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Charged hydrogenic, helium, and helium-hydrogenic molecular chains in a strong magnetic field

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A nonrelativistic classification of charged molecular hydrogenic, helium, and mixed helium-hydrogenic chains with one or two electrons which can exist in a strong magnetic field $B \lesssim 10^{16}$ G is given. It is shown that for both $1e$-$2e$ cases at the strongest studied magnetic fields the longest hydrogenic chain contains at most five protons, indicating the existence of $H_5{}^{4+}$ and $H_5{}^{3+}$ ions, respectively. In the case of the helium chains, the longest chains can exist at the strongest studied magnetic fields with three and four α particles for $1e$-$2e$ cases with the possible existence of $He_3{}^{5+}$ and $He_4{}^{6+}$, respectively. For mixed helium-hydrogenic chains, the number of heavy centers can reach five for the highest magnetic fields studied. In general, for a fixed magnetic field, two-electron chains are more bound than one-electron chains.

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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 past two decades (see, for example, the review papers [1–3]). This attention is motivated by both pure theoretical interest and by possible practical applications in astrophysics. From the point of theory, such studies would lead to the creation of a theory of atoms and molecules in a magnetic field similar to standard atomic-molecular physics. In practice, even the basic elements of such a theory—a knowledge of the energy levels of the simplest Coulomb systems which can exist in a magnetic field—can be important for interpretation of the spectra of white dwarfs, where the surface magnetic field ranges over $B \approx 10^6$–10^9 G; neutron stars, where the surface magnetic field varies over $B \approx 10^{12}$–10^{13} G; and even values of $B \approx 10^{14}$–10^{16} G for the case of magnetars.

It was conjectured long ago [4,5] that unusual chemical compounds can appear in a strong magnetic field. In particular, it was suggested by Ruderman [5] and then further developed (see [2] and references therein) that the presence of a strong magnetic field can lead to the formation of linear hydrogenic neutral molecules (linear chains) situated along magnetic lines. It was assumed that in the ground state all electrons are in the same spin state with all spins antiparallel to the magnetic field line. To avoid a contradiction with the Pauli principle, it was further assumed that all electrons have different magnetic quantum numbers, as a characteristic of the ground state. This assumption seems obviously correct in the case of atoms and atomic ions, where the electrons are close to each other. However, it is not that obvious for the case of molecules for which the electrons are situated in far distant places in space. All of them (or, at least, some of them) can be in the same quantum state, with the same spin projection and magnetic quantum number [6]. This situation was observed for H_2 [7] and $H_3{}^+$ [8], where in a domain of large magnetic fields the ground state was given by the state of the maximal total spin but with the electrons having the same zero magnetic quantum number (see discussion that follows). In [5] qualitative arguments were presented that such chains can be of any length and, thus, can contain arbitrarily many protons. It seems that such a picture is oversimplified; it intrinsically assumes that the magnetic field is "infinitely" strong. For instance, for any exotic chain (which does not exist in the field-free case), there must be a certain threshold magnetic field for it to begin to exist. It is possible that such a threshold magnetic field is beyond realistic magnetic fields that occur in nature. This phenomenon is absent in the qualitative theory [5]. Thus, some very general features of Ruderman's picture only, like the growth of the binding energies, shrinking of the size of the molecules with increasing magnetic field, and maximal total electronic spin can hold for realistic high magnetic fields.

It is well known that in the absence of a magnetic field, in general, the hydrogenic linear chains (polymers) do not exist; the only exceptions are the two shortest ones, $H_2{}^+$ and H_2.[1] Therefore, for each other chain there must be a threshold magnetic field from which the chain begins to exist if it is realized. It seems natural to assume that the threshold magnetic field grows with the length of the chain, which is defined by the number of heavy particles therein. At the moment, only $H_2{}^+$ and H_2—the shortest chains—are studied in detail (see, e.g., [3] and [7], respectively). The results are far more sophisticated than those predicted in a simple qualitative picture in [5]. For example, the H_2 molecule does *not* exist at a large domain of strong magnetic fields.

The aim of this article is to provide a classification of one- and two-electron linear molecular systems made from protons and/or α particles in nonrelativistic consideration, which can exist in a strong magnetic field of $10^2 \leqslant B \leqslant 10^7$ a.u. ($=2.35 \times 10^{16}$ G). To make the classification complete, we include a description of the (meta)stability of each existing

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[1] The H_3^+ ion exists in triangular geometry.

system with an indication of possible decay modes. A realization of such an aim implies a detailed quantitative study of hydrogen, helium, and mixed helium-hydrogen linear chains with one or two electrons. Since our study is limited to the question of the existence of a particular Coulomb system, the most attention is paid to an exploration of the ground state. The spectroscopy of each particular chain (classification of states, radiative transitions, etc.) is not discussed and is left for a future study.

It is shown in the one-electron case, depending on the magnetic field strength, that the hydrogenic systems ${H_2}^+$, ${H_3}^{2+}$, ${H_4}^{3+}$, and even ${H_5}^{4+}$ can exist in linear geometry. It is also shown that, as the magnetic field grows, the exotic helium-hydrogenic chains ${He_2}^{3+}$, $(HeH)^{2+}$, $(HHeH)^{3+}$, $(HeHHe)^{4+}$, and ${He_3}^{5+}$ begin to exist in linear geometry (for a brief review, see [6]). For all magnetic fields the system ${H_2}^+$ (as well as the hydrogen atom) is stable, whereas the system ${H_3}^{2+}$ becomes stable at $B \gtrsim 10^{13}$ G. A detailed review of the current status of some one-electron hydrogenic molecular systems, both traditional and exotic, that might exist in a magnetic field at $B \geqslant 10^9$ G up to the Schwinger limit can be found in [3]. For the two-electron case, depending on the magnetic field strength, the hydrogenic chains H_2, ${H_3}^+$, ${H_4}^{2+}$, and at most ${H_5}^{3+}$ can exist in linear geometry, as well as the two-electron helium chains ${He_2}^{2+}$, ${He_3}^{4+}$, and ${He_4}^{6+}$, and the mixed hydrogen-helium chains $(HeH)^+$, $(HHeH)^{2+}$, $(HeHHe)^{3+}$, $(HHeHeH)^{4+}$, $(HeHHHe)^{4+}$, $(HHHeHH)^{4+}$, $(HHeHHeH)^{5+}$, and $(HeHeHHeHe)^{7+}$. The overall study is made in the framework of a nonrelativistic consideration by solving the Schroedinger equation. It is also assumed that the Born-Oppenheimer approximation of zero order holds, which implies that the positions of positively charged heavy particles are kept fixed (they are assumed to be infinitely massive). Relativistic corrections are always neglected, assuming that the longitudinal motion of electrons is nonrelativistic for magnetic field $\lesssim 10^{16}$ G while there are no relativistic corrections to the energies of transverse motion because the spectra of nonrelativistic and relativistic harmonic oscillators coincide (we call it the "Duncan argument"; for a discussion see [9]). Some preliminary results were announced in [6]. We perform such a nonrelativistic consideration with infinitely massive positively charged centers as a first basic step toward a realistic theory of simple positively charged molecular species in a strong magnetic field. In turn, it could be considered an important ingredient in a theory of gases, liquids, and solids made from these species. In our understanding, such a theory, even on the basic level, is needed for the construction of a meaningful model of a neutron star atmosphere.

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. ONE-ELECTRON HYDROGENIC CHAINS

A. Generalities

Let us consider the electron and n infinitely massive particles (protons) situated on a line that coincides with the magnetic line (see Fig. 1). We call this system a linear finite chain of size n. If for such a system a bound state can be found, it implies the existence of the ion $H_n^{(n-1)+}$ in linear geometry.

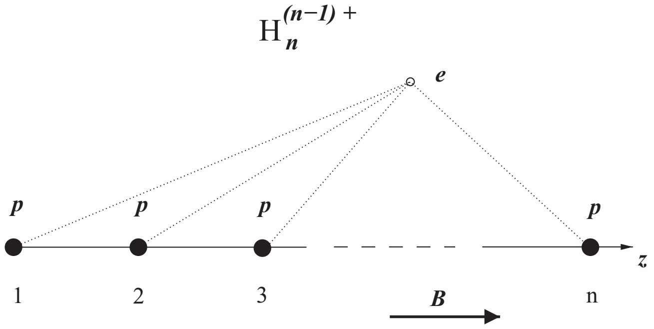

FIG. 1. $H_n^{(n-1)+}$ linear molecular ion in parallel configuration with a magnetic field $\mathbf{B}$ oriented along the z axis.

The Hamiltonian that describes this system when the magnetic field is oriented along the z direction, $\mathbf{B} = (0, 0, B)$, is[2]

$$\mathcal{H}_n = (\hat{\mathbf{p}} + \mathcal{A})^2 - 2\sum_{i=1,n}\frac{Z_i}{r_i} + \sum_{\substack{i\neq j\\ i,j=1,n}}\frac{Z_iZ_j}{R_{ij}} + 2\mathbf{B}\cdot\mathbf{S} \tag{1}$$

(see Fig. 1 for the geometrical setting and notations), where $Z_i = Z_j = 1$ in the case of protons, $\hat{\mathbf{p}} = -i\nabla$ is the momentum of the electron, $\mathbf{S}$ is the operator of the spin, r_i is the distance from the electron to the ith proton, and R_{ij} is the distance between the ith and jth protons. The vector potential $\mathcal{A}$ corresponds to the constant uniform magnetic field $\mathbf{B}$. It is chosen to be in the symmetric gauge,

$$\mathcal{A} = \frac{1}{2}(\mathbf{B} \times \mathbf{r}) = \frac{B}{2}(-y,\ x,\ 0). \tag{2}$$

Finally, the Hamiltonian can be written as

$$\mathcal{H}_n = \left(-\nabla^2 + \frac{B^2}{4}\rho^2\right) - 2\sum_{i=1}^{n}\frac{Z_i}{r_i} + \sum_{\substack{i\neq j\\ i,j=1}}^{n}\frac{Z_iZ_j}{R_{ij}} + B(\hat{L}_z + 2\hat{S}_z), \tag{3}$$

where $\hat{L}_z$ and $\hat{S}_z$ are the z components of the total angular momentum and total spin operators, respectively, and $\rho = \sqrt{x^2 + y^2}$. Both $\hat{L}_z$ and $\hat{S}_z$ are integrals of motion. Thus, the operators $\hat{L}_z$ and $\hat{S}_z$ in Eq. (3) can be replaced by their eigenvalues m and m_s, respectively. Since we are interested in the ground state for which $m = 0$ and $m_s = -1/2$, the last term in Eq. (3) can be omitted and the reference point for energy becomes $-B$.

