetic fields. The ion \( \text{H}_3^+ \) constitutes the simplest one-electron polyatomic molecular ion in a strong magnetic field. The \( \text{H}_3^+ \) ion has been proposed as being the most abundant chemical compound in the atmosphere of the isolated neutron star 1E1207.4-5209 [5]. A detailed review of the current status of one-electron molecular systems, both traditional and exotic, that might exist in a magnetic field \( B \geq 10^9 \, \text{G} \) can be found in [3].

The molecular ion \( \text{H}_3^+ \) is the simplest stable two-electron polyatomic molecular ion. It has a long history since its discovery by J.J. Thomson [6]. Its exceptional importance in astrophysics related to interstellar media explains the great interest in this ion from astronomy, astrophysics and chemistry communities (for a detailed review, see [7]). For all these reasons, there have been extensive theoretical and experimental works on this molecular ion since the pioneering (semi-quantitative) work by Coulson [8].

The first variational calculations [9] of the total energy of the molecular ion \( \text{H}_3^+ \) showed that the equilibrium configuration might be either linear or equilateral triangular. However, this was not well-established until 1964 [10] when it was shown that the equilibrium configuration for the state of the lowest total energy is an equilateral triangular configuration, while the linear configuration of the \( \text{H}_3^+ \) ion may occur in excited state(s). Since that time a large number of excited states has been studied [11] (for a general review, see [7]). In particular, it has been found that there exists a single spin-triplet state which appears in a linear
configuration $3\Sigma_u$. This is also the unique known state of H$_3^+$ in the linear configuration. No spin-triplet states have been found for a triangular (spacial) configurations so far.

Although the molecular ion H$_3^+$ is characterized by the equilateral triangular configuration as being the optimal in field-free case, it is expected that in a magnetic field $B \approx 0.2$ a.u. (see below) a linear configuration, parallel to a magnetic field direction, gives the lower total energy and becomes the optimal configuration. Somehow, a similar phenomenon already happened for the one-electron exotic molecular ion H$_3^{2+}$ [12] where the optimal configuration is triangular at $10^8 \lesssim B \lesssim 10^{11}$ G and becomes linear parallel at $B \approx 10^{11}$ G. It is worth noting that for H$_3^+$ in field-free case the difference between the total energy of the ground state (triangular configuration) and of the lowest linear configuration is very small, $\approx 0.13$ Ry, in comparison to characteristic energies in a magnetic field.

To the best of our knowledge there exists a single attempt to explore the molecular ion H$_3^+$ in a magnetic field [13]. We repeated all numerical calculations of this work following its guidelines with use of its formulas (see below, Tables I, V, VI) - in fact, no single number from [13] was confirmed. However, in [13] it was made a qualitative statement that with a magnetic field increase the transition from equilateral stable equilibrium configuration to linear equilibrium configuration may occur. This statement we confirm. We predict that this transition takes place at a magnetic field $\approx 0.2$ a.u. A detailed study of a triangular configuration and of this transition will be published elsewhere [14].

Atomic units are used throughout ($\hbar=m_e=e=1$), although energies are expressed in Rydbergs (Ry). The magnetic field $B$ is given in a.u. with a conversion factor $B_0 = 2.35 \times 10^9$ G.

II. GENERALITIES

Let us consider a system of three protons and two electrons (pppee) placed in a uniform constant magnetic field. If for such a system a bound state is developed it corresponds to the molecular ion H$_3^+$. We assume that the protons are infinitely massive (the Born-Oppenheimer approximation of zero order). They are situated along the magnetic field direction forming a linear chain (we call it “the parallel configuration”). The Hamiltonian which describes this system when the magnetic field is oriented along the $z$ direction, $\mathbf{B} = (0, 0, B)$ is [29]

$$
\mathcal{H} = \sum_{\ell=1}^{2} (\hat{p}_\ell + A_\ell)^2 - \sum_{\ell=1,2}^{\kappa=A,B,C} \frac{2}{r_{\ell\kappa}} + \frac{2}{r_{12}} + \frac{2}{R_+} + \frac{2}{R_-} + \frac{2}{R_+ + R_-} + 2\mathbf{B} \cdot \mathbf{S},
$$

(1)
FIG. 1: Geometrical setting for the $H^+_3$ ion in linear configuration parallel to a magnetic field directed along $z$-axis. The protons (marked by bullets) are situated on the $z$-line at distances $R_\pm$ from the central proton which is placed at the origin.

(see Fig. 1 for the geometrical setting and notations), where $\mathbf{p}_\ell = -i\nabla_\ell$ is the 3-vector of the momentum of the $\ell$th electron, the index $\kappa$ runs over protons $A, B$ and $C$, $r_{12}$ is the interelectron distance and $\mathbf{S} = \hat{s}_1 + \hat{s}_2$ is the operator of the total spin. $\mathcal{A}_\ell$ is a vector potential which corresponds to the constant uniform magnetic field $\mathbf{B}$. It is chosen to be in the symmetric gauge,

$$\mathcal{A}_\ell = \frac{1}{2}(\mathbf{B} \times \mathbf{r}_\ell) = \frac{B}{2}(-y_\ell, x_\ell, 0).$$

Finally, the Hamiltonian can be written as

$$\mathcal{H} = \sum_{\ell=1}^2 \left(-\nabla_\ell^2 + \frac{B^2}{4\rho_\ell^2}\right) - \sum_{\ell=1,2} \sum_{\kappa=A,B,C} \frac{2}{r_{1\kappa}} + \frac{2}{r_{12}} + \frac{2}{R_+} + \frac{2}{R_-} + \frac{2}{R_+ + R_-} + B(\hat{L}_z + 2\hat{S}_z),$$

where $\hat{L}_z = \hat{l}_{z1} + \hat{l}_{z2}$ and $\hat{S}_z = \hat{s}_{z1} + \hat{s}_{z2}$ are the $z$-components of the total angular momentum and total spin, respectively, and $\rho_\ell = \sqrt{x_\ell^2 + y_\ell^2}$.

The problem under study is characterized by three conserved quantities: (i) the operator of the $z$-component of the total angular momentum (projection of the angular momentum on the magnetic field direction) giving rise to the magnetic quantum number $m$, (ii) the spatial parity operator $P(\vec{r}_1 \to -\vec{r}_1, \vec{r}_2 \to -\vec{r}_2)$ which has eigenvalues $p = \pm 1$ (gerade/ungerade) (iii) the operator of the $z$-component of the total spin (projection of the total spin on the magnetic field direction) giving rise to the total spin projection $m_s$. Hence, any eigenstate
has three explicit quantum numbers assigned: the magnetic quantum number \( m \), the total spin projection \( m_s \) and the parity \( p \). For the case of two electrons the total spin projection \( m_s \) takes values \( 0, \pm 1 \).

