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H_3^+ molecular ion in a magnetic field: Linear parallel configuration

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A detailed study of the ground state of the H_3^+ molecular ion in linear configuration, parallel to the magnetic field direction, and its low-lying Σ, Π, and Δ states is carried out for magnetic fields $B=0-4.414\times10^{13}$ 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 γ 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 $B\lesssim5\times10^8$ 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 $5\times10^{10}\lesssim B\lesssim4.414\times10^{13}$ 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 significant attention during the last two decades (see, in particular, the review papers in [1–3]). It has been motivated by both pure theoretical interest and possible practical applications in astrophysics and solid-state physics. In particular, knowledge of the energy levels can be important for interpretation of the spectra of white dwarfs (where the surface magnetic field is in the range $B\approx10^6-10^9$ G) and neutron stars where a surface magnetic field varies in the range $B\approx10^{12}-10^{13}$ G, and even can be $B\approx10^{14}-10^{16}$ G for the case of magnetars.

Recently, it was announced that in a sufficiently strong magnetic field $B\gtrsim10^{11}$ G the exotic molecular ion H_3^{2+} can exist in linear configuration with protons situated along the magnetic line [4] (for a discussion see the review in [3]). In general, it is a metastable long-living system which decays to $H_2^+ + p$. However, at $B\gtrsim10^{13}$ G the ion H_3^{2+} becomes stable. This system does not exist without or for weak magnetic fields. The ion H_3^{2+} constitutes the simplest one-electron polyatomic molecular ion in a strong magnetic field. The H_3^{2+} 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 $B\geqslant10^9$ G can be found in [3].

The molecular ion H_3^+ is the simplest stable two-electron polyatomic molecular ion. It has a long history since its discovery by Thomson [6]. Its exceptional importance in astrophysics related to interstellar media explains the great interest in this ion by the 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 (semiquantitative) work by Coulson [8].

The first variational calculations [9] of the total energy of the molecular ion 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 H_3^+ ion may occur in excited state(s). Since that time, a large number of excited states have 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 triangular (spatial) configurations so far.

Although the molecular ion H_3^+ is characterized by the equilateral triangular configuration as being optimal in the field-free case, it is expected that in a magnetic field $B\approx0.2$ 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 $10^8\lesssim B\lesssim10^{11}$ G and becomes linear parallel at $B\approx10^{11}$ G. It is worth noting that for H_3^+ in the field-free case the difference between the total energy of the ground state (triangular configuration) and of the lowest linear configuration is very small, ≈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, and VI)—in fact, no single number from [13] was confirmed. However, in [13] a qualitative statement was made that with a magnetic field increase a transition from an equilateral stable equilibrium configuration to a linear equilibrium configuration may occur. This statement we confirm. We predict that this transition takes place at a magnetic field ≈0.2 a.u. A detailed study of the 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

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B is given in a.u. with a conversion factor $B_0=2.35\times10^9$ 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[1]

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

(see Fig. 1 for the geometrical setting and notations), where $\hat{\mathbf{p}}_\ell=-i\boldsymbol{\nabla}_\ell$ is the 3-vector of the momentum of the ℓth electron, the index κ runs over protons A, B, and C, r_{12} is the interelectron distance, and $\mathbf{S}=\hat{\mathbf{s}}_1+\hat{\mathbf{s}}_2$ 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,

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

Finally, the Hamiltonian can be written as

$$\mathcal{H} = \sum_{\ell=1}^{2}\left(-\nabla_\ell^2 + \frac{B^2}{4}\rho_\ell^2\right) - \sum_{\substack{\ell=1,2\\ \kappa=A,B,C}} \frac{2}{r_{\ell\kappa}} + \frac{2}{r_{12}} + \frac{2}{R_+} + \frac{2}{R_-} + \frac{2}{R_+ + R_-} + B(\hat{L}_z + 2\hat{S}_z), \tag{3}$$

where $\hat{L}_z=\hat{l}_{z_1}+\hat{l}_{z_2}$ and $\hat{S}_z=\hat{s}_{z_1}+\hat{s}_{z_2}$ 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 $p=\pm1$ (gerade and ungerade), and (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 the values 0, ±1.