In the equilibrium configuration the problem is characterized by two integrals of motion: (i) angular momentum projection m on the magnetic field direction (z direction) and (ii) spatial parity p. The problem for parallel symmetric configuration is characterized by the z parity, $P_z(z \to -z)$, with eigenvalues $\sigma = \pm 1$. One can relate the magnetic quantum number m, spatial parity p, and z parity σ as follows:

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

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

In the case that m is even, both parities coincide ($p = \sigma$). Thus, any eigenstate has two definite quantum numbers: the magnetic quantum number m and the parity p with respect $\vec{r} \to -\vec{r}$. Therefore, the space of eigenstates is split into subspaces (sectors), each of which is characterized by definite m and σ, or m and p. The notation for the states is based on the following convention: the first number corresponds to the number of the excitation, the "principal quantum number" (e.g., the number 1 is assigned to the ground state); then a Greek letter σ, π, δ corresponds to $m = 0, -1, -2$, respectively, with subscript g (u) for gerade (ungerade) corresponding to positive (negative) eigenvalues of the spacial parity operator P. Thus, the $1\sigma_g$ state is the ground state, and its coordinate eigenfunction is nodeless.

B. Method

The variational method is used for a study of Hamiltonian (3). Trial functions are chosen following the physics relevance arguments [10]. Their explicit expression is a linear superposition of K terms given by

$$\psi^{(\text{trial})}_{n,K} = \sum_{k=1}^{K} A_k \left\{ e^{-\sum_{i=1}^{n} \alpha_{k,i} r_i} \right\}_k e^{-B\beta_k \frac{\rho^2}{4}} \tag{4}$$

(see [3]), where A_k and $\alpha_{k,i}$, β_k are linear and nonlinear parameters, respectively. Interproton distances R are considered as variational parameters as well. The notation {} indicates the symmetrization of identical nuclei of the expression inside the brackets. Usually, a certain physical meaning is given to each term in Eq. (4). For example, one term had all $\alpha_{k,i}$ equal as an analog of the Heitler-London wave function for the $H_2{}^+$ ion, describing the coherent interaction of the electron with all protons. For another term when all values of $\alpha_{k,i}$, except for one, vanish, it is an analog of the Hund-Mulliken wave function, describing the incoherent interaction of the electron with all protons. All other terms are different nonlinear superpositions of these two—an analog of the Guillemin-Zener wave function for the $H_2{}^+$ ion. We call a term for which all $\alpha_{k,i}$ are different and unconstrained the *general term*. Needless to say, in each particular term in Eq. (4) the parameters are chosen in such a way that ensures the normalizability of this term as the overall function.

Calculations were performed using the minimization package MINUIT from CERNLIB. Two-dimensional integration was carried out using a dynamical partitioning procedure: a domain of integration is manually divided into subdomains following an integrand profile with a localization of domains of large gradients of the integrand. Each subdomain is integrated (for details, see, e.g., [3]). Numerical integration of subdomains is done with a relative accuracy of $\sim 10^{-9}$–10^{-10} by use of the adaptive D01FCF routine from NAGLIB.

1. $n = 1$

This case was considered for the sake of completeness. It is known that the hydrogen atom exists for any magnetic field strength. It is the least bound system among one-electron systems. The results for the H atom at $B = 10^6$, 10^7 a.u. are calculated with a ten-parameter variational trial function, which is a modification of the function introduced in [10,11]. It is described elsewhere.

2. $n = 2$

The results for $H_2{}^+$ ion are found with a three-term trial function (4), which depends on the ten free parameters including the interproton distance R, which is a linear superposition of the Heitler-London, Hund-Mulliken, and Guillemin-Zener (general term) wave functions. For $B \leqslant 10^4$ a.u., results are from [3].

3. $n = 3$

The results for the $H_3{}^{2+}$ ion are found with a three-term trial function (4), which depends on 22 free parameters including two interproton distances R, which is a linear superposition of the Heitler-London, Hund-Mulliken, and a type of the Guillemin-Zener (general term) wave functions. For $B \leqslant 10^4$ a.u., results are from [3].

4. $n = 4$

Results for the $H_4{}^{3+}$ ion are found with a one-term trial function (4), which depends on the seven free parameters including three interproton distances R, two of which are assumed to be equal (symmetric configuration). For $B \leqslant 10^4$ a.u., the results obtained with three- and seven-term trial function (4) can be found in [3]. They lead to slightly better binding energies but do not change the qualitative picture.

5. $n = 5$

It is the first study of this system. The results for the $H_5{}^{4+}$ ion are obtained using a two-term trial function (4), which depends on the 15 free parameters including four interproton distances R, two pairs of which are assumed to be equal (symmetric configuration). In fact, it implies that a linear superposition of two general terms is taken. It is worth noting that the one-term trial function at $B = 10^7$ a.u. already gives a clear indication of the existence of the $H_5{}^{4+}$ ion with binding energy $E_b = 206.11$ Ry and equilibrium distances $R_1 = 0.053$ a.u., $R_2 = 0.032$ a.u. The smallest magnetic field for which a minimum of the total energy surface in R was observed is 5×10^6 a.u. The $H_5{}^{4+}$ ion for these magnetic fields looks like the $H_3{}^{2+}$ ion bound with a far-distant proton from each side.

6. $n = 6$

No indication of the existence of the $H_6{}^{5+}$ ion in the domain $B \leqslant 10^7$ a.u. was found.

C. Results

The results of the calculations are presented in Tables I and II and illustrated in Fig. 2. Two traditional field-free case systems H and $H_2{}^+$ exist for all studied magnetic fields $B \leqslant 10^7$ a.u. The first exotic molecular system $H_3{}^{2+}$ appears at $B \sim 10^2$ a.u. and exists for larger magnetic fields. Another exotic molecular system, $H_4{}^{3+}$, appears at $B \sim 10^4$ a.u. and the last exotic molecular system, $H_5{}^{4+}$, appears at $B \sim 5 \times 10^6$ a.u. No other one-electron molecular hydrogenic systems are seen for $B \leqslant 10^7$ a.u. For $n > 1$, the optimal geometry of any molecular system is linear and aligned along the magnetic field. Thus, such a system forms a finite chain.

TABLE I. Binding energies (in rydbergs) for the ground state $1\sigma_g$ of one-electron hydrogenic linear systems (finite chains) in a magnetic field. Binding energies for the ground state $1s_0$ of the H atom at $0 \leqslant B \leqslant 10^2$ a.u. are from [11].

B(a.u.) System	0	1	10	10^2	10^4	10^6	10^7
H	1.0	1.662	3.495	7.564	27.10	73.96	108.86
$H_2{}^+$	1.2053	1.9499	4.3498	10.291	45.799	139.91	217.75
$H_3{}^{2+}$				8.639	45.408	160.17	263.80
$H_4{}^{3+}$					34.922	142.75	251.71
$H_5{}^{4+}$							206.15

It was checked that the configuration is stable with respect to small deviations from linearity. All studied finite chains are characterized by two features: with a magnetic field growth, (i) their total energies increase and (ii) their lengths decrease—each system becomes more bound and compact.

For all studied magnetic fields, the systems H and $H_2{}^+$ are stable: the H atom has no decay channels, although the total energy of the $H_2{}^+$ ion is always less than the total energy of the H atom. Furthermore, for $B \lesssim 1.5 \times 10^4$ a.u., the $H_2{}^+$ ion has a smaller total energy then the $H_3{}^{2+}$ ion when it exists; these two finite chains are the only ones that exist in this domain. The $H_3{}^{2+}$ ion never dissociates to $H + 2p$ but it always dissociates to $H_2{}^+ + p$. For higher magnetic fields ($B \gtrsim 1.5 \times 10^4$ a.u.), the $H_3{}^{2+}$ ion becomes stable as well. It is characterized by the smallest total energy for these magnetic fields. Another exotic molecular system, $H_4{}^{3+}$, never dissociates to $H + 3p$, but it dissociates to $H_2{}^+ + p$ for $10^4 < B < 10^6$ a.u. For magnetic fields $B \gtrsim 10^6$ a.u., the total energy of $H_4{}^{3+}$ is smaller than that of $H_2{}^+$ and the latter dissociation channel does not exist. For all studied magnetic fields $B \leqslant 10^7$ a.u., the system $H_4{}^{3+}$ can dissociate to $H_3{}^{2+}$, although the energy difference between such systems decreases gradually as the magnetic field increases. A smooth extrapolation indicates that, at the magnetic field $B \sim 2 \times 10^8$ a.u., there is a crossing for which the total energies of $H_3{}^{2+}$ and $H_4{}^{3+}$ become equal. The system $H_5{}^{4+}$ can dissociate to all finite chains except for the single-proton one: the H atom. Summarizing, one can state that there are two one-electron finite hydrogenic chains characterized by the lowest total energy for different magnetic fields: it is the $H_2{}^+$ system at $0 \lesssim B \lesssim 1.5 \times 10^4$ a.u. and the $H_3{}^{2+}$ ion at $1.5 \times 10^4 \lesssim B \lesssim 10^7$ a.u.