As a magnetic field increases a contribution from the Zeeman term (interaction of spin with magnetic field, \( \mathbf{B} \cdot \mathbf{S} \)) becomes more and more important. It seems natural to assume that for small magnetic fields a spin-singlet state is a state of a lowest total energy, while for large magnetic fields it should be a spin-triplet state with \( m_s = -1 \), where the electron spins are antiparallel to the magnetic field direction \( \mathbf{B} \). The total space of eigenstates is split into subspaces (sectors), each of them is characterized by definite values of \( m \), \( p \) and \( m_s \). It is worth noting that the Hamiltonian \( \mathcal{H} \) is invariant with respect to reflections \( z_1 \to -z_1 \) and \( z_2 \to -z_2 \) (\( z \)-parity operator \( P_z \)). Hence, any eigenstate is characterized by the quantum numbers \( \sigma_N = \pm 1 \) for positive/negative \( z \)-parity (this symmetry accounts for the interchange of the nuclei \( A \) and \( C \) if they are situated symmetrically with respect to \( B \)).

In order to classify eigenstates we follow the convention widely accepted in molecular physics using the quantum numbers \( m, p \) and the total spin \( S \) without indication to the value of \( m_s \). Eventually, the notation is \( 2S+1M_p \), where \( 2S+1 \) is the spin multiplicity which is equal to \( 1 \) for spin-singlet state \( (S=0) \) and \( 3 \) for spin-triplet \( (S=1) \), as for the label \( M \) we use Greek letters \( \Sigma, \Pi, \Delta \) that mark the states with \( |m| = 0, 1, 2, ..., \) respectively, and the subscript \( p \) (the spatial parity quantum number) takes gerade/ungerade\((g/u)\) labels describing positive \( p = +1 \) and negative \( p = -1 \) parity, respectively. There exists a relation between the quantum numbers corresponding to the \( z \)-parity (interchange of nuclei \( A \) and \( C \)) and the spatial parity:

\[
p = (-1)^{|m|} \sigma_N.
\]

Present consideration is limited to the states with magnetic quantum numbers \( m = 0, -1, -2 \) because the total energy of the lowest energy state (the ground state) for any sector with \( m > 0 \) is always larger than anyone with \( m \leq 0 \).

As a method to explore the problem we use the variational procedure. The recipe of choice of trial functions is based on physical arguments \[15\]. As a result the trial function for a lowest energy state with magnetic quantum number \( m \) is chosen in the form

\[
\psi^{(\text{trial})} = \rho_1^{m} e^{i \phi_1} e^{-r_{12} + \alpha_1 r_{1A} - \alpha_2 r_{1B} - \alpha_3 r_{1C} - \alpha_4 r_{2A} - \alpha_5 r_{2B} - \alpha_6 r_{2C} - B\beta_1 \frac{r_{1A}^2}{4} - B\beta_2 \frac{r_{1B}^2}{4} - B\beta_3 \frac{r_{1C}^2}{4}} \times (1 + \sigma_e P_{12} + \sigma_{AC} P_{AC}) (1 + \sigma_{AB} P_{AB} + \sigma_{BC} P_{BC})
\]

\[
(4)
\]
where \( \sigma_e = \pm 1 \) stands for spin singlet \((+)\) and triplet states \((-)\), while \( \sigma_N = 1, -1 \) stands for nuclear gerade and ungerade states, respectively. The \( P_{12} \) is the permutation operator for electrons \((1 \leftrightarrow 2)\) and \( P_{ij}, i, j = A, B, C \) is the operator which interchanges the two protons \( i \) and \( j \). For \( S_3 \)-permutationally symmetric case (all protons are identical) \( \sigma_N = \sigma_{Na} = \pm 1 \). \( \alpha_{1-6}, \beta_{1-2} \) and \( \gamma \) as well as \( R_+, R_- \) are variational parameters. Their total number is eleven.

It is worth emphasizing that in the trial function \( (4) \) the interelectron interaction is included explicitly in the exponential form \( e^{\gamma r_{12}} \).

Calculations were performed using the minimization package MINUIT from CERN-LIB. Multidimensional integration was carried out using a dynamical partitioning procedure: a domain of integration was divided into subdomains following an integrand profile and then each subdomain was integrated separately (for details, see, e.g., [3]). Numerical integration was done with a relative accuracy of \( \sim 10^{-6} - 10^{-7} \) by use of the adaptive D01FCF routine from NAG-LIB. A process of minimization for each given magnetic field and for any particular state was quite time-consuming due to a complicated profile of the total energy surface in the parameter space but when a minimum is found it took a few minutes to compute a variational energy.
III. RESULTS

We carry out a detailed study of $\Sigma, \Pi, \Delta$ low-lying states with a particular emphasis of the state which has the lowest total energy for a given magnetic field - the ground state.

A. $m = 0$

For the case $m = 0$ we consider four subspaces in the Hilbert space, $S = 0$ ($m_s = 0$, spin singlet states), $S = 1$ (spin triplet states) at $m_s = -1$, $\sigma_N = 1$ (gerade states) and $\sigma_N = -1$ (ungerade states).

1. $^1\Sigma_g$ state ($S = 0, \sigma_N = 1$)

For field-free case the system (pppee) in linear configuration (all protons are situated on a line, see, Fig.1) the state $^1\Sigma_g$ is the lowest total energy state which is characterized by a shallow minimum (see, e.g., [7]). However, in spite of developing a minimum for a linear chain the system is unstable towards any deviation from linearity. Hence, this state is globally unstable. It is worth noting that the true ground state does exist and it corresponds to the equilateral triangular configuration (the protons form equilateral triangle) with the total energy $E_T = -2.6877$ Ry and the side of triangle $a_{eq} = 1.65$ a.u. (see [16] and also [17]) [30]. A situation is not so different when a magnetic field is not strong, $B \lesssim 0.2$ a.u.: a linear parallel configuration with the protons situated along a magnetic line is characterized by well-pronounced minimum but a stability towards a deviation from linearity does not occur and a global bound state $^1\Sigma_g$ does not exist. However, with a magnetic field growth, at $B \geq 0.2$ a.u. the system (pppee) becomes stable towards small deviations from parallel configuration and the $^1\Sigma_g$ state exists (being an excited state, see below).

We made a detailed study of the state $^1\Sigma_g$ of the $H_3^+$ ion in the linear parallel configuration, with a particular emphasis of the symmetric case $R_+ = R_- \equiv R$ (see Fig. 1), as well as small deviations from this configuration in a wide domain of magnetic fields $0 \leq B \leq 10000$ a.u. (see Table II). Finally, for the linear parallel configuration the variational trial function $\psi_{\text{trial}}$ [1] with $\sigma_e = 1$, $\sigma_N = 1$ and $m = 0$ was used. It depends on eleven variational parameters. A simple, obvious generalization of (1) is used to study
TABLE I: The H$^{+}_3$ ion in the state $^{1}\Sigma_g$ and a comparison with 2e systems H$_2$ and H$^{-}$: Total $E_T$ and binding (double-ionization) $E_I$ energies, equilibrium distance $R_{eq}$ (in a.u.) as well as the total energies of final states of dissociation and ionization channels of H$^{+}_3$ are shown; all energies are in Ry. * the energy and equilibrium distance of H$^{+}_3$ for these magnetic fields is for a case when a linear configuration is kept externally (see text), $^b$ [13], $^c$ our re-calculation based on the trial function from [13] (see text). Total energies for the H$_2$ molecule in $^{1}\Sigma_g$ state as well as H$^{+}_2$ and H$^{2+}_3$ ions in $1\sigma_g$ state in a magnetic field taken from [18], [19] and [20], respectively. Total energies for the ground state of the H atom and for the H$^{-}$ ion in a magnetic field from [21] and [22], respectively. The ground state energy of H$^{-}$ in field-free case from [23].

