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$He_2{}^+$ molecular ion and the He^- atomic ion in strong magnetic fields

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We study the question of existence, i.e., stability with respect to dissociation of the spin-quartet permutation- and reflection-symmetric ${}^4(-3)^+{}_g$ ($S_z = -3/2, M = -3$) state of the ($\alpha\alpha eee$) Coulomb system: the $He_2{}^+$ molecular ion, placed in a magnetic field $0 \leqslant B \leqslant 10\,000$ a.u. We assume that the α particles are infinitely massive (Born-Oppenheimer approximation of zero order) and adopt the parallel configuration, when the molecular axis and the magnetic field direction coincide, as the optimal configuration. The study of the stability is performed variationally with a physically adequate trial function. To achieve this goal, we explore several helium-containing compounds in strong magnetic fields, in particular; we study the spin-quartet ground state of the He^- ion and the ground (spin-triplet) state of the helium atom, both for a magnetic field in $100 \leqslant B \leqslant 10\,000$ a.u. The main result is that the $He_2{}^+$ molecular ion in the state ${}^4(-3)^+{}_g$ is stable towards *all* possible decay modes for magnetic fields $B \gtrsim 120$ a.u. and with the magnetic field increase the ion becomes more tightly bound and compact with a cigar-type form of electronic cloud. At $B = 1000$ a.u., the dissociation energy of $He_2{}^+$ into $He^- + \alpha$ is ~702 eV and the dissociation energy for the decay channel to $He + \alpha + e$ is ~729 eV, and both energies are in the energy window for one of the observed absorption features of the isolated neutron star 1E1207.4-5209.

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I. INTRODUCTION

It seems obvious that the chemical composition of the atmosphere of a magnetic white dwarf or a magnetized neutron star cannot be established as long as we lack reliable information about the behavior of many-body Coulomb systems, especially about simple molecules and atoms in the presence of strong magnetic fields. So far, only hydrogen- and helium-like atomic systems, and $H_2{}^+$-type molecular systems, have been studied to a certain depth. There are indications that in addition to traditional atoms and molecules, other nonstandard, exotic atomic and molecular systems can also exist in strong magnetic fields (see, for example, Refs. [1,2]). In a recent discovery [3], it was found that even the He^- atomic ion becomes stable for magnetic fields $B \gtrsim 0.13$ a.u. with the spin doublet state ${}^2(-1)^+$ as ground state at first, and then for $B \gtrsim 0.74$ a.u. all electron spins get aligned and antiparallel to a magnetic field direction: The corresponding state ${}^4(-3)^+$ becomes the ground state of the system (see also Ref. [4]). It happens in spite of the fact that helium belongs to the most inert (closed-shell) atomic systems. Needless to say, helium has a rich chemistry even in the absence of intense magnetic fields (see, e.g., Ref. [5]).

Usually, investigations of the Coulomb systems in strong magnetic fields (unreachable in the laboratory) are justified by the fact there exists a strong magnetic field on the surface of many neutron stars $B \sim 10^{11\text{–}13}$ G and of some highly magnetized white dwarfs $B \sim 10^{8\text{–}9}$ G; see, e.g., Ref. [6]. In general, magnetic fields can reach $B \sim 10^{15}$ G, or even higher, in the case of the so-called magnetars, the neutron stars with anomalously large surface magnetic fields. While there is the evidence for the presence of helium in the atmosphere of magnetic white dwarfs [7], there is no similar understanding about helium in any form in atmospheres of neutron stars or their chemical content in general that can satisfactorily explain the observations.

The discovery of absorption features at ~0.7 and ~1.4 keV in the x-ray spectrum of the isolated neutron star 1E1207.4-5209 by Chandra X-ray Observatory [8] and its further confirmation by XMM-Newton X-ray Observatory [9] motivated us to perform studies of atoms and molecules in a strong magnetic field. At present, there is a number of neutron stars whose atmospheres are characterized by absorption features: All of them are waiting to be solidly explained. These observations make clear that a detailed study of traditional atomic-molecular systems is needed, as well as for a search for new exotic chemical compounds which exist in a strong magnetic field only (see, e.g., Refs. [10–13]).

As a result of such investigations, a model of the helium-hydrogenic molecular atmosphere of the neutron star 1E1207.4-5209 was proposed which is based on the assumption that the most abundant components in the atmosphere are the exotic molecular ions $He_2{}^{3+}$ and $H_3{}^{2+}$, with the presence of He^+,$(HeH)^{2+}$,$H_2{}^+$ subject to a surface magnetic field $\approx 4.4 \times 10^{13}$ G (see Ref. [14]). Conjectures about the absence of hydrogen envelopes in some neutron stars have also motivated the study of atmospheres composed of neutral helium. However, those simple models appear to be in conflict with observations. Models of atmosphere, composed with a large abundance of molecular systems containing helium, have been later suggested (see Refs. [14,15] and references therein). For reasons which are not completely clear to the present authors, it has been emphasized [15] that the $He_2{}^+$ molecule has to play a particularly important role. This molecular system exists in a field-free case in the spin-doublet, nuclei-permutation-antisymmetric (u), reflection-symmetric (with respect to any plane containing the internuclear axis) (+) ground state ${}^20_u^+$ [16], usually denoted as ${}^2\Sigma_u^+$. It is a rather compact system characterized by a small dissociation energy ~2.5 eV into $He^+({}^2S) + He({}^1S)$, see Table I. The lowest spin-doublet, nuclei-permutation-symmetric (g) excited state

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TABLE I. $He_2{}^+$, field-free case: First row → energy and equilibrium distance ($\star$) for the ground state $^2\Sigma_u$ and excited state $^2\Sigma_g$ calculated with a trial function (9). Second row → the energies calculated at the equilibrium distance taken from Refs. [37,38]. Third row → energy (rounded) and equilibrium distance for $^2\Sigma_u$ from Ref. [37] [a] and for $^2\Sigma_g$ from Ref. [38] [b].

$^2\Sigma_u$		$^2\Sigma_g$	
E (a.u.)	R_{eq} (a.u.)	E (a.u.)	R_{eq} (a.u.)
−4.955243	2.15 ($\star$)	−4.8653	8.61 ($\star$)
−4.953765	2.042	−4.8651	8.742
−4.994644	2.042[a]	−4.9036	8.742[b]

TABLE II. Total energies and equilibrium distances (in a.u.) for spin $S = 1/2$ states of the $He_2{}^+$ ion in a magnetic field $B = 100$ a.u., in parallel configuration calculated with a trial function (9). For $M = -1$ the configuration, $m_1,m_2,m_3 = -1,0,0$ was used in the trial function. The energy of the spin-3/2 state ($M = -3$ with $m_1,m_2,m_3 = 0,-1,-2$) included for comparison.

	$S = 1/2$				$S = 3/2$
	$M = 0$		$M = -1$		$M = -3$
	g	u	g	u	g
E (a.u.)	76.13	76.27	69.57	66.84	−22.46
R (a.u.)	1.85	0.79	0.279	0.79	0.432

$^20^+{}_g$ [16], usually denoted as $^2\Sigma_g^+$, is repulsive. It is essentially unbound with shallow van der Waals minimum at large internuclear distance; see Ref. [5] and references therein. It took us a number of years to perform a quantitative study of this particular system in the presence of a strong magnetic field, which is the subject of the present work. We are not aware of any similar previous study.

It is quite common in the field-free case that the ground state of simple atoms and molecules be characterized by the lowest possible total electron spin. Since the first qualitative studies of atomic and molecular systems [17–22], it became clear that in sufficiently strong magnetic fields the ground state is eventually realized by a state where the spins of all electrons are antiparallel to the magnetic field direction. Thus, the total electron spin takes maximal value as well as its total projection. It implies that the ground state depends on the magnetic field strength: There exists one (or several) threshold (critical) magnetic field(s) for which one type of ground state changes to another one. This phenomenon was quantitatively observed for the first time for the H_2 molecule. It was shown that spin-singlet ground state $^1\Sigma_g$, for small magnetic field, changes for intermediate fields $B \gtrsim 0.2$ a.u. to the unbound (repulsive) $^3\Sigma_u$ state as the ground state (precisely in the domain of magnetic fields typical of magnetic white dwarfs), while for stronger magnetic fields $B \gtrsim 12.3$ a.u., the ground state of the hydrogen molecule is realized by spin-triplet state $^3\Pi_u$ (see Ref. [23] and references therein). Another recent example, which was mentioned above, is the case of the He^- atomic ion where the ground state is realized first by the spin doublet state $^2(-1)^+$ for $B \gtrsim 0.13$ a.u., and later by the spin-quartet state $^4(-3)^+$, for magnetic fields $B \gtrsim 0.74$ a.u., where all electron spins are aligned antiparallel to a magnetic field direction. In general, the phenomenon of change of the ground-state nature with a magnetic field strength in traditional atomic systems was known since a time ago; see, e.g., Ref. [24] and reference therein.