III. TWO-ELECTRON HYDROGENIC CHAINS

A. Generalities

Let us consider a system of two electrons and n infinitely massive protons situated on a line that coincides with the magnetic line (see Fig. 3). It is called a $2e$ linear finite chain of size n. If for such a system a bound state can be found, it implies the existence of the ion $H_n^{(n-2)+}$ in linear geometry. Sometimes, we say that this system is "in the parallel configuration." Also, it implies that the corresponding finite chain exists. It can be stable or metastable.

The Hamiltonian that describes the system of two electrons and n protons when the magnetic field is oriented along the z direction, $\mathbf{B} = (0, 0, B)$, is [12]

$$\mathcal{H}_n = \sum_{\ell=1}^{2} (\hat{\mathbf{p}}_\ell + \mathcal{A}_\ell)^2 - 2 \sum_{\substack{\ell=1,2\\ i=1,n}} \frac{Z_i}{r_{\ell i}} + \frac{2}{\mathrm{r}_{12}} + \sum_{\substack{i\neq j\\ i,j=1,n}} \frac{Z_i Z_j}{R_{ij}} + 2\mathbf{B}\cdot\mathbf{S} \tag{5}$$

(see Fig. 3 for the geometrical setting and notation), where $Z_i = Z_j = 1$ in the case of protons; $\hat{\mathbf{p}}_\ell = -i\nabla_\ell$ is the momentum of the ℓth electron; $r_{\ell i}$ is the distance from the ℓth electron to the ith proton; R_{ij} is the distance between ith and jth proton; $\mathrm{r}_{12} = |\vec{r}_1 - \vec{r}_2|$ is the interelectron distance, where $\vec{r}_1$ ($\vec{r}_2$) is the position from the center of the chain (mid-point with respect to the end-situated protons) of the first (second) electron; and $\mathbf{S} = \mathbf{S}_1 + \mathbf{S}_2$ is the operator of the total spin. The vector potential $\mathcal{A}_\ell$ corresponds to the constant uniform magnetic field $\mathbf{B}$ written in the symmetric gauge (2). Finally, the Hamiltonian can be written as

$$\mathcal{H}_n = \sum_{\ell=1}^{2} \left(-\nabla_\ell^2 + \frac{B^2}{4}\rho_\ell^2\right) - 2 \sum_{\substack{\ell=1,2\\ i=1,n}} \frac{Z_i}{r_{\ell i}} + \frac{2}{\mathrm{r}_{12}} + \sum_{\substack{i\neq j\\ i,j=1,n}} \frac{Z_i Z_j}{R_{i,j}} + B(\hat{L}_z + 2\hat{S}_z), \tag{6}$$

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 $\rho_\ell = \sqrt{x_\ell^2 + y_\ell^2}$. All performed calculations

TABLE II. Interproton equilibrium distances (in a.u.) for the ground state $1\sigma_g$ of the one-electron hydrogenic linear systems (finite chains) in a strong magnetic field. All configurations have center of symmetry; symmetric interproton distances are not displayed.

B(a.u.) System	0	1	10	10^2	10^4	10^6	10^7
$H_2{}^+$ (R)	1.997	1.752	0.957	0.448	0.118	0.045	0.032
$H_3{}^{2+}$ (R, R)				0.579, –	0.130, –	0.044, –	0.029, –
$H_4{}^{3+}$ (R_1, R_2, R_1)					0.214, 0.138, –	0.056, 0.044, –	0.034, 0.028, –
$H_5{}^{4+}$ (R_1, R_2, R_2, R_1)							0.053, 0.032, –, –

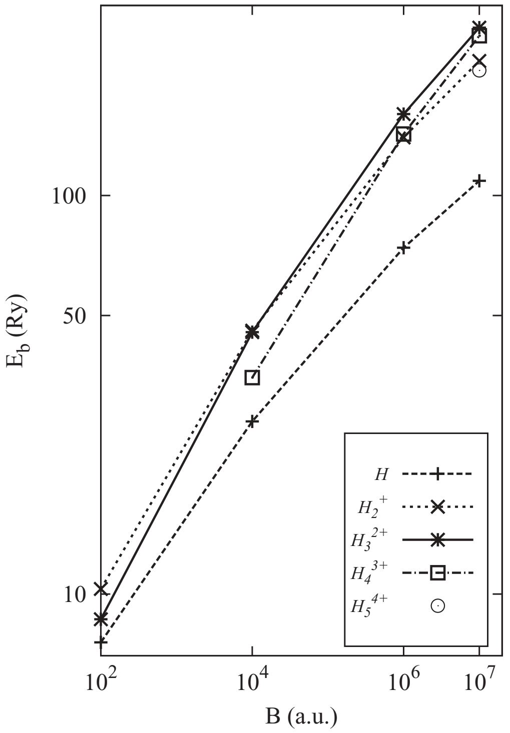

FIG. 2. Binding energies E_b for the one-electron hydrogenic linear molecular ions in parallel configuration vs a magnetic field **B**.

indicated a symmetry property of a chain: in the optimal geometry a chain has a center of symmetry. Hence, for any proton there is a partner situated symmetrically with respect to this center. We consider this property as intrinsic of any chain.

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 $p = 1$ (-1) for gerade (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 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 the state of lowest total energy, while for larger magnetic fields it should be a spin-triplet state with $m_s = -1$, where the electron spins are antiparallel to the magnetic field direction **B**. The total space of the eigenstates is split into subspaces (sectors), each of which is characterized by definite values of m, p, and m_s. It is worth noting that the Hamiltonian $\mathcal{H}_n$ is invariant with respect to reflections P_z: $z_1 \to -z_1$ and $z_2 \to -z_2$, with eigenvalues $\sigma_N = \pm 1$, for a symmetric chain.

In order to classify eigenstates we follow the convention widely accepted in molecular physics that uses the quantum numbers m, p and the total spin S without indication of 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 ($S = 1$). For the label M, we use Greek letters Σ, Π, and Δ, which mark the states with $|m| = 0, 1, 2, \ldots$, respectively, but implying that m takes negative values and the subscript p (the spatial parity quantum number) takes gerade g and ungerade 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 and the spatial parity:

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

The present consideration is limited to the states with magnetic quantum numbers $m = 0, -1$ because the total energy of the lowest energy state in any sector with $m > 0$ is always larger than one with $m \leqslant 0$. A study of states with different values for m is necessary to identify the state of lowest total energy. For large magnetic fields for all studied two-electron chains, this state was characterized by $m = -1$ in agreement with Ruderman's hypothesis.

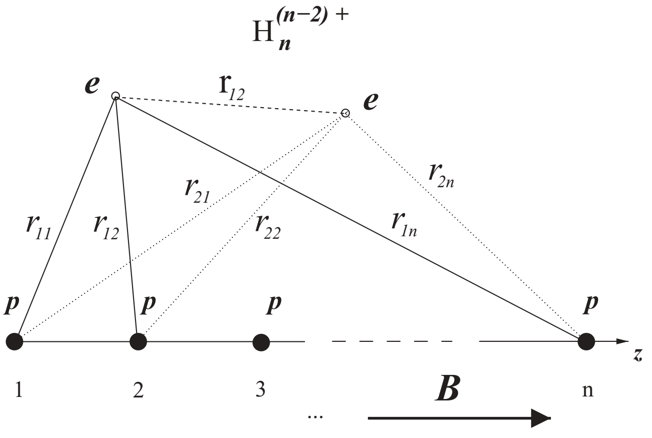

FIG. 3. $H_n^{(n-2)+}$ linear molecular ion in parallel configuration with a magnetic field **B** oriented along the z axis.

B. Method

As a method to explore the problem, we use the variational procedure. The recipe of choice of trial functions is based on physical arguments [10]. As a result, the trial function for the lowest energy state with magnetic quantum number m is chosen in the form

$$\psi^{(trial)} = (1 + \sigma_e P_{12}) \rho_1^{|m|} e^{im\phi_1} \sum_{k=1}^{K} A_k \left\{ e^{-\sum_{\substack{\ell=1,2 \\ i=1,n}} \alpha_{k,\ell i} r_{\ell i}} \right\}_k \times e^{\gamma_k \mathrm{r}_{12} - B\beta_{k,1} \frac{\rho_1^2}{4} - B\beta_{k,2} \frac{\rho_2^2}{4}} , \tag{7}$$

where $\sigma_e = \pm 1$ stands for spin-singlet (+) and spin-triplet states (−), and {} indicates the symmetrization of identical nuclei of the expression inside the brackets; P_{12} is the permutation operator for the electrons ($1 \leftrightarrow 2$). The parameters

$\alpha_{k,ij}$, $\beta_{k,1-2}$, and γ_k as well as interproton distances $R_{ij} = R_{ji}$ are variational parameters. For each term with fixed k, their total number is $2n + 4$, including the linear parameter A_k. In addition, we have $n - 1$ interproton distances. It is worth emphasizing that in trial function (7) the interelectron interaction is included explicitly in the exponential form $e^{\gamma r_{12}}$.

Calculations are performed using the minimization package MINUIT from CERNLIB. Multidimensional integration is carried out using a dynamical partitioning procedure: a domain of integration is manually divided into subdomains following an integrand profile with a localization of domains of large gradients of the integrand. Each subdomain is integrated separately using a parallelization procedure (for details, see, e.g., [3]). Numerical integration of subdomains is 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; when a minimum is found it takes several seconds of CPU time to compute a variational energy.

1. $n = 1$

This case corresponds to the negative hydrogen ion H^- and is mentioned for the sake of completeness. It is known that the negative hydrogen ion H^- exists for any magnetic field strength [13]. At zero and small magnetic fields $B < 5 \times 10^{-2}$ a.u., the spin-singlet state $^1 0$ is the ground state. If $B > 5 \times 10^{-2}$ a.u., the spin-triplet state $^3(-1)$, which does not exist in the absence of a magnetic field, becomes bound and the ground state. Although this result is checked quantitatively for magnetic fields up to 4000 a.u. [13,14], it is quite likely that it holds for higher magnetic fields. It is the least bound system among two-electron systems made from protons. However, the H^- ion is stable for studied magnetic fields: the dissociation $H^- \to H + e$ is prohibited.