| B (a.u.) | $E_T$ | $E_I$ | $R_{eq}$ | $E_T$(H$_2$) | $E_T$(H$^{+}_3$ + H) | $E_T$(H$^{2+}_3$ + e) | $E_T$(H$^{-}$) |
|----------|-------|-------|----------|-------------|-------------------|-------------------|--------------|
| 0°       | -2.5519 | 1.540 | -2.55$^a$ | -            | -                 | -                 | -             |
| 0.2°     | -2.5229 | 1.513 | -1.793$^b$ | -1.7807     | -1.6122           | -0.00358          | -             |
| 1        | -2.0692 | 4.0692 | 1.361     | -3.6024     | -                 | -                 | -             |
| 5        | 2.9597  | 7.0403 | 0.918     | 3.6024      | -                 | -                 | -             |
| 10       | 10.8168 | 9.1832 | 0.746     | 11.778      | 12.1554           | 16.6084           | 15.7613       |
| 11.154$^b$ | 11.153$^c$ | 0.736 | 12.034    | 0.587       | 30.082            | -                 | -             |
| 20       | 27.966  | 12.034 | 0.587     | 30.082      | -                 | -                 | -             |
| 100      | 177.59  | 22.410 | 0.336     | 181.014     | 182.145           | 190.361           | 190.872       |
| 1000     | 1948.41 | 51.586 | 0.160     | 1961.99     | 1979.22           | 1981.569          | -             |
| 10000    | 19889.6 | 108.45 | 0.083     | 19926.25    | 19954.60          | -                 | -             |

$^a$This data can be extracted from [7], p.427

slightly deviated configurations when stability of the linear system was checked.

The variational calculations demonstrate in very clear way the existence of a minimum in the total energy surface $E_T(R_+, R_-)$ for the (pppee) system for all magnetic fields ranging $B = 0 - 10000$ a.u. Minimum always corresponds to the symmetric case $R_{eq}^+ = R_{eq}^- = R_{eq}$ of the linear parallel configuration. For $B < 0.2$ a.u. stability is lost with respect to deviations from linearity. This indicates a ”limited” existence of the molecular ion H$^{+}_3$ in the state $^{1}\Sigma_g$ for these magnetic fields. It exists if in some way a linear configuration is supported.
externally.

Table I displays the results for the total $E_T$ and the double ionization, $E_I = 2B - E_T$, energies, as well as for the internuclear equilibrium distance $R_{eq}$ for the state $^1\Sigma_g$. We find that with an increase of the magnetic field strength the total energy grows more or less linearly with a magnetic field, the system becomes more and more bound (both double ionization and dissociation energies increase) and more compact (the internuclear equilibrium distances $R_{eq}^\pm$ and a size of the system $L_{eq} = R_{eq}^+ + R_{eq}^-$ decrease).

An important characterization of the system is given by a description of possible dissociation and ionization channels together with their behavior as a function of a magnetic field. There are three dominant dissociation channels: (i) $H_3^+ \rightarrow H_2 + p$, (ii) $H_3^+ \rightarrow H_2^+ + H$ and (iii) $H_3^+ \rightarrow H^- + p + p$ (see Table I) as well as two sub-dominant channels $H_3^+ \rightarrow H_2^+ + p + e$ (ionization) and $H_3^+ \rightarrow H + H + p$ (dissociation). Last two channels are characterized by higher ionization-dissociation energies than the channel $H_3^+ \rightarrow H_2^+ + H$ and thus they are not considered. There are two single-ionization processes $H_3^+ \rightarrow H_2^+ + p + e$ and $H_3^+ \rightarrow H_3^{2+} + e$ (see Table I). The second one occurs only at $B > 10$ a.u. where the $H_3^{2+}$ ion can exist, it becomes a dominant single-ionization process at $B > 10000$ a.u. where $E_T(H_3^{2+}) < E_T(H_2^+)$. The total energy of the final state compounds after dissociation for different magnetic fields is shown in Table I. It is interesting to mention that at $B > 100$ a.u. the dissociation $H_3^+ \rightarrow H_3^{2+} + e$ dominates over $H_3^+ \rightarrow H^- + p + p$.

A comparison of the total energy of the ground state of $H_3^+$ for each studied magnetic field with the total energy of the products of dissociation or ionization (see Table I) leads to a conclusion that the total energy of the $H_3^+$ ion is always the smallest among them. Thus, the $H_3^+$ ion in the state $^1\Sigma_g$ is stable for all magnetic fields towards all possible dissociation or ionization channels. A smallest dissociation energy corresponds to the channel $H_3^+ \rightarrow H_2 + p$, which then is followed by $H_3^+ \rightarrow H_2^+ + H$. It is worth noting that the largest dissociation energy corresponds to the channel $H_3^+ \rightarrow H^- + p + p$. In general, the dissociation energy (the difference between the energies of the final and initial states) increases monotonously with a magnetic field growth. It is quite interesting that the difference in total energies of the final compounds of two major dissociation channels (i) and (ii) grows extremely slow with the magnetic field increase reaching 1.1 Ry at $B = 100$ a.u.

A conclusion can be drawn that the $H_3^+$ molecular ion in the state $^1\Sigma_g$ exists for $B \lesssim 0.2$ a.u. if a linear parallel configuration of protons is somehow supported externally, e.g. by
placing a system to an (sub)-atomic trap. However, for larger magnetic fields it exists as an excited state which is stable towards small deviations from linearity. It is worth noting that for the magnetic field \( B = 0.2 \text{ a.u.} \) the total energy well contains at least one longitudinal vibrational state. The vibrational energy is calculated following the same procedure which is used for \( \text{H}_3^{2+} \) ion [20] and it is equal to 0.035 Ry.

2. \( ^3\Sigma_u \) state \((S = 1, \sigma_N = -1)\)

In field-free case the state \( ^3\Sigma_u \) of the system \((pppee)\) is (i) the only state of the \( \text{H}_3^+ \) ion in linear configuration which is known so far and also (ii) it is the only known spin-triplet state of \( \text{H}_3^+ \) (for a review of this state see [24] and references therein). For this state several vibrational states exist. The linear symmetric configuration \( R_+ = R_- \) is stable towards any small deviations, in particular, from linearity. The state \( ^3\Sigma_u \) is stable with respect to the decay \( \text{H}_3^+ \rightarrow \text{H}_2^+ + \text{H} \) (see [25]). Also there is no decay channel \( \text{H}_3^+(^3\Sigma_u) \rightarrow \text{H}_2(1\Sigma_g) + p \).

A detailed variational study of the \( ^3\Sigma_u \) state of the \( \text{H}_3^+ \) molecular ion is done for \( 0 \leq B \leq 10000 \text{ a.u.} \) (see Table II). It turns out that for all studied magnetic fields the total energy surface displays a minimum which corresponds to a linear parallel configuration. Furthermore, always this minimum appears in the symmetric configuration \( R_+ = R_- \equiv R \). For this particular configuration the variational trial function \( \psi^{\text{trial}} \) with \( \sigma_e = -1, \sigma_N = -1 \) and \( m = 0 \) is used which depends on ten variational parameters. Field-free case is studied separately with 23-parametric trial function which is a linear superposition of \( \psi^{\text{trial}} \) and its three different degenerations [31]. This sufficiently simple function allows to reproduce three significant digits in total energy (see Table II). It is separately checked that the linear parallel symmetric equilibrium configuration is stable towards all possible small deviations.

