Stable He^- can Exist in a Strong Magnetic Field

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The existence of bound states of the system (α, e, e, e) in a magnetic field B is studied using the variational method. It is shown that for $B \gtrsim 0.13$ a.u. this system gets bound with total energy below the one of the (α, e, e) system. It manifests the existence of the stable He^- atomic ion. Its ground state is a spin doublet $^2(-1)^+$ at 0.74 a.u. $\gtrsim B \gtrsim 0.13$ a.u. and it becomes a spin quartet $^4(-3)^+$ for larger magnetic fields. For 0.8 a.u. $\gtrsim B \gtrsim 0.7$ a.u. the He^- ion has two (stable) bound states $^2(-1)^+$ and $^4(-3)^+$.

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Astrophysical objects such as magnetic white dwarfs may have surface magnetic fields of 10^8–10^{10} G ($\sim$0.1–10 a.u.) while neutron stars typically reach 10^{12}–10^{13} G ($\sim 10^3$–10^4 a.u.) or even 10^{15} G ($\sim 10^6$ a.u.) in the so-called magnetars. In the presence of such strong magnetic fields the chemical properties of atoms and molecules change dramatically. In particular, it makes possible the formation of unusual chemical compounds such as the H_3^{++} ion at $B \gtrsim 10^{10}$ G [1] (for a review see [2] about one-electron molecular systems, and [3] about two-electron atomic-molecular systems, and references therein). A separate question of interest concerns the existence of negative atomic ions in a magnetic field. An immediate observation is that the induced quadrupole moment—charge interaction of the atomic core with an electron is repulsive: it can influence binding. Thus, it was quite a striking theoretical result that the simplest negative atomic ion H^-, which possesses the single bound state [4], develops an infinite number of bound states in the presence of a magnetic field [5]. A similar situation may occur for the case of the negative atomic ion He^- which does not seem to have a stable bound state in the field-free case [6,7], but can become bound in a magnetic field.

The goal of this Letter is to explore the possibility of having stable bound states of the 1-center Coulomb system (α, e, e, e) in a magnetic field checking the existence of the negative ion He^-. Our main motivation to study the negative ion He^- in a magnetic field comes from the recently observed spectra of white dwarfs which indicate the presence of atomic helium on the surface of some of these astrophysical magnetized objects, see, e.g., [8]. Therefore, the existence of He^- ions can be of relevance to interpret the observed absorption features in the spectra. In this Letter atomic units ($\hbar = e = m_e = 1$) are used throughout, and the magnetic field is measured in units of $B_0 = 2.35 \times 10^9$ G.

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

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

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. Z is the nuclear charge (for He^- $Z = 2$). 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.

The variational method is used to explore the problem. The recipe for choosing the trial function is based on arguments of physical relevance: the trial function should support the symmetries of the system, has to reproduce the Coulomb singularities of the potential correctly, and reproduce the asymptotic behavior at large distances (see, e.g., [2,9,10]). It implies that electron-electron interaction plays an important role; thus, the correlation should be introduced into trial functions in exponential form $\sim \exp(\alpha r_{ij})$, where α is a variational parameter.

Following the above, a trial function for the spin 1/2 lowest energy state is chosen in the form

$$\psi(\vec{r}_1, \vec{r}_2, \vec{r}_3) = \mathcal{A}[\phi(\vec{r}_1, \vec{r}_2, \vec{r}_3)\chi], \quad (2)$$

where χ is the spin eigenfunction, $\mathcal{A}$ is the three-particle antisymmetrizer

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

and $\phi(\vec{r}_1, \vec{r}_2, \vec{r}_3)$ is the explicitly correlated orbital function

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

where M_k is the magnetic quantum number of the kth electron, and α_k, β_k, and α_{kj} are nonlinear variational parameters. In total, the trial function (2) contains 9 variational parameters. The function (2) is a properly antisymmetrized product of $1s$ Slater-type orbitals, the lowest Landau orbitals, and the exponential correlation factors $\sim \exp(\alpha r_{kj})$. We expect the ground state to be realized by different states depending on the domain of magnetic fields: guided by an analogy with the case of the lithium atom in a magnetic field (for a discussion, see [11]), we assume the spin 1/2 states $^2(0)^+$, $^2(-1)^+$ to correspond to the ground state for small and intermediate magnetic fields, respectively, while the spin 3/2 state $^4(-3)^+$ is the ground state for the large magnetic fields.

