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Two-dimensional hydrogen negative ion in a magnetic field*

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Making use of the adiabatic hyperspherical approach, we report a calculation for the energy spectrum of the ground and low-excited states of a two-dimensional hydrogen negative ion H^- in a magnetic field. The results show that the ground and low-excited states of H^- in low-dimensional space are more stable than those in three-dimensional space and there may exist more bound states.

Keywords: hydrogen negative ion, energy spectrum
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1. Introduction

The hydrogen negative ion (H^-) is one of the simplest nontrivial three-body atomic systems, which cannot be solved exactly. H^- consists of a single positive ion and two electrons which are bound to the positive ion. They can be used as a test for the theoretical description of electron–electron interaction.

Due to its importance in astrophysics, many studies of the H^- ion have been performed during the last years.[1−10] With the advancement of modern semiconductor techniques, it has been possible to fabricate low-dimensional structures like quantum wells, quantum wires and quantum dots, sometimes referred to as an artificial atom.[11−14] An artificial atom is essentially a number of electrons confined in a potential well. Similar systems may be obtained by confining an atom, a molecule or such objects. Spatial confinement leads to the appearance of new properties of quantum systems in low-dimensional space. Two-dimensional hydrogen atoms have been a subject of active research during the last years. Several articles have been published on this problem in the framework of non-relativistic quantum mechanics. On the other hand, external perturbation of a system, such as the application of an electric or a magnetic field, can provide much valuable information about the hydrogen negative ion. However, to our knowledge, there are only few studies on the hydrogen negative ion in low-dimensional space.[15] Hence, in this paper, in order to obtain a better understanding of the features of the ground and low-excited states in low-dimensional space, we will calculate the energy spectrum of the ground and low-excited states of the hydrogen negative ion in a two-dimensional (2D) space by using the adiabatic hyperspherical approach.[16]

The adiabatic hyperspherical approach is a powerful tool for investigating the weakly bound states,[17] where a hyperradius and a number of angular variables are introduced. The hyperradius measures the size of the triangle with the two electrons and the positron as vertices, while the angular variables determine the shape and orientation of the triangle. The main advantage of this approach is the reduction of the multidimensional Schrödinger equation into a set of coupled second-order differential equations with a set of effective potentials for determining the eigenenergies. In 1984 adiabatic hyperspherical approximations were used to calculate the energies of the lowest single states of H^- and He in a uniform magnetic field.[18] They have been shown to provide both qualitative insights and quantitatively accurate predictions for low-energy two-electron states.[19]

We consider a system consisting of two electrons and a nucleus of charge e in a homogeneous magnetic field B along the z-axis. We assume that the electrons

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are confined more strongly in one direction than the other two directions under magnetic fields, and we neglect the finite mass of the nucleus. Hence we focus on two electrons with mass m_e moving in a 2D space. We choose the symmetric gauge vector potentials for the electrons as $\boldsymbol{A}_i = (B/2)(-y_i, x_i, 0)$. The Hamiltonian for the H^- is given by

$$H = \sum_{i=1}^{2}(-\nabla_i^2 + \gamma^2 r_i^2) + 2\gamma(L_z + g_e\sigma_z) + V_c, \quad (1)$$

with

$$V_c = -\frac{2}{r_1} - \frac{2}{r_2} + \frac{2}{r_{12}}, \quad (2)$$

where $\boldsymbol{r}_i$ is the radius vector of the electron i with respect to the nucleus, L_z and σ_z are the z components of the total angular momentum and spin respectively, and g_e is the electronic g-factor, $r_{12} = |\boldsymbol{r}_1 - \boldsymbol{r}_2|$ is the distance between electrons 1 and 2. In Eq. (1) we have $r_1^2 = x_1^2 + y_1^2$, etc. In the present work, the energy is in Rydberg units, with 1Ry=13.6058eV, and the magnetic field strength ($\gamma = B/B_0$) is in units of $B_0 = 2\alpha^2 m_e c^2/(eh) \simeq 4.70 \times 10^5$T.

