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Lowest energy levels of H^-, He, and Li^+ in intense magnetic fields*

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We present rough variational upper-bound estimates of some low-lying bound-state energy levels of two-electron systems, including H^-, He, and Li^+, in magnetic fields B above 10^{10} G, a regime that is relevant to recent astrophysical studies of pulsars. The simple trial wave functions that we use in the Rayleigh-Ritz calculations consist of single antisymmetrized products of single-particle orbitals which are predominantly *magnetic* in their spatial character. Most importantly, our results indicate that in the regime $10^{10} \lesssim B \lesssim 10^{13}$ G the H^- ion has at least one singlet and one triplet bound state; at 2×10^{12} G, e.g., the ionization energy of the triplet ground state of H^- is greater than 12 eV. (The number of bound states of H^- in this regime of B may be much greater; moreover, the number of levels and their depths is expected to increase monotonically with B.) These results appear to contradict a recent indication that there might not be any bound states of H^- above 10^{10} G. For $B\rightarrow\infty$ we also present the approximate leading asymptotic terms for the total (nonrelativistic) energies and corresponding ionization energies of some low-lying states of two-electron systems with nuclear charge $Z\geq 2$.

I. INTRODUCTION

The supposition that intense magnetic fields B of order 10^{12} G exist within pulsars[1] has stimulated interest in the structure of atoms under these conditions. We report here[2] variational upper-bound estimates of some low-lying bound-state energy levels of two-electron systems, including H^-, He, and Li^+, in magnetic fields above 10^{10} G; H^- and He may be particularly important from an astrophysical viewpoint.

The trial wave functions Ψ_t used in the Rayleigh-Ritz calculations are constructed from single-particle orbitals that are based on an adiabatic approximation, described below, in which the magnetic interaction assumes a dominant role over the Coulomb interaction in setting the character of the solutions. For the atomic systems considered this approach is expected to lead to reasonably accurate trial wave functions for B above approximately 10^{10} G. We have considered states of both singlet and triplet symmetry with various values of M, the conserved eigenvalue of the z component of the total orbital angular momentum. Ψ_t is written as a single antisymmetrized product of these orthogonal "magnetic" orbitals; for each case, we have included the determinantal configuration which we expect represents the principal contribution to the lowest state of given symmetry. This form of Ψ_t is still simple enough to enable us to carry through the calculations of the expectation value of the Hamiltonian analytically.

As the field B rises above about 5×10^9 G, the Larmor radius for the motion of an electron in the plane perpendicular to the magnetic field becomes less than the Bohr radius for hydrogen, and the magnetic interaction of the electron in a hydrogen atom begins to dominate over its Coulomb interaction with the proton. In the adiabatic approach one neglects the effects of the Coulomb interaction with regard to this cyclotron motion of the electron in the plane perpendicular to B. At sufficiently high values of B, this same approach will be valid for all electrons, including the innermost, in a many-electron atom. Note, however, that by the time the Larmor radius of an electron is comparable to its Compton wavelength, which occurs for $B\approx 3\times10^{13}$ G, relativistic effects, which we do not consider, are expected to play an important role.

Perhaps surprisingly, even with these simple trial wave functions, the H^- ion is shown to have at least one singlet and one triplet bound state in the range $10^{10}\lesssim B\lesssim 10^{13}$ G. Beyond about 10^{13} G our energy estimates for H^- do not indicate that H^- is bound, but we attribute this to inadequacies in the wave function for H^- in this limit, as discussed in Sec. II. Actually there may be many more bound states of H^- in this intense-magnetic-field regime than the two presented here; moreover, the number of levels and their depths are expected to increase monotonically with B. The existence of bound states of H^- in this intense-magnetic-field regime appears to contradict the recent indication[3] that H^- becomes unbound above 10^{10} G. This conclusion is based on energy estimates with Ψ_t a linear combination of functions, the radial parts of which are Slater orbitals and which thereby stress the spherical "Coulomb" character of the problem. While appropriate for lower magnetic fields, these orbitals are not separately particularly suitable for intense magnetic fields, $B \gtrsim 10^9$ G, where the wave function is highly distorted, being much more tightly bound in the plane perpendicular to B than along the z axis. A very large number of Slater orbitals and large l values would be required to reproduce such behavior, and therefore the decrease in the binding energy of H^- in this region reported in Ref. 3 is perhaps merely reflecting the inadequacy of the Ψ_t. This is confirmed by the fact that the decrease is pushed up to higher values of B when the number of orbitals is increased.[4]

