# High accuracy calculation of the hydrogen negative ion in strong magnetic fields*

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Using a full configuration-interaction method with Hylleraas–Gaussian basis function, this paper investigates the $1^1 0^+$, $1^1(-1)^+$ and $1^1(-2)^+$ states of the hydrogen negative ion in strong magnetic fields. The total energies, electron detachment energies and derivatives of the total energy with respect to the magnetic field are presented as functions of magnetic field over a wide range of field strengths. Compared with the available theoretical data, the accuracy for the energies is enhanced significantly. The field regimes $3 < \gamma < 4$ and $0.02 < \gamma < 0.05$, in which the $1^1(-1)^+$ and $1^1(-2)^+$ states start to become bound, respectively, are also determined based on the calculated electron detachment energies.

**Keywords:** strong magnetic field, hydrogen negative ion, total energy, electron detachment energy

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## 1. Introduction

Since the astrophysical discovery of strong magnetic fields on the surfaces of white dwarf stars ($10^2$–$10^5$ T) and neutron stars ($10^7$–$10^9$ T)[1–3] in the 1970s, the properties of atoms in strong magnetic fields have attracted increasing interest of researchers. In order to identify the spectra from these astrophysical objects, it is essential to possess an accurate knowledge of the properties of atoms subjected to strong magnetic fields. However, the study of atoms embedded in a strong magnetic field is quite complicated. Under such extreme conditions, magnetic and Coulomb effects are of nearly equal importance: neither can be treated as a perturbation of the other. Even so, considerable research effort has been dedicated to this subject. For the hydrogen atom, the calculations have reached a very complete level.[4–8] Rösner *et al.*[5] have studied the spectrum of the hydrogen atom exposed to strong magnetic fields, which has been successfully used to identify the observed spectra from many magnetic white dwarf stars. Kravchenko *et al.*[6,7] presented the exact solutions for the ground state and several excited states of the hydrogen atom in a uniform magnetic field of arbitrary strength.

Compared with the hydrogen atom, we find that the problem of the $H^-$ atomic ion is more complex because of the existence of electron-electron repulsion. Despite this, much work has been performed on this problem. In the absence of the magnetic field, it has been proved that there exists only one bound state for the $H^-$ ion,[9] while an infinite number of bound states exists in the presence of a magnetic field.[10] Henry *et al.*[11] studied this issue with a variational approach in the low and intermediate field regime for the first time. Mueller *et al.*[12] presented rough variational upper-bound estimates of some low-lying bound-state energy levels in the high field regime. Larsen[13–15] has done detailed work on the $H^-$ ion in strong magnetic fields. In Ref. [14] he gave the binding energies of the $1^1 0^+$ state in the field regime $\gamma = 0$–5 and those of the $1^3(-3)^+$ state in the field regime $\gamma = 0$–3. In Ref. [15] he provided the binding energies of the $1^1 0^+$, $1^3(-1)^+$ and $1^3(-2)^+$ states in the field regime $\gamma = 20$–1000. Park and Starace[16] presented the upper and lower bounds for the total energies and binding energies of the $1^1 0^+$ state using Chandrasekar-type wave functions in low fields. Vincke and Baye[17] improved the previous results and showed the importance of the correlation effect. They calculated the binding energies of the lowest singlet and triplet states for a few field strengths with a simple Slater-determinant basis. Furthermore, Larsen and McCann[18,19] also described the lowest singlet and triplet states in a broad field regime. In particular, Al-Hujaj and Schmelcher[20] used anisotropic Gaussian-type basis sets in cylindri-

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cal coordinates to calculate the total energies and electron detachment energies for the ground state and the first few excited states in strong magnetic fields with high precision.

In this paper, we investigate the $H^-$ ion in strong magnetic fields with Hylleraas–Gaussian basis, which was put forward by Wang *et al.*[21,22] The lower total energies and higher electron detachment energies of $1^1 0^+$, $1^1(-1)^+$ and $1^1(-2)^+$ states are obtained by using a full configuration interaction (CI) method. Atomic units are used throughout this paper.