Table II shows the results for the total \( E_T \) and the internuclear equilibrium distance \( R_{eq} \) for the \( ^3\Sigma_u \) state for different magnetic fields. With an increase of the magnetic field the total energy decreases, the system becomes more bound - double ionization energy increases [32] and more compact (the internuclear equilibrium distance decreases). A major emphasis of our study of the state \( ^3\Sigma_u \) is the domain \( 0.2 \lesssim B \lesssim 20 \text{ a.u.} \) where this state becomes the ground state of the \( \text{H}_3^+ \) ion in parallel configuration and likely the global ground state of the ion.

As for the dissociation channel \( \text{H}_3^+(^3\Sigma_u) \rightarrow \text{H}_2^+(1\sigma_g) + \text{H}(1s) \) (with electrons in spin-triplet
TABLE II: \( \text{H}_3^+ \) ion in the state \( ^3\Sigma_u \): total energy (in Ry), equilibrium distance (in a.u.) and the energy of the lowest longitudinal vibrational state \( E_{vib}^0 \), rotational \( E_{rot}^0 \) and bending \( E_{bend}^0 \). Total energy of \( \text{H}_3^+(1\sigma_g) + \text{H}(1s) \) (in Ry) in ground state with spin of each electron antiparallel to \( B \) from [19] and [21], respectively, shown for comparison.

| \( B \) (a.u.) | \( E_T \) | \( R_{eq} \) | \( E_{vib}^0 \) | \( E_{rot}^0 \) | \( E_{bend}^0 \) | \( E_T \) (\( \text{H}_3^+(1\sigma_g) + \text{H}(1s) \)) |
|----------------|----------|---------|--------------|-------------|--------------|--------------------------------------------------|
| 0              | -2.2297  | 2.457   |              |             |              | -2.2052                                          |
| 0.1            | -2.3968  | 2.416   |              |              |              |                                                  |
| 0.2            | -2.5991  | 2.440   | 0.012        | 0.0037      | 0.014        | -2.5734                                          |
| 0.5            | -3.0387  | 2.273   |              |              |              |                                                  |
| 1              | -3.6584  | 2.125   | 0.019        | 0.015       | 0.028        | -3.6122                                          |
| 10             | -7.9064  | 1.216   | 0.048        | 0.095       | 0.17         | -7.8446                                          |
| 20             | -10.110  | 1.00    | 0.063        | 0.16        | 0.26         | -10.082                                          |
| 100            | -17.527  | 0.645   |              |              |              | -17.855                                          |
| 1000           | -35.987  | 0.372   |              |              |              | -38.01                                           |
| 10000          | -67.169  | 0.235   |              |              |              | -73.75                                           |

\( ^a \)Our calculations (see text)

\( ^b \)Rounded data from [25] and [21]

state) the total energy of the final state is slightly higher than \( E_T (\text{H}_3^+) \) for the magnetic fields \( 0.2 \lesssim B \lesssim 20 \) a.u.; the energy difference varies from 0.03 Ry to 0.06 Ry depending on a magnetic field strength, see Table III remaining very small. Hence, although \( \text{H}_3^+(^3\Sigma_u) \) is stable with respect to this dissociation channel it turns out to be a weakly bound state. The dissociation may occur at \( B > 20 \) a.u. with photon emission at the final state. We do not mention a dissociation channel to \( \text{H}_2(^3\Sigma_u) + p \) due to a probable non-existence of the \( \text{H}_2 \) molecule in the domain \( 0.2 \lesssim B \lesssim 20 \) a.u. (see e.g. [18]).

In the domain \( 0.2 \lesssim B \lesssim 20 \) a.u. the total energy well corresponding to the \( ^3\Sigma_u \) state contains at least one longitudinal vibrational state (see Table II). Its energy grows with a magnetic field increase. It is calculated the lowest rotational energy as well as the lowest bending energies using the same formulas as for \( \text{H}_3^{++} \) [20]. All these energies grow with a magnetic field increase. The interesting observation is that for each magnetic field in the domain \( 1 < B < 20 \) a.u. the following hierarchy of these energies holds:

\( E_{vib}^0 < E_{rot}^0 < E_{bend}^0 \),

contrary to the hierarchy at \( 0.2 \lesssim B \lesssim 1 \) a.u.

\( E_{rot}^0 < E_{vib}^0 < E_{bend}^0 \).
Hence, the bending energy is the highest to the contrary the hierarchy at the field-free case where the longitudinal vibrational energy is the highest (see e.g. [24]),

\[ E_{0}^{\text{rot}} < E_{0}^{\text{bend}} < E_{0}^{\text{vib}}. \]

Finite-proton-mass effects might change the binding energies. So far, it is not completely clear how such effects can be calculated quantitatively. At present, a size of their contribution might be estimated by values of the energies of the normal modes - the lowest vibrational, rotational and bending energies. Their contribution to the binding-dissociation energies grows with a magnetic field increase (see Table II) and may reach 10-20% for the magnetic fields close to the Schwinger limit (for discussions and references see [3]).

A comparison of the total energies of the \( \text{H}_3^+ \) ion for the states \( ^1\Sigma_g \) and \( ^3\Sigma_u \) (see Tables II and III) shows that at \( B \approx 0.2 \) a.u. the energy crossing between these two states occurs. It implies that for linear parallel configuration the lowest energy state for \( B \lesssim 0.2 \) a.u. is the \( ^1\Sigma_g \) state while for \( B \gtrsim 0.2 \) a.u. the state \( ^3\Sigma_u \) gets the lowest total energy becoming the ground state. Hence, one can state that in the domain \( 0.2 \lesssim B \lesssim 20 \) a.u. the state \( ^3\Sigma_u \) is the ground state (see below a description of \( \Pi \) and \( \Delta \) states). In this region of the magnetic fields the linear parallel configuration for the state \( ^3\Sigma_u \) is stable towards small deviations. It was demonstrated by calculating the corresponding curvatures and then the lowest vibrational, rotational and bending energies. It is worth noting that these energies (see Table II) turned to be small in comparison to the \( E_T = -E_I \) which implies small finite-proton-mass effects.