2. $n = 2$

In a domain of non-ultra-high magnetic fields, the H_2 molecule was studied in detail in [7]. It was shown that the lowest total energy state depends on the magnetic field strength. It evolves from the spin-singlet state $^1\Sigma_g$ at $0 \leqslant B \lesssim 0.18$ a.u. to a repulsive spin-triplet state $^3\Sigma_u$ (unbound state) for $0.18 \lesssim B \lesssim 12.3$ a.u. and, finally, to a strongly bound spin-triplet state $^3\Pi_u$. Hence, there exists quite a large domain of magnetic fields where the H_2 molecule is unbound that are represented by two hydrogen atoms in the same electron spin state but situated at an infinite distance from each other. The optimal geometry of the H_2 molecule (when it exists) always corresponds to the elongation along a magnetic line for the $^1\Sigma_g$ state, thus forming a finite chain. It is assumed that the chain in the $^3\Pi_u$ state is stable toward the deviation from linearity. This assumption seems well justified from a physics point of view for large magnetic fields: any deviation from linearity leads to a sharp increase in the total energy due to nonvanishing rotational energy. This chain is stable (when it exists) for all studied magnetic fields. However, this chain always has a total energy higher than the $H_3{}^+$ chain (see following discussion) and thus is less preferable energetically. Calculations for the $^3\Pi_u$ state of H_2 using a single function of the form of Eq. (7) for which all α parameters are different (general term) are presented in Tables III and IV.

3. $n = 3$

In [8] it is shown that the H_3^+ molecular ion exists in a magnetic field as a bound state. For $B \gtrsim 0.2$ a.u., the ground-state geometry is linearly realized, parallel to the magnetic field line configuration. Thus, the three-proton finite chain occurs. In the domain $0.2 \lesssim B \lesssim 20$ a.u., the ground state is realized by the $^3\Sigma_u$ state and it is weakly bound. However, at $B > 20$ a.u., the ground state $^3\Pi_u$ is strongly bound and the chain is stable.

4. $n = 4$

In the field-free case, the system $4p2e$ does not display any binding. However, for magnetic fields $B \gtrsim 2000$ a.u., it becomes bound in the linear configuration aligned along the magnetic line with the $^3\Pi_u$ state as the ground state. Hence, the molecular ion $H_4{}^{2+}$ begins to exist. Its total energy is lower systematically than the total energy of $H_3{}^+$. Hence, the molecular ion $H_4{}^{2+}$ is stable. With an increase of the magnetic field strength, the total energy at the equilibrium position decreases, and the system becomes more bound (in this case, the double ionization energy is $E_I = -E_T$, which increases with B) and more compact (the internuclear equilibrium distance decreases with B). Eventually, we state that the finite chain $H_4{}^{2+}$ is always stable. For magnetic fields $1 \lesssim B \lesssim 2000$ a.u., the state $^3\Pi_u$ is bound but the ground state corresponds to an unbound system in the repulsive $^3\Sigma_u$ state: it consists of two $H_2{}^+$ ions at infinite distance from each other.

5. $n = 5$

In the field-free case the system $5p2e$ does not display any binding. However, for magnetic fields $B \gtrsim 5000$ a.u., it becomes bound in the linear configuration aligned along the magnetic line with the $^3\Pi_u$ state as the ground state; hence, the molecular ion $H_5{}^{3+}$ begins to exist. For $5000 \lesssim B \lesssim 10^6$ a.u., the $H_5{}^{3+}$ molecular ion decays to $H_4{}^{2+} + p$. At magnetic fields $B \gtrsim 10^6$ a.u., the molecular ion $H_5{}^{3+}$ becomes stable.

6. $n = 6$

No indication of the bound state of the $6p2e$ system is found for even the highest magnetic field studied.

C. Results

The results of the calculations are presented in Tables III and IV and illustrated in Fig. 4. Three traditional ions for the field-free case systems, H^-, H_2, and $H_3{}^+$, continue to exist at magnetic fields of $10^2 \leqslant B \leqslant 10^7$ a.u. The first exotic molecular system, $H_4{}^{2+}$, appears at $\sim 2 \times 10^3$ a.u. in linear configuration and exists for all larger magnetic fields. Another exotic molecular system, $H_5{}^{3+}$, appears at a slightly larger magnetic field, $\sim 5 \times 10^3$ a.u. No other two-electron molecular hydrogenic system is seen in the domain $B \leqslant 10^7$ a.u. At large magnetic fields the ground state of all studied systems is the spin-triplet state with spin projection $m_s = -1$ and total magnetic quantum number $m = -1$, in agreement with the

TABLE III. Double ionization energies E_I in rydbergs ($E_T = -E_I$) for the ground state $^3\Pi_u$ of the two-electron hydrogenic systems (finite chains) in a strong magnetic field. Energy in brackets means that the state $^3\Pi_u$ is bound but the ground state corresponds to an unbound state. The magnetic field $B_{\mathrm{Schwinger}} = 4.414 \times 10^{13}$ G $= 1.878 \times 10^4$ a.u. corresponds to the so-called nonrelativistic threshold for which the electron cyclotron energy equals the electron rest mass.

B(a.u.)						
System	10^2	10^3	10^4	4.414×10^{13} (G)	10^6	10^7
H^-	8.35	16.95	30.1	35.4	82.5	121.4
H_2	16.473[a]	35.632	71.42	85.00	219.9	330.3
$H_3{}^+$	18.915	44.538	95.21	115.19	324.2	529.8
$H_4{}^{2+}$	(17.601)	(43.917)	99.80	122.34	367.7	636.0
$H_5{}^{3+}$			91.70	114.34	383.2	687.7

[a] From [7].

Ruderman hypothesis. For $n > 1$, the optimal geometry of the molecular system is linear, and the system is aligned along magnetic field. Thus, each molecular system forms a finite chain. It is checked that such a linear configuration is stable with respect to small vibrations and its vibrational energies can be calculated. However, we were not able to check the stability of the configuration with respect to small deviations from linearity and to calculate the rotational energies. All studied finite chains are characterized by two features: with magnetic field growth, (i) their binding energies increase and (ii) their longitudinal lengths decrease; each system becomes more bound and compact. For all studied magnetic fields $B \gtrsim 10^2$ a.u., the systems H^- and H_2 are stable. They are characterized by much smaller binding energies in comparison with other systems. Thus, their significance for thermodynamics at a fixed magnetic field seems limited.

It is worth emphasizing that among two-electron hydrogenic finite chains the system $H_3{}^+$ has the lowest total energy in the domain $10^2 \lesssim B \lesssim 2 \times 10^3$ a.u.; at larger magnetic fields $2 \times 10^3 \lesssim B \lesssim 10^6$ a.u., the finite chain $H_4{}^{2+}$ gets the lowest total energy and eventually, at $B \gtrsim 10^6$ a.u., the molecular ion $H_5{}^{3+}$ (the longest hydrogenic chain) is characterized by the lowest total energy. Interestingly, in the domain $10^6 \lesssim B \lesssim 10^7$ a.u., *all* two-electron finite hydrogen chains are stable.

IV. ONE-ELECTRON HELIUM AND HELIUM-HYDROGEN CHAINS

A. Generalities

Let us now consider molecular systems composed of one electron and a finite number n of infinitely massive protons and/or α particles as charged centers, situated on a line which coincides with the direction of a homogeneous magnetic field. The geometrical arrangement is similar to that depicted in Fig. 1, except for the fact that charged centers can be either protons or α particles. If found, bound states of such systems are called one-electron helium or helium-hydrogen chains. In the present review, only one-electron helium or helium-hydrogen chains with $n = 1, 2, 3$ were included.

Following similar considerations as for the case of hydrogenic chains (see Sec. II), the Hamiltonian which describes the one-electron helium (helium-hydrogen) chains in a magnetic field oriented along the z direction, $\mathbf{B} = (0, 0, B)$, is given by Hamiltonian (3) with $Z_i, Z_j = 1$ or 2, depending on each particular system. Since we are interested in the ground state for which $m = 0$ and $m_s = -1/2$, the last term in Hamiltonian (3) can be omitted and the reference point for energy becomes equal to $-B$.

B. Method

The variational method is used for a study of the helium (helium-hydrogen) chains described by Hamiltonian (3). Trial functions are chosen following physics relevance arguments [10]. Their explicit expressions are linear superpositions of K terms given by functions of the class (4), where A_k and $\alpha_{k,i}$, β_k are linear and nonlinear parameters, respectively. Internuclear distances R are considered as variational parameters as well. In this case the notation {} in Eq. (4) indicates the symmetrization of the expression inside the brackets with respect to the permutations of the identical charged centers; for example, for the system $(HHeH)^{3+}$ it means permutation with respect to the external protons. As for the case of hydrogenic chains, each term in Eq. (4) has a certain physical meaning (see

TABLE IV. Interproton equilibrium distances (in a.u.) for the ground state $^3\Pi_u$ of the two-electron hydrogenic linear systems (finite chains) in a strong magnetic field. All configurations have center of symmetry and symmetric interproton distances are not displayed. ^{s} from [7]. Distances in brackets indicate that the state $^3\Pi_u$ is bound but the ground state corresponds to an unbound state.