In addition to solid-state applications,[5] the present adiabatic approach has been used previously[6] in the pulsar context to estimate the ground-state and corresponding ionization energies for atoms with $Z \leq 10$. In these calculations Ψ_t was restricted to Hartree product form, with exchange contributions included in rough fashion; for two electron systems, and particularly H^-, where exchange interactions play an important role, an antisymmetrized Ψ_t is expected to be more reliable. Results have also been obtained for heavy atoms. In a "strong" B-field regime, that is, $10^9 Z^{4/3} B < 10^{10} Z^3$ G, a one-dimensional Thomas-Fermi–like model was found to be valid,[7,8] but a statistical model is, of course, untrustworthy for a two-electron system, and is not even valid for negative ions. (This model has also been extended to atoms under pressure in the pulsar crust.[9]) At still higher values of B, $B \gg 10^{10} Z^3$ G, approximations to the leading terms in the ground-state energies were obtained,[8] but the simple wave functions used are of a form most reliable for heavy atoms and ions, and, moreover, the asymptotic limit that was derived is not approached, for Z of the order of 2, until B is above 10^{12} G. Finally, we note that recent calculations indicate that it is extremely favorable on energetic grounds for many-electron atoms to combine to form one-dimensional molecules, and even long filaments containing many atoms.[6,10] Whether or not this conclusion is also valid for two-electron systems is unclear, but, in any case, it would be useful to study the atomic case.

II. VARIATIONAL CALCULATION

The nucleus with charge Ze is assumed infinitely massive. B is uniform and oriented along the z axis and is assumed strong enough for a complete Paschen-Back effect with the spin-orbit interaction neglected. The Hamiltonian for the two electrons is then written

$$H = H^{(0)}(\vec{r}_1, \vec{p}_1; \vec{s}_1) + H^{(0)}(\vec{r}_2, \vec{p}_2; \vec{s}_2) + e^2/|\vec{r}_1 - \vec{r}_2|, \tag{1}$$

where $\vec{s}_1$ and $\vec{s}_2$ are the electron spins and $H^{(0)}$, the Hamiltonian for a hydrogenlike system in a magnetic field including the interaction of the electron's spin with B, can be expressed as[11]

$$H^{(0)} = p^2/2\mu + \tfrac{1}{2}\omega_c l_z + \tfrac{1}{8}\mu\omega_c^2\rho^2 - Ze^2/r + \omega_c s_z, \tag{2}$$

where $\omega_c \equiv eB/\mu c$ is the angular Larmor frequency, μ is the electron mass, and l_z and s_z are the respective z components of the orbital and spin angular momentum operators. The operators representing the projection along the z axis of the total orbital and spin angular momentum, $L_z = l_{z_1} + l_{z_2}$ and $S_z = s_{z_1} + s_{z_2}$, respectively, as well as the operators $\vec{S}^2 = (\vec{s}_1 + \vec{s}_2)^2$ and parity, all commute with H, and the corresponding eigenvalues $(M; S, M_S; \Pi)$ are good quantum numbers for solutions of Eq. (1). (We note that this notation is slightly different from that used in Ref. 3.) The eigenfunctions of both H and $H^{(0)}$ factor into spatial and spin wave functions. The spatial wave functions are written $\Psi(\vec{r}_1, \vec{r}_2)$ and $\Psi^{(0)}(\vec{r})$, respectively. The eigenvalues are written $E = E_{\text{spat}} + \hbar\omega_c M_S$ and $E^{(0)} = E^{(0)}_{\text{spat}} + \hbar\omega_c m_s$, where $m_s\hbar = \pm\frac{1}{2}\hbar$ is the eigenvalue of s_z, and we have decomposed the energies into spatial and spin contributions.