The aim of this article is to perform a variational study of the $He_2{}^+$ molecular ion subject to a strong magnetic field in the state $^4(-3)^+{}_g$, when all electron spins get oriented antiparallel to the magnetic field direction and the electronic total angular momentum projection is equal to $M = -3$,[1] and to show that the system is *stable* towards all possible decays or dissociation. Further, it is naturally assumed that $^4(-3)^+{}_g$ is the ground state. Due to extreme technical complexity, we do not discuss other states of $He_2{}^+$ and leave the question about evolution of the type of the ground state with magnetic field changes for a future publication. However, for a strong magnetic field of $B = 100$ a.u., we carried out variational calculations for the energy of the spin $S = 1/2$ states with $M = 0,-1$, both gerade and ungerade. A comparison with the energy of the spin $S = 3/2$ state, indicates indeed, that for this magnetic field, the spin $S = 3/2$ realizes the (unstable) ground state of $He_2{}^+$, see Table II. Since our study is limited to the question of the existence and stability of this system in a certain state, our main attention is devoted to the exploration of all possible decay channels. A natural assumption about the optimal (equilibrium) configuration with minimal total energy is one which is achieved in the parallel configuration, where the internuclear axis connecting the two massive α particles (He nuclei) is situated along the magnetic line.

Another aim of the article is to continue to study the He^- atomic ion in spin-quartet state $^4(-3)^+$ for strong magnetic fields $B \geqslant 1$ a.u., which was initiated in Ref. [3]. This study is necessary due to the possible decay mode $He_2{}^+$ into $He^- + \alpha$.

The consideration is nonrelativistic, based on a variational solution of the Schrödinger equation. The magnetic field strength is restricted to magnetic fields $B \leqslant 10\,000$ a.u. ($=2.35 \times 10^{13}$ G) below the relativistic Schwinger limit. Also, it is based on the Born-Oppenheimer approximation of zeroth order: The particles of positive charge (α particles) are assumed to be infinitely massive.

Atomic units are used throughout ($\hbar = m_e = e = 1$). The magnetic field B is given in a.u., with $B_0 = 2.35 \times 10^9$ G. For energies given in eV, the conversion 1 a.u. = 27.2 eV was used. All energies which are mentioned in the article are the total energies (with spin terms included) if it is not indicated otherwise.

II. $He_2{}^+$ HAMILTONIAN

The nonrelativistic Hamiltonian for a three-electron diatomic molecule with fixed nuclei A,B in uniform constant

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[1] To avoid a contradiction with the Pauli principle, and thus the appearance of the Pauli forces, it is further assumed that all three electrons have different magnetic quantum numbers, i.e., $m_1 = 0$, $m_2 = -1$, $m_3 = -2$.

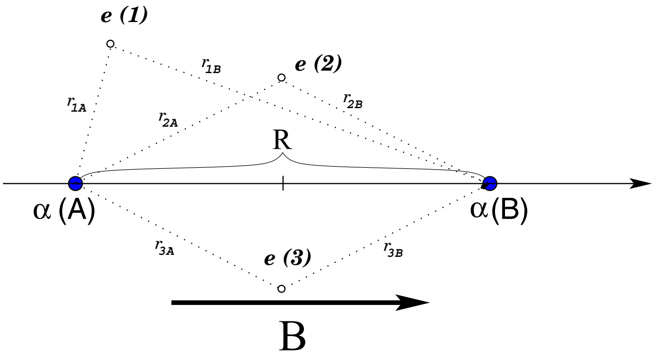

FIG. 1. Geometrical setting and notations for the $He_2{}^+$ molecular ion in the presence of a magnetic field **B** aligned parallel to the molecular axis.

magnetic field $\boldsymbol{B} = B\boldsymbol{e}_z$, directed along z axis with vector potential in the symmetric gauge $\mathbf{A} = \frac{1}{2}\mathbf{B} \times \mathbf{r}$ is given by

$$\mathcal{H} = -\sum_{i=1}^{3}\left(\frac{1}{2}\nabla_i^2 + \sum_{\eta=\mathsf{A},\mathsf{B}} \frac{Z_\eta}{r_{i\eta}}\right) + \sum_{i=1}^{3}\sum_{j>i}^{3} \frac{1}{r_{ij}} + \frac{B^2}{8}\sum_{i=1}^{3} {\rho_i}^2 + \frac{B}{2}(\hat{L}_z + 2\hat{S}_z) + \frac{Z_\mathsf{A} Z_\mathsf{B}}{R}, \qquad (1)$$

where ∇_i is the 3-vector of the momentum of the ith electron, Z_η is the charge of the nucleus $\eta = \mathsf{A},\mathsf{B}$, the terms $-Z_\eta/r_{i\,\eta}$, correspond to the Coulomb interactions of the electrons with each charged nuclei ($r_{i\,\eta} = |\boldsymbol{r}_{i\,\eta}|$ is the distance between the ith electron and the η nuclei), the three terms $1/r_{ij}$ ($j > i = 1\ldots3$) are the interelectron Coulomb repulsive interactions ($r_{i\,j}$ are the distances between the i,jth electrons), and the term $+Z_\mathsf{A} Z_\mathsf{B}/R$ is the classical Coulomb repulsion energy between the nuclei, where R is the internuclear distance (see Fig. 1 for notations). The Hamiltonian (1) includes the paramagnetic terms $\frac{1}{2}\,\boldsymbol{B}\cdot\boldsymbol{l}_i$ the spin Zeeman term $\boldsymbol{B}\cdot\boldsymbol{s}_i$ for the interaction of the magnetic field with the spin, and the diamagnetic term $\frac{\boldsymbol{B}^2}{8}{\rho_i}^2$, with ${\rho_i}^2 = x_i^2 + y_i^2$ for each electron, $i = 1,2,3$. If the magnetic field is directed along the z direction and parallel to the internuclear axis, the component of the total angular momentum along the z-axis M, the total spin S, the z projection of the total spin S_z, and the total z parity Π_z are conserved quantities. Sometimes in the text the spectroscopic notation $\nu^{2S+1}M^{\Pi_z}$ (with standard labels $\Sigma,\Pi,\Delta\ldots$ for $|M| = 0,1,2,$ etc.) is used for the electronic states. Here ν stands for the degree of excitation for given (fixed) symmetry. In our case of a homonuclear diatomic molecule, an additional subscript g or u (gerade or ungerade) indicates a symmetric or antisymmetric state with respect to the permutation of the identical nuclei.

III. GROUND STATE IN A STRONG MAGNETIC FIELD (GENERALITIES)

Before approaching concrete calculations, a description of the ground state of a Coulomb system of k electrons and several heavy charged centers in a strong magnetic field should be given. In fact, a complete qualitative picture was presented in the pioneering works by Kadomtsev-Kudryavtsev [17–20] and Ruderman [21,22]:

(i) All spins of electrons are oriented antiparallel to the magnetic field direction. Hence, the total electronic spin projection is $-\frac{k}{2}$.

(ii) All heavy centers are situated on a magnetic line. Hence, there is no gyration.

(iii) Electronic magnetic quantum numbers are different and take values $0,-1,-2,\ldots,-(k-1)$; hence, the total magnetic quantum number of the system $M = -\frac{k(k-1)}{2}$. This configuration does not contradict to the Pauli principle and implies vanishing Pauli forces.

We are not familiar with a rigorous proof of the validity of these observations in general.

For hydrogen atom, $k = 1$, validity of this observation, see item (iii), was explicitly checked by Ruder *et al.* [25] and for other one-electron systems in Ref. [1]; it was shown that the ground state corresponds to $M = 0$. For a helium atom, it was checked in Ref. [26], where the ground state was of $(1s_0 2p_{-1})$ type, thus $M = -1$, and for a lithium atom, it was of $(1s_0 2p_{-1} 3d_{-2})$ type, thus $M = -3$ [27], as well as for He^- [3]. For two-electron molecules H_2,HeH^+,$He_2{}^{++}$, it was checked that lowest energy occurs at $M = -1$ compared to $M = 0,-2$; see Refs. [2,23,28].

IV. TRIAL FUNCTIONS (GENERAL)

The variational method is used to study the state ${}^4(-3)^+{}_g$ of the $He_2{}^+$ molecular ion (with infinitely massive centers) placed in a uniform magnetic field parallel to the molecular z axis. In general, the wave function of the electronic Hamiltonian (1) with two identical nuclei can be written in the form

$$\psi(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3) = (1 + \sigma_N\, P_{\mathsf{AB}})\mathcal{A}[\,\phi(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)\chi\,], \qquad (2)$$

where χ is a three-electron spin eigenfunction corresponding either to a total electronic spin $S = 1/2$ or $S = 3/2$. Here $\mathbf{r}_{1,2,3}$ are position vectors of the first, second, and third electrons, respectively; see Fig. 1. The function $\phi(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)$ is a three-particle orbital function, and P_{AB} is the permutation operator of the two identical nuclei ($\sigma_N = \pm 1$ for gerade and ungerade states, respectively). The operator $\mathcal{A}$ is the three-particle antisymmetrizer:

$$\mathcal{A} = 1 - P_{12} - P_{13} - P_{23} + P_{231} + P_{312}. \qquad (3)$$

Here, P_{ij} represents the permutation $i \leftrightarrow j$, and P_{ijk} stands for the permutation of 123 into ijk. For strong magnetic fields which are typically present in the atmosphere of neutron stars, a natural expectation is that the ground state corresponds to the case when all electron spins are aligned antiparallel to the magnetic field, i.e., $S_z = -3/2$, and thus with the three-electron spin eigenfunction χ being totally symmetric. In this case, when $S_z = -3/2$, the trial function is written as

$$\psi^{S_z=-3/2}(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3) = (1 + \sigma_N\, P_{\mathsf{AB}})\mathcal{A}[\phi(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)]\beta(1)\beta(2)\beta(3), \qquad (4)$$

with $\phi(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)$ being a properly chosen orbital function, which then antisymmetrized by $\mathcal{A}$. Here $\beta(i)$, $i = 1,2,3$ is spin-down function of ith electron (see below).