B(a.u.)						
System	10^2	10^3	10^4	4.414×10^{13} (G)	10^6	10^7
H_2 (R)	0.38^s	0.19	0.102	0.087	0.038	0.034
$H_3{}^+$ (R, R)	0.395, –	0.183, –	0.093, –	0.078, –	0.030, –	0.023, –
$H_4{}^{2+}$ (R_1, R_2, R_1)	(0.51, 0.38, –)	(0.215, 0.174, –)	0.103, 0.086, –	0.092, 0.075, –	0.030, 0.018, –	0.020, 0.013, –
$H_5{}^{3+}$ (R_1, R_2, R_2, R_1)	–	–	0.184, 0.134, –, –	0.160, 0.110, –, –	0.035, 0.025, –, –	0.023, 0.018, –, –

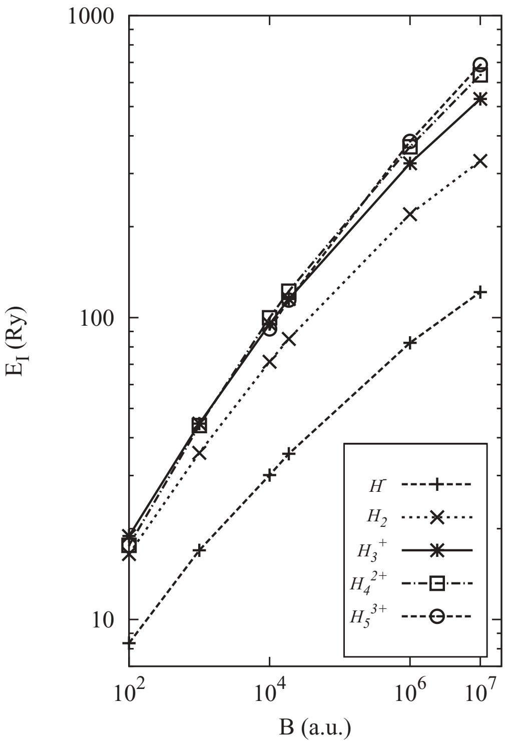

FIG. 4. Ionization energies E_I for the two-electron hydrogenic linear molecular ions in parallel configuration vs magnetic field **B**.

Sec. II). In the following, we describe the different chains studied.

1. $n = 1$

(αe). This case corresponds to the simplest one-electron helium system. It is known that the positive atomic ion of helium exists for any magnetic field strength. Furthermore, it is the only one-electron helium system that exists for magnetic fields of strength $B \lesssim 10$ a.u. The following results presented for the ground state $1s_0$ of the He^+ atomic ion (see Table V) were obtained with a seven-parameter variational trial function introduced in [11] for a study of the H atom.

2. $n = 2$

(i) ($\alpha\alpha e$). Accurate variational calculations in equilibrium configuration (parallel to the magnetic field) for the ground state $1\sigma_g$ of the system ${He_2}^{3+}$ were carried out in detail in [3,15] for the range of magnetic fields $10^2 \lesssim B \lesssim B_{\text{Schwinger}}$ a.u.. A three-term trial function of the form of Eq. (4) which depends on ten free parameters, including the internuclear distance R, is used in the calculations. It is the same linear superposition of the Heitler-London, Hund-Mulliken, and Guillemin-Zener wave functions which was used to study the ${H_2}^+$ molecular ion (see Sec. II). It was found that for magnetic fields $10^2 \lesssim B \lesssim 10^3$ a.u., the system ${He_2}^{3+}$ is unstable toward the decay to $He^+ + \alpha$. Nonetheless, at $B \gtrsim 10^4$ a.u., this compound becomes the system with the lowest total energy among the one-electron helium (helium-hydrogen) chains. In [15], the lowest vibrational and rotational energies for this system were also calculated.

(ii) (αpe). The first indication of the existence of the hybrid system $(HeH)^{2+}$, for magnetic fields $B \gtrsim 10^4$ a.u., was established in [3,15], where accurate variational calculations for the ground state 1σ of the system $(HeH)^{2+}$ were carried out. Variational calculations are performed with a three-term trial function of the type of Eq. (4). In [3,15] it was also demonstrated that the equilibrium configuration corresponds to the situation when the molecular axis (the line connecting the proton and the α particle) is parallel to the magnetic field. For the narrow range of magnetic fields $10^4 \lesssim B \lesssim B_{\text{Schwinger}}$ a.u., the system $(HeH)^{2+}$ is found to be a long-lived metastable state decaying to $He^+ + p$. For magnetic fields larger than $B_{\text{Schwinger}}$, the system becomes stable toward the decay to $He^+ + p$.

3. $n = 3$

(i) ($\alpha\alpha\alpha e$). It seems it is for the first time we see an indication of the possible existence of the exotic molecular ion ${He_3}^{5+}$ for magnetic fields $B \gtrsim 10^6$ a.u. For this system, a three-term trial function of the form of Eq. (4) is used for its variational study. It depends on 22 free parameters, including two internuclear distances $R_{1,2}$. This function is the same linear superposition of the Heitler-London, Hund-Mulliken, and a type of the Guillemin-Zener wave functions, which was used to study the H_3^{2+} molecular ion (see Sec. II). It is found that the system ($\alpha\alpha\alpha e$) begins to exist as a bound state (i.e., displays a minimum in the corresponding potential energy surface for finite internuclear distances) at magnetic fields $B \gtrsim 10^6$ a.u. in the linear symmetric configuration (for which the two internuclear distances are equal, $R_1 = R_2$) parallel to the magnetic field direction. The ground state is $1\sigma_g$.

TABLE V. Binding energies (in rydbergs) for the ground state $1\sigma_g$ of the one-electron helium and helium-hydrogenic linear systems (finite chains) in a magnetic field [the ground state for $(HeH)^{2+}$ is 1σ]. For He_3^{5+}: $E_b = 86.76$Ry, $R_{eq} = 0.202$ a.u. at $B = 10^{14}$ G; while for $B_{\text{Schwinger}}$ there is no minimum.

B(a.u.) System	1	10	10^2	10^4	4.414×10^{13} (G)	10^6	10^7
He^+	4.8820	8.7801	19.109	78.426	92.528	226.66	345.17
${He_2}^{3+}$			16.516	86.233	105.121	305.11	507.31
${He_3}^{5+}$						227.83	417.15
$(HeH)^{2+}$				77.303	92.858	251.32	402.10
$(HHeH)^{3+}$				64.747	79.69	233.71	392.47
$(HeHHe)^{4+}$					70.76	230.38	408.58

TABLE VI. Internuclear equilibrium distances (in a.u.) for the ground state $1\sigma_g$ of the one-electron helium and helium-hydrogenic linear systems (finite chains) in a strong magnetic field [the ground state for $(\mathrm{HeH})^{2+}$ is 1σ]. For all configurations that have center of symmetry, symmetric internuclear distances are not displayed.

B(a.u.) System	10^2	10^4	4.414×10^{13} (G)	10^6	10^7
$\mathrm{He_2}^{3+}$ (R)	0.779	0.150	0.126	0.049	0.032
$\mathrm{He_3}^{5+}$ (R, R)				0.070, –	0.041, –
$(\mathrm{HeH})^{2+}$ (R)		0.142	0.119	0.048	0.032
$(\mathrm{HHeH})^{3+}$ (R, R)		0.227, –	0.184, –	0.058, –	0.035, –
$(\mathrm{HeHHe})^{4+}$ (R, R)			0.170, –	0.051, –	0.031, –

(ii) ($p\alpha pe$). The first indications of the existence of the exotic trilinear molecular ion $(\mathrm{H\text{-}He\text{-}H})^{3+}$ for magnetic fields $B \gtrsim B_{\mathrm{Schwinger}}$ were given in [3,15]. For this system, a three-term trial function of the form of Eq. (4), which depends on 14 free parameters including two internuclear distances $R_{1,2}$, is used in the variational calculations. The results clearly show the appearance of a minimum in the potential energy surface of the (αppe) system for the symmetric configuration of the charged centers (p-α-p) with $R_1 = R_2$. The ground state is the type $1\sigma_g$. An indication of the existence of nonsymmetric configuration (α-p-p) was not observed.

(iii) ($\alpha p\alpha e$). The first indications of the existence of the exotic trilinear molecular ion $(\mathrm{He\text{-}H\text{-}He})^{4+}$ for magnetic fields $B \gtrsim B_{\mathrm{Schwinger}}$ were given in [3,15]. For this system, a three-term trial function of the form of Eq. (4), which depends on 14 free parameters including two internuclear distances R_1, R_2, is used in the variational calculations. The results show the appearance of a minimum in the potential energy surface of the ($\alpha\alpha pe$) system for the symmetric configuration of the charged centers (α-p-α) with $R_1 = R_2$. The ground state is $1\sigma_g$. An indication of the existence of nonsymmetric configuration (α-α-p) was not observed.

4. $n = 4$

No binding is detected for systems ($\alpha\alpha\alpha\alpha e$), ($\alpha pp\alpha e$), or ($p\alpha\alpha pe$) for even the highest studied magnetic field, $\sim 10^7$ a.u.