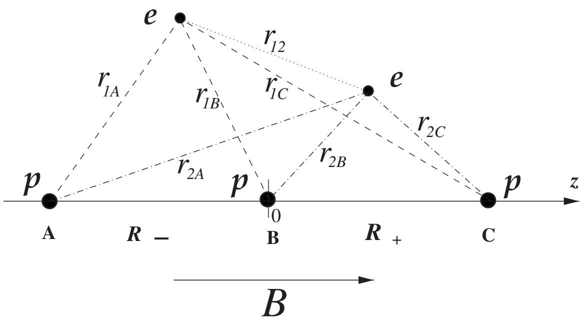

FIG. 1. Geometrical setting for the H_3^+ ion in linear configuration parallel to a magnetic field directed along z axis. The protons (marked by bullets) are situated on the z line at distances $R_\pm$ from the central proton, which is placed at the origin.

As a magnetic field increases the 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 characterized by definite values of m, p, and m_s. It is worth noting that the Hamiltonian $\mathcal{H}$ is invariant with respect to the 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 $\sigma_N=\pm1$ for positive and 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 as to the value of m_s. Eventually, the notation is ${}^{2S+1}M_p$, where $2S+1$ is the spin multiplicity which is equal to 1 for the spin-singlet state ($S=0$) and 3 for the spin-triplet state ($S=1$). As for the label M we use the Greek letters Σ, Π, and Δ, which mark the states with $|m|=0,1,2,\ldots$, respectively, and the subscript p (the spatial parity quantum number) takes gerade and ungerade (g and 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:

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

The 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 one with $m\leqslant0$.

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

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[1] The Hamiltonian is normalized by multiplying by a factor of 2 in order to get the energies in rydbergs.

$$\psi^{(trial)} = (1+\sigma_e P_{12})(1+\sigma_N P_{AC})(1+\sigma_{N_a} P_{AB}+\sigma_{N_a} P_{BC})\rho_1^{|m|} e^{im\phi_1} e^{\gamma r_{12}} e^{-\alpha_1 r_{1A}-\alpha_2 r_{1B}-\alpha_3 r_{1C}-\alpha_4 r_{2A}-\alpha_5 r_{2B}-\alpha_6 r_{2C}-B\beta_1\rho_1^2/4-B\beta_2\rho_2^2/4}, \quad (4)$$

where $\sigma_e = \pm 1$ stands for spin singlet (+) and triplet (−) states, while $\sigma_N = 1$ and -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), $\sigma_N = \sigma_{N_a} = \pm 1$. α_{1-6}, β_{1-2}, and γ as well as R_+, R_- are variational parameters. Their total number is 11. 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 the complicated profile of the total energy surface in the parameter space but when a minimum was found it took a few minutes to compute the variational energy.

III. RESULTS

We carry out a detailed study of Σ, Π, and Δ low-lying states with a particular emphasis on 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 the 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 an equilateral triangle) with total energy $E_T = -2.6877$ Ry and the side of triangle $a_{eq} = 1.65$ a.u. (see [16] and also [17]).[2] The situation is not so different when the 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 a well-pronounced minimum but stability towards a deviation from linearity does not occur and a global bound state ${}^1\Sigma_g$ does not exist. However, with magnetic field growth, at $B \gtrsim 0.2$ a.u. the system ($pppee$) becomes stable towards small deviations from a 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 on 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 $0 \leqslant B \leqslant 10\,000$ a.u. (see Table I). Finally, for the linear parallel configuration the variational trial function ψ^{trial}, Eq. (4), with $\sigma_e = 1$, $\sigma_N = 1$, and $m = 0$ was used. It depends on 11 variational parameters. A simple, obvious generalization of Eq. (4) is used to study slightly deviated configurations when stability of the linear system was checked.

The variational calculations demonstrate in a 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 in the range $B = 0-10\,000$ a.u. The 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 the linear configuration is supported externally.

Table I displays the results for the total, E_T, and 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 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 magnetic field. There are three dominant dissociation channels: (i) $H_3^+ \to H_2 + p$, (ii) $H_3^+ \to H_2^+ + H$, and (iii) $H_3^+ \to H^- + p + p$ (see Table I) as well as two subdominant channels $H_3^+ \to H_2^+ + p + e$ (ionization) and $H_3^+ \to H + H + p$ (dissociation). The last two channels are characterized by