On the other hand, for states of the total spin projection $S_z = -1/2$ ($S = 1/2$) we have two linearly independent spin eigenfunctions:

$$\chi_1 = \frac{1}{\sqrt{2}}[\beta(1)\alpha(2)\beta(3) - \alpha(1)\beta(2)\beta(3)]\,, \tag{5}$$

$$\chi_2 = \frac{1}{\sqrt{6}}[2\beta(1)\beta(2)\alpha(3) - \beta(1)\alpha(2)\beta(3) - \alpha(1)\beta(2)\beta(3)], \tag{6}$$

where $\alpha(i)(\beta(i))$, $i = 1,2,3$ are spin-up (spin-down) functions of the ith electron. So, the general form of a spin projection $S_z = -1/2$ function has the form

$$\Phi = \phi_1(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)\chi_1 + \phi_2(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)\chi_2, \tag{7}$$

where $\phi_1(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)$ and $\phi_2(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)$ are orbital functions. In particular, we can choose these functions to be proportional and write

$$\Phi = \phi(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)(\chi_1 + a\chi_2), \tag{8}$$

where a is a variational parameter.[2] Thus, the trial function for states of spin $S_z = -1/2$ can be written as [cf. (2)]

$$\psi^{S_z=-1/2}(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3) = (1+\sigma_N\, P_{\mathsf{AB}})\mathcal{A}[\,\phi(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)(\chi_1 + a\chi_2)], \tag{9}$$

with $\phi(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)$ being a properly chosen orbital function.

V. TRIAL FUNCTIONS (COORDINATE PARTS)

Variational trial functions are designed following physical relevance arguments. In particular, we construct wave functions which allow us to reproduce both the Coulomb singularities of the potential and the correct asymptotic behavior at large distances (see, e.g., Ref. [30]). Following such criterion, we propose the function

$$\phi(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3) = \prod_{k=1}^{3}\left(\rho_k^{|m_k|} e^{i m_k \phi_k} e^{-\alpha_{k,\mathsf{A}} r_{k\mathsf{A}} - \alpha_{k,\mathsf{B}} r_{k\mathsf{B}}} e^{-\frac{B}{4}\beta_k \rho_k^2}\right) \times e^{\alpha_{12} r_{12} + \alpha_{13} r_{13} + \alpha_{23} r_{23}}, \tag{10}$$

which is a type of product of Guillemin-Zener-type molecular orbital functions multiplied by the product of Landau-type orbitals for an electron in a magnetic field. Here $\alpha_{k,\mathsf{A}},\alpha_{k,\mathsf{B}}$ and β_k, $k = 1,2,3$ are parameters. In the case of the fully polarized state $S = 3/2$ and in order to avoid a contradiction with the Pauli principle, it is further assumed that all electrons have different magnetic quantum numbers in a certain minimal way: $m_1 = 0$, $m_2 = -1$, $m_3 = -2$; hence, the total electronic quantum number is $M = -3$. It was already discussed in Ref. [2] that this assumption seems obviously correct in the case of atoms and atomic ions, where the electrons are sufficiently close to each other, but not that obvious for the case of molecules for which the electrons are spread 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. This situation was observed for H_2 and $H_3{}^+$, where in a domain of large magnetic fields the ground state was given by the state of maximal total spin but with the electrons having the same zero magnetic quantum number (see Ref. [2] and references therein). However, for very strong fields the state of minimal total energy always corresponds to the situation described above with all electrons having different magnetic quantum numbers.

In (10) the variational parameters $\alpha_{k,\mathsf{A}},\alpha_{k,\mathsf{B}}$ ($k = 1,2,3$) have the meaning of screening (or antiscreening) factors (charges) for the nucleus A,B respectively, as is seen from the kth electron. The variational parameters β_k are screening (or antiscreening) factors for the magnetic field seen from kth electron, and the parameters $\alpha_{ij}, i < j = 1\ldots 3$ "measure" the screening (or antiscreening) of the interelectron interaction. In total, the trial function (10) has 12 variational parameters in addition to the internuclear distance R which can also be considered as a variational parameter.

The calculation of the variational energy using the trial function (4)–(10) involves two major parts: (i) nine-dimensional numerical integrations which were implemented by an adaptive multidimensional integration routine (*cubature*) [31] and (ii) a minimizer which was implemented with the minimization package TMINUIT from CERN-lib (an old version of TMINUITMINIMIZER in the ROOT system [32], which allows fixing or releasing parameters, was recovered and adapted to our purposes). The nine-dimensional integrations were carried out using a dynamical partitioning procedure: The domain of integration is manually divided into subdomains following the profile of the integrand. Then each subdomain is integrated using the routine CUBATURE. In total, we have a subdivision to ~2000 subregions for the numerator and ~2000 for the denominator in the variational energy. With a maximal number of sampling points $\sim 2 \times 10^8$ for the numerical integrations (it guarantees the relative accuracy $\sim 10^{-3}$ to 10^{-4} in integration) for each subregion, the time needed for one evaluation of the variational energy takes 5×10^4 s with 96 processors. It was checked that this procedure stabilizes the estimated accuracy to be reliable in the first two decimal digits. However, in order to localize a domain, where minimal parameters are, the minimization procedure with much fewer sample points was used in each subdomain and a single evaluation of the energy usually took ~15–20 min. Once a domain is roughly localized, the number of sample points was increased by factor $\sim 10^2$ and minimization was repeated. Final evaluation was made with 2×10^8 sampling points and for the strongest fields $B = 100, 1000, 10\,000$ a.u. it was even 5×10^8 with a subdivision of seven subintervals in each z domain. Typically, a minimization procedure required several hundred evaluations. Computations were performed in parallel with a cluster KAREN (ICN, UNAM) with 96 Intel Xeon processors at ~2.70 GHz.

VI. DECAY CHANNELS AND DISSOCIATION

In this section, we analyze different decay channels of the $S_z = -3/2$, $M = -3$ state ${}^4(-3)^+_g$ of the $He_2{}^+$ molecular ion in a magnetic field in the range $1\ \text{a.u.} \leqslant B \leqslant 10\,000\ \text{a.u.}$ Possible decay channels that we consider for the system

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[2] A similar treatment was used for the study of the Li atom in a magnetic field in Ref. [29].

TABLE III. Variational results for the total energy and equilibrium distance of the *spin-quartet* state ${}^4(-3)^+{}_g$ with total angular momentum projection $M = -3$ of the $He_2{}^+$ molecular ion in a magnetic field and comparison with the total energy of different subsystems. For helium atom the ground-state energy $E_T[1^3(-1)^+]$ [33] for $B \lesssim 100$ a.u. was used, while for $B \geqslant 1000$ a.u., the ansatz (16) was used (see Sec. VIII). Energies for He^- in the state ${}^4(-3)^+$ at $B = 100$–$10\,000$ a.u. were calculated for the present study using the trial function (13) (see Sec. VII), while for $B = 1$ a.u. it was taken from Ref. [3]. For He^+ the energies are from the scaling relation (11) with use of data from Ref. [34] (with electron-spin-Zeeman contribution included). For $He_2{}^{2+}$ energies from Ref. [36], and for $He_2{}^{3+}$ results from Ref. [1] with the (single)-electron-spin-Zeeman contribution added. All molecular systems assumed parallel configuration as optimal. All energies are in a.u.

B	$He_2{}^+[{}^4(-3)^+{}_g]$		He^-	He^+	$He_2{}^{3+}$	$He_2{}^{2+}$	He
(a.u.)	E_T	R_{eq}	$E_T[{}^4(-3)^+]$	$E_T(1s_0)$	$E_T(1\sigma_g)$	$E_T({}^3\Pi_u^+)$	$E_T[1^3(-1)^+]$
1	−4.02	2.18	−3.04	−2.4410		−3.3745	−2.9655
100	−22.46	0.432	−13.38	−9.5605	−8.2581	−16.9917	−13.1048
1000	−53.98	0.196	−28.18	−20.2707	−19.6338	−40.2462	−27.1738
10 000	−114.9	0.098	−55.41	−39.5107	−43.1165	−87.255	−53.2011

$(\alpha\alpha eee)$ placed in a magnetic field are

$$\begin{array}{rll} He_2{}^+ & \to He + He^+ & (a) \\ & \to He^- + \alpha & (b) \\ & \to He + \alpha + e & (c) \\ & \to He^+ + He^+ + e & (d) \\ & \to He_2{}^{2+} + e & (e) \\ & \to He_2{}^{3+} + e + e & (f). \end{array}$$

A few remarks emerge immediately: In the cases where there are free electrons[3] in the decay channel [channels (c)–(f)] we can assume that the electrons are in the ground state $n = 0, s_z = -1/2, m < 0$ which yields $E = 0$ (regardless of the magnetic quantum number m carried by the electron, where the spin contribution is included). In the Born-Oppenheimer approximation, the energy of a free α particle in a magnetic field is zero by assumption. Also, it is known that the helium atom exists for any magnetic field strength. For magnetic fields $0 \leqslant B \lesssim 0.75$ a.u. the spin-singlet state 1^10^+ is the ground state. For $B \gtrsim 0.75$ a.u., the spin-triplet state (with $M = -1$) $1^3(-1)^+$ becomes the ground state. For the He atom in a magnetic field $B \leqslant 100$ a.u., the corresponding total energies collected in Table III were taken from Refs. [26,33]. Such energies were calculated for the infinite nuclear mass approximation and include the spin contributions $B\,s_z$ for each electron. For magnetic fields $B = 1000$ and 10 000 a.u., a simple variational ansatz with five variational parameters was used to estimate the value of the energy of the spin-triplet state of helium (see Sec. VIII below for more details).