For the states $^2(0)^+$, $^2(-1)^+$ of the total spin $S = 1/2$ we have two linearly independent spin functions of mixed symmetry

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

and

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

where $\boldsymbol{\alpha}(i)$, $\boldsymbol{\beta}(i)$ are spin-up, spin-down eigenfunctions of the ith electron. The spin function χ in (2) is chosen as

$$\chi = \chi_1 + c\chi_2,$$

(for discussions see [12,13]), where c is the variational parameter. For the entire range of studied magnetic fields, c is different but close to zero. For the spin $S = 3/2$ state $^4(-3)^+$ with $M_1 + M_2 + M_3 = -3$, the spin part corresponds to the totally symmetric spin function $\chi = \boldsymbol{\beta}(1)\boldsymbol{\beta}(2)\boldsymbol{\beta}(3)$, and the orbital part $\phi(\vec{r}_1, \vec{r}_2, \vec{r}_3)$ is antisymmetrized by applying the operator $\mathcal{A}$ [Eq. (3)].

The variational energy has a quite complicated profile in the parameter space: use of standard minimization strategies did not allow us to find a minimum reasonably fast. As a result, most of the minimization was performed manually using the procedure SCAN from the minimization package MINUIT from CERN-LIB. Nine-dimensional integrals which appear in the functional of energy are calculated numerically using a "state-of-the-art"dynamical partitioning procedure based on division of the integration domain following the profile of the integrand, separating domains with large gradients. Each subdomain was integrated separately in parallel and with controlled absolute or relative accuracy (for details, see, e.g., [2]). Numerical integration of every subdomain is done with a relative accuracy of $\sim 10^{-2}$–10^{-4} using an adaptive routine [14]. Parallelization is implemented using the MPI library MPICH. Computations are performed on a Linux cluster with 96 Xeon processors at 2.67 GHz each, and 12 Gb RAM.

The existence of a chemical compound is established when the system possesses at least one stable bound state. If such a bound state exists, it is characterized by a positive ionization energy, i.e., the minimal amount of energy which is necessary to add to the system to separate it into two or more subsystems. In particular, the one-particle ionization energy is defined as the energy needed to move an electron to infinity. A bound state of He^- is characterized by definite values of the total magnetic quantum number and z projection of the total spin (M, S_z). Then, such a state is stable if its total energy is smaller than the sum of energies of two subsystems (He-atom $+e$), i.e., if

$$E_T^{\mathrm{He}^-}(M, S_z) < E_T^{\mathrm{He}}(M', S_z') + E_T^{e^-}(M_{e^-}, S_{z_{e^-}}), \quad (7)$$

where $E_T^{\mathrm{He}}(M', S_z')$ and $E_T^{e^-}(M_{e^-}, S_{z_{e^-}})$ are the total energies of the He atom and the electron, respectively (see Ref. [15]). The condition (7) must be valid for all possible decay channels satisfying the conservation of the quantum numbers

$$M = M' + M_{e^-}, \qquad S_z = S_z' + S_{z_{e^-}}, \quad (8)$$

which are valid in the nonrelativistic approximation. For an electron in a magnetic field, the total energy of the Landau levels is given by

$$E_T^{e^-}(M_{e^-}, S_{z_{e^-}}) = (M_{e^-} + |M_{e^-}| + 2S_{z_{e^-}} + 1)\frac{B}{2}, \quad (9)$$

and for nonpositive values of the magnetic quantum number M_{e^-}, the Landau levels are infinitely degenerate:

$$E_T^{e^-}(M_{e^-} \le 0, S_{z_{e^-}}) = (2S_{z_{e^-}} + 1)\frac{B}{2}. \quad (10)$$

Hence, for an electron with z-spin projection antiparallel to the magnetic field and zero (or negative) magnetic quantum number, $E_T^{e^-}(M_{e^-} \le 0, S_{z_{e^-}} = -1/2) = 0$, whereas an electron with z-spin projection parallel to the magnetic field and zero or negative magnetic quantum number has $E_T^{e^-}(M_{e^-} < 0, S_{z_{e^-}} = +1/2) = B$.

State $^2(0)^+$.—The state $^2(0)^+$ of the system (α, e, e, e) in a magnetic field of strength B is described by the trial function (2) with $M_1 = M_2 = M_3 = 0$ [see Eq. (4)]. Since this state $^2(0)^+$ is the ground state for the lithium atom for weak magnetic fields [11], it is natural to assume that the system (α, e, e, e) can also develop a stable ground state with this symmetry in a magnetic field. However, our results show that the total energy of this state always lies well above the He ground state 1^10^+ in the whole domain of magnetic fields studied (see Table I and Fig. 1). Thus,

TABLE I. Total energies in a.u. (Hartrees) for the states $^2(0)^+$, $^2(-1)^+$, and $^4(-3)^+$ for the system (α, e, e, e) obtained with trial function (2). For comparison, the total energies of the He-atom states 1^10^+, 1^30^+, and $1^3(-1)^+$ are included.