First, we briefly discuss the form of the spatial eigenfunctions $\Psi^{(0)}(\vec{r})$ and corresponding eigenvalues $E^{(0)}$ of $H^{(0)}$ given in Eq. (2) for intense magnetic fields. These solutions are the basis functions used to construct trial solutions for the two-electron case. In the adiabatic limit previously described, the motion of the electron in the perpendicular plane is taken to be independent of the Coulomb field; the solutions for the perpendicular motion are therefore the Landau magnetic wave functions,[12] with corresponding eigenvalues (excluding the spin contribution)

$$\epsilon_\perp = \hbar\omega_c(n_\rho + \tfrac{1}{2}m + \tfrac{1}{2}|m| + \tfrac{1}{2}), \tag{3}$$

where the quantum numbers for the perpendicular motion are $n_\rho = 0, 1, 2, \ldots$, which denotes the number of nodes along the ρ direction, and $m\hbar = 0, \pm\hbar, \pm 2\hbar, \ldots$, which is the eigenvalue of l_z. As is well known, each energy level in Eq. (3) is infinitely degenerate. For intense magnetic fields, the separation $\hbar\omega_c$ between energy levels in Eq. (3) is large compared to Coulomb binding energies, and the Coulomb interaction will not cause significant mixing between states of different n_ρ. (At 10^{12} G, e.g., $\hbar\omega_c \approx 10^4$ eV.) We therefore choose states with $n_\rho = 0$ and express $\Psi^{(0)}$ in terms of the normalized ground-state Landau wave functions ($n_\rho = 0, m = 0, -1, -2, \ldots$) as

$$\Psi_m^{(0)}(\vec{r}) = \Phi_{0,m}(\rho, \phi) f(z), \tag{4}$$

where we suppress the m dependence of $f(z)$, the first index of Φ denotes the value of n_ρ, and[12]

$$\Phi_{0,m} = (\pi\hat{\rho}^2 |m|!)^{-1/2} (\rho/\hat{\rho})^{|m|} e^{-\rho^2/2\hat{\rho}^2} e^{im\phi}, \tag{5}$$

with $\hat{\rho} \equiv (2\hbar c/eB)^{1/2}$ the cyclotron radius. (This definition of $\hat{\rho}$ is consistent with that of Ref. 8, but differs by the factor $\sqrt{2}$ from that in Refs. 4 and 6.) Note that the parity of $\Phi_{0,m}$ is $(-1)^m$. This form of the solutions $\Psi_m^{(0)}$ becomes exact in the limit $B \to \infty$. Upon substitution of (4) into the Schrödinger equation, multiplication by $\Phi_{0,m}^*$, and integration over variables ρ, ϕ, we obtain a one-dimensional Schrödinger equation for $f(z)$

$$[p_z^2/2\mu + V_{|m|}(z)] f(z) = \epsilon_{\parallel}^{|m|} f(z), \tag{6}$$

where the effective potential $V_{|m|}(z)$ is given by

$$V_{|m|}(z) = -Ze^2 \int\int |\Phi_{0,m}|^2 (\rho^2 + z^2)^{-1/2} \rho \, d\rho \, d\phi. \tag{7a}$$

Since for the states in question $\epsilon_\perp = \frac{1}{2}\hbar\omega_c$, the eigenvalues $E^{(0)}$ [more precisely, because of the steps leading to Eq. (6) these are upper bounds on the energies] are then approximated by

$$E^{(0)} = \tfrac{1}{2}\hbar\omega_c + \epsilon_{\parallel}^{|m|} + m_s \hbar. \tag{7b}$$