To obtain the energy of the He^+ ion, we use the basic result of Surmelian and O'Connel for hydrogen-like atoms

$$E(Z,B) = Z^2 E(1, B/Z^2), \qquad (11)$$

and use the data of Ref. [34] for the binding energies of hydrogen in a magnetic field (recalling that instead of the total energy E_T, in Ref. [34] the authors reported the energies $E_b = (1 + m + |m|)\gamma/2 - E$, which coincide with the binding energies $\epsilon = \gamma/2 - E$ for $m < 0$). The Zeeman contribution to the total energy $B\,s_z$ due to the spin of the electron is not taken into account in the results appearing in Ref. [34]. Such contribution for the case of a spin antiparallel to the magnetic field ($s_z = -\frac{1}{2}$) is $E_{\rm spin} = -B/2$ a.u. and was added to the results collected in Table III to obtain the total energies of He^+.

In the molecular system $(\alpha\alpha e)$ ($He_2{}^{3+}$ molecular ion), accurate variational calculations in equilibrium configuration parallel to the magnetic field for the ground state $1\sigma_g$ were carried out in detail in Refs. [1,35] for the range of magnetic fields 100 a.u. $\lesssim B \lesssim B_{\rm Schwinger}$ where $B_{\rm Schwinger} = 4.414 \times 10^{13}$ G is the nonrelativistic limit. It was found that for magnetic fields $10^2 \lesssim B \lesssim 10^3$ a.u. the system $He_2{}^{3+}$ is unstable toward decay to $He^+ + \alpha$. Thus, in principle we can neglect in our considerations the decay channel (e) above. 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 (for details, see Ref. [1]).

For the molecular system $(\alpha\alpha ee)$ $He_2{}^{2+}$ molecular ion, this molecule was studied in detail in Ref. [36] in the domain of magnetic fields $B = 0 - B_{\rm Schwinger}$. It was shown that the lowest total energy state depends on the magnetic field strength and evolves from the spin-singlet ${}^1\Sigma_g$ metastable state at $0 \leqslant B \lesssim 0.85$ a.u. to a repulsive spin triplet ${}^3\Sigma_u$ (unbound state) for $0.85 \lesssim B \lesssim 1100$ a.u. and then to a strongly bound triplet state ${}^3\Pi_u$ 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.

VII. He^- REVISITED

In order to have a complete understanding about the stability of the molecular $He_2{}^+$ ion in magnetic fields, we need to extend the study on the He^- atomic ion [three electron atomic system (α,e,e,e)] in magnetic fields to the regime of very strong fields $B \gg 1$a.u. In this section, we review the basic notions for the study of the He^- ion in magnetic fields. In Ref. [3] it was found that the ground state of He^- in a magnetic field is realized by a spin-doublet ${}^2(-1)^+$ at 0.74 a.u. $\gtrsim B \gtrsim 0.13$ a.u.

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[3] For the total energy of a free electron E_e (excluding the spin contribution) in the magnetic field in the symmetric gauge, the z component of the angular momentum L_z is conserved and the electron Landau levels are $E_e = \hbar\omega_B(n + 1/2)$, where $n = n_\rho + \frac{|m|+m}{2} = 0,1,2\ldots$ All $m \leqslant 0$ states are degenerate. Here $\omega_B = \frac{eB}{m_e c}$ is the cyclotron frequency.

and it becomes a fully polarized spin-quartet $^4(-3)^+$ for larger magnetic fields. Thus, we will extend that study of the He$^-$ ion in strong magnetic fields, in the fully polarized, spin quartet $S = 3/2$, state only. For more details, the reader is referred to Ref. [3].

The nonrelativistic Hamiltonian for an atomic system of three-electron and one infinitely massive center of charge Z in a magnetic field (directed along the z axis and taken in the symmetric gauge) is

$$\mathcal{H} = -\sum_{k=1}^{3}\left(\frac{1}{2}\nabla_k^2 + \frac{Z}{r_k}\right) + \sum_{k=1}^{3}\sum_{j>k}^{3}\frac{1}{r_{kj}} + \frac{B^2}{8}\sum_{k=1}^{3}{\rho_k}^2 + \frac{B}{2}(\hat{L}_z + 2\hat{S}_z), \qquad (12)$$

where ∇_k is the 3-vector momentum of the kth electron, r_k is the distance between the kth electron and the nucleus, ρ_k is the distance of the kth electron to the z axis, and r_{kj} $(k,j = 1,2,3)$ are the interelectron distances. $\hat{L}_z$ and $\hat{S}_z$ are the z components of the total angular momentum and total spin operators, respectively. Both $\hat{L}_z$ and $\hat{S}_z$ are integrals of motion and can be replaced in (1) by their eigenvalues M and S_z respectively. For He$^-$ the nuclear charge is $Z = 2$. The total spin $\hat{S}$ and z-parity $\hat{\Pi}_z$ are also conserved quantities. The spectroscopic notation $\nu^{2S+1}M^{\Pi_z}$ is used to mark the states, where Π_z denotes the z parity eigenvalue ($\pm$), and the quantum number ν labels the degree of excitation. For states with the same symmetry, for the lowest energy states at $\nu = 1$ the notation is $^{2S+1}M^{\Pi_z}$. We always consider states with $\nu = 1$ and $S_z = -S$ assuming they correspond to the lowest total energy states of a given symmetry in a magnetic field.

A. Trial functions

The spin $S = 3/2$ state $^4(-3)^+$ of the system (α,e,e,e) in a magnetic field is described by the trial function

$$\psi(\vec{r}_1,\vec{r}_2,\vec{r}_3) = \mathcal{A}[\,\phi(\vec{r}_1,\vec{r}_2,\vec{r}_3)\,], \qquad (13)$$

where $\mathcal{A}$ is the three-particle antisymmetrizer (3) and $\phi(\vec{r}_1,\vec{r}_2,\vec{r}_3)$ is the explicitly correlated orbital function

$$\phi(\vec{r}_1,\vec{r}_2,\vec{r}_3) = \left(\prod_{k=1}^{3}\rho_k^{|M_k|}e^{iM_k\phi_k}e^{-\alpha_k r_k - \frac{B}{4}\beta_k\rho_k^2}\right) \times e^{\alpha_{12}r_{12}+\alpha_{13}r_{13}+\alpha_{23}r_{23}}, \qquad (14)$$

where M_k is the magnetic quantum number and α_k, β_k, and α_{kj} are nonlinear variational parameters for each electron $k = 1,2,3$. In total, the trial function (13) contains nine variational parameters. The function (13) is a properly antisymmetrized product of 1s Slater-type orbitals, the lowest Landau orbitals, and the exponential correlation factors $\sim\exp(\alpha\, r_{kj})$.

The spin 3/2 state $^4(-3)^+$ of the system (α,e,e,e) in a magnetic field is described by the trial function (13) with $M_1 = 0$, $M_2 = -1$, $M_3 = -2$. Due to the spin Zeeman contribution, the energy of this (spin $S = 3/2$) state decreases rapidly and monotonically with the magnetic field increase and becomes the (stable) ground state for $B \gtrsim 0.7$ a.u.

In Ref. [3], we made a study of the (α,e,e,e) atomic system in magnetic fields $B \leqslant 100$ a.u. Here we extend that study for magnetic fields up to $B = 10\,000$ a.u. In particular, we improve the value of the total energy at $B = 100$ a.u. from $E_T = -13.29$ a.u. (as quoted in Ref. [3]) to $E_T = -13.38$ a.u., i.e., by $\sim$0.1 a.u. (see Table III).

The variational method used to find the energy of the system with the trial function (13) involves two major procedures of numerical minimization and integration. This was already described above for the case of the ${\rm He_2}^+$ molecular ion (see Sec. V). In particular, for strong magnetic fields, a reliable minimization depends on the accuracy of the variational energies, i.e., on the accuracy of the numerical nine-dimensional integrations. Our strategy to find the minimal energy was first to make approaching minimizations with relatively low accuracy in the integrations and then followed by a manual scanning of the energy dependence on each variational parameter with high accuracy in the numerical integrations. For our final results, we used a partition of the integration domain into 4800 subregions for the numerator and 4800 subregions for the denominator using 5×10^8 sample points for each numerical integration. A single evaluation of the energy takes about 14 h of wall clock time using a cluster KAREN (ICN, UNAM) with 120 processors.