	He^-	He^-	He^-	He	He	He
B a.u.	$E[^2(0)^+]$ $M=0$, $S_z=-1/2$	$E[^2(-1)^+]$ $M=-1$ $S_z=-1/2$	$E[^4(-3)^+]$ $M=-3$, $S_z=-3/2$	$E(1^10^+)$ $M=0$, $S_z=0$	$E(1^30^+)$ $M=0$, $S_z=-1$	$E[1^3(-1)^+]$ $M=-1$, $S_z=-1$
0.1	−2.871	−2.892		−2.901 740[c]	−2.258 237[c]	–
0.16	−2.861	−2.905		−2.898 290[a]	−2.296 318[a]	−2.325 189[b]
0.24	−2.848	−2.904		−2.892 404[c]	−2.339 571[c]	−2.402 393[b]
0.40	−2.816	−2.899	−2.563	−2.872 874[c]	−2.412 731[c]	−2.540 763[b]
0.50	−2.794	−2.887	−2.650	−2.855 859[a]	−2.454 347[a]	−2.620 021[b]
0.8	−2.713	−2.836	−2.891	−2.788 425[c]	−2.573 620[c]	−2.835 619[b]
1.0	−2.652	−2.794	−3.034	−2.730 373[c]	−2.650 658[c]	−2.965 504[b]
1.6		−2.658	−3.394	−2.508 81[c]	−2.867 620[a]	−3.308 774[b]
2.0			−3.606	−2.330 65[c]	−2.999 708[a]	−3.508 911[b]
5.0			−4.764	−0.575 5[c]	−3.768 199[a]	−4.625 491[b]
10.0			−5.999	3.064 582[a]	−4.627 450[a]	−5.839 475[b]
20.0			−7.614	11.267 051[a]	−5.772 448[a]	−7.440 556[b]
50.0			−10.46	38.076 320[a]	−7.815 256[a]	−10.284 10[b]
100.0			−13.29	84.918 313[a]	−9.843 074[a]	−13.104 78[b]

[a]Ref. [16], Becken: 1999.
[b]Ref. [17], Becken: 2000.
[c]Ref. [18], Hesse: 2004.

this state is metastable, being unstable towards decay $He^-[^2(0)^+] \rightarrow He(1^10^+) + e$. The total energy of this metastable state grows monotonically with an increase of the magnetic field strength (see Table I and Fig. 1).

State $^2(-1)^+$.—The state $^2(-1)^+$ of the system (α, e, e, e) in a magnetic field is described by the trial function (2) with $M_1 = M_2 = 0$, $M_3 = -1$ [see Eq. (4)]. This state

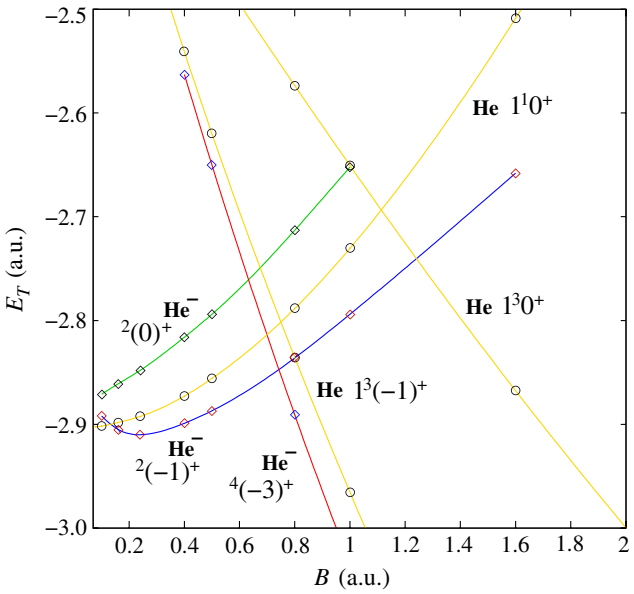

FIG. 1 (color online). Total energies (in a.u.) for the states $^2(0)^+$, $^2(-1)^+$ and $^4(-3)^+$ of the negative ion He^- (open diamonds) in comparison to the energies of the lowest He-atom states 1^10^+, 1^30^+, $1^3(-1)^+$ (open circles) in a magnetic field B.

becomes the lowest energy (ground) state of the lithium atom for intermediate magnetic fields (see, e.g., [11]). The state $^2(-1)^+$ for He^- gets bound for all magnetic fields studied. Its variational energies are shown at Table I for 1.6 a.u. $> B >$ 0.1 a.u. These energies are always below the total energies of the state $^2(0)^+$. Qualitatively, the total energy of the state $^2(-1)^+$ displays a minimum at $B \simeq$ 0.25 a.u. and then grows monotonically with a magnetic field increase (see Fig. 1). For magnetic fields $B \gtrsim$ 0.13 a.u. this state turns out to be stable towards decay $He^-[^2(-1)^+] \rightarrow He(1^10^+) + e$, since its total energy lies below the energy of the He ground state 1^10^+ for all magnetic fields (see Fig. 1). However, for magnetic fields $B \gtrsim 0.8$ a.u. the state $^2(-1)^+$ of the system (α, e, e, e) becomes metastable: (α, e, e, e) decays to (α, e, e) + e.