## 2. Theory and method

In the following work, we assume that the nuclear mass is infinite and the magnetic field is oriented along the $z$ axis. Then the non-relativistic Hamiltonian for a hydrogen negative ion in a homogeneous magnetic field can be written in cylindrical coordinates as

$$H = \sum_{i=1}^{2} -\frac{1}{2}\left[\frac{1}{\rho_i}\frac{\partial}{\partial\rho_i}\left(\rho_i\frac{\partial}{\partial\rho_i}\right) + \frac{1}{\rho_i^2}\frac{\partial^2}{\partial\phi_i^2} + \frac{\partial^2}{\partial z_i^2}\right] + \sum_{i=1}^{2}\left[-\frac{1}{\sqrt{\rho_i^2+z_i^2}} + \frac{1}{8}\gamma^2\rho_i^2\right] + \frac{\gamma}{2}(L_z+2S_z) + \frac{1}{\sqrt{\rho_1^2+\rho_2^2-2\rho_1\rho_2\cos(\varphi_1-\varphi_2)+(z_1-z_2)^2}}. \quad (1)$$

The magnetic field strength is characterized by $\gamma = B/B_0$, where $B_0 = 2.35\times10^5$ T. Here, the Hamiltonian system possesses four conserved quantities, including the square of the total spin $S^2$, the $z$-component of the total spin $S_z$, the $z$-component of the total angular momentum $L_z$ and the $z$-component of the total parity $\Pi_z$.

In our calculations, the wave function for singlet states can be expanded as

$$\Psi(1,2) = \sum_{ijk} c_{ij} r_{12}^k [f_i(\rho_1,\varphi_1,z_1)\, g_j(\rho_2,\varphi_2,z_2) + f_i(\rho_2,\varphi_2,z_2)\, g_j(\rho_1,\varphi_1,z_1)], \quad (2)$$

where $c_{ij}$ is the expansion coefficient and $r_{12}$ is the interelectron distance. Additionally, $f$ and $g$ are one-particle anisotropic Gaussian basis functions[23]

$$\Phi_i(\rho,\varphi,z) = \rho^{n_{\rho i}} z^{n_{zi}} \mathrm{e}^{-\alpha_i\rho^2-\beta_i z^2}\mathrm{e}^{\mathrm{i}\, m_i\varphi}, \quad (3)$$

where the nonlinear variational parameters $\alpha_i$ and $\beta_i$ are positive and must be carefully optimized through a direct two-particle optimization procedure and a one-particle optimization procedure at given field strength. The exponents $n_{\rho i}$ and $n_{zi}$ obey the following rules:[23]

$$n_{\rho i} = |m_i| + 2k_i \quad (k_i = 0,1,2,\ldots, m_i = \ldots,-2,-1,0,1,2,\ldots),$$
$$n_{zi} = \pi_{zi} + 2l_i \quad (l_i = 0,1,2,\ldots, \pi_{zi} = 0,1). \quad (4)$$

The basis combining the $r_{12}^k$ term with the anisotropic Gaussian basis is called the Hylleraas–Gaussian basis, which is the key ingredient of this work. In Eq. (2), the $r_{12}^k$ term needs to be replaced by an approximate expansion of Gaussian-type geminals[24]

$$r_{12}^k \approx \sum_{\upsilon=0} b_\upsilon \left(1-\mathrm{e}^{-\tau_\upsilon r_{12}^2}\right) \quad \left(k = 0, \frac{1}{2}, 1, \ldots\right). \quad (5)$$

Only in this way can it extend the derivations of the matrix elements with the anisotropic Gaussian basis to the Hylleraas–Gaussian basis case. To label the different states of the $H^-$ ion at a specific magnetic field, we employ the standard spectroscopic notation $\upsilon^{2S+1}M^{\Pi_z}$, where $\upsilon$ denotes the degree of excitation.