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

TABLE I. 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 and equilibrium distance R_{eq} (in a.u.) as well as the total energies of the final states of the dissociation and ionization channels of H_3^+ are shown; all energies are in Ry. Total energies for the H_2 molecule in $^1\Sigma_g$ state, as well as H_2^+ and H_3^{2+} ions in the $1\sigma_g$ state, in a magnetic field taken from [18–20], 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}	$E_T(H_2)$	$E_T(H_2^+ + H)$	$E_T(H_3^{2+} + e)$	$E_T(H^-)$
0[a]	−2.5519		1.540				−1.0555
	−2.55[b]						
0.2[a]	−2.5229		1.513				
1	−2.0692	4.0692	1.361	−1.7807	−1.6122		−0.00358
	−1.7993[c]						
	−1.7195[d]		1.402				
5	2.9597	7.0403	0.918	3.6024			
	3.2893[c]						
	3.2888[d]		0.929				
10	10.8168	9.1832	0.746	11.778	12.1554	16.6084	15.7613
	11.154[c]						
	11.153[d]		0.736				
20	27.966	12.034	0.587		30.082		
	28.317[c]						
	28.316[d]		0.576				
100	177.59	22.410	0.336	181.014	182.145	191.361	190.872
1000	1948.41	51.586	0.160		1961.99	1979.22	1981.569
10000	19891.6	108.45	0.083		19926.25	19954.60	

[a] The energy and equilibrium distance of H_3^+ for these magnetic fields is for the case when a linear configuration is kept externally (see text).

[b] These data can be extracted from [7], p. 427.

[c] Reference [13].

[d] Our recalculations based on the trial function from [13] (see text).

higher ionization-dissociation energies than the channel $H_3^+ \to H_2^+ + H$, and thus they are not considered. There are two single-ionization processes $H_3^+ \to H_2^+ + p + e$ and $H_3^+ \to H_3^{2+} + e$ (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 $B > 10\,000$ 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 $H_3^+ \to H_3^{2+} + e$ dominates over $H_3^+ \to H^- + p + p$.

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 the 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. The smallest dissociation energy corresponds to the channel $H_3^+ \to H_2 + p$, which then is followed by $H_3^+ \to H_2^+ + H$. It is worth noting that the largest dissociation energy corresponds to the channel $H_3^+ \to H^- + p + p$. In general, the dissociation energy (the difference between the energies of the final and initial states) increases monotonously with 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 $B = 0.2$ 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 H_3^{2+} ion [20] and it is equal to 0.035 Ry.

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

In the field-free case the state $^3\Sigma_u$ of the system ($pppee$) is (i) the only state of the H_3^+ ion in linear configuration which is known so far and also (ii) it is the only known spin-triplet state of 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

TABLE II. H_3^+ ion in the state $^3\Sigma_u$: total energy (in Ry), equilibrium distance (in a.u.) and energy of the lowest longitudinal vibrational state E_0^{vib}, rotational E_0^{rot}, and bending E_0^{bend}. The total energy of $H_2^+(1\sigma_g)$ $+H(1s)$ (in Ry) in the ground state with spin of each electron antiparallel to B from [19] and [21], respectively, is shown for comparison.

B (a.u.)	E_T	R_{eq}	E_0^{vib}	E_0^{rot}	E_0^{bend}	$E_T[H_2^+(1\sigma_g)+H(1s)]$
0	−2.2297[a]	2.457[a]				−2.2052
	−2.2322[b]	2.454[b]				
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 [25,24].

linearity. The state $^3\Sigma_u$ is stable with respect to the decay $H_3^+ \to H_2^+ + H$ (see [25]). Also there is no decay channel $H_3^+(^3\Sigma_u) \to H_2(^1\Sigma_g)+p$.

A detailed variational study of the $^3\Sigma_u$ state of the H_3^+ molecular ion is done for $0 \leqslant B \leqslant 10\,000$ a.u. (see Table II). It turns out that for all magnetic fields studied the total energy surface displays a minimum which corresponds to a linear parallel configuration. Furthermore, this minimum always appears in the symmetric configuration $R_+ = R_- \equiv R$. For this particular configuration the variational trial function ψ^{trial}, Eq. (4), with $\sigma_e=-1$, $\sigma_N=-1$, and $m=0$ is used which depends on ten variational parameters. The field-free case is studied separately with a 23-parametric trial function which is a linear superposition of Eq. (4) and its three different degenerations.[3] This sufficiently simple function allows us to reproduce three significant digits in the 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 and the system becomes more bound—the double-ionization energy increases[4] and becomes more compact (the internuclear equilibrium distance decreases). A major emphasis of our study of the state $^3\Sigma_u$ is the domain $0.2 \lesssim B \lesssim 20$ a.u. where this state becomes the ground state of the H_3^+ ion in parallel configuration and likely the global ground state of the ion.