The low-lying eigenvalues of Eq. (6) for $|m| \leq 5$ have been numerically calculated[13] at two values of B (2×10^9 and 2×10^{12} G). Since $|\Phi_{0,m}|^2 \rho$ is sharply peaked in ρ at the value $\rho = \hat{\rho}_m \equiv \hat{\rho}(|m| + \frac{1}{2})^{1/2}$, we can replace $(\rho^2 + z^2)^{-1/2}$ in Eq. (7a) by $(\hat{\rho}_m^2 + z^2)^{-1/2}$. The further replacement by the (lower-bound) estimate $(\hat{\rho}_m + |z|)^{-1}$ leads to the much simpler and still reasonably accurate one-dimensional Coulomb-like potential

$$V_{|m|}(z) \simeq -Ze^2/(|z| + \hat{\rho}_m).$$

The eigenvalue spectrum for this latter potential has been studied previously,[14] and the principal results are the following: Provided $\hat{\rho}_m < a_0$, which is of course true for the intense-field limit, the energy levels of this potential for a given value of m include, in addition to an infinite sequence of levels which approximate the Bohr levels, one deep level corresponding to a state with $f(z)$ nodeless. The leading term in the energy of this deep level is given by

$$\epsilon_{\parallel}^{|m|} \simeq -4Z^2 E_H \ln^2(a_0/Z\hat{\rho}_m), \tag{8a}$$

where $E_H \equiv 13.6$ eV. The results of Ref. 13 also show the existence of this deep level for the exact potential $V_{|m|}(z)$. An approximate variational estimate of this deep-level energy for the exact $V_{|m|}(z)$ can be obtained simply with the trial function $f_t(z) = N_z e^{-\alpha z^2}$, where α is a variational parameter and N_z is the normalization factor. As $B \to \infty$, the leading asymptotic term in the result, in this approximation, is

$$\epsilon_{\parallel}^{|m|} \simeq -(8/\pi) Z^2 E_H \ln^2(a_0/Z\hat{\rho}_m). \tag{8b}$$

[This follows from the nonasymptotic variational expression given in Eq. (13).] This asymptotic expression will be compared with comparable expressions for two-electron systems.

The trial spatial wave function, $\Psi_t(\vec{r}_1, \vec{r}_2)$, which we use to calculate the expectation of H given in Eq. (1), is taken to be a spatially symmetric (for singlet states) or antisymmetric (for triplet states) product of the lowest adiabatic solutions $\Psi_m^{(0)}$ consistent with the Pauli principle. If the electron-electron interaction were completely neglected, the lowest singlet state would place both electrons in the adiabatic state with $m = 0$ and with nodeless $f(z)$; the lowest triplet state would have the electrons described by adiabatic solutions with $m = 0$ and -1 and with nodeless $f(z)$. [As seen from Eq. (8b), there is some loss in binding energy if we place the second electron in the adiabatic state with other than $m = 0$, as will be necessary if we choose a nodeless $f(z)$; however, it is much less than the loss that would occur if the second electron were placed in the adiabatic state with $m = 0$ and with an $f(z)$ which is not nodeless. The energy of such a state is approximately $-E_H$, as compared to the deep binding of the nodeless $f(z)$.] The energy spectrum would also include a series of singlet and triplet states in which one or both electrons had higher values of $|m|$.