Our results for the spin 3/2 state $^4(-3)^+$ of the system (α,e,e,e) in magnetic fields $B = 100,1000,10\,000$ a.u. are collected in Table III below. These results indicate that as the magnetic field increases, the total energy of the He$^-$ ion in the $^4(-3)^+$ state decreases, but at a slower rate in comparison to the total energy of the ${\rm He_2}^+$ molecular ion in the $^4(-3)^+$ state. Also, our results confirm that as the magnetic field increases, the total energy of the He$^-$ ion in the $^4(-3)^+$ state decreases more rapidly than the total energy of the He atom in the spin triplet state $1^3(-1)^+$ and, therefore, becoming more stable toward decay into He$^-$ → He + α [see below for our extended calculations of the He atom in the spin triplet state $1^3(-1)^+$].

VIII. He ATOM IN STRONG MAGNETIC FIELDS REVISITED

The assertion on the stability of the molecular ion ${\rm He_2}^+$ in strong magnetic fields requires a full understanding of the helium atom and other helium species in the presence of a strong magnetic field. It is known that the helium atom exists for any magnetic field strength. Its ground state is realized by a singlet spin state 1^1S at zero and small magnetic fields $0 \leqslant B \leqslant 0.75$ a.u. For larger magnetic fields, the ground state is realized by the fully polarized spin triplet state $1^3(-1)^+$ [26]. Despite the fact that the helium atom in magnetic fields is one of the most studied systems, all such studies that we are familiar with are limited to magnetic fields up to $B = 100$ a.u. (see, e.g., Ref. [26]). For higher magnetic fields (up to the Schwinger limit $B_{\rm rel} = 4.414 \times 10^{13}$ G ~ 18783 a.u.), the relativistic corrections to the energy seem to be relatively small. Thus, we extend the study of the helium atom up to the largest magnetic field $B = 10^4$ a.u. considered in the present study. In particular, a full understanding of the He atom in the spin triplet (ground) state $1^3(-1)^+$ at magnetic fields $10\,000 \geqslant B \geqslant 100$ a.u. is necessary.

A. Hamiltonian

The nonrelativistic Hamiltonian which described the helium atom with an infinitely massive nucleus of charge $Z = 2$

in a magnetic field oriented along the z axis is given by

$$\mathcal{H} = -\sum_{k=1}^{2}\left(\frac{1}{2}\nabla_k^2 + \frac{Z}{r_k}\right) + \frac{1}{r_{12}} + \frac{B^2}{8}\sum_{k=1}^{2}{\rho_k}^2 + \frac{B}{2}(\hat{L}_z + 2\hat{S}_z), \tag{15}$$

where the symmetric gauge $\mathbf{A} = \frac{1}{2}\mathbf{B}\times\mathbf{r}$ was used, and ∇_k is the 3-vector momentum of the kth electron, r_k is the distance between the kth electron and the nucleus, ρ_k is the distance of the kth electron to the z axis, and r_{12} is the interelectron distance. $\hat{L}_z$ and $\hat{S}_z$ are the z components of the total angular momentum and total spin operators, respectively. Both $\hat{L}_z$ and $\hat{S}_z$ are integrals of motion and can be replaced in (15) by their eigenvalues M and S_z respectively. The total spin $\hat{S}$ and z-parity $\hat{\Pi}_z$ are also conserved quantities. The spectroscopic notation $\nu^{2S+1}M^{\Pi_z}$ is used to mark the states, Π_z denotes the z parity eigenvalue ($\pm$), and the quantum number ν labels the degree of excitation. For states with the same symmetry, for the lowest energy states at $\nu = 1$ the notation is ${}^{2S+1}M^{\Pi_z}$.

B. Trial functions

To study the ground state of the Hamiltonian (15), we use the variational method with trial functions chosen according to the criterion of physical relevance. The trial functions for the low-lying states of (15) can be written as

$$\Psi = (1 + \sigma_e P_{12})\big(\rho_1^{|m_1|}e^{im_1\phi_1}\rho_2^{|m_2|} \times e^{im_2\phi_2}e^{-\alpha_1 r_1 - \alpha_2 r_2 - \frac{B}{4}(\beta_1\rho_1^2 + \beta_2\rho_2^2) + \alpha_{12}r_{12}}\big), \tag{16}$$

where P_{12} is the permutation operator for the electrons ($1 \leftrightarrow 2$), $\sigma_e = \pm 1$ corresponds to the spin singlet ($\sigma_e = 1$) and the spin triplet ($\sigma_e = -1$) eigenstates, and $m_{1,2}$ are the magnetic quantum numbers of electrons (1,2 respectively). The trial function (16) depends on five variational parameters which account for effective screened charges of the nucleus $\alpha_{1,2}$ (as seen by electrons 1, 2), of the electrons moving in the magnetic field $\beta_{1,2}$, and of one of the electrons as seen from the other α_{12}.

The ground state of the helium atom at strong magnetic fields is realized by the spin triplet state $1^3(-1)^+$ corresponding to $\sigma_e = -1$ and $m_1 = 0$, $m_2 = -1$ ($M = m_1 + m_2$) in (16). This simple ansatz gives an energy $E_T = -12.8215$ a.u. at $B = 100$ a.u., which compared to the most accurate result $E_T = -13.1048$ a.u. in Ref. [33] indicates that the relative difference provided by this trial function is $\sim$2%. The total energy of the triplet state $1^3(-1)^+$ decreases as the magnetic field increases. For a magnetic field $B = 1000$ a.u. our variational trial function gives an energy of $E_T = -27.1738$ a.u., while at $B = 10\,000$ a.u. it gives an energy of $E_T = -53.2011$ a.u. It is worth noticing that the total energy of helium in the spin triplet state $1^3(-1)^+$ lies higher than the total energy of the He^- ion in the fully polarized state ${}^4(-3)^+$, and the energy difference increases with an increase of the magnetic field.

The variational method used to find the energy of the helium atom with the trial function (16) involves two major procedures of numerical minimization (MINUIT) and multidimensional numerical integration (CUBATURE). Because of the axial symmetry of the problem, the dimensionality reduces to five. The integrations are performed in double cylindrical coordinates ($z_1,\rho_1,z_2,\rho_2,\phi$) (where ϕ is the relative azimuthal angle between the electrons). The manual partitioning includes five subdomains in each z coordinate, three subdomains in each ρ coordinate, and one domain for ϕ. The maximal number of sample points used to evaluate the numerical integrations is 5×10^7. Our results for this system are presented in Table III (see below).

IX. RESULTS

A. Field-free case: Low-lying states

We have carried out variational calculations for the field-free ground state ${}^2\Sigma_u^+$ state as well as for the weakly bound excited state ${}^2\Sigma_g^+$ state of $He_2{}^+$. The aim of this study is mainly to have an estimate of the accuracy of our variational calculations. Previous studies on one- and two-electron Coulomb systems in strong magnetic fields have shown that simple trial functions of the type (10) which are built following the criterion of physical adequacy have led to very accurate results for such systems (see Refs. [1,2]).

The results for the energy of the states ${}^2\Sigma_u$ and ${}^2\Sigma_g$ using the trial function (9) are collected in the Table I. From such results, and comparing to the most accurate results to date for such states [37,38], we can conclude that the energies obtained with our 10-parameter trial function have a relative accuracy of $\sim$1%. It is worth to note that the level of accuracy provided by the trial function (9) is sufficiently high to observe the shallow minimum of the ${}^2\Sigma_g$ state, though the equilibrium distance seems to be slightly shifted in comparison to the results of Ref. [38].

In a magnetic field one can expect a relatively slow decrease in accuracy as the magnetic field increases. A similar comparison for the energies of the helium atom in a magnetic field $B \leqslant 100$ a.u. obtained (a) with the two-electron, five-parameter trial function (16) and (b) with the more accurate energies using a Gaussian basis set method with $\sim$4300 two-particle functions [33] leads to the conclusion that even at $B = 100$ a.u. the relative accuracy is $\sim$2%. Thus, we can estimate that our results for the $He_2{}^+$ ion in magnetic fields $B \lesssim 100$ a.u. have an accuracy of $\sim$2% with a small decrease for higher magnetic fields. To confirm this conjecture, a separate study would be necessary.

B. $B = 1$ a.u.

We begin our analysis for the total energy and equilibrium distance for the spin $S = -3/2$ state with $M = -3$ corresponding to the Hamiltonian (1) for a magnetic field $B = 1$ a.u.