C. Results

The results of the ground-state calculations are presented in Tables V and VI and illustrated in Fig. 5. The positive atomic ion of helium, He^+, is the only system that exists for all studied magnetic fields $0 \leqslant B \leqslant 10^7$ a.u. At $B \sim 10^2$ a.u., the first exotic molecular system $\mathrm{He_2}^{3+}$ appears, being unstable toward decay to $\mathrm{He}^+ + \alpha$ in the range of magnetic fields $10^2 \lesssim B \lesssim 2 \times 10^4$ a.u. For larger magnetic fields $B \gtrsim 2 \times 10^4$ a.u., the system $\mathrm{He_2}^{3+}$ becomes the most bound one-electron system among the systems made from protons and/or α particles and it is stable. Two exotic molecular systems begin to exist at about the same magnetic field, $B \sim 10^4$ a.u., namely, the hybrid molecular ion $(\mathrm{HeH})^{2+}$, followed by the trilinear symmetric molecular system $(\mathrm{H\text{-}He\text{-}H})^{3+}$, which are unstable toward decay to $\mathrm{He}^+ + \mathrm{p}$ and $\mathrm{He}^+ + 2\mathrm{p}$, respectively. Remarkably, the system $(\mathrm{HeH})^{2+}$ rapidly becomes stable for magnetic fields $B \gtrsim 2 \times 10^4$ a.u. The system $(\mathrm{H\text{-}He\text{-}H})^{3+}$ becomes more bound than He^+ for magnetic fields $B \gtrsim 5 \times 10^5$ a.u. but remains unstable toward decay to $(\mathrm{HeH})^{2+} + p$ in the range of magnetic fields $5 \times 10^5 \lesssim B \leqslant 10^7$ a.u. It never dissociates to $\mathrm{H}_2^+ + \alpha$. Another exotic symmetric molecular system, $(\mathrm{He\text{-}H\text{-}He})^{4+}$, appears at $B \sim B_{\mathrm{Schwinger}}$, being unstable toward decay to $(\mathrm{HeH})^{2+} + \alpha$ for magnetic fields $B_{\mathrm{Schwinger}} \lesssim B \leqslant 6.5 \times 10^6$ a.u., as well as toward decay to $\mathrm{He_2}^{3+} + \mathrm{p}$ for all magnetic fields studied. It is worth noting that, in spite of the greater Coulomb repulsion, the system $(\mathrm{He\text{-}H\text{-}He})^{4+}$ becomes more bound than $(\mathrm{H\text{-}He\text{-}H})^{3+}$ for magnetic fields $B \gtrsim 1.8 \times 10^6$ a.u. The last exotic molecular system, $\mathrm{He_3}^{5+}$, appears at $B \gtrsim 10^6$ a.u. This system is unstable with respect to decay into $\mathrm{He_2}^{3+} + \alpha$. The present level of available computational resources does allow a reliable conclusion to be drawn about this molecular system at larger magnetic fields. No more one-electron helium-hydrogenic systems are seen for the range of magnetic fields studied at $B \leqslant 10^7$ a.u.

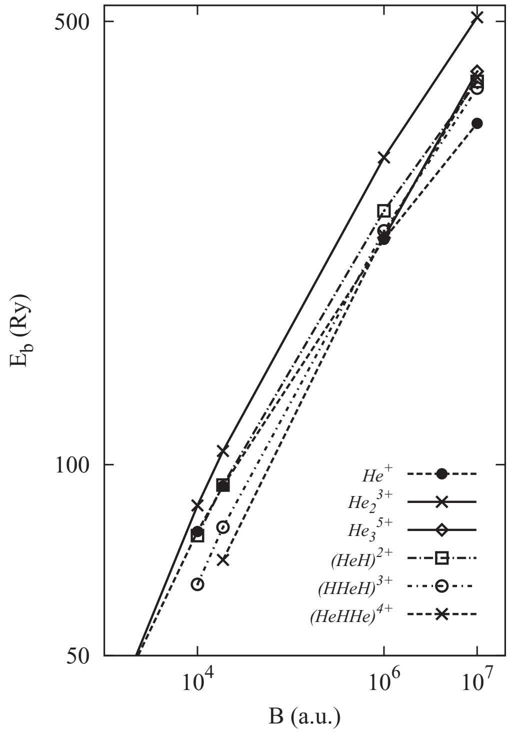

FIG. 5. Binding energies E_b for the one-electron helium-hydrogen linear molecular ions in parallel configuration vs a magnetic field $\mathbf{B}$.

Concrete variational calculations for the chains ${He_2}^{3+}$ and $(HeH)^{2+}$ demonstrate that the optimal geometry of the molecular systems is linear and aligned along the magnetic field, and it is stable with respect to small deviations from linearity. This is understood by simple argument since any slight deviation from the magnetic field direction leads to a large increase in the rotational energy. Therefore, it is natural to assume that all other studied linear chains are also stable with respect to small deviations from linearity.

All studied finite chains are characterized by two features: with a magnetic field growth, (i) their total energies increase and (ii) their equilibrium size decreases; each system becomes more bound and compact.

Summarizing, one can state that among the one-electron helium-hydrogen chains there are two helium systems characterized by the lowest total energy for different magnetic fields: the He^+ ion at $0 \lesssim B \lesssim 2 \times 10^3$ a.u. and the ${He_2}^{3+}$ chain at $2 \times 10^3 \lesssim B \lesssim 10^7$ a.u.

V. TWO-ELECTRON HELIUM AND HELIUM-HYDROGEN CHAINS

A. Generalities

Let us consider systems of two electrons and n infinitely massive α particles situated on a line that coincides with the magnetic line. If a bound state is found, the system is called a $2e$ linear helium chain of length n, indicating the existence of the ion $He_n^{(2n-2)+}$ in linear geometry.

The Hamiltonian that describes systems of two electrons and a number of α particles with a magnetic field oriented along the z direction, $\mathbf{B} = (0, 0, B)$, is given by Hamiltonian (6) with $Z_i = Z_j = 2$.

All performed calculations show that in the optimal geometry the chain possesses a symmetry property similar to that for two-electron hydrogenic chains: for any α particle there is a partner situated symmetrically with respect to the center of the chain.

We also study mixed systems: out of n heavy centers, some have the charge 2 (α particles) and some have the charge 1 (protons). If a bound state is found, the system is called a $2e$ linear helium-hydrogen chain of length n.

B. Method

For these systems we follow a treatment similar to that for the case of two-electron hydrogenic chains. The variational procedure is used to explore the problem. Physical relevance arguments are followed to choose the trial function (see, e.g., [10]), which is given by function (7).

1. $n = 1$

(αee). This case is only mentioned for the sake of completeness. It is known that the helium atom exists for any magnetic field strength [18]. At zero field and for small magnetic fields $B \lesssim 0.75$ a.u., the spin-singlet state $1^1 0^+$ is the ground state. For $B \gtrsim 0.75$ a.u., the spin-triplet state $1^3(-1)^+$ becomes the ground state. The neutral helium atom is the least bound system among two-electron Coulomb systems made from α particles (see Tables VII and VIII).

2. $n = 2$

(i) ($\alpha\alpha ee$). The ${He_2}^{2+}$ molecule was studied in detail in [16] in a magnetic field $B = 0$–4.414×10^{13} G. It was shown that the lowest total energy state depends on the magnetic field strength. Similarly to the case of *ppee*, it evolves from the spin-singlet ${}^1\Sigma_g$ metastable state at $0 \leqslant B \lesssim 0.85$ a.u. to a repulsive spin-triplet ${}^3\Sigma_u$ state (unbound state) for $0.85 \lesssim B \lesssim 1100$ a.u. and, finally, to a strongly bound spin-triplet ${}^3\Pi_u$ state. Hence, there exists quite a large domain of magnetic fields where the ${He_2}^{2+}$ molecule is unbound and represented by two atomic helium ions in the same electron spin state but situated at an infinite distance from each other. The optimal geometry of the ${He_2}^{2+}$ molecule (when it exists) always corresponds to the elongation along a magnetic line forming a finite chain. It is assumed that the chain in the ${}^3\Pi_u$ state is stable toward the deviation from linearity. This chain is stable (or metastable) for all studied magnetic fields. However, this chain has a total energy higher than the ${He_3}^{4+}$ chain (see following discussion) for $B \gtrsim 3 \times 10^4$ a.u. and, thus, is less preferable energetically.

(ii) (αpee). This system is the simplest $2e$ mixed helium-hydrogen system. A detailed study of the low-lying electronic states ${}^1\Sigma$, ${}^3\Sigma$, ${}^3\Pi$, and ${}^3\Delta$ of the HeH^+ ion was carried out in [17]. The ground state evolves from the spin-singlet ${}^1\Sigma$ state for small magnetic fields $B \lesssim 0.5$ a.u. to the spin-triplet ${}^3\Sigma$ (unbound or weakly bound) state for intermediate fields

TABLE VII. Double ionization energies E_I in rydbergs for the ground state ${}^3\Pi_u$ of the two-electron helium and helium-hydrogenic linear systems (finite chains) in a strong magnetic field [the ground state for $(HeH)^+$ is ${}^3\Pi$].

System \ B(a.u.)	10^2	10^3	10^4	4.414×10^{13} (G)	10^5	10^6	10^7
He	25.65	54.37	106.4	126.0	191.4	319.7	494.3
${He_2}^{2+}$	33.98	80.49	174.51	212.14	343.47	616.68	1016.75
${He_3}^{4+}$	26.58	68.93	163.90	202.60	352.50	684.19	1212.40
${He_4}^{6+}$					272.07	576.85	1089.89
HeH^+	28.36	64.24	133.49	160.50	253.22	440.24	709.65
$(H\text{-}He\text{-}H)^{2+}$			142.40	172.58	279.39	509.99	843.38
$(He\text{-}H\text{-}He)^{3+}$			153.62	190.22	320.63	603.91	1029.95
$(H\text{-}He\text{-}He\text{-}H)^{4+}$					275.	585.0	979.1
$(He\text{-}H\text{-}H\text{-}He)^{4+}$					223.	510.4	885.2

TABLE VIII. Internuclear equilibrium distances (in a.u.) for the ground state $^3\Pi_u$ of the two-electron helium linear systems (finite chains) in a strong magnetic field [the ground state for $(\mathrm{HeH})^+$ is the $^3\Pi$ state]. All configurations [except for $(\mathrm{HeH})^+$] have center of symmetry, and symmetric internuclear distances are not displayed.