We expect that this approximate description of the low-lying states for a two-electron neutral atom in the intense-field limit continues to provide a reasonable description of the true solutions when the electron-electron interaction is included. This is based first on the fact that approximate calculations[8] of the leading asymptotic term for the ground-state energies of heavy atoms yield a value of 1/3 for the ratio of the magnitude of the total electron-electron interaction energy to the electron-nucleus interaction energy.[15] Second the electron probability distributions corresponding to the ground-state adiabatic solutions are roughly confined to thin cylindrical shells of radii $\hat{\rho}_m$, width $\hat{\rho}$, and length a_0/Z. From classical electrostatics the interaction energy of repulsion of two such shells, each of total charge $-e$ (either with the same or different radii), always remains a fraction of the interaction energy of attraction of both shells with the point charge nucleus of charge $+2e$ at the origin, and this remains valid in the limit $B\rightarrow\infty$ when the ratio of the cylinder's radius to length goes to zero, because $\hat{\rho}$ and $\hat{\rho}_m$ scale with B in the same way.

Analogous arguments will of course apply to positive two-electron ions such as Li^+. However, for the negative H^- ion the situation is not as straightforward. Firstly, in the strict $B\rightarrow\infty$ limit the repulsive energy of two cylindrical shells, each of charge $-e$, ultimately becomes greater than their net attractive energy with the single proton. It is not then surprising that our results, based on our particular trial function, do not, in the limit $B\rightarrow\infty$, prove that any bound states of H^- exist. (The results for H^- do, however, still give binding for B in the range $10^{10}\lesssim B\lesssim 10^{13}$ G when the corresponding cylindrical shells are not quite one dimensional.) As B increases, other configurations will become important in Ψ_t, configurations with larger values of $|m|$, which represent electrons occupying "cylinders" of larger radii and which thereby increase the ρ extension of the wave function. It is expected that H^- will continue to have bound states. Once the intense-field regime is achieved there is no apparent reason for H^- becoming unbound; on the contrary, as B increases further the principal effect of the magnetic field at this stage is to confine the electrons, at least with regard to their perpendicular motion.

In the trial functions, the $f(z)$ are taken, for simplicity, to be Gaussian functions, with the values of the parameters in the exponents to be determined variationally in the final energy estimates. Although the correct dependence of the $f(z)$ from Eq. (6) is asymptotically exponential, we choose the Gaussian form which permits us to quite easily carry out analytically all the integrals involved in the estimation of $\langle H\rangle$. With these basis functions the eigenvalues $M\hbar$ of L_z reduce to m_1+m_2 (m_1 and m_2 are not, of course, separately good quantum numbers), and the upper bounds to the total-energy eigenvalues, including the spin energies, are then given by

$$E\leqslant\hbar\omega_c+E_z+\hbar\omega_c M_s\,, \tag{9a}$$

where the first term represents $2\epsilon_\perp$ and where E_z is the expectation value with respect to $\Psi_m^{(0)}(\vec{r})$,

$$E_z=\left\langle\frac{p_{z_1}^2}{2\mu}+\frac{p_{z_2}^2}{2\mu}-\frac{Ze^2}{r_1}-\frac{Ze^2}{r_2}+\frac{e^2}{|\vec{r}_1-\vec{r}_2|}\right\rangle. \tag{9b}$$

We have evaluated Eq. (9b) for the lowest singlet state with $M=0$ and even parity, using the trial function

$$\Psi_t(M=0,S=0)=\Phi_{0,0}(\rho_1)\Phi_{0,0}(\rho_2)f_1(z_1)f_1(z_2), \tag{10}$$

and the lowest triplet (−) and singlet (+) states with $M=-1$ and odd parity, with

$$\Psi_t(M=-1,S=1,0)=2^{-1/2}[\Phi_{0,0}(\rho_1)\Phi_{0,-1}(\rho_2,\phi_2)\times f_1(z_1)f_2(z_2)\mp(1\leftrightarrow 2)], \tag{11}$$

where f_1 and f_2 are the normalized even-parity Gaussian functions

$$f_1(z)=(\alpha/\pi)^{1/4}e^{-\alpha z^2},$$
$$f_2(z)=(\beta/\pi)^{1/4}e^{-\beta z^2}. \tag{12}$$

Note that for the forms of Ψ_t under consideration, we have $\Pi=(-1)^M$.