Instead of the radius vector $\boldsymbol{r}_i$ we use the Jacobi coordinates $\boldsymbol{\xi}_1 = (\boldsymbol{r}_1 - \boldsymbol{r}_2)/\sqrt{2}$ and $\boldsymbol{\xi}_2 = (\boldsymbol{r}_1 + \boldsymbol{r}_2)/\sqrt{2}$ to describe the electron's motion. In this coordinate system, Eq.(1) can be rewritten as

$$H = \sum_{i=1}^{2}(-\nabla_{\xi_i}^2 + \gamma^2 \xi_i^2) + 2\gamma(L_z + g_e\sigma_z) + V_c. \quad (3)$$

This particular set of Jacobi coordinates will be referred to as the α-set. In this coordinate system, the Schrödinger equation takes the form

$$\left[\sum_{i=1}^{2}(-\nabla_{\xi_i}^2 + \gamma^2\xi_i^2) + 2\gamma(L_z + g_e\sigma_z) + V_c - E\right]\Psi(\boldsymbol{\xi}_1, \boldsymbol{\xi}_2) = 0. \quad (4)$$

There is another possible Jacobi coordinate set: the β-set, where $\boldsymbol{\xi}_1^{(\beta)} = \boldsymbol{r}_1$ and $\boldsymbol{\xi}_2^{(\beta)} = -\boldsymbol{r}_2$. We notice that the Schrödinger equation (5) can be written in terms of β-set Jacobi coordinates as well. The superscripts in the coordinates will not be specified unless such a distinction is needed in the discussion.

From ξ, it is straightforward to introduce the hyperspherical coordinates

$$\xi = \sqrt{\xi_1^2 + \xi_2^2}, \tan\phi = \xi_2/\xi_1, \quad (5)$$

where ξ is the hyperradius and ϕ is the hyperangle. Thus the two vectors $\boldsymbol{\xi}_1$ and $\boldsymbol{\xi}_2$ are replaced by four coordinates (ξ, Ω), where $\Omega = (\phi, \varphi_1, \varphi_2)$ denotes collectively the three angles, with φ_i being the polar angle of the vector $\boldsymbol{\xi}_i$.

With an arbitrary set of hyperspherical coordinates $(\xi, \phi, \varphi_1, \varphi_2)$, the Schrödinger equation (4) for relative motion reads

$$\left[-\left(\frac{1}{\xi^3}\frac{\mathrm{d}}{\mathrm{d}\xi}\xi^3\frac{\mathrm{d}}{\mathrm{d}\xi} - \frac{\Lambda^2(\Omega)}{\xi^2}\right) + \frac{C(\Omega)}{\xi} + \gamma^2\xi^2 + 2\gamma(L_z + g_e\sigma_z) - E\right]\Psi(\xi, \Omega) = 0, \quad (6)$$

where

$$\Lambda^2(\Omega) = -\frac{\partial^2}{\partial\phi^2} + \left(\frac{\sin\phi}{\cos\phi} - \frac{\cos\phi}{\sin\phi}\right)\frac{\partial}{\partial\phi} + \frac{\hat{l}^2(\varphi_1)}{\cos^2\phi} + \frac{\hat{l}^2(\varphi_2)}{\sin^2\phi} \quad (7)$$

is the grand orbital operator, $\hat{l}(\varphi_1) = -\mathrm{i}\partial/\partial\varphi_1$, etc. and

$$C(\Omega) = \left[\frac{2}{\cos\phi^\alpha} - \frac{2}{\cos\phi^\beta} - \frac{2}{\sin\phi^\beta}\right] \quad (8)$$

is the fictitious electric charge, i.e. $C(\Omega)/\xi$ is the total Coulomb interaction potential among the charged particles. The eigenvalues and eigenfunctions for the $\Lambda^2(\Omega)$ operator are known as follows:

$$\Lambda^2(\Omega)Y_{[K]}(\Omega) = \lambda_{[K]}(\lambda_{[K]} + 2)Y_{[K]}(\Omega), \quad (9)$$

where

$$\lambda_{[K]} = 2m + |l_1| + |l_2|, \quad (10)$$

and the eigenfunctions are

$$Y_{[K]} = N_m^{l_1 l_2} P_m^{l_1 l_2}(\phi)\mathrm{e}^{\mathrm{i}l_1\varphi_1}\mathrm{e}^{\mathrm{i}l_2\varphi_2}, \quad (11)$$

where $[K]$ denotes the set of quantum numbers, $[K] = (l_1,\ l_2,\ m)$, with m related to the polynomial functions in angle ϕ, $l_1 + l_2 = L$, $N_m^{l_1 l_2}$ is the normalization constant and $P_m^{l_1 l_2}(\phi)$ is a Jacobi polynomial. In coordinate $\alpha-$set, the particle exchange symmetry is automatic, i.e. l_1=odd for spin triplet states of two electrons and l_1=even for spin single states of two electrons.