System \ B(a.u.)	10^2	10^3	10^4	4.414×10^{13} (G)	10^5	10^6	10^7
$\mathrm{He}_2{}^{2+}(R)$	0.463	0.212	0.106	0.0902	0.060	0.0353	0.023
$\mathrm{He}_3{}^{4+}(R, R)$	0.67, –	0.27, –	0.122, –	0.116, –	0.063,–	0.0358,–	0.023,–
$\mathrm{He}_4{}^{6+}(R_1, R_2, R_1)$					0.089,0.060,–	0.047, 0.037,–	0.030,0.023,–
HeH^+	0.440	0.203	0.104	0.092	0.0585	0.0356	0.0238
$(\mathrm{H\text{-}He\text{-}H})^{2+}(R_1, R_1)$			0.105, –	0.092, –	0.059,–	0.035,–	0.022,–
$(\mathrm{He\text{-}H\text{-}He})^{3+}(R_1, R_1)$			0.095, –	0.081, –	0.051,–	0.030,–	0.018,–
$(\mathrm{H\text{-}He\text{-}He\text{-}H})^{4+}$ (R_1, R_2, R_1)					0.07, 0.10,–	0.047, 0.030,–	0.027, 0.015,–
$(\mathrm{He\text{-}H\text{-}H\text{-}He})^{4+}$ (R_1, R_2, R_1)					0.08, 0.12,–	0.041, 0.025,–	0.025, 0.019,–

and to the spin-triplet strongly bound $^3\Pi$ state for $B \gtrsim 15$ a.u. When the HeH^+ molecular ion exists, it is stable with respect to dissociation. In the domain $B \gtrsim 15$ a.u., the optimal geometry is linear and parallel: the ion is elongated along a magnetic line. Hence, the chain is formed. With a magnetic field increase, the chain gets more bound and more compact. At magnetic fields $B < 10^4$ a.u., the double ionization energy E_I of the HeH^+ ion is smaller but comparable to that of the $\mathrm{He}_2{}^{2+}$ ion. However, for $B > 10^4$ a.u., E_I gets, in fact, the smallest value among $2e$ helium-contained molecular ions.

3. $n = 3$

(i) $(\alpha\alpha\alpha ee)$. In the field-free case, the system $(\alpha\alpha\alpha ee)$ does not display any binding. However, for magnetic fields $B \gtrsim 100$ a.u., the $\mathrm{He}_3{}^{4+}$ molecule becomes bound in the linear configuration aligned along the magnetic line. For $100 \lesssim B \lesssim 1000$ a.u., the $^3\Sigma_u$ state is the ground state [19]. This state is a metastable state for any magnetic field; its total energy lies above the total energies of its lowest dissociation channel. For $B \gtrsim 1000$ a.u., the state $^3\Pi_u$ is the ground state. For magnetic fields $1000 \lesssim B \lesssim 3 \times 10^4$ a.u., the total energy of the dominant dissociation channel $\mathrm{He}_3{}^{4+} \to \mathrm{He}_2{}^{2+}(^3\Pi_u) + \alpha$ is lower than the total energy of the $\mathrm{He}_3{}^{4+}$ ion in the $^3\Pi_u$ state. Thus, in this range of magnetic fields, the ion $\mathrm{He}_3{}^{4+}(^3\Pi_u)$ is a metastable state toward the lowest channel of decay. Hence, for magnetic fields $B \gtrsim 3 \times 10^4$ a.u., the molecular ion $\mathrm{He}_3{}^{4+}$ is stable in the $^3\Pi_u$ state. With an increase of the magnetic field strength, the total energy at the equilibrium position decreases, and the system becomes more bound (in this case, the double ionization energy is $E_I = -E_T$; it increases with B) and more compact (the internuclear equilibrium distance decreases with B).

(ii) $(p\alpha pee)$. In the field-free case, the system $(p\alpha pee)$ does not display any binding. However, for magnetic fields $B \gtrsim 10^4$ a.u., the $(\mathrm{H\text{-}He\text{-}H})^{2+}$ ion becomes bound in the linear configuration aligned along the magnetic line with the $^3\Pi_u$ state as the ground state. This ion is stable.

(iii) $(\alpha p\alpha ee)$. In the field-free case, the system $(\alpha p\alpha ee)$ does not display any binding. However, for magnetic fields $B \gtrsim 10^4$ a.u., the $(\mathrm{He\text{-}H\text{-}He})^{3+}$ ion becomes bound in the linear configuration aligned along the magnetic line with the $^3\Pi_u$ state as the ground state. This ion is unstable toward a decay to $\mathrm{He}_2{}^{2+}(^3\Pi_u) + p$; however, at $B > 10^6$ a.u., the ion $(\mathrm{He\text{-}H\text{-}He})^{3+}$ becomes stable.

4. $n = 4$

(i) $(4\alpha 2e)$. In the field-free case, the system $(4\alpha 2e)$ does not display any binding. However, for magnetic fields $B \gtrsim 10^5$ a.u., the $\mathrm{He}_4{}^{6+}$ molecule becomes bound in the linear configuration aligned along the magnetic line with the $^3\Pi_u$ state as the ground state. With an increase of the magnetic field strength, the total energy at the equilibrium position decreases, and the system becomes more bound (in this case, the double ionization energy is $E_I = -E_T$; it increases with B) and more compact (the internuclear equilibrium distance decreases with B). For magnetic fields $B \gtrsim 10^5$ a.u., the total energy of the dominant dissociation channel $\mathrm{He}_3^{4+}(^3\Pi_u) + \alpha$ is lower than the total energy of the $\mathrm{He}_4^{6+}(^3\Pi_u)$ ion. Thus, the ion $\mathrm{He}_4^{6+}(^3\Pi_u)$ is a metastable state toward the lowest channel of decay. It is also unstable toward decay to $\mathrm{He}_2{}^{2+}(^3\Pi_u) + 2\alpha$ for magnetic fields $10^5 \lesssim B \lesssim 2 \times 10^6$ a.u.

(ii) $(p\alpha\alpha p2e)$. In the field-free case, the system $(p\alpha\alpha p2e)$ does not display any binding. However, for magnetic fields $B > 10^5$ a.u., the $(\mathrm{H\text{-}He\text{-}He\text{-}H})^{4+}$ molecule becomes bound in the linear configuration aligned along the magnetic line with the $^3\Pi_u$ state as the ground state. With an increase of the magnetic field strength, the system becomes more bound (the double ionization energy increases with B) and more compact; that is, both the internuclear equilibrium distance R_1 between a proton and the closest α particle, and the distance R_2 between the two α particles, decrease with B. For magnetic fields $B \gtrsim 10^5$ a.u., the total energy of the dominant dissociation channel $\mathrm{He}_2{}^{2+}(^3\Pi_u) + 2p$ is lower than the total energy of the $(\mathrm{H\text{-}He\text{-}He\text{-}H})^{4+}$ ion. Thus, the $(\mathrm{H\text{-}He\text{-}He\text{-}H})^{4+}$ is a metastable state toward the lowest channel of decay.

(iii) $(\alpha pp\alpha 2e)$. In the field-free case, the system $(\alpha pp\alpha 2e)$ does not display any binding. However, for magnetic fields $B > 10^5$ a.u., the $(\mathrm{He\text{-}H\text{-}H\text{-}He})^{4+}$ molecular ion becomes bound in the linear configuration aligned along the magnetic line with the $^3\Pi_u$ state as the ground state. With an increase of

TABLE IX. Two-electron five-center molecular ions (finite chains) in a magnetic field in ${}^3\Pi_u$ state-symmetric, spin-triplet configuration parallel to the magnetic field direction. E_T and E_I are total and double ionization energy, respectively. For unbound states a characteristic total energy is indicated.

		$E_T = -E_I$ (Ry)	
Composition	Configuration	$B = 10^6$ a.u.	$B = 10^7$ a.u.
$1\alpha\ 4p$	H-H-He-H-H	Unbound ~ -450	Bound -866.0 ($R_1 = 0.0228$, $R_2 = 0.0203$ a.u.)
$2\alpha\ 3p$	He-H-H-H-He	Bound -414.5	Bound -792.6
	H-He-H-He-H	Bound -485.3	Bound -873.9 ($R_1 = 0.0306$, $R_2 = 0.0189$ a.u.)
$3\alpha\ 2p$	He-H-He-H-He	Unbound ~ -420	"Bound"[a] ~ -860.0 ($R_1 = 0.023$, $R_2 = 0.018$ a.u.)
	H-He-He-He-H	Unbound ~ -620	Unbound ~ -1055
$4\alpha\ 1p$	He-He-H-He-He	Unbound ~ -380	Bound -862.4 ($R_1 = 0.0356$, $R_2 = 0.0195$ a.u.)

[a] "Bound" means that the potential surface of the $3\alpha\ 2p$ system has a local minimum which corresponds to the configuration $\alpha - p - \alpha - p - \alpha$ where the global minimum corresponds to the configuration $p - \alpha - \alpha - \alpha - p$.

the magnetic field strength, the system becomes more bound (the double ionization energy increases with B) and more compact; that is, both the internuclear equilibrium distance R_1 between a proton and the closest α particle, and the distance R_2 between the two protons, decrease with B. For magnetic fields $B \gtrsim 10^5$ a.u., the total energy of the dominant dissociation channel $\mathrm{He}_2{}^{2+}({}^3\Pi_u) + 2p$ is lower than the total energy of the (He-H-H-He)$^{4+}$ molecular ion and, thus, is a metastable state toward the lowest channel of decay.

5. $n = 5$

The results of the analysis of five-center, two-electron systems are shown in Table IX. An indication of binding of the proton-free systems ($5\alpha 2e$) is not found for the whole domain of studied magnetic fields, whereas ($4\alpha p 2e$) becomes bound at $B \sim 10^7$ a.u. and is unstable, decaying toward many different finite chains. The system ($3\alpha 2p 2e$) is unbound, although a particular configuration ($\alpha p \alpha p \alpha 2e$) displays a minimum in the potential curve. The two α-contained systems are bound in both symmetric configurations—($p\alpha p \alpha p 2e$) and ($\alpha p p p \alpha 2e$)—while the latter one is more bound even for a magnetic field $B \sim 10^6$ a.u. This system is unstable with a dominant decay mode to ($\alpha p \alpha 2e$). One α-contained system ($pp\alpha pp 2e$) is bound at $\sim 10^7$ a.u. and it is stable. It is worth noting that the system $5p2e$ is bound for magnetic fields $B \gtrsim 10^4$ a.u. (see Table III and our earlier discussion).

6. $n = 6$

An indication of the bound state of any six-center system is not found even for the highest magnetic field studied.