As for the dissociation channel $H_3^+(^3\Sigma_u) \to H_2^+(1\sigma_g)$ $+H(1s)$ (with electrons in the spin-triplet state) the total energy of the final state is slightly higher than $E_T(H_3^+)$ for magnetic fields $0.2 \lesssim B \lesssim 20$ a.u.; the energy difference varies from 0.03 Ry to 0.06 Ry depending on the magnetic field strength (see Table II), remaining very small. Hence, although $H_3^+(^3\Sigma_u)$ 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 $H_2(^3\Sigma_u)+p$ due to a probable nonexistence of the 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 corresponding well to the $^3\Sigma_u$ state contains at least one longitudinal vibrational state (see Table II). Its energy grows with a magnetic field increase. The lowest rotational energy is calculated as well as the lowest bending energies using the same formulas as for H_3^{2+} [20]. All these energies grow with a magnetic field increase. The interesting observation is that for each magnetic field in the domain $1 < B \lesssim 20$ a.u. the following hierarchy of these energies holds:

$$E_0^{vib} < E_0^{rot} < E_0^{bend},$$

contrary to the hierarchy at $0.2 \lesssim B \lesssim 1$ a.u.,

$$E_0^{rot} < E_0^{vib} < E_0^{bend}.$$

Hence, in the above domain of magnetic fields the bending energy is the highest to the contrary the hierarchy in the field-free case where the longitudinal vibrational energy is the highest (see, e.g., [24]),

$$E_0^{rot} < E_0^{bend} < E_0^{vib}.$$

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, the 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)

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

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

TABLE III. $H_3{}^+$ ion in the state $^3\Sigma_g$: total energy in Ry and equilibrium distance in a.u. (in field-free case 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

TABLE IV. $H_3{}^+$ 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 $H_3{}^+$ (in the 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

and may reach 10%–20% for magnetic fields close to the Schwinger limit (for discussions and references see [3]).

A comparison of the total energies of the $H_3{}^+$ ion for the states $^1\Sigma_g$ and $^3\Sigma_u$ (see Tables I and II) 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 the Π and Δ 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 out to be small in comparison to $E_T=-E_I$ which implies small finite-proton-mass effects.

However, the $^3\Sigma_u$ state as a ground state is weakly bound—the energy needed for dissociation to $H_2{}^+(1\sigma_g)+H(1s)$ with electron spins antiparallel to $\mathbf{B}$ 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 $B \sim 0.2$ 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 $^3\Sigma_u$.

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

In the field-free case the state $^3\Sigma_g$ of the $H_3{}^+$ 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 a linear parallel configuration. A detailed variational study of the state $^3\Sigma_g$ of the $H_3{}^+$ molecular ion in linear parallel configuration is done for the domain $1 \leqslant B \leqslant 10\,000$ a.u. (see Table III). The trial function ψ^{trial}, Eq. (4), at $\sigma_e=-1$, $\sigma_N=1$, and $m=0$ is used; it depends on 11 variational parameters.

The calculations indicate clearly the existence of a minimum in the total energy surface $E_T(R_+,R_-)$ of $H_3{}^+$ for all magnetic fields studied $B=1-10\,000$ 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. 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 $H_3{}^+$ 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 $H_3{}^+$ molecular ion in linear parallel configuration is done for $1 \leqslant B \leqslant 10\,000$ a.u. (see Table IV). The trial function ψ^{trial}, Eq. (4), at $\sigma_e=1$, $\sigma_N=-1$, and $m=0$ is used for it which depends on 11 variational parameters.

The variational calculations indicate clearly the existence of a minimum in the total energy surface $E_T(R_+,R_-)$ of $H_3{}^+$ for magnetic fields in the range $B=1-10\,000$ 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 (the 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 $H_3{}^+$ molecular ion in linear configuration does not exist for the 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 $10^9 \leqslant B \leqslant 4.414 \times 10^{13}$ G using the variational trial function ψ^{trial}, Eq. (4), with $\sigma_e=-1$, $\sigma_N=1$, and $m=-1$. It depends on 11 variational parameters.

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^{vib} and total energies of dissociation channels. The total energy $E_T[H_2(^3\Pi_u)]$ is from [18] for $B=1,10,100$ a.u., while for $B=20,1000,10\,000$ a.u. and 4.414×10^{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(1*s*) from [3,26].

B (a.u.)	E_T	R_{eq}	E_0^{vib}	$E_T[H_2(^3\Pi_u)]$	$E_T[H_2^+(1\pi_u)+H(1s)]$	$E_T[H_2^+(1\sigma_g)+H(2p_{-1})]$
1	−3.036	1.896		−2.9686	−2.6825	−2.8631
	−2.953[a]					
	−2.817[b]	2.040				
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
4.414×10^{13} G	−115.19	0.078		−84.96	−73.59	−79.86

[a] Reference [13].