The grand angular momentum operator $\Lambda^2(\Omega)$ has the same form in terms of two set of Jacobi coordinates, i.e.

$$\Lambda^2(\Omega^\alpha) = \Lambda^2(\Omega^\beta), \quad (12)$$

therefore, the hyperspherical harmonics in different sets of hyperangles are simply the different representations. The eigenfunctions in one set can be expanded in terms of eigenfunctions of the other set with $\lambda_{[K]} = \lambda_{[K']}$,

$$Y_{[K]}(\Omega^i) = \sum_{[K']} B_{[K],[K']}Y_{[K]}(\Omega^j), \quad (13)$$

where the expansion coefficients $B_{[K],[K']}$ can be evaluated from

$$B_{[K],[K']} = \int \mathrm{d}\Omega^j Y^*_{[K]}(\Omega^i) Y_{[K]}(\Omega^j). \tag{14}$$

These coefficients are called the transformation bracket and a program for their evaluation has been published.[20] These transformation brackets are useful when we evaluate integrals involving functions of different sets of Jacobi coordinates.

Since the set of hyperspherical harmonics forms a complete set on each hyperspherical surface, the solution of the Schrödinger equation can be expanded as

$$\Psi_L = \sum_{[K]} R_{[K]}(\xi) Y_{[K]}(\Omega). \tag{15}$$

By projecting out the hyperspherical harmonics, a set of coupled second-order hyperradial differential equations is obtained:

$$\begin{aligned} &\left[-\left(\frac{1}{\xi^3} \frac{\mathrm{d}}{\mathrm{d}\xi} \xi^3 \frac{\mathrm{d}}{\mathrm{d}\xi} - \frac{\lambda_{[K]}(\lambda_{[K]}+2)}{\xi^2} \right) \right. \\ &\left. + \gamma^2 \xi^2 + 2\gamma(L_z + g_e \sigma_z) - E \right] R_{[K]}(\xi) \\ &- \frac{1}{\xi} \sum_{[K']} U_{[K],[K']} R_{[K']}(\xi) = 0, \end{aligned} \tag{16}$$

where

$$U_{[K],[K']} = \left\langle Y_{[K]}(\Omega) \left| C \right| Y_{[K']}(\Omega) \right\rangle, \tag{17}$$

is the matrix element of the effective charge C evaluated between two hyperspherical harmonics:

$$R_{n\lambda}(\xi) = N_{\mathrm{n}\lambda} (\beta\xi^2)^{\lambda/2} L^{\lambda}_{\mathrm{n}}(\beta\xi^2) \mathrm{e}^{-\beta\xi^2/2}, \tag{18}$$

where $N_{\mathrm{n}\lambda}$ is the normalization constant, L^{λ}_{n} is a Laguerre polynomial and β is a variational parameter used to minimize the energy of the low-lying states. Equation (16) can be solved to obtain the eigenvalues if convergence can be achieved by using a reasonable truncated set of hyperspherical harmonics. This method has been applied by a number of authors to H^- and He[21,22] in three-dimensional space.

The accuracy of the solutions depends on how large the model space is. Since we are interested only in the low-lying states and in the qualitative aspect, the model space adopted is neither very large, to facilitate numerical calculation, nor very small, to assure the qualitative accuracy. This is achieved by extending the dimension of the model space step by step: in each step the new results are compared with the previous results from a smaller space, until satisfactory convergence is achieved. The dimensions of our space is taken to be the maximum number of Laguerre polynomials $N_{\mathrm{LP}} = 8$ and the maximum number of hyperspherical harmonics $N_{\mathrm{HH}} = 256$.

Let ^{2S+1}L denote the quantum state, because the total orbital angular momentum L and the spin σ of two electrons are the good quantum numbers. Using the above method, we have performed numerical calculations for the energy levels of both singlet and triplet S, P and D states of H^- in a 2D quantum well with $\gamma \leq 0.1 \times 10^{-3}$Ry in Table 1.

In Table 1, firstly, we find that the energy level ordering is in good agreement with those of the 3D case.[3] However, the energy values of 2D H^- is lower than those of 3D H^-.[7] Hence, there may exist more bound states in 2D space. Secondly, we find that when $\gamma \leq 0.1 \times 10^{-3}$Ry, as the magnetic field strength increases, the energy values of the S states increase and those of the P and D states decrease. This is due to the negative term $2\gamma L_z$ which brings levels with higher γ below those with lower γ when $L \neq 0$. Finally, we find that the energy value of the ^{1}D state is much lower than that of the ^{3}D state and this point is different from the 3D case.[3] From the analysis of quantum mechanics symmetry, our result is reasonable.[16]

On the other hand, as shown in Table 1, the energy spectrum of low-lying states varies not only in the values but also in the level ordering as γ changes from 0.0 to 0.1×10^{-3}Ry. As illustrated in Table 1, an important aspect of the effect of magnetic fields is the crossing between different states of a 