C. Results

The results of the calculations are presented in Tables VII–IX and illustrated in Fig. 6. Three traditional systems, He, $\mathrm{He}_2{}^{2+}$, and HeH^+, exist for all studied magnetic fields $10^2 \leqslant B \leqslant 10^7$ a.u. The first exotic molecular system, $\mathrm{He}_3{}^{4+}$, appears at ~ 100 a.u. in linear configuration and exists for larger magnetic fields. For $100 \lesssim B \lesssim 5 \times 10^4$ a.u., the $\mathrm{He}_3{}^{4+}$ ground state is a metastable state with respect to its lowest dissociation channel. For magnetic fields $B > 5 \times 10^4$ a.u., the ground state of system $\mathrm{He}_3{}^{4+}$ becomes a strongly bound state. Another exotic molecular system, $\mathrm{He}_4{}^{6+}$, appears at $\sim 10^5$ a.u. as a metastable state. No other two-electron molecular helium systems are seen for $B \leqslant 10^7$ a.u. At large magnetic field, the ground state of all studied systems is the spin-triplet state with spin projection $m_s = -1$ and total magnetic quantum number $m = -1$. For $n > 1$, the optimal geometry of the molecular system is linear, and the system is aligned along the magnetic field. Thus, each molecular system forms a finite chain. Such a linear configuration is concluded to be stable with respect to small vibrations, and its vibrational energies can be calculated. However, we were not able to check the stability of the configuration with respect to small deviations from linearity or to calculate the rotational energies. All studied finite chains are characterized by two features: with magnetic field growth, (i) their binding energies increase and (ii) their longitudinal lengths decrease; each system becomes more bound and compact.

It is worth noting that, among two-electron helium finite chains, the system $\mathrm{He}_2{}^{2+}$ in spin-triplet ${}^3\Pi_u$ state has the lowest total energy in the domain $10^2 \lesssim B \lesssim 3 \times 10^4$ a.u.,

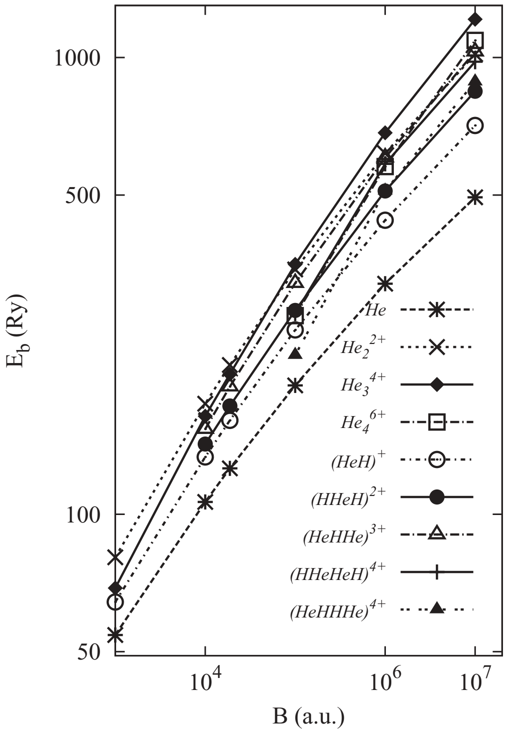

FIG. 6. Double ionization energies E_I for the two-electron helium-hydrogen linear molecular ions in parallel configuration vs a magnetic field **B**.

whereas at larger magnetic fields of $3 \times 10^4 \lesssim B \lesssim 10^7$ a.u., the finite chain He_3^{4+} in spin-triplet $^3\Pi_u$ state acquires the lowest total energy. In the domain $2 \times 10^6 \lesssim B \lesssim 10^7$ a.u., all studied two-electron finite helium chains that were studied become stable with the only exception of He_4^{6+}.

VI. CONCLUSIONS

A complete nonrelativistic classification of one- and two-electron finite molecular chains (polymers) made out of protons and/or α particles in a strong magnetic field is presented. It is naturally assumed that the ground state of any one-electron chain is $1\sigma_g$ (or 1σ for nonsymmetric systems), whereas for any two-electron chain the ground state is spin-triplet $^3\Pi_u$ (or $^3\Pi$ for nonsymmetric systems). All calculations were carried out in variational methods with state-of-the-art trial functions. Protons and α particles are assumed to be infinitely massive and situated along a magnetic line.

The existence of three magnetic field thresholds is clearly seen:[3]

$$B_t^{(1)} \sim 10^2 \text{ a.u.}, \quad B_t^{(2)} \sim 10^4 \text{ a.u.}, \quad B_t^{(3)} \sim 10^6 \text{ a.u.}$$

At magnetic fields $B \lesssim 10^2$ a.u., only the traditional ions, atoms, and molecules can exist, and the chains are not well pronounced—they are very short and contain at most two heavy particles. However, at $10^2 < B < 10^4$ a.u., several new exotic ions appear in addition to the traditional ones. All ions immediately form strongly bound linear chains aligned along a magnetic field. At $B \sim 10^4$ a.u., several more new exotic ions appear, quickly forming linear chains. Then a similar appearance of new exotic ions happens at $B \sim 10^6$ a.u. It is quite interesting that the ions which already appeared (existed) below some magnetic field threshold, become stable above the threshold. It is worth noting that for a fixed magnetic field the neutral systems are always the least bound ones.

In conclusion we present a list of 1-2e proton and/or α particle-contained ions for which certain magnetic fields exist where they are stable: H, $H_2{}^+$, $H_3{}^{2+}$, He^+, $He_2{}^{3+}$, $(HeH)^{2+}$, and H^-, H_2, $H_3{}^+$, $H_4{}^{2+}$, $H_5{}^{3+}$, He, $He_2{}^+$, $He_3{}^{4+}$, $(HeH)^+$, $(HHeH)^{2+}$, $(HeHHe)^{3+}$, $(HHHeHH)^{4+}$. These are among the 25 Coulomb 1-2e systems which (can) exist in a magnetic field (see Tables I–IX).

All presented results were obtained in a nonrelativistic way with an assumption that masses of heavy particles are infinite. They can be considered an indication of a new atom-molecular physics in magnetic fields $B \gtrsim 10^2$ a.u. This study encourages us to explore finite mass effects in a magnetic field. This issue looks quite complicated technically due to the absence of a separation of variables (see, e.g., [20]), especially in the case of more than two particles and nonzero total charge of the system. Those two cases are exactly the ones that are the most important from the point of view of obtained results: the most bound systems usually contain more than two bodies and are charged. Another important issue is related to relativistic corrections of our nonrelativistic results. Although in our understanding the Duncan qualitative argument [9] is physically sound, it should be improved and, eventually, it needs to be checked quantitatively. The current authors plan to study both issues in the near future.

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[3] A notion of the existence of the molecule in the Born-Oppenheimer approximation is ambiguous (for a discussion, see [12]). In one definition it is enough for the existence if a potential curve has a minimum; in the other one the existence of at least one vibrational and one rotational state is required. We follow the first definition, however, localizing a moment of the appearance of the minimum of the potential curve very approximately.

[1] M. A. Liberman and B. Johansson, Sov. Phys. Usp. Fiz. Nauk **165**, 121 (1995) [Sov. Phys. Usp. **38**, 117 (1995)].

[2] D. Lai, Rev. Mod. Phys. **73**, 629 (2001), e-print arXiv:astro-ph/0009333.

[3] A. V. Turbiner and J. C. López Vieyra, Phys. Rep. **424**, 309 (2006).

[4] B. B. Kadomtsev and V. S. Kudryavtsev, Pis'ma Zh. Eksp. Teor. Fiz. **13**, **15**, 61 (1971) [Sov. Phys. JETP Lett. **13**, **9**, 42 (1971)]; Zh. Eksp. Teor. Fiz. **62**, 144 (1972) [Sov. Phys. JETP **35**, 76 (1972)].

[5] M. Ruderman, Phys. Rev. Lett. **27**, 1306 (1971); in *IAU Symposium 53, Physics of Dense Matter*, edited by C. J. Hansen (Reidel, Dordrecht, 1974), p. 117.

[6] A. V. Turbiner, Astrophys. Space Sci. **308**, 267 (2007).

[7] T. Detmer, P. Schmelcher, and L. S. Cederbaum, Phys. Rev. A **57**, 1767 (1998).

[8] A. V. Turbiner, N. L. Guevara, and J. C. López Vieyra, Astrophys. Space Sci. **308**, 493 (2007); Phys. Rev. A **75**, 053408 (2007), e-print arXiv:physics/0606083.

[9] Robert C. Duncan, e-print arXiv:astro-ph/0002442.

[10] 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)]; Sc.D. thesis, ITEP, Moscow, 1989 (unpublished).

[11] A. Y. Potekhin and A. V. Turbiner, Phys. Rev. A **63**, 065402 (2001), e-print arXiv:physics/0101050.

[12] G. Herzberg, *Molecular Spectra and Molecular Structure. I. Spectra of Diatomic Molecules*, 2nd ed. (Krieger, Malabar, FL, 1989).

[13] O.-A. Al Hujaj and P. Schmelcher, Phys. Rev. A **61**, 063413 (2000).

[14] A. V. Turbiner, J. C. López Vieyra, and N. L. Guevara (unpublished).

[15] A. V. Turbiner and J. C. López Vieyra, Int. J. Mod. Phys. A **22**, 1605 (2007).

[16] A. V. Turbiner and N. L. Guevara, Phys. Rev. A **74**, 063419 (2006), e-print arXiv:astro-th/0610928.

[17] A. V. Turbiner and N. L. Guevara, J. Phys. B **40**, 3249 (2007), e-print arXiv:physics/0703090.

[18] W. Becker and P. Schmelcher, J. Phys. B **33**, 545 (2000).

[19] A. V. Turbiner, J. C. López Vieyra, and N. L. Guevara (unpublished).

[20] L. P. Gor'kov and I. E. Dzyaloshinskii, Sov. Phys. JETP **26**, 449 (1968).