[b] Our recalculations using the trial function from [13] (see text).

The variational calculations indicate clearly the existence of a minimum in the total energy surface $E_T(R_+,R_-)$ of H_3^+ for magnetic fields in the range $B=10^9-4.414\times10^{13}$ G. The minimum always corresponds to a linear parallel configuration at $R_+=R_-\equiv R$. Its stability towards small deviations from equilibrium in linear parallel configuration was investigated. For this state we are not aware how to check quantitatively the stability towards deviations from a linear parallel configuration. However, physical arguments based on perturbation theory estimates indicate 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 decreases and the system becomes more bound (the double-ionization energy increases) and more compact (the internuclear equilibrium distance decreases).

The total energy of the final states for the dissociation channels $H_3^+\to H_2^+(1\pi_u)+H(1s)$, $H_3^+\to H_2^+(1\sigma_g)+H(2p_{-1})$ and $H_3^+\to H_2(^3\Pi_u)+p$ 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. The dominant dissociation channel is $H_3^+\to H_2(^3\Pi_u)+p$. For all three channels the dissociation energy grows monotonously as the magnetic field increases. For the dominant channel $H_3^+\to H_2(^3\Pi_u)+p$ it reaches 30.3 Ry at the Schwinger limit 4.414×10^{13} G, while for the channel $H_3^+\to H_2^+(1\pi_u)+H(1s)$ for this magnetic field ≈35 Ry is required to dissociate. For magnetic fields $5\times10^{10}\lesssim B\lesssim4.414\times10^{13}$ 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 $^3\Sigma_u$ states which occurs at $B\approx20$ a.u. It shows that the ground state of H_3^+ for $B\gtrsim20$ a.u. is given by the $^3\Pi_u$ state (see below a study of Δ states which are characterized by the higher total energies), while the $^3\Sigma_u$ state is the ground state for $0.2\lesssim B\lesssim20$ 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 the spin-singlet $^1\Sigma_g$

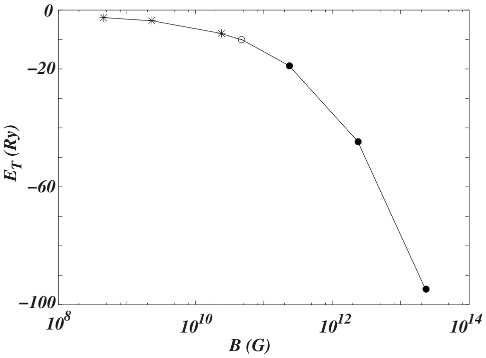

FIG. 2. Ground-state energy of H_3^+ vs magnetic field: $^3\Sigma_u$ (stars) and $^3\Pi_u$ (bullets); the point of crossing of these states is marked by an open circle.

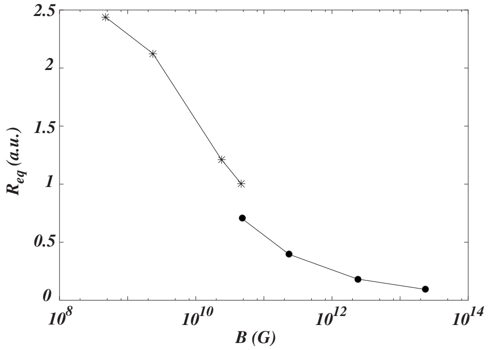

FIG. 3. Equilibrium distance for the ground state: ${}^3\Sigma_u$ (stars) and ${}^3\Pi_u$ (bullets).

state for small magnetic fields $B \lesssim 0.2$ a.u. (not shown in Figs. 2 and 3) to the spin-triplet ${}^3\Sigma_u$ state for intermediate fields and to the spin-triplet ${}^3\Pi_u$ state for $B \gtrsim 20$ a.u. The total energy decreases monotonously and smoothly as the magnetic field grows. 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 $\langle |z_1| \rangle$: it reduces monotonously from ≈ 1.9 a.u. at $B = 0.2$ a.u. to ≈ 0.1 a.u. at $B = 10\,000$ a.u. with a small discontinuity at $B \approx 20$ a.u. Perhaps, it is worth noting that the average distance between two electrons, $\langle r_{12} \rangle$ is also reduced as the magnetic field grows in about 20 times between 0.2 a.u. and 10 000 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 the 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. 5(a) and 5(b) the valleys and the total energy behavior (profile) along the valley for $B = 100$ a.u. for the ${}^3\Pi_u$ 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, $1 \leqslant B \leqslant 10\,000$ a.u. (see Table VI). The variational trial function ψ^{trial} with $\sigma_e = 1$, $\sigma_N = 1$, and $m = -1$ is used for this state; it depends on ten variational parameters.