III. DISCUSSION

A schematic diagram of the lowest energy levels of Eq. (1) for H^- from $B=0$ to intense magnetic fields is shown in Fig. 1. At $B=0$ there is only one bound state, a singlet state with a binding energy of 0.75 eV. At intermediate magnetic-field strengths other singlet and triplet states will abruptly become bound. In order to determine whether a given state of H^- is bound, that is, whether its ionization energy $I(\mathrm{H}^-)=E^{(0)}(\mathrm{H})-E(\mathrm{H}^-)$ is positive, we must compare the energy of H^- with the lowest energy of a hydrogen atom in the magnetic field plus a free electron in the magnetic field, for the same set of good quantum numbers $(M;S,M_s;\Pi)$. For comparison then we have included in Fig. 1 the lowest-energy states of a free electron, $E_{\mathrm{el}}=\hbar\omega_c(m_s+\frac{1}{2})$, with $m_s=\pm\frac{1}{2}$, and the lowest energy levels of a hydrogen atom, $E^{(0)}=\hbar\omega_c(m_s+\frac{1}{2})+\epsilon_\parallel^0$, again with $m_s=\pm\frac{1}{2}$. In addition to the adiabatic calculations of Ref. 13, which are expected to be quite accurate at the higher values of B, the lowest eigenvalues of $H^{(0)}$ have also been calculated over the range 10^7–10^{11} G with a variety of other approaches.[16-18] These results appear to agree quite well and appear to have converged, and we have used these results for $E^{(0)}(\mathrm{H})$ for $B<10^{12}$ G and our results for $E(\mathrm{H}^-)$ to estimate the ionization energies of the states of H^-.

Our estimates of E_z for H^- are variational upper bounds. Provided the energy results for hydrogen are accurate, our estimates of the ionization energies of H^- will then represent variational lower bounds—the second electron can only be more tightly bound than in our estimates. For the triplet states under consideration, $(M;S,M_s;\Pi)$ reduces to $(-1;1,M_s;-)$, with $M_s=1,0,-1$; the cal-

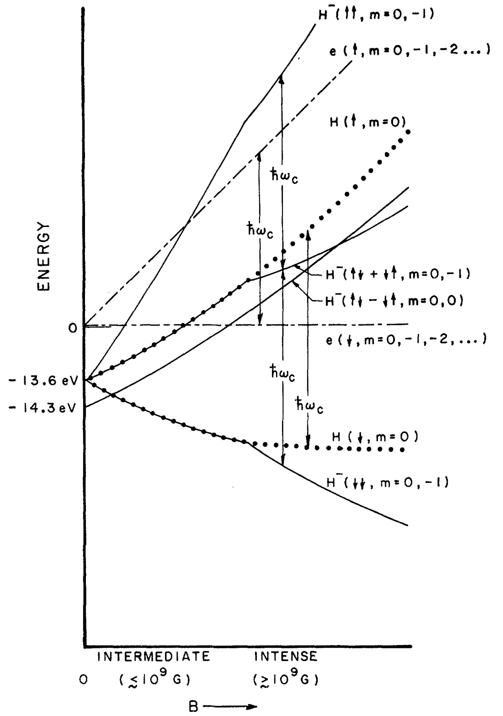

FIG. 1. Schematic diagram of the energies of some low-lying states of an electron, a hydrogen atom, and a hydrogen ion as a function of the magnetic-field strength B. The designations of intermediate and intense B are very approximate. The various curves are labeled by the electron-spin projections and the distributions of m values (↑ denotes a spin projection parallel to $\vec{B}$). For clarity, the binding energy of the singlet H^- state, represented by the separation of the H^-(↑↓−↓↑, $m=0,0$) and H(↑, $m=0$) curves [since the corresponding e(↓) curve has zero energy] and equal to 0.75 eV at $B=0$, is shown on a greatly enlarged scale. This has also been done for the triplet H^- states beyond the point at which they first become bound. We have also indicated the energy separation $\hbar\omega_c \equiv eB/\mu c$ between curves for e, H, and H^- corresponding to different electron spin projections for one or both electrons.