However, the \( ^3\Sigma_u \) state as a ground state is weakly bound - energy needed for dissociation to \( \text{H}_2^+(1\sigma_g) + \text{H}(1s) \) with electron spins antiparallel to \( \text{B} \) is very small. This weak boundness can be considered as a consequence of the fact that electrons are in the same quantum state, thus the Pauli repulsion plays an essential role leading to a large exchange energy. It is worth emphasizing that at \( B \approx 0.2 \) a.u. the total energy of the global ground state given by a triangular configuration [14] coincides approximately to the total energies of the states \( ^1\Sigma_g \) and \( ^3\Sigma_u \).
TABLE III: \( \mathrm{H}_3^+ \) ion in the state \( ^3\Sigma_g \): Total energy (in Ry) and equilibrium distance in (a.u.) (in field-free \( \mathrm{H}_3^+ \) the state \( ^3\Sigma_g \) does not exist).

| B(a.u.) | \( E_T \) | \( R_{eq} \) |
|---------|----------|-------------|
| 1       | -3.3256  | 5.139       |
| 10      | -6.9315  | 3.063       |
| 100     | -14.834  | 1.958       |
| 1000    | -29.66   | 1.35        |
| 10000   | -54.55   | 0.94        |

3. \( ^3\Sigma_g \) state \( (S = 1, \sigma_N = 1) \)

In field-free case the state \( ^3\Sigma_g \) of the \( \mathrm{H}_3^+ \) ion in linear configuration does not exist - the total energy surface does not reveal a minimum or even irregularity which would correspond to this state. However, when a magnetic field is imposed this state may appear. It happens already at \( B = 1 \) a.u. where the total energy surface \( E_T(R_+, R_-) \) of this state displays a well-pronounced minimum for linear parallel configuration. A detailed variational study of the state \( ^3\Sigma_g \) of the \( \mathrm{H}_3^+ \) molecular ion in linear parallel configuration is done for the domain \( 1 \leq B \leq 10000 \) a.u. (see Table III). The trial function \( \psi^{\text{trial}}(\Pi) \) at \( \sigma_e = -1, \sigma_N = 1 \) and \( m = 0 \) is used, it depends on eleven variational parameters.

The calculations indicate clearly the existence of a minimum in the total energy surface \( E_T(R_+, R_-) \) of \( \mathrm{H}_3^+ \) for all studied magnetic fields \( B = 1 - 10000 \) a.u. The minimum always occurs for the symmetric configuration \( R_+ = R_- \equiv R \). The results are presented in Table III. With an increase of the magnetic field strength the total energy decreases. The system becomes more bound: the double ionization energy \( E_I \) grows [26]. Also the system gradually becomes more compact - the internuclear equilibrium distance gradually decreases.

4. \( ^1\Sigma_u \) state \( (S = 0, \sigma_N = -1) \)

Similar to the state \( ^3\Sigma_g \) in the field-free case the state \( ^1\Sigma_u \) of the \( \mathrm{H}_3^+ \) ion in linear configuration does not exist. However, when a magnetic field is imposed this state can occur. Similar to the state \( ^3\Sigma_g \) it happens already at \( B = 1 \) a.u. where the total energy surface of this state displays a minimum. A detailed variational study of the state \( ^1\Sigma_u \) of the \( \mathrm{H}_3^+ \) molecular ion in linear parallel configuration is done for \( 1 \leq B \leq 10000 \) a.u. (see Table IV). The trial function \( \psi^{\text{trial}}(\Pi) \) at \( \sigma_e = 1, \sigma_N = -1 \) and \( m = 0 \) is used for it which
TABLE IV: \( \text{H}_3^+ \) ion in the state \( ^1\Sigma_u \): total \( E_T \) and double-ionization energies \( E_I \) (in Ry), and equilibrium distance (in a.u.) of \( \text{H}_3^+ \) (in field-free case this state does not exist).

| \( B \) (a.u.) | \( E_T \) | \( E_I \) | \( R_{eq} \) |
|------------|--------|--------|---------|
| 1          | -1.3256 | 3.3256 | 4.632   |
| 10         | 13.0545 | 6.9454 | 2.563   |
| 100        | 185.150 | 14.85  | 1.651   |
| 1000       | 1970.36 | 29.64  | 1.494   |
| 10000      | 19945.6 | 54.42  | 1.328   |

depends on eleven variational parameters.

The variational calculations indicate clearly the existence of a minimum in the total energy surface \( E_T(R_+, R_-) \) of \( \text{H}_3^+ \) for magnetic fields ranging \( B = 1 - 10000 \) a.u. The minimum always occurs for the symmetric configuration \( R_+ = R_- \equiv R \). In Table IV the results for the total \( E_T \) and double ionization energies \( (E_I = 2B - E_T) \) as well as the internuclear equilibrium distance \( R_{eq} \) are shown. With an increase of the magnetic field strength the total energy increases, the system becomes more bound (double ionization energy increases) and gradually more compact (the internuclear equilibrium distance globally decreases).

B. \( m = -1 \)

For the case \( m = -1 \) four subspaces are studied: \( S = 0 \) (spin singlet states) and \( S = 1 \) (spin triplet states) with \( m_s = -1 \), and parities \( \sigma_N = 1 \) and \( \sigma_N = -1 \), respectively. All these states do not exist in the field-free case.

1. \( ^3\Pi_u \) state \((S = 1, \sigma_N = 1)\)

The spin-triplet state \( ^3\Pi_u \) of the \( \text{H}_3^+ \) molecular ion in linear configuration does not exist for field-free case. However, when a magnetic field is imposed a minimum on the total energy surface \( E_T(R_+, R_-) \) can occur. This state is studied in the domain of magnetic fields \( 10^9 \leq B \leq 4.414 \times 10^{13} \) G using the variational trial function \( \psi_{\text{trial}}^{(4)} \) with \( \sigma_e = -1 \), \( \sigma_N = 1 \) and \( m = -1 \). It depends on eleven variational parameters.

The variational calculations indicate clearly the existence of a minimum in the total energy surface \( E_T(R_+, R_-) \) of \( \text{H}_3^+ \) for magnetic fields ranging \( B = 1 - 4.414 \times 10^{13} \) G. The
TABLE V: $H_3^+$ ion for the state $^3\Pi_u$: total energy $E_T$ (in Ry), equilibrium distance $R_{eq}$ (in a.u.) and the energy of the lowest longitudinal vibrational state $E_{0\text{vib}}^{\text{ub}}$. $^a$ Our re-calculations using the trial function from [13] (see text). The total energy $E_T(H_2(3\Pi_u))$ is from [18] for $B = 1, 10, 100$ a.u., while for $B = 20, 1000, 10000$ a.u. and $4.414 \times 10^{13}$ G the total energy is calculated using the present technique (it will be described elsewhere). Data for $H_2^+(1\pi_u)$ and H(1s) from [3] and [26].

| B(a.u.) | $E_T$    | $R_{eq}$ | $E_{0\text{vib}}^{\text{ub}}$ | $E_T(H_2(3\Pi_u))$ | $E_T(H_2^+(1\pi_u) + H(1s))$ | $E_T(H_2^+(1\sigma_g) + H(2p_{-1}))$ |
|--------|----------|----------|-------------------------------|---------------------|--------------------------------|-----------------------------------|
| 1      | -3.036   | 1.896    | -2.9686                       | -2.6825             | -2.8631                        |                                   |
|        | -2.953 $^a$ |         |                               |                     |                                |                                   |
|        | -2.817 $^b$ | 2.049    |                               |                     |                                |                                   |
| 5      | -5.654   | 1.163    |                              |                     |                                |                                   |
|        | -5.802 $^a$ |         |                               |                     |                                |                                   |
|        | -5.463 $^b$ | 1.176    |                               |                     |                                |                                   |
| 10     | -7.647   | 0.898    | -6.9325                       | -6.1980             | -6.5995                        |                                   |
|        | -7.803 $^a$ |         |                               |                     |                                |                                   |
|        | -7.307 $^b$ | 0.910    |                               |                     |                                |                                   |
| 20     | -9.944   | 0.706    | 0.135                         | -8.934              | -8.036                         | -8.582                           |
|        | -10.475 $^a$ |         |                               |                     |                                |                                   |
|        | -9.752 $^b$ | 0.7 $^b$ |                               |                     |                                |                                   |
| 100    | -18.915  | 0.395    | 0.343                         | -16.473             | -14.452                        | -15.547                          |
| 1000   | -44.538  | 0.183    | 1.105                         | -35.444             | -31.353                        | -33.976                          |
| 10000  | -95.214  | 0.093    | 3.147                         | -71.39              | -62.023                        | -67.356                          |
| 4.414 $\times 10^{13}$ G | -115.19  | 0.078    | -84.96                        | -73.59              | -79.86                         |                                   |