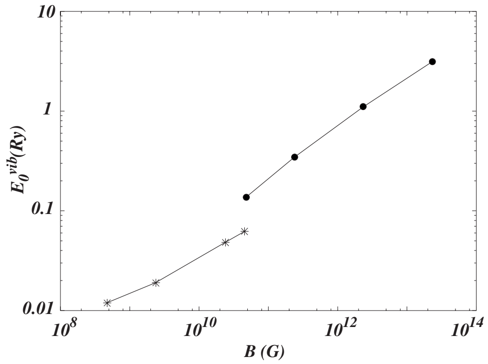

FIG. 4. Energy of the lowest longitudinal vibrational state E_0^{vib} for the ground state: ${}^3\Sigma_u$ (stars) and ${}^3\Pi_u$ (bullets).

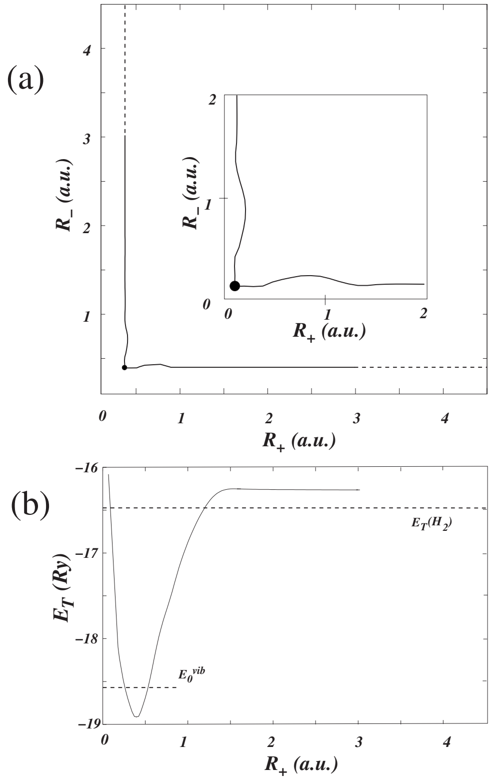

FIG. 5. Valleys of the total energy (a) and the profile (b) for $B = 100$ a.u. of the ground state ${}^3\Pi_u$.

The results obtained indicate clearly the existence of a minimum in the total energy $E_T(R)$ of H_3^+ for all magnetic

TABLE VI. 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.).

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

[a] Reference [13].

[b] Our recalculations using the trial function from [13] (see text).

TABLE VII. 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

fields in the range $B=1-10\,000$ 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 and the system becomes more bound (the double-ionization energies increase) and more compact (the internuclear equilibrium distance decreases).

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

A detailed study is carried out of the state $^1\Pi_g$ of the H_3^+ molecular ion in symmetric configuration $R_+=R_-\equiv R$ in the domain of magnetic fields, 1 a.u.$\leqslant B \leqslant 10\,000$ a.u. (see Table VII). For this state our variational trial function ψ^{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 the magnetic field grows; the system becomes more bound (the double-ionization energies increase) and more compact (the internuclear equilibrium distance decreases).

4. $^3\Pi_g$ state ($S=1$, $\sigma_N=-1$)

A detailed study is carried out of 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 a.u.$\leqslant B \leqslant 10\,000$ a.u. (see Table VIII). For this state our variational trial function ψ^{trial}, Eq. (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 increases while the internuclear equilibrium distance R_{eq} decreases as the magnetic field grows; the system becomes more bound (the double-ionization energy increases) and more compact (the internuclear equilibrium distance decreases).

TABLE VIII. 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

TABLE IX. H_3^+ ion for the state $^1\Delta_g$: total E_T and double-ionization E_I energies in Ry and equilibrium distance R_{eq} in a.u.

B (a.u.)	E_T	E_I	R_{eq}
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

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.

A detailed study is carried out of the states of the symmetric configuration $R_+=R_-\equiv R$ in the domain of magnetic fields $1 \leqslant B \leqslant 10\,000$ a.u. For each of these four states $^1\Delta_g$, $^3\Delta_g$, $^1\Delta_u$, and $^3\Delta_u$ the trial function ψ^{trial}, Eq. (4), 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 H_3^+ for magnetic fields in the range $B=1-10\,000$ 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 and the system becomes more bound (the double-ionization energy increases) and more compact (the internuclear equilibrium distance decreases).