Hence, the state $^2(-1)^+$ realizes the stable bound state of the system (α, e, e, e) for magnetic fields 0.8 a.u. $\gtrsim B \gtrsim$ 0.13 a.u. Eventually, it becomes the ground state of the He^--ion for 0.74 a.u. $\gtrsim B \gtrsim$ 0.13 a.u. and the first (stable) excited state for 0.8 a.u. $\gtrsim B \gtrsim$ 0.74 a.u. (see below).

State $^4(-3)^+$.—The spin 3/2 state $^4(-3)^+$ of the system (α, e, e, e) in a magnetic field is described by the trial function (2) with $M_1 = 0$, $M_2 = -1$, $M_3 = -2$ [see Eq. (4)]. Because of the spin Zeeman contribution, the energy of this (spin $S = 3/2$) state decreases rapidly and monotonically with the magnetic field increase (see Fig. 1 and Table I). Based on pure energy considerations, one can see that the system (α, e, e, e) in the state $^4(-3)^+$ gets stable for $B \gtrsim 0.7$ a.u.

At $B \simeq 0.7$ a.u. the total energy of the state $^4(-3)^+$ of He^- coincides with the total energy of the state 1^10^+ of the He atom. Hence, this state becomes the first excited state of

TABLE II. Total energies in a.u. for the Li atom in a magnetic field for the states $^2(-1)^+$, $^2(-1)^+$, and $^4(-3)^+$ obtained with (2) and compared with [15].

B a.u.	$E(1^20^+)$		$E(1^2(-1)^+)$		$E(1^4(-3)^+)$	
	(2)	[15]	(2)	[15]	(2)	[15]
0.0	−7.455[a]	−7.477766[b]	−7.406	−7.407126[b]		−5.142319[b]
1.0		−7.458550[b]	−7.701	−7.716679[b]	−6.567	−6.582361[b]
5.0		−6.136918[b]		−7.002346[b]		−9.591769[b]

[a]Ref. [12], Turbiner: 2009.
[b]Ref. [15], Al-Hujaj: 2004.

the He^- ion, while the ground state is $^2(-1)^+$. The total energy of the state $^4(-3)^+$ continues to decrease with the magnetic field increase. At $B \simeq 0.74$ a.u. it intersects with the total energy of the state $^2(-1)^+$ and becomes the ground state of the He^- ion for larger magnetic fields. In the domain 0.8 a.u. $\gtrsim B \gtrsim$ 0.74 a.u. the He^- ion has two stable states: $^4(-3)^+$ as the ground state and $^2(-1)^+$ as the first excited state. At $B \simeq 0.8$ a.u. the latter state gets metastable decaying to $He[1^3(-1)^+] + e$. Thus, for larger magnetic fields $B \gtrsim 0.8$ a.u. the He^- ion has a single stable bound state $^4(-3)^+$.

Lithium.—In order to have an independent estimate of the accuracy reached, we have made some test calculations with the trial function (2) for the $^20^+$, $^2(-1)^+$ and for tightly bound $^4(-3)^+$ states of the lithium atom in a magnetic field. Our results are presented in the Table II where we include previous results [15] to compare with.

Conclusions.— We have shown that the system (α, e, e, e) in a magnetic field has at least one stable bound state for magnetic fields $B \gtrsim 0.13$ a.u. This manifests the existence of the stable He^- atomic ion. For values of the magnetic field in $0.80 \gtrsim B \gtrsim 0.70$ a.u. the system displays two stable bound states with the ground state being realized at first by the state $^2(-1)^+$ for magnetic fields up to $B \simeq$ 0.74 a.u., followed by the state $^4(-3)^+$ as the stable ground state for $B \gtrsim 0.74$ a.u., while the state $^2(-1)^+$ becomes the excited state. For magnetic fields $B \gtrsim 0.80$ a.u. the negative ion He^- has a single stable bound state. All this shows that the closed shell argument does not work in a magnetic field.

It is worth noting that the energy of bound-free transitions grows very slowly with the magnetic field increase from $\sim$0.8 eV for $\sim 10^9$ G [for the state $^2(-1)^+$] to $\sim$4.9 eV for $\sim 10^{11}$ G [for the state $^4(-3)^+$]. Hence, it may be visible in the infrared or optical part of the spectra of radiation of a cold magnetic white dwarf.

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