minimum always corresponds to a linear parallel configuration at $R_+ = R_- \equiv R$. It was investigated its stability towards small deviation from equilibrium in linear parallel configuration. For this state we are not aware how to check quantitatively a stability towards deviations from linear parallel configuration. However, physical arguments based on perturbation theory estimates indicate to the stability. Table V contains the results for the total $E_T$ and the internuclear equilibrium distance $R_{eq}$. With an increase of the magnetic field strength the total energy decrease, the system becomes more bound (double ionization energy increases [26]) and more compact (the internuclear equilibrium distance decreases).

The total energy of the final states for the dissociation channels $H_3^+ \rightarrow H_2^+(1\pi_u) + H(1s)$, $H_3^+ \rightarrow H_2^+(1\sigma_g) + H(2p_{-1})$ and $H_3^+ \rightarrow H_2(3\Pi_u) + p$ with electron spins antiparallel to the magnetic field direction for different magnetic fields is shown in Table V. For all studied magnetic fields the total energy of both dissociation channels to $H_2^+(1\pi_u) + H(1s), H_2^+(1\sigma_g) + H(2p_{-1})$ and $H_2(3\Pi_u)$ are always higher than the total energy of the $H_3^+$ ion in the $^3\Pi_u$
state. Thus, the ion \( H_3^+(3\Pi_u) \) is stable towards these decays for all studied magnetic fields. Dominant dissociation channel is \( H_3^+ \rightarrow H_2(3\Pi_u) + p \). For all three channels the dissociation energy grows monotonously as a magnetic field increases. For the dominant channel \( H_3^+ \rightarrow H_2(3\Pi_u) + p \) it reaches 30.3 Ry at the Schwinger limit \( 4.414 \times 10^{13} \) G, while for the channel \( H_3^+ \rightarrow H_2^+(1\pi_u) + H(1s) \) for this magnetic field it is required \( \approx 35 \) Ry to dissociate. For magnetic fields \( 5 \times 10^{10} \lesssim B \lesssim 4.414 \times 10^{13} \) G there exists at least one longitudinal vibrational state (see Table V).

We made an analysis of the total energies for all spin-triplet states. One can see that there is a crossing between the \( 3\Pi_u \) and the \( 3\Sigma_u \) states which occurs at \( B \approx 20 \) a.u. It shows that the ground state of \( H_3^+ \) for \( B \gtrsim 20 \) a.u. is given by the \( 3\Pi_u \) state (see below a study of \( \Delta \) states which are characterized by the higher total energies). While the \( 3\Sigma_u \) state is the ground state for \( 0.2 \lesssim B \lesssim 20 \) a.u. In Figs. 2 and 3 the evolution of the total energy and the equilibrium distance, respectively, of the ground state with the magnetic field strength are plotted. The ground state evolves from spin-singlet \( 1\Sigma_g \) for small magnetic fields \( B \lesssim 0.2 \) a.u. (not shown in Figs. 2, 3) to spin-triplet \( 3\Sigma_u \) for intermediate fields and to spin-triplet \( 3\Pi_u \) state for \( B \gtrsim 20 \) a.u. The total energy decreases monotonously and smoothly as magnetic field growth. The equilibrium distance decreases as well, but having a discontinuous behavior at \( B \approx 20 \) a.u. - in the transition from \( 3\Sigma_u \) to \( 3\Pi_u \) states. Similar behavior is displayed by \( < |z_1| > \): it reduces monotonously from \( \approx 1.9 \) a.u. at \( B = 0.2 \) a.u. to \( \approx 0.1 \) a.u. at \( B = 10000 \) a.u. with a small discontinuity at \( B \approx 20 \) a.u. Perhaps, it is worth noting that the average distance between two electrons \( < r_{12} > \) is also reduced as a magnetic field grows in about 20 times between 0.2 a.u. and 10000 a.u. At large magnetic fields the transverse size of the electronic cloud coincides approximately with the Larmor radius. In Fig. 4 the energy of the lowest longitudinal vibrational state of the ground state for \( 5 \times 10^8 \lesssim B \lesssim 4.414 \times 10^{13} \) G is presented. It grows monotonously as a magnetic field increases suffering a discontinuity at \( B \approx 20 \) a.u. - in the transition from \( 3\Sigma_u \) to \( 3\Pi_u \) states. In Figs. 5a,b the valleys and the total energy behavior (profile) along the valley for \( B = 100 \) a.u. for \( 3\Pi_u \) state, respectively, are shown. Similar behavior takes place for the valleys and the total energy profile for \( 3\Pi_u \) state for other magnetic fields in the domain \( 5 \times 10^{10} \lesssim B \lesssim 4.414 \times 10^{13} \) G.
2. $^{1}\Pi_u$ state ($S = 0$, $\sigma_N = 1$)

A detailed study of the state $^{1}\Pi_u$ of the H$_3^+$ molecular ion in symmetric configuration $R_+ = R_- \equiv R$ is carried out in the domain of magnetic fields $1 \leq B \leq 10000$ a.u. (see Table V). The variational trial function $\psi^{trial}$ with $\sigma_e = 1$, $\sigma_N = 1$ and $m = -1$ is used for
FIG. 4: Energy of the lowest longitudinal vibrational state $E_{0}^{\text{vib}}$ for the ground state: $^3\Sigma_u$ (stars) and $^3\Pi_u$ (bullets).

this state, it depends on ten variational parameters.

The obtained results indicate clearly the existence of a minimum in the total energy $E_T(R)$ of $\text{H}_3^+$ for all magnetic fields ranging $B = 1 - 10000$ a.u. Table VI shows the total $E_T$ and double ionization energies ($E_I = 2B - E_T$), as well as the internuclear equilibrium distance $R_{eq}$ for the $^1\Pi_u$ state. It is found that with an increase of the magnetic field strength the total energy increases, the system becomes more bound (double ionization energies increase) and more compact (the internuclear equilibrium distance decreases).