For this magnetic field, the total energy of the spin-quartet, $M = -3$ state obtained with the trial function (4)–(10) is $E_T^{He_2{}^+}[{}^4(-3)^+] = -4.02$ a.u. with an equilibrium distance $R_{eq} = 2.18$ a.u. (see Table III). The lowest energy state of He corresponding to the triplet state, and $M = -1$, has a total energy $E_T^{He}[1^3(-1)^+] = -2.9655$ a.u., and the total energy of the ground state of He^+ ion is $E_T^{He^+}(1s_0) = -2.4410$ a.u. From these considerations, it is clear that for this magnetic field the state ${}^4(-3)^+{}_g$ of $He_2{}^+$ is unstable toward decay [channel (a)] to

$$\mathrm{He_2}^+\left[{}^4(-3)^+{}_g\right] \to \mathrm{He}[1^3(-1)^+] + \mathrm{He}^+(1s_0)\,, \tag{17}$$

since the total energy of the subproducts $E_T^{\mathrm{He}}[1^3(-1)^+] + E_T^{\mathrm{He}^+}(1s_0) = -5.4065$ a.u. is essentially lower than the total energy of the spin-quartet $M = -3$ state of $\mathrm{He_2}^+$. It is also noteworthy to mention that the lowest state of He^+ with $|m| = 2$ has a total energy of $E_T^{\mathrm{He}^+}(3d_{-2}) = -0.7930$ a.u. (including the contribution from the spin Zeeman term) and, for this case, the state ${}^4(-3)^+$ of $\mathrm{He_2}^+$ is stable toward the (M-conserved) decay into

$$\mathrm{He_2}^+\left[{}^4(-3)^+{}_g\right] \nrightarrow \mathrm{He}[1^3(-1)^+] + \mathrm{He}^+(3d_{-2}), \tag{18}$$

since the total energy of the subproducts is $E_T^{\mathrm{He}}[1^3(-1)^+{}_g] + E_T^{\mathrm{He}^+}(3d_{-2}) = -3.7585$ a.u. Thus, $\mathrm{He_2}^+$ in the state ${}^4(-3)^+{}_g$ is a metastable state.

For this magnetic field $\mathrm{He_2}^+[{}^4(-3)^+{}_g]$ is also unstable toward decay into two $\mathrm{He}^+(1s_0)$ ions plus an electron infinitely separated [decay channel (d)]. This separated system has a total energy -4.8820 a.u. On the other side, following the results summarized in Table III, $\mathrm{He_2}^+[{}^4(-3)^+{}_g]$ is stable toward decays into $\mathrm{He}^-[{}^4(-3)^+] + \alpha$ [channel (b)] or $\mathrm{He}[1^3(-1)^+] + \alpha + e$ [channel (c)]. Decay channels (e) and (f) are not possible since the systems $\mathrm{He_2}^{2+}$ and $\mathrm{He_2}^{3+}$ either do not exist or are unstable. For $B = 1$ a.u., the lowest energy state of the two electron molecular ion $\mathrm{He_2}^{2+}$ corresponds to a purely repulsive spin-triplet (unbound) state ${}^3\Sigma_u$ (for $0.85 \lesssim B \lesssim 1100$ a.u. this system does not exist in the four-body bound state; it exists in a form of two separated helium ions He^+ situated at an infinitely large distance from each other), and the one electron molecular ion $\mathrm{He_2}^{3+}$ in its ground state $1\sigma_g$ is unstable toward decay into $\mathrm{He}^+ + \alpha$.

C. $B = 100$ a.u.

We continue our analysis for a magnetic field $B = 100$ a.u. For this magnetic field, the total energy of the quartet state with $M = -3$ belonging to the Hamiltonian (1) is $E_T^{\mathrm{He_2}^+}[{}^4(-3)^+{}_g] = -22.46$ a.u. with an equilibrium distance $R_{\mathrm{eq}} = 0.432$ a.u. (see Table III).

For this magnetic field, the lowest energy state of He is the triplet state with magnetic quantum number $M = -1$, and has a total energy $E_T^{\mathrm{He}}[1^3(-1)^+] = -13.1048$ a.u., while the total energy of the ground state of the He^+ ion is $E_T^{\mathrm{He}^+}(1s_0) = -9.5605$ a.u. (including the spin Zeeman contribution). From this, we can conclude that the state ${}^4(-3)^+{}_g$ is still unstable toward decay (17), since the total energy of the subproducts is $E_T^{\mathrm{He}}[1^3(-1)^+] + E_T^{\mathrm{He}^+}(1s_0) = -22.6653$ a.u., which is slightly smaller than the total energy of the quartet $M = -3$ state of $\mathrm{He_2}^+$. However, it is clear from this comparison that for some $B > 100$ a.u. the state ${}^4(-3)^+$ of $\mathrm{He_2}^+$ becomes stable toward decay into $\mathrm{He} + \mathrm{He}^+$ (see below).

Following the results summarized in Table III, we conclude that $\mathrm{He_2}^+[{}^4(-3)^+{}_g]$ is stable toward decays into $\mathrm{He}^-[{}^4(-3)^+] + \alpha$ [channel (b)] or $\mathrm{He}[1^3(-1)^+] + \alpha + e$ [channel (c)] or $\mathrm{He}^+(1s_0) + \mathrm{He}^+(1s_0) + e$ [channel (d)] since the total energies of the corresponding separated subsystems in all these channels are above the total energy of the quartet state. Decay channels (e) and (f) are also not possible, since for this magnetic field the lowest energy state of the two electron molecular ion $\mathrm{He_2}^{2+}$ corresponds to a purely repulsive triplet state ${}^3\Sigma_u$, and the system $\mathrm{He_2}^{3+}$ in its ground state $1\sigma_g$ is unstable toward decay into $\mathrm{He}^+ + \alpha$.

D. $B = 1000$ a.u.

Our variational result for the total energy of the quartet state with $M = -3$ belonging to the Hamiltonian (1) for a magnetic field $B = 1000$ a.u. is $E_T^{\mathrm{He_2}^+}[{}^4(-3)^+{}_g] = -53.98$ a.u. with an equilibrium distance $R_{\mathrm{eq}} = 0.196$ a.u. (see Table III).

Now, for the main decay channel (a) the total energy of the subproducts is $E_T^{\mathrm{He}}[1^3(-1)^+] + E_T^{\mathrm{He}^+}(1s_0) = -47.4445$ a.u. which lies higher than the total energy of the quartet state of $\mathrm{He_2}^+$, and thus, the molecular ion $\mathrm{He_2}^+$ is stable toward decay to $\mathrm{He_2}^+ \to \mathrm{He} + \mathrm{He}^+$. The dissociation energy for this channel is 6.54 a.u. = 177.8 eV at $B = 1000$ a.u.

For the case of channel (b), a direct comparison of the total energies of $\mathrm{He_2}^+$ and He^- at $B = 1000$ a.u. (for He^- we made an extension of the results in Ref. [3] at $B = 1000$ a.u.) indicates that $\mathrm{He_2}^+$ is also stable toward decay to $\mathrm{He_2}^+ \nrightarrow \mathrm{He}^- + \alpha$ with a dissociation energy of $\sim$701.8 eV. For the case of channel (c) $\mathrm{He_2}^+ \to \mathrm{He} + \alpha + e$, the total energy of the subproducts of this decay is larger than the total energy of the $\mathrm{He_2}^+$ ion in the quartet state. So, the system is also stable toward this decay channel with a dissociation energy of $\sim$729.1 eV. For the case of channel (d) $\mathrm{He_2}^+ \to \mathrm{He}^+ + \mathrm{He}^+ + e$, the total energy of the subproducts of this decay is larger than the total energy of the $\mathrm{He_2}^+$ ion in the quartet state. The dissociation energy in this case is $\sim$365.5 eV. For the case of channel (e) $\mathrm{He_2}^+ \to \mathrm{He_2}^{2+}({}^3\Pi_u^+) + e$, at $B = 1000$ a.u. the total energy of the subproducts of this decay is larger than the total energy of the $\mathrm{He_2}^+$ ion in the quartet state. However, we should remember that for this magnetic field the ground state of the two-electron molecular ion $\mathrm{He_2}^{2+}$ is realized by a repulsive spin triplet state ${}^3\Sigma_u$ state [for $0.85 \lesssim B \lesssim 1100$ a.u. this system exists in the form of two helium ions He^+ situated at an infinitely large distance from each other, i.e., case (d)], and the strongly bound triplet state ${}^3\Pi_u$ state becomes the ground state at $B \gtrsim 1100$ a.u. (see Ref. [36]).

For the case of channel (f) $\mathrm{He_2}^+ \to \mathrm{He_2}^{3+}(1\sigma_g) + 2e$, at $B = 1000$ a.u. the total energy of the subproducts of this decay is larger than the total energy of the $\mathrm{He_2}^+$ ion in the quartet state, and the corresponding dissociation energy is $\sim$934.2 eV. For this magnetic field the ion $\mathrm{He_2}^{3+}$ is stable toward $\mathrm{He_2}^{3+} \to \mathrm{He}^+ + \alpha$ and it is the most bound one-electron system made from protons and/or α particles for $B > 1000$ a.u.

E. $B = 10\,000$ a.u.

Our variational result for the total energy of the quartet state with $M = -3$ belonging to the Hamiltonian (1) for a magnetic field $B = 10\,000$ a.u. is $E_T^{\mathrm{He_2}^+}[{}^4(-3)^+{}_g] = -114.9$ a.u. with an equilibrium distance $R_{\mathrm{eq}} = 0.098$ a.u. (see Table III). At this magnetic field, the numerical integrations with different accuracies (maximal number of points) indicate that the energy has a relative accuracy of 0.1 a.u. This may result in differences of a few eV in the transition energies.

For the main decay channel (a), the total energy of the subproducts is $E_T^{\mathrm{He}}[1^3(-1)^+] + E_T^{\mathrm{He}^+}(1s_0) = -92.7118$ a.u.