IV. CONCLUSION

We study the low-lying energy states of H_3^+ molecular ions in linear configuration parallel to a magnetic field from 0 up to 4.414×10^{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 in Fig. 6. In the field-free case there exist only two eigenstates in a linear configuration, but many more eigenstates in a linear parallel configuration can appear when a magnetic field is imposed.

TABLE X. 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	R_{eq}
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
4.414×10^{13} G	−106.02	0.09

TABLE XI. $H_3{}^+$ 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. $H_3{}^+$ 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

In general, for all states studied, as the magnetic field increases, the equilibrium internuclear distance 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 a spin-singlet (unstable towards a deviation from linearity) $^1\Sigma_g$ state for weak magnetic fields $B \lesssim 0.2$ a.u. to a spin-triplet (stable towards a deviation from linearity) $^3\Sigma_u$ state for intermediate fields and eventually to a 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 $B \lesssim 0.2$ 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.[5] The $H_3{}^+$ ion in the $^3\Sigma_u$ state is weakly bound. For all magnetic fields studied the total energy surface corresponding well 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 $0.18 \lesssim B \lesssim 15.6$ 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 $0.85 \lesssim B \lesssim 1100$ a.u. [28].

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

It is interesting to note that at $B=1000$ a.u. the $H_3{}^+$ ion exists with $^3\Pi_u$ as the ground state ($E_T=-44.54$ a.u.) with two possible excited states $^3\Delta_g$ ($E_T=-40.38$ a.u.) and $^3\Sigma_u$ ($E_T=-35.99$ a.u.) with energies below the threshold of dissociation to $H_2(^3\Pi_u)+p$ ($E_T=-35.44$ a.u.). For larger magnetic fields the situation becomes different. For instance, at $B=10\,000$ a.u. for the $H_3{}^+$ ion ($E_T=-95.21$ a.u.) only one excited state $^3\Delta_g$ ($E_T=-87.49$ a.u.) exists with energy below the dissociation threshold to $H_2(^3\Pi_u)+p$ ($E_T=-71.39$ a.u.).

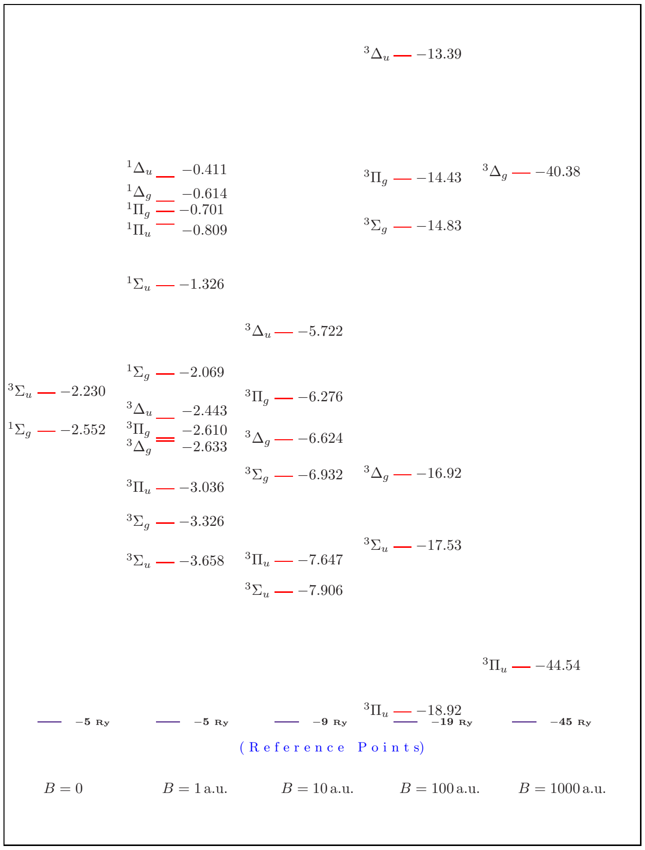

FIG. 6. (Color online) Total energy of the low-lying levels for $B=0$, 1, 10, 100, and 1000 a.u. (the energy scale is kept the same for all magnetic fields presented, but the reference points depend on them).