## 3. Results and discussion

The total energies and electron detachment energies of $1^1 0^+$, $1^1(-1)^+$ and $1^1(-2)^+$ states have been calculated as functions of magnetic field with Hylleraas–Gaussian basis. The highly accurate results are presented in Tables 1–3. In order to obtain the electron detachment energy, namely one-electron ionization energy

$$I(H^-) = T - E, \quad (6)$$

we have to compute the one-electron ionization threshold

$$T = \gamma - I(H), \quad (7)$$

where the binding energy of the ground state of hydrogen $I(H)$ at magnetic field $\gamma$ is given by Kravchenko *et al.*[6] For $1^1 0^+$, $1^1(-1)^+$ and $1^1(-2)^+$ states, the identical one-electron ionization threshold is provided in the last column of Table 1. In addition, we also calculate the derivatives of the total energy with respect to the magnetic field of $1^1 0^+$, $1^1(-1)^+$ and $1^1(-2)^+$ states (see Tables 1–3), which reflect the changing relationship between total energies and field strengths, by means of the Hellman–Feynman theorem

$$\frac{\partial E}{\partial\gamma} = \left\langle \Psi \left| \frac{\partial H}{\partial\gamma} \right| \Psi \right\rangle. \quad (8)$$

Exploiting the obtained total energies and derivatives of the total energy at selected magnetic field values,

one can estimate the total energies for values $\gamma$ in between based on Hermite interpolation. And the finer the grid of the selected magnetic field values is, the higher the achieved accuracy of interpolation is.

Table 1 shows the results of $1^1 0^+$ state. We compare the results with those obtained by other methods. Our field-free total energy is –0.52774673, which is much closer to –0.527751016544377196503 calculated by Drake *et al.*[25] in Hylleraas coordinates. But, the electron detachment energy at zero field obtained by Drake *et al.* is a little bit higher than ours. Except for this, our electron detachment energies are generally higher than those published data[14,16,18,20]. Compared with the calculation with Gaussian basis,[20] our energies are about $(1.98-2.00)\times10^{-4}$ above in the field regime $0 \le \gamma < 0.001$, about $(1.84-2.92)\times10^{-4}$ above in the field regime $0.001 \le \gamma \le 1$, and about $(2.05-5.79)\times10^{-4}$ above in the field regime $1 < \gamma \le 100$. However, it should be pointed out that Hylleraas-like function is more efficient at zero and low fields.[26–28] However, there is not related work on $H^-$ ion published at low fields for comparison.

**Table 1.** Total energy $E$, electron detachment energy $I$ and derivative of the total energy $\partial E/\partial\gamma$ of $1^1 0^+$ state as functions of magnetic field strength $\gamma$.

| $\gamma$ | $E$ | $I$ | $I^{[20]}$ | $I^{[25]}$ | $I^{[16]}$ | $I^{[14]}$ | $I^{[18]}$ | $\partial E/\partial\gamma$ | $T$ |
|---|---|---|---|---|---|---|---|---|---|
| 0 | −0.52774673 | 0.02774673 | 0.02754875 | 0.027751 | | | | 0.00000000 | −0.50000000 |
| 0.0008 | −0.52774498 | 0.02814514 | 0.02794446 | | | | | 0.00317584 | −0.49959984 |
| 0.001 | −0.52774279 | 0.02824304 | 0.02804078 | | 0.02735 | | | 0.00396936 | −0.49949975 |
| 0.002 | −0.52773712 | 0.02873812 | 0.02853877 | | 0.02785 | | | 0.00792574 | −0.49899900 |
| 0.005 | −0.52769417 | 0.03020042 | 0.03000425 | | 0.0293 | | | 0.01975019 | −0.49749375 |
| 0.008 | −0.52762077 | 0.03163677 | 0.03142473 | | | | | 0.03144091 | −0.49598400 |
| 0.01 | −0.52754683 | 0.03257183 | 0.03237472 | | 0.0317 | | | 0.03909497 | −0.49497500 |
| 0.02 | −0.52697467 | 0.03707463 | 0.03687014 | | 0.0362 | | | 0.07534053 | −0.48990004 |
| 0.05 | −0.52332420 | 0.04894749 | 0.04876375 | | | | | 0.16328434 | −0.47437671 |
| 0.08 | −0.51739859 | 0.05898758 | 0.05874669 | | | | | 0.22924867 | −0.45841100 |
| 0.1 | −0.51244917 | 0.06492269 | 0.06470874 | | | 0.0634 | | 0.26522837 | −0.44752648 |
| 0.2 | −0.47893274 | 0.08855118 | 0.08830200 | | | 0.08685 | | 0.39446558 | −0.39038157 |
| 0.5 | −0.32832661 | 0.13111607 | 0.13083820 | | | | 0.130 | 0.58095536 | −0.19721054 |
| 0.8 | −0.13965117 | 0.15736777 | 0.15710667 | | | | | 0.66841077 | 0.01771661 |
| 1 | −0.00208009 | 0.17091119 | 0.17061922 | | | | 0.1695 | 0.70569923 | 0.16883110 |
| 2 | 0.75957246 | 0.21821363 | 0.21788123 | | | | 0.2175 | 0.80181279 | 0.97778609 |
| 4 | | | | | | | | | 2.71920198 |
| 5 | 3.32300770 | 0.29659343 | 0.2961625 | | | | 0.2955 | 0.88734312 | 3.61960113 |
| 8 | 6.03465624 | 0.34595877 | 0.3455713 | | | | | 0.91677460 | 6.38061500 |
| 10 | 7.88019482 | 0.37200802 | 0.3715626 | | | | 0.371 | 0.92809137 | 8.25220284 |
| 20 | 17.31930735 | 0.46529413 | 0.464715 | | | | 0.463 | 0.95479220 | 17.78460148 |
| 50 | 46.35918681 | 0.62295248 | 0.622747 | | | | 0.618 | 0.97602357 | 46.98213929 |
| 80 | 75.75329355 | 0.72242930 | 0.721953 | | | | | 0.98280316 | 76.47572285 |
| 100 | 95.43564823 | 0.77454753 | 0.773977 | | | | 0.7665 | 0.98532954 | 96.21019576 |