3. $^1\Pi_g$ state ($S = 0$, $\sigma_N = -1$)

It is carried out a detailed study for the state $^1\Pi_g$ of the $\text{H}_3^+$ molecular ion in symmetric configuration $R_+ = R_- \equiv R$ in the domain of magnetic fields $1$ a.u. $\leq B \leq 10000$ a.u. (see Table VII). For this state our variational trial function $\psi_{\text{trial}}$ with $\sigma_e = 1$, $\sigma_N = -1$ and $m = -1$ depends on ten variational parameters. The total $E_T$ and double ionization $E_I = 2B - E_T$ energies increase while the internuclear equilibrium distance $R_{eq}$ decreases as a magnetic field grows; the system becomes more bound (double ionization energies increase) and more compact (the internuclear equilibrium distance decreases).
A detailed study is carried out for the state $^3\Pi_g$ of the H$_3^+$ molecular ion in symmetric configuration $R_+ = R_\equiv R$ in the domain of magnetic fields $1 \text{ a.u.} \leq B \leq 10000 \text{ a.u.}$ (see Table VIII). For this state our variational trial function $\psi^{\text{trial}}$ (4) with $\sigma_e = -1$, $\sigma_N = -1$ and $m = -1$ depends on ten variational parameters. The total $E_T$ energy decreases and the double ionization $E_I$ energy [26] increases while the internuclear equilibrium distance

FIG. 5: Valleys of the total energy (a) and the profile (b) for $B = 100 \text{ a.u.}$ of the ground state $^3\Pi_u$. 

4. $^3\Pi_g$ state ($S = 1$, $\sigma_N = -1$)
TABLE VI: $\text{H}_3^+$ ion in the state $^1\Pi_u$: total $E_T$ and double-ionization $E_I$ energies (in Ry) and equilibrium distance $R_{eq}$ (in a.u.). $^a$ Ref. [13], $^b$ our re-calculations using the trial function from [13] (see text).

| B(a.u.) | $E_T$  | $E_I$  | $R_{eq}$ |
|---------|--------|--------|----------|
| 1       | -0.809 | 2.809  | 1.995    |
|         | -0.561 $^a$ |        |          |
|         | -0.511 $^b$ |        | 2.233    |
| 5       | 4.747  | 5.253  | 1.232    |
|         | 5.025  $^a$ |        |          |
|         | 5.051  $^b$ |        | 1.262    |
| 10      | 13.028 | 6.972  | 0.967    |
|         | 13.346 $^a$ |        |          |
|         | 13.346 $^b$ |        | 0.963    |
| 20      | 30.708 | 9.292  | 0.750    |
|         | 31.078 $^a$ |        |          |
|         | 31.081 $^b$ |        | 0.738    |
| 100     | 182.23 | 17.77  | 0.419    |
| 1000    | 1957.77 | 42.23  | 0.191    |
| 10000   | 19909.0 | 91.0   | 0.098    |

TABLE VII: $\text{H}_3^+$ ion in the state $^1\Pi_g$: total energy $E_T$ in Ry and equilibrium distance $R_{eq}$ in a.u.

| B(a.u.) | $E_T$  | $E_I$  | $R_{eq}$ |
|---------|--------|--------|----------|
| 1       | -0.701 | 2.701  | 3.176    |
| 10      | 13.669 | 6.331  | 1.441    |
| 100     | 185.413 | 14.587 | 0.741    |
| 1000    | 1969.42 | 30.58  | 0.421    |
| 10000   | 19942.1 | 57.9   | 0.273    |

$R_{eq}$ decreases as a magnetic field grows; the system becomes more bound (double ionization energy increases) and more compact (the internuclear equilibrium distance decreases).

TABLE VIII: $\text{H}_3^+$ ion in the state $^3\Pi_g$: total energy $E_T$ in Ry and equilibrium distance $R_{eq}$ in a.u.

| B(a.u.) | $E_T$  | $R_{eq}$ |
|---------|--------|----------|
| 1       | -2.6095 | 2.700    |
| 10      | -6.276  | 1.487    |
| 100     | -14.429 | 0.838    |
| 1000    | -30.44  | 0.447    |
| 10000   | -57.8   | 0.27     |
C. \( m = -2 \)

In the \( m = -2 \) subspace we study four subspaces: \( S = 0 \) (spin singlet states), \( S = 1 \) (spin triplet states with \( m_s = -1 \)), \( \sigma_N = 1 \) and \( \sigma_N = -1 \) and the lowest energy state in each of them. All these states do not exist in the field-free case.

It is carried out a detailed study for the states of the symmetric configuration \( R_+ = R_- \equiv R \) in the domain of magnetic fields \( 1 \leq B \leq 10000 \) a.u. For each of these four states \( ^1\Delta_g, ^3\Delta_g, ^1\Delta_u, ^3\Delta_u \) the trial function \( \psi_{trial} \) at \( m = -2 \) depends on ten variational parameters. All four states indicate clearly the existence of a minimum in the total energy \( E_T(R) \) of \( \text{H}_3^+ \) for magnetic fields ranging \( B = 1 - 10000 \) a.u. Tables IX - XII show the results. For these states with an increase of the magnetic field strength the total energy increases for the spin-singlet states and decreases for spin-triplet states, the system becomes more bound (double ionization energy increases) and more compact (the internuclear equilibrium distance decreases).

**TABLE IX:** The \( \text{H}_3^+ \) ion for the state \( ^1\Delta_g \): total energy \( E_T \) and double-ionization energy \( E_I \) in Ry and equilibrium distance \( R_{eq} \) in a.u.

| \( B \) (a.u.) | \( E_T \) (Ry) | \( E_I \) (Ry) | \( R_{eq} \) (a.u.) |
|----------------|----------------|----------------|------------------|
| 1              | -0.6136        | 2.6136         | 2.206            |
| 10             | 13.499         | 6.501          | 1.027            |
| 100            | 183.325        | 16.675         | 0.433            |
| 1000           | 1960.19        | 39.81          | 0.191            |
| 10000          | 19913.6        | 86.4           | 0.10             |

**TABLE X:** The \( \text{H}_3^+ \) ion in the state \( ^3\Delta_g \): total energy \( E_T \) in Ry and equilibrium distance \( R_{eq} \) in a.u.

| \( B \) (a.u.) | \( E_T \) (Ry) | \( R_{eq} \) (a.u.) |
|----------------|----------------|-------------------|
| 1              | -2.633         | 2.179             |
| 10             | -6.624         | 1.013             |
| 100            | -16.92         | 0.432             |
| 1000           | -40.38         | 0.197             |
| 10000          | -87.49         | 0.099             |
| \( 4.414 \times 10^{13} \) G | -106.02    | 0.09              |

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TABLE XI: The H$_3^+$ ion in the state $^1\Delta_u$: total energy $E_T$ in Ry and equilibrium distance $R_{eq}$ in a.u.

| B(a.u.) | $E_T$ | $E_I$ | $R_{eq}$ |
|--------|-------|-------|---------|
| 1      | -0.4107 | 2.4107 | 3.316   |
| 10     | 14.281  | 5.719  | 1.514   |
| 100    | 186.602 | 13.398 | 0.775   |
| 1000   | 1972.08 | 27.92  | 0.401   |
| 10000  | 19945.7 | 54.3   | 0.273   |

TABLE XII: The H$_3^+$ ion in the state $^3\Delta_u$: total energy $E_T$ in Ry and equilibrium distance $R_{eq}$ in a.u.

| B(a.u.) | $E_T$ | $R_{eq}$ |
|--------|-------|---------|
| 1      | -2.443 | 4.494   |
| 10     | -5.722 | 1.600   |
| 100    | -13.39 | 0.804   |
| 1000   | -28.41 | 0.449   |
| 10000  | -54.4  | 0.28    |

IV. CONCLUSION

We study the low-lying energy states of H$_3^+$ molecular ion in linear configuration parallel to a magnetic field from 0 up to $4.414 \times 10^{13}$ G using the variational method in the Born-Oppenheimer approximation. The total energy curves display a well pronounced minimum at finite internuclear distances at $R_+ = R_-$ for the lowest states with magnetic quantum numbers $m = 0, -1, -2$, total spins $S = 0, 1$ ($m_s = -1$) and parity $p = \pm 1$. A level distribution for several magnetic field strengths is shown on Fig. 6. If in field-free case there exist only two eigenstates in a linear configuration, but many more states in linear parallel configuration can appear when a magnetic field is imposed.