culation of $I(H^-)$ involves a comparison of the total energy $E(H^-)$ of H^- with the total energy of a hydrogen atom with quantum numbers $m=0$ and m_s plus the energy of a free electron with quantum numbers $m=-1$ and m_s', where $m_s+m_s'=M_s$. For the lowest-energy configuration of a hydrogen atom plus free electron with a value of $M<0$, the electron in the hydrogen atom will have the value $m=0$, while the free electron will assume the value $m=M$—which has the same energy as a free electron with $m=0$. For the singlet state under consideration, (0; 0, 0; +), the calculation of $I(H^-)$ involves comparison of $E(H^-)$ with the total energy of a hydrogen atom with quantum numbers $m=0$ and m_s plus the energy of a free electron with quantum numbers $m=0$ and m_s', where $m_s+m_s'=0$. Consequently, it should be clear that there is no spin contribution to $I(H^-)$ for either the triplet or singlet state.

The points shown in Fig. 1 where the triplet states of H^- have a discontinuous change in derivative, that is, first become bound, are chosen relatively arbitrarily; a much more careful calculation would be required to reliably locate where this occurs. The result for the energy of the singlet state lies above that of the corresponding triplet state for intense B, which then implies a crossing point at some lower value of B, as shown. This result could, however, be due merely to a particularly poor choice for the trial wave function of the singlet case. We note that the results of Ref. 3 show the singlet state (0; 0, 0; +) is unbound for intermediate B from $B \gtrsim 10^8$ G to the upper limit of B for which results are presented, $B=3.3\times10^9$ G, and hence if these results are correct the energy curve of the singlet state would join that of the appropriate $H+e^-$ state in this intermediate regime. Also, the point at which the triplet state (−1; 1, −1; −) first becomes bound is given in Ref. 3 as $B \cong 4\times10^8$ G.

Estimates of E_z [Eq. (9b)] for H^- for the states (0; 0, 0; +) and (−1; 1, −1; −) are presented[19] in Table I for B from 10^{10} to 5×10^{13} G. The ionization energy of these states is simply $-E_z+\epsilon_\parallel^0$, and values are included in Table I if results for $\epsilon_\parallel^0$ are available. The ionization energies for the triplet state of H^- are largest, indicating that the negative electron-electron exchange contribution outweighs the slight loss in binding of the $m=-1$ electron. For the singlet state with $M=-1$ the ionization energies are never positive. In general, however, we would expect singlet and triplet states of H^- with arbitrary values of $M<0$ to eventually become bound, and also the number of such states for given M to increase with B. The decrease in ionization energy of H^- that we obtain in going from 0.5×10^{12} G to 2×10^{12} G, for both the singlet and triplet cases, is presumably not real but rather a reflection of the crudeness of the trial function, commented on previously, for such strong B fields.

Results for E_z for He and Li^+ are presented[19] in Table II. Unfortunately, accurate estimates of $\epsilon_\parallel^0$ for $Z=2, 3$ are not available, and hence we cannot reliably estimate the ionization energies. Rough estimates of the ionization energies can be obtained, however, by comparison of E_z with the simple variational estimate of $\epsilon_\parallel^0$ described earlier. Using the Gaussian form for $f(z)$ with parameter α, the total variational expression for the energy [in contrast to the minimized leading asymptotic result in Eq. (8b)] is

TABLE I. Variational upper-bound estimates E_z [Eq. (9b)] of the binding energy of the bound triplet $(-1;1,-1;-)$ and singlet $(0;0,0;+)$ states of H^- at various values of the magnetic field B. We are using the notation $(M;S,M_S;\Pi)$. Also included in column 4, if available, are estimates of $\epsilon_{\parallel}^0$ [Eq. (6)] the binding energy for the lowest $m=0$ state of H. These results are obtained by extrapolating from the results in Refs. 16–18. In columns 5 and 6 we have listed the corresponding ionization energies for the singlet and triplet states of H^-. (Values are included only if a bound state is found.)