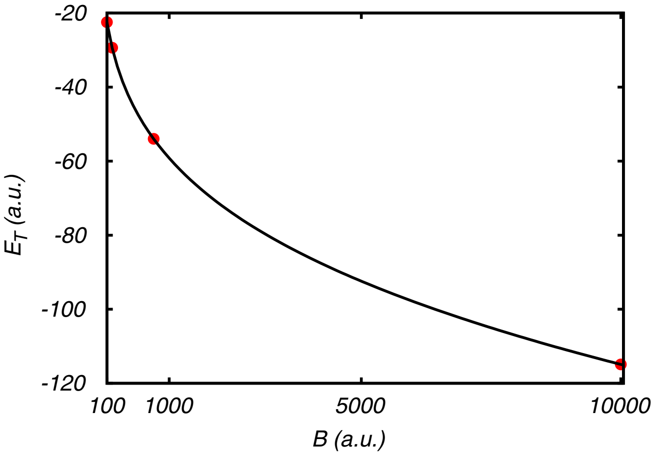

FIG. 2. Total energy E_T of the $He_2{}^+$ ion in the spin-quartet state $^4(-3)^+$ as a function of the magnetic field B; the continuous line is the fit $E_T(B) = -2.7582\log^2(B) + 18.078\log(B) - 47.4006$.

which lies higher than the total energy of the quartet state of $He_2{}^+$, and thus, the molecular ion $He_2{}^+$ is stable toward decay to $He_2{}^+ \to He + He^+$. The corresponding dissociation energy for this channel is 22.2 a.u. = 603.5 eV at $B = 10\,000$ a.u.

For the case of channel (b), a direct comparison of the total energies of $He_2{}^+$ and He^- at $B = 10\,000$ a.u. (in Sec. VII, we carried out an extension of the results in Ref. [3] for He^- up to $B = 10\,000$ a.u.) indicates that $He_2{}^+$ is also stable toward decay to $He_2{}^+ \nrightarrow He^- + \alpha$ with a dissociation energy of ∼1618 eV. For the case of channel (c) $He_2{}^+ \to He + \alpha + e$, the total energy of the subproducts of this decay is larger than the total energy of the $He_2{}^+$ ion in the quartet state. So, the system is also stable toward this decay channel with a dissociation energy of ∼1678 eV. For the case of channel (d) $He_2{}^+ \to He^+ + He^+ + e$, the total energy of the subproducts of this decay is larger than the total energy of the $He_2{}^+$ ion in the quartet state. The dissociation energy in this case is ∼976 eV. For the case of channel (e) $He_2{}^+ \to He_2{}^{2+}(^3\Pi_u^+) + e$, at $B = 10\,000$ a.u. the total energy of the subproducts of this decay is larger than the total energy of the $He_2{}^+$ ion in the quartet state, and the corresponding dissociation energy is ∼752 eV.

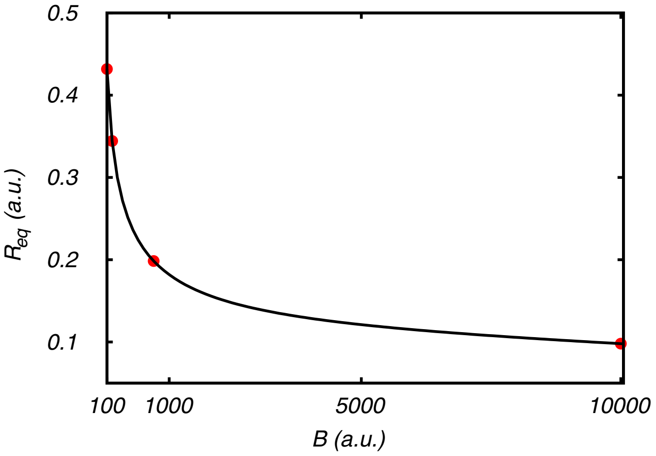

FIG. 3. Equilibrium distance of the $He_2{}^+$ ion in the spin-quartet state $^4(-3)^+$ as a function of the magnetic field, the continuous line is the fit $R_{\rm eq}(B) = 0.01262\log^2(B) - 0.24654\log(B) + 1.29830$.

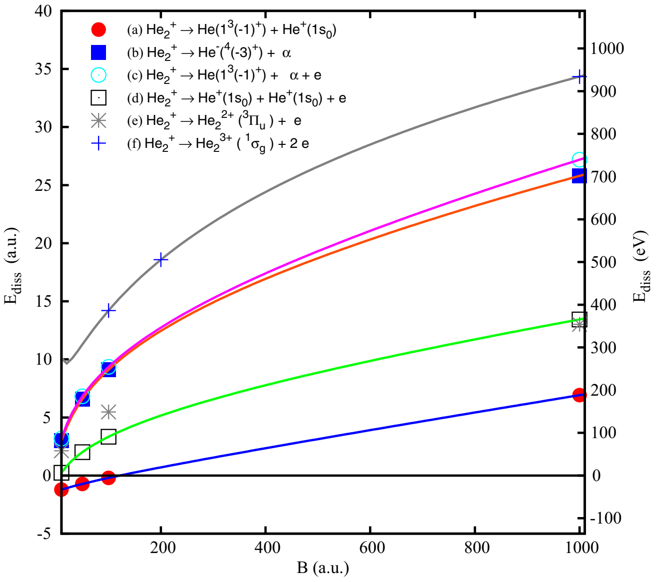

FIG. 4. Dissociation energies of the $He_2{}^+$ ion in the spin-quartet state$^4(-3)^+{}_g$ as a function of the magnetic field $10 \lesssim B \leqslant 1000$ a.u. toward different decay channels.

For the case (f) $He_2{}^+ \to He_2{}^{3+}(1\sigma_g) + 2e$, at $B = 10\,000$ a.u. the total energy of the subproducts of this decay is larger than the total energy of the $He_2{}^+$ ion in the quartet state, and the corresponding dissociation energy is ∼1953 eV.

The total energy of the $He_2{}^+$ ion in the quartet state $^4(-3)^+{}_g$ as a function of the magnetic field is presented in Fig. 2. This figure shows that as the magnetic field is increased, the system becomes more bound. The internuclear equilibrium distance of the $He_2{}^+$ ion in the quartet state $^4(-3)^+$ as a function of the magnetic field is presented in Fig. 3. This figure shows that as the magnetic field is increased, the system becomes more compact. We have plotted in Figs. 4 and 5 the dissociation energies, (i.e., difference of total energies between the state $^4(-3)^+{}_g$ of $He_2{}^+$ and the energy of the final products) for the different decay channels described in Sec. VI. This plot shows that the ion $He_2{}^+$ in the state $^4(-3)^+$ becomes more bound with respect to all dissociation channels as the magnetic field increases and, more important, that the dissociation energies at $B \sim 1000$ a.u. lie in the window 0.1–1 keV, which is the window of observed absorption features in the spectrum of the isolated neutron star 1E1207.4-5209 (see Refs. [8,9]).

In order to have a hint about the critical magnetic field at which the state $^4(-3)^+{}_g$ of $He_2{}^+$ becomes the ground state of the Coulomb system $(\alpha\alpha eee)$, we have collected in Table IV a list of atomic and molecular Coulomb systems made out of hydrogen and/or α particles, as well as the lithium atom, and the corresponding critical magnetic fields at which the ground state is realized by a state with all spins oriented antiparallel to the magnetic field. A simple analysis of this table indicates that for atomic systems [with more than one electron (He, He^-, Li)] the critical magnetic field is rather weak, being $B_{\rm crit} \sim 0.75$–2.21 a.u. For molecular-type systems, there seem

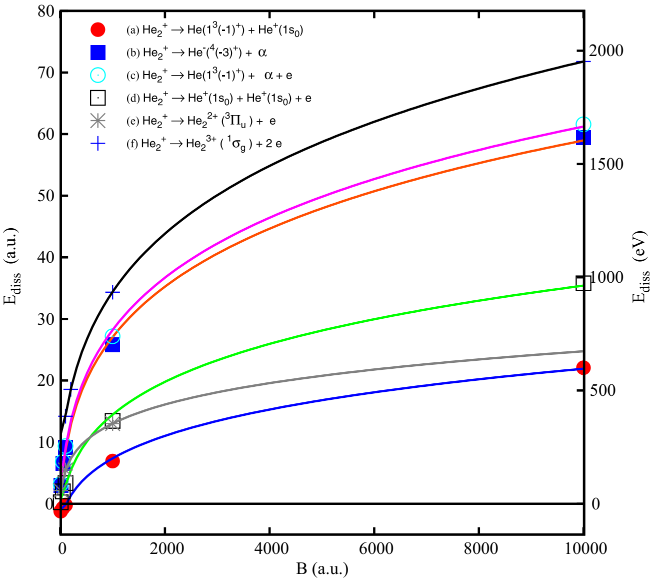

FIG. 5. Dissociation of the $He_2{}^+$ ion in the spin-quartet state $^4(-3)^+{}_g$ as a function of the magnetic field $10 \lesssim B \leqslant 10\,000$ a.u. towards different decay channels (same as Fig. 4 but extended up to $B = 10\,000$ a.u.).

to be two typical ranges of values for the critical magnetic field, i.e., $B_{\text{crit}} \sim 10$–20 a.u. and $B_{\text{crit}} \sim 1000$–2000 a.u., which is much larger than for the atomic-type systems. Perhaps this phenomenon can be explained by the fact that electrons in a molecular system are further apart than in the case of atoms. So, if this tendency is also valid for the case of the $He_2{}^+$ molecular ion, then it is very likely that the state $^4(-3)^+{}_g$ becomes the ground state for magnetic fields $B \gtrsim 1000$ a.u. Of course, a detailed study of other states of the $He_2{}^+$ molecular ion is needed in order to establish this conjecture.