Due to the complicated interplay of the different interactions,[20] the $1^1(-1)^+$ and $1^1(-2)^+$ states are not bound at low fields but bound at sufficiently strong fields. Above some critical field strengths, the nuclear-electron attraction and correlation effect overcome the influence of the electron-electron repulsion, so that the $1^1(-1)^+$ and $1^1(-2)^+$ states become bound. Table 2 displays the results of $1^1(-1)^+$ state. It becomes bound in the field regime $\gamma \approx 3-4$. Compared with the data of Ref. [20], our electron detachment energies are about $(0.87-3.02)\times10^{-4}$ above in the field regime $5 \le \gamma \le 100$. Furthermore, we also present the energy value for $\gamma = 4$. Here, it should be mentioned that the total energy at $\gamma = 5$ in Ref. [20], which is considerably lower than ours, can not give rise to the relative electron detachment energy. Most probably, this total energy value is incorrect.

**Table 2.** Total energy $E$, electron detachment energy $I$ and derivative of the total energy $\partial E/\partial\gamma$ of $1^1(-1)^+$ state as functions of magnetic field strength $\gamma$.

| $\gamma$ | $E$ | $I$ | $I^{[20]}$ | $I^{[19]}$ | $\partial E/\partial\gamma$ |
|---|---|---|---|---|---|
| 4 | 2.71913821 | 0.00006377 | | | 0.89298673 |
| 5 | 3.61937309 | 0.00022805 | 0.0001312 | | 0.90666475 |
| 8 | 6.37951468 | 0.00110032 | 0.0009946 | | 0.93051081 |
| 10 | 8.25035887 | 0.00184397 | 0.0017574 | | 0.93995254 |
| 20 | 17.77800026 | 0.00660122 | 0.0063920 | | 0.96167255 |
| 50 | 46.96079888 | 0.02134041 | 0.0210500 | | 0.97938993 |
| 80 | 76.44111515 | 0.03460770 | 0.0343060 | | 0.98516279 |
| 100 | 96.16760731 | 0.04258845 | 0.0424020 | 0.01405 | 0.98730863 |

Table 3 lists the results of $1^1(-2)^+$ state. It becomes bound in the field regime $\gamma \approx 0.02 - 0.05$. For all considered field strengths, our electron detachment energies are systematically higher than those reported in the literature. Compared to the results of Al-Hujaj and Schmelcher,[20] the energies are improved by about $(0.13 - 0.63)\times10^{-4}$ in the field regime $0.1 \leq \gamma \leq 1$ and about $(0.76 - 1.15)\times10^{-4}$ in the field regime $1 < \gamma \leq 50$. Moreover, the energies for $\gamma = 0.05$ and $\gamma = 0.08$ are also achieved.