In general, for all studied states, as the magnetic field increases the equilibrium internuclear distances $R_{eq}$ decreases and the system becomes more compact, while the total energies of spin-singlet states increase whereas that of spin-triplet states decrease.

The state of the lowest total energy in linear parallel configuration depends on the magnetic field strength. It evolves from spin-singlet (unstable towards a deviation from linearity) $^1\Sigma_g$ for weak magnetic fields $B \lesssim 0.2$ a.u. to spin-triplet (stable towards a deviation from linearity) $^3\Sigma_u$ for intermediate fields and eventually to spin-triplet $^3\Pi_u$ state for $B \gtrsim 20$ a.u. which remains the ground state until the Schwinger limit $B = 4.414 \times 10^{13}$ G. It is worth
emphasizing that for weak magnetic fields, $B \lesssim 0.2 \text{ a.u.}$, the global ground state is given by a triangular configuration \[14\] and then, for larger magnetic fields, the global stable ground state corresponds to a linear parallel configuration \[33\]. The $H_3^+$ ion in the $3\Sigma_u$ state is weakly bound. For all studied magnetic fields the total energy surface well corresponding to the ground state contains at least one longitudinal vibrational state.

It is interesting to compare the evolution of the ground state for $H_3^+$ with magnetic field change with that of other two-electron systems (see \[27\] and references therein). For atomic type $H^-$ and $He$ systems there is no domain of magnetic field where the spin-triplet, $m = 0$ state is the ground state: for weak fields the ground state is the spin-singlet, $m = 0$ state and then it becomes the spin-triplet, $m = -1$ state for large fields. For the hydrogen molecule the $3\Sigma_u$ state is unbound for all magnetic fields unlike the case of $H_3^+$. It implies that the $H_2$ molecule does not exist as a bound system for $0.18 \lesssim B \lesssim 15.6 \text{ a.u.}$, where the unbound state $3\Sigma_u$ has the lowest total energy at infinitely-large distance between protons. A similar situation occurs for the $He_2^{2+}$-ion: it does not exist as a bound system for $0.85 \lesssim B \lesssim 1100 \text{ a.u.} \[28\].

What is the lowest-lying excited state for weak magnetic fields $B \lesssim 0.2 \text{ a.u.}$ is not clear yet. This question, and also the whole domain $B \lesssim 0.2 \text{ a.u.}$, will be studied elsewhere. In the domain of magnetic fields $0.2 \leq B \leq 5 \text{ a.u.}$ the lowest-lying excited state is $3\Sigma_g$, then for $B \gtrsim 5 \text{ a.u.}$ the lowest-lying excited state is $3\Pi_u$. For $B \gtrsim 20 \text{ a.u.}$, where the $3\Pi_u$ state becomes the ground state, the lowest-lying excited state is $3\Sigma_u$. However, at $B \gtrsim 1000 \text{ a.u.}$ until the Schwinger limit the lowest-lying excited state is $3\Delta_g$.

It is interesting to note that at $B = 1000 \text{ a.u.}$ the $H_3^+$ ion exists with $3\Pi_u$ as the ground state ($E_T = -44.54 \text{ a.u.}$) with two possible excited states: $3\Delta_g$ ($E_T = -40.38 \text{ a.u.}$) and $3\Sigma_u$ ($E_T = -35.99 \text{ a.u.}$) with energies below the threshold of dissociation to $H_2(3\Pi_u) + p$ ($E_T = -35.44 \text{ a.u.}$). For larger magnetic fields the situation becomes different. For instance, at $B = 10000 \text{ a.u.}$ for the $H_3^+$ ion ($E_T = -95.21 \text{ a.u.}$) only one excited state, $3\Delta_g$ ($E_T = -87.45 \text{ a.u.}$), exists with energy below the dissociation threshold to $H_2(3\Pi_u) + p$ ($E_T = -71.39 \text{ a.u.}$). Similar situation holds up to the Schwinger limit $B = 4.414 \times 10^{13} \text{ G}$: a single excited state $3\Delta_g$ lies below the dissociation threshold.

It is found that many states in linear configuration which do not exist for $B = 0$ begin to be bound at relatively small magnetic field $B \approx 0.2 \text{ a.u.}$ A study of the existence of the bound states which might appear in a spacial configuration is our goal for a future study.
Another goal is related to a study of transition amplitudes for different electronic states.

Present consideration is based on the use of a simple variational trial function (1). This function can be easily generalized and extended in the same way as was done in a variational study of various one-electron systems in a strong magnetic field (see [3]). This will allow to improve the present results and might be done in future. However, we are not sure that such a study is crucially important. It is related to a fact that typical accuracies in astronomical observations of neutron star radiation would not be higher $\sim 10^{-3} - 10^{-4}$ unlike to spectroscopical accuracies in laboratory where they can be by several orders of magnitude higher.

**Acknowledgments**

The first author is grateful to A. Alijah, T. Oka and J. Tennyson for introduction to the subject of the $\mathrm{H}_3^+$ ion, helpful discussions and interest to the present work. We thank D. Page for careful reading of the manuscript. Computations were performed on a dual DELL PC with two Xeon processors of 2.8 GHz each (ICN), 54-node FENOMEC and 32-node TOCHTLI clusters (UNAM) and a dual DELL PC with two Xeon processors of 3.06 GHz each (CINVESTAV). This work was supported in part by CONACyT grant \texttt{47899-E} and PAPIIT grant \texttt{IN121106} (Mexico).

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[29] The Hamiltonian is normalized by multiplying on the factor 2 in order to get the energies in Rydbergs

[30] If the same simple 7-parametric function (4) is used for the equilateral triangular configuration it gives $E_T = -2.676 \text{Ry}$ and $a_{eq} = 1.64 \text{a.u.}$ [14] which is in quite good agreement with the results from [16]

[31] Each degeneration is made in such a way that six different $\alpha$’s in (4) are divided into three pairs and then inside of each pair the $\alpha$’s are kept equal. Hence, instead of six varying parameters $\alpha$’s in (4) we get a degeneration where only three $\alpha$’s are varied.

[32] For spin-triplet states, $m_s = -1$ the double ionization energy is equal to $E_I = -E_T$

[33] In order to make such a claim that the state of the lowest energy corresponds by a linear parallel configuration we make a very natural physically assumption that there are no any other spacial configuration which may provide a lower total energy. But in order to be rigorous we must investigate the total energy surface for all possible spacial configurations.
FIG. 6: Total energy of the low-lying levels for $B = 0, 1, 10, 100$ and 1000 a.u. (energy scale is kept the same for all presented magnetic fields but the reference points depend on them)