F. Spin-1/2 states

As for the spin $S = 1/2$ states of $He_2{}^+$, we have calculated the total energy of some states with $M = 0, -1$ for both gerade and ungerade parities at the magnetic field $B = 100$ a.u. (see Table II). It is clear from such results that for high magnetic fields $B > 100$ a.u., these states will lay much higher in energy than the fully polarized $S = 3/2$ state that we consider in our study. For spin $S = 1/2$ states, the contribution to the total energy coming from the spin-Zeeman term is $E_{\text{Zeeman}}^{S_z=-1/2} = -B/2$ a.u., while it is $E_{\text{Zeeman}}^{S_z=-3/2} = -3/2B$ a.u. for the spin $S = 3/2$ fully polarized state. Thus, considering only the spin-Zeeman contribution to the total energy, the states with spin

TABLE IV. Critical magnetic field for different Coulomb systems for which the ground state becomes a state with maximal electronic spin: All electron spins are antiparallel to the magnetic field. Results taken from Refs. [1–3,26,36].

System	Ground state	M	S_z	B_{crit} (a.u.)
He^+	$1s_0$	0	$-1/2$	$\geqslant 0$
$He_2{}^{3+}$	$1\sigma_g$	0	$-1/2$	$\geqslant 10$
He	$1^3(-1)^+$	-1	-1	$\gtrsim 0.75$
H_2	$^3\Pi_u$	-1	-1	$\gtrsim 12.3$
$He_2{}^{2+}$	$^3\Pi_u$	-1	-1	$\gtrsim 1100$
$H_3{}^+$	$^3\Pi_u$	-1	-1	$\gtrsim 20$
$H_4{}^{2+}$	$^3\Pi_u$	-1	-1	$\gtrsim 2000$
HeH^+	$^3\Pi_u$	-1	-1	$\gtrsim 15$
$He_3{}^{4+}$	$^3\Pi_u$	-1	-1	$\gtrsim 1000$
He^-	$^4(-3)^+$	-3	$-3/2$	$\gtrsim 0.74$
Li	$^4(-3)^+$	-3	$-3/2$	$\gtrsim 2.21$

TABLE V. $He_2{}^+$ in a strong magnetic field. State $^4(-3)^+{}_g$ variational parameters for the trial function (10), α parameters are in $[\text{a.u.}]^{-1}$. For the evaluation of the variational total energy, 5×10^8 was the maximal number of sample points used for the numerical integration in each subdomain in the manual partitioning. Triple cylindrical coordinates were used with two subdomains in each of the three ρ coordinates and seven subdomains in each of the three z coordinates. The integration routine CUBATURE [31] was used.

	Magnetic field B in a.u.		
Parameter	100	1000	10 000
$\alpha_{1,\text{A}}$	0.93175	1.975	3.59
$\alpha_{1,\text{B}}$	3.34641	3.9	4.28
$\alpha_{2,\text{A}}$	1.41717	1.9	2.5
$\alpha_{2,\text{B}}$	2.0076	3.059	4.36
$\alpha_{3,\text{A}}$	1.53986	2.09	2.32
$\alpha_{3,\text{B}}$	1.03391	1.82	3.1
α_{12}	0.58803	0.46	0.38
α_{13}	0.23269	0.16	0.08
α_{23}	0.17702	0.15	0.2
β_1	0.81948	0.93	0.98
β_2	0.87464	0.94	0.983
β_3	0.90583	0.957	0.989
R_{eq} (a.u.)	0.43177	0.1985	0.098
E_T (a.u.)	-22.460	-53.978	-114.908

TABLE VI. He^- in a strong magnetic field. State $^4(-3)^+{}_g$ variational parameters for the trial function (14), α parameters are in $[\text{a.u.}]^{-1}$. For the evaluation of the variational total energy, 5×10^8 was the maximal number of sample points used for the numerical integration in each subdomain in the manual partitioning. Triple cylindrical coordinates were used with two subdomains in each of the three ρ coordinates, five subdomains in two z coordinates, and three subdomains in the third z coordinate which integrated over the half line. The integration routine CUBATURE [31] was used.

	Magnetic field B in a.u.		
Parameter	100	1000	10 000
α_1	2.86366	4.30183	5.32027
α_2	1.91669	3.09290	3.79174
α_3	1.20906	1.67689	2.48690
α_{12}	-0.13497	0.06847	0.37195
α_{13}	-0.12987	0.02558	-0.04966
α_{23}	-0.11967	0.05634	-0.08924
β_1	0.84414	0.92115	0.97709
β_2	0.91848	0.95373	0.99092
β_3	0.96952	0.98367	0.99470
E	-13.3772	-28.1756	-55.4053

TABLE VII. He atom in a strong magnetic field. Spin triplet state $1^3(-1)^+$ variational parameters for the trial function (16), α parameters are in [a.u.]$^{-1}$.

	Magnetic field B in a.u.		
Parameter	100	1000	10 000
α_1	2.107315	3.085664	4.589369
α_2	2.952063	4.151930	5.887318
α_{12}	0.145703	0.117778	0.227942
β_1	0.895958	0.958737	0.986090
β_2	0.825659	0.930747	0.977742
E	−12.8215	−27.1738	−53.2011

$S = 1/2$ are about $\Delta E_T \sim B$ a.u. higher that the spin $S = 3/2$ states.

Finally, and for the sake of completeness, we present in Tables V, VI and VII the variational parameters corresponding to the systems $He_2{}^+$, He^-, and He for magnetic fields 100, 1000, and 10000 a.u.

X. CONCLUSIONS

We have studied the stability of the molecular Coulomb system formed by two infinitely massive α particles and three electrons ($\alpha\alpha eee$) in the range of magnetic fields $0 \leqslant B \leqslant 10\,000$ a.u., in a state where all electron spins are oriented antiparallel to the magnetic field direction; hence, $S_z = -3/2$. It was further assumed that in the ground state, in order to suppress the appearance of the Pauli force, all electrons should have different magnetic quantum numbers; in particular, if these are equal to $m_1 = 0$, $m_2 = -1$, $m_3 = -2$, the total magnetic quantum number $M = -3$. This choice looks natural physically. The parallel configuration, for which both the molecular axis and the magnetic field direction coincide, was adopted as the optimal configuration with minimal total energy. The stability toward possible decay channels was studied variationally, using trial functions (4) and (10). We found that for all studied magnetic fields $1 \leqslant B \leqslant 10\,000$ a.u., there exists a well-pronounced minimum in the potential curve of total energy versus the internuclear distance R at some $R = R_{\text{eq}}$. The equilibrium distance R_{eq} decreases with the magnetic field increase; hence, the system becomes more compact at large magnetic fields. At the same, time the total energy is getting more negative, while the binding energy increases, making the system more bound. For $B \gtrsim 120$ a.u., the $He_2{}^+$ molecular ion in the state ${}^4(-3)^+_g$ becomes stable towards all possible decay channels [see Fig. 4]. In other words, the molecular system $He_2{}^+$ becomes the most bound helium specie with three electrons. It also hints at the possible relevance of other helium chains like He_2, He_3, or even the hybrid molecules like the neutral HeH, for the chemistry in a strong magnetic field.

Studying the evolution of the ground state with the magnetic field change in different Coulomb systems, with different number of electrons, we found that there is always a specific, well-defined state of maximal total spin projection, which becomes the ground state at large magnetic fields. For one-electron systems, this state has $S_z = -1/2$ and $M = m_1 = 0$. For two-electron systems, it has $S_z = -1$ and $M = -1$ with $m_1 = 0, m_2 = -1$; see Table II. For two studied three-electron systems, Li and He^-, it was the state $S_z = -3/2$ and $M = -3$ [3]. It seems natural to assume that this state will be the ground state for $He_2{}^+$ for a certain *critical* magnetic field; see Sec. III. In order to find this critical magnetic field, it is necessary to explore other states of $He_2{}^+$, in particular, spin-quartet gerade and ungerade states with different total electron angular momentum ${}^4(0,-1,-2,-4)^+_{g,u}$. This will be done elsewhere.

Concluding we have to state that at $B = 1000$ a.u., the dissociation energy with respect to the main decay channel $He_2{}^+[{}^4(-3)^+] \to He[1^3(-1)^+] + He^+(1s_0)$ reaches $E_{\text{diss}} \simeq 6.54$ a.u. ($\sim$178 eV), while the dissociation energy for the decay channel (b) into $He^- + \alpha$ is $\sim$25.8 a.u. $\simeq$ 702 eV and the dissociation energy for the decay channel (c) into $He + \alpha + e$ is $\sim$26.8 a.u. $\simeq$ 729 eV. Thus, the two latter energies are in the energy window for one of the absorption features observed for the isolated neutron star 1E1207.4-5209.

We found that in a strong magnetic field $B \gtrsim 120$ a.u., the molecular ion $He_2{}^+$ is the most bound system among the atomic and molecular systems containing helium and up to three electrons. Thus, this molecule may play a particularly important role in the description of atmosphere of strongly magnetized neutron stars, as was hinted at in Ref. [15].

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