**Table 3.** Total energy $E$, electron detachment energy $I$ and derivative of the total energy $\partial E/\partial\gamma$ of $1^1(-2)^+$ state as functions of magnetic field strength $\gamma$.

| $\gamma$ | $E$ | $I$ | $I^{[20]}$ | $I^{[19]}$ | $\partial E/\partial\gamma$ |
|---|---|---|---|---|---|
| 0.05 | −0.47438619 | 0.00000948 | | | 0.52416528 |
| 0.08 | −0.45845758 | 0.00004658 | | | 0.53791096 |
| 0.1 | −0.44761131 | 0.00008483 | 0.00002201 | | 0.54698951 |
| 0.2 | −0.39083997 | 0.00045840 | 0.00044576 | | 0.58758591 |
| 0.5 | −0.19995685 | 0.00274631 | 0.00272262 | | 0.67750310 |
| 0.8 | 0.01220652 | 0.00551009 | 0.00546981 | | 0.73296837 |
| 1 | 0.16153522 | 0.00729589 | 0.00724788 | 0.0015 | 0.75920046 |
| 2 | 0.96298123 | 0.01480486 | 0.01472889 | | 0.83266790 |
| 5 | 3.59043513 | 0.02916600 | 0.02906590 | | 0.90314433 |
| 8 | 6.34203470 | 0.03858030 | 0.03848190 | | 0.92813190 |
| 10 | 8.20859573 | 0.04360711 | 0.04350280 | 0.006 | 0.93781584 |
| 20 | 17.72272424 | 0.06187724 | 0.06176200 | | 0.96075714 |
| 50 | 46.88811112 | 0.09402818 | 0.09391600 | | 0.97904722 |

As can be seen from Tables 1–3, the total energies and electron detachment energies both increase monotonically with increasing field strength for all states considered here. Besides, it can also be found that the $1^10^+$ state is stronger bound than the $1^1(-2)^+$ state, while the $1^1(-2)^+$ state is stronger bound than the $1^1(-1)^+$ state in the regime $0 \leq \gamma \leq 50$. These two facts are consistent with the observations of Al-Hujaj and Schmelcher. In addition, Fig. 1 also indicates that the derivatives of the total energy with respect to the magnetic field of $1^10^+$, $1^1(-1)^+$ and $1^1(-2)^+$ states increase and approach each other with the increasing magnetic field in the regime $0.0008 \leq \gamma \leq 50$.

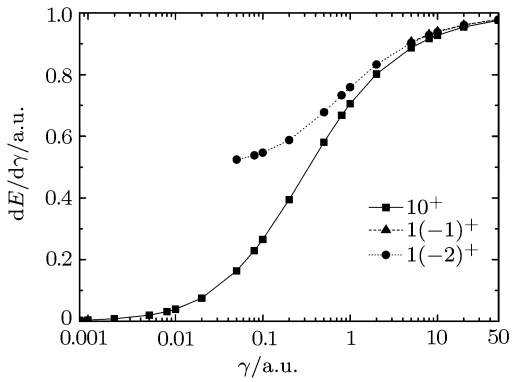



**Fig. 1.** The derivatives of the total energy with respect to the magnetic field of $1^10^+$, $1^1(-1)^+$ and $1^1(-2)^+$ states.

## 4. Conclusions

In summary, we have studied the $1^1 0^+$, $1^1(-1)^+$ and $1^1(-2)^+$ states of the $H^-$ ion in strong magnetic fields by use of a full CI method. The total energies, electron detachment energies and derivatives of the total energy with respect to the magnetic field are calculated with Hylleraas–Gaussian basis function in cylindrical coordinates. The accuracy for the energies, in comparison with the available theoretical data in the literature, is enhanced significantly. These accurate data can be used to analyse the spectra of some white dwarf stars whose spectra could not be completely accounted for with hydrogen atom. In the absence of the magnetic field, only the $1^1 0^+$ state is bound.[9] The field regimes $3 < \gamma < 4$ and $0.02 < \gamma < 0.05$, in which the $1^1(-1)^+$ and $1^1(-2)^+$ states start to become bound, respectively, are also determined according to the calculated electron detachment energies. Hylleraas–Gaussian basis function taking the electron correlation into consideration is the key element of this work, due to the fact that electron correlation plays an important role in the bound states of the $H^-$ ion.

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