B (10^{12} G)	H^- $-E_z$ (eV) $(-1;1,-1;-)$	$(0;0,0;+)$	H $-\epsilon_{\parallel}^0$ (eV)	Ionization energy of H^- (eV) $(-1;\ 1,-1;-)$	$(0;0,0;+)$
0.01	38.5	37.2	35	3.5	2.2
0.05	68	65	62.6	5.4	2.4
0.10	85	82	78	7.0	4.0
0.5	138	133	125	13	8.0
1.0	168	162			
2.0	202	195	190 [a]	12	5.0
5.0	254	245			
10.0	299	288			
50.0	425	407			

[a] Reference 13.

$$\epsilon_{\parallel}^m \simeq Z E_{\mathrm{H}}\left(\frac{a_0}{\hat{\rho}_m}\right)\frac{1}{\sqrt{\pi}}\left[\frac{\sqrt{\pi}}{Z}\left(\frac{a_0}{\hat{\rho}_m}\right)x - \frac{2(2x)^{1/2}}{(1-2x)^{1/2}}\ln\frac{1+(1-2x)^{1/2}}{1-(1-2x)^{1/2}}\right], \tag{13}$$

where $x \equiv \alpha/\hat{\rho}_m^2$ should then be varied to obtain the minimum energy.

As $B \to \infty$ the approximate leading asymptotic term in the energy E_z, minimized with respect to parameter(s) in the trial wave function, is independent of the values of S_z and M for the three states considered, reducing to

$$E_z \simeq -\frac{[4-(\sqrt{2}/Z)]^2}{\pi} Z^2 E_{\mathrm{H}} \ln^2\frac{a_0}{Z\hat{\rho}},$$

where the minimized variational parameter(s) is given by

$$\alpha \simeq \frac{(2\sqrt{2}-1/Z)^2}{\pi}\frac{Z^2}{a_0^2}\ln^2\frac{a_0}{Z\hat{\rho}}.$$

(Roughly, the extension along z is given in terms of α as $\alpha^{-1/2}$.) For the states with $M=-1$, the two variational parameters are both set equal to the above value. If we compare these energies with the approximate asymptotic energy $\epsilon_{\parallel}^0$ of a hydrogenlike ion of nuclear charge Z [Eq. (8b)] we see that all three states are bound for $Z \geqslant 2$. (As discussed previously these results do not apply for H^-.) Admittedly, with an approximate estimate of the energy of hydrogen it is hazardous to

TABLE II. Variational upper-bound estimates E_z [Eq. (9b)] of the binding energy of the triplet $(-1;1,-1,-)$, singlet $(0;0,0;+)$, and singlet $(-1;0,0;-)$ states of He and Li^+ at various values of the magnetic field B.

	$-E_z$ (eV)					
		He			Li^+	
B (10^{12} G)	$(-1;1,-1;-)$	$(0;0,0;+)$	$(-1;0,0;-)$	$(-1;1,-1;-)$	$(0;0,0;+)$	$(-1;0,0;-)$
0.01	107	118	91	180	207	161
0.05	200	219	171	347	396	313
0.10	258	282	222	453	515	410
0.5	450	488	393	816	918	744
1.0	563	609	494	1040	1160	948
5.0	913	978	811	1740	1920	1600
10.0	1104	1180	988	2140	2350	1980
50.0	1662	1763	1504	3320	3620	3100

estimate ionization energies, but, to the extent that relativistic corrections are not yet important, the form of the dependence may well be correct.

Finally, on the basis of these results, which indicate such large values for the ionization energy of H^-, we end by speculating that there may exist more negative ions, including possibly the H^{--} ion, in the presence of intense B fields.

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