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[5] In order to make such a claim that the state of the lowest energy corresponds to a linear parallel configuration we make a very natural physical assumption that there are no other spatial configurations which may provide a lower total energy. But in order to be rigorous we must investigate the total energy surface for all possible spatial configurations.

A similar situation holds up to the Schwinger limit $B=4.414\times 10^{13}$ 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 $B\approx 0.2$ a.u. A study of the existence of the bound states which might appear in a spatial configuration is our goal for a future study. The another goal is related to a study of transition amplitudes for different electronic states.

The present consideration is based on the use of a simple variational trial function (4). 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 improvement of the present results and might be done in the future. However, we are not sure that such a study is crucially important. It is related to the fact that typical accuracies in astronomical observations of neutron star radiation would not be higher than $10^{-3}-10^{-4}$, unlike spectroscopical accuracies in the laboratory where they can be by several orders of magnitude higher.

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[1] M. A. Liberman and B. Johansson, Usp. Fiz. Nauk **165**, 121 (1995) [Phys. Usp. **38**, 117 (1995)].
[2] D. Lai, Rev. Mod. Phys. **73**, 629 (2001).
[3] A. V. Turbiner and J. C. López Vieyra, Phys. Rep. **424**, 309 (2006).
[4] A. Turbiner, J. C. López Vieyra, and U. Solis H., Pis'ma Zh. Eksp. Teor. Fiz. **69**, 800 (1999) [JETP Lett. **69**, 844 (1999)].
[5] A. V. Turbiner and J. C. López Vieyra, Mod. Phys. Lett. A **19**, 1919 (2004).
[6] J. J. Thomson, Philos. Mag. **21**, 225 (1911); **24**, 209 (1912).
[7] J. Tennyson, Rep. Prog. Phys. **57**, 421 (1995).
[8] C. A. Coulson, Proc. Cambridge Philos. Soc. **31**, 244 (1935).
[9] J. Hirschfelder, H. Eyring, and N. Rosen, J. Chem. Phys. **4**, 130 (1935); J. Hirschfelder, *ibid.* **6**, 795 (1938).
[10] R. E. Christoffersen, J. Chem. Phys. **41**, 960 (1964).
[11] L. J. Schaad and W. V. Hicks, J. Chem. Phys. **72**, 3909 (1974).
[12] J. C. López Vieyra and A. V. Turbiner, Phys. Rev. A **66**, 023409 (2002).
[13] C. S. Warke and A. K. Dutta, Phys. Rev. A **16**, 1747 (1977).
[14] A. V. Turbiner and N. Guevara (unpublished).
[15] A. V. Turbiner, Zh. Eksp. Teor. Fiz. **79**, 1719 (1980) [Sov. Phys. JETP **52**, 868 (1980)]; Usp. Fiz. Nauk **144**, 35 (1984) [Sov. Phys. Usp. **27**, 668 (1984)]; Yad. Fiz. **46**, 204 (1987) [Sov. J. Nucl. Phys. **46**, 125 (1987)]; Doctor of Sciences thesis, ITEP, Moscow, 1989.
[16] J. B. Anderson, J. Chem. Phys. **96**, 3702 (1992).
[17] W. Cencek, J. Rychlewski, R. Jaquet, and W. Kutzelnigg, J. Chem. Phys. **108**, 2831 (1998).
[18] T. Detmer, P. Schmelcher, F. K. Diakonos, and L. S. Cederbaum, Phys. Rev. A **56**, 1825 (1997).
[19] A. V. Turbiner and J. C. López Vieyra, Phys. Rev. A **69**, 053413 (2004).
[20] A. V. Turbiner, J. C. López Vieyra, and N. L. Guevara, Phys. Rev. A **72**, 023403 (2005).
[21] A. Y. Potekhin and A. V. Turbiner, Phys. Rev. A **63**, 065402 (2001).
[22] O.-A. Al-Hujaj and P. Schmelcher, Phys. Rev. A **61**, 063413 (2000).
[23] C. L. Pekeris, Phys. Rev. **126**, 1470 (1962).
[24] A. Alijah and A. J. C. Varandas, Philos. Trans. R. Soc. London, Ser. A **364**, 2889 (2006).
[25] A. Preiskorn, D. Frye, and E. Clementi, J. Chem. Phys. **94**, 7204 (1991).
[26] J. C. López Vieyra and A. V. Turbiner, Int. J. Mod. Phys. A (to be published).
[27] A. V. Turbiner, Astrophys. Space Sci. (to be published).
[28] A. V. Turbiner and N. L. Guevara, Phys. Rev. A **74**, 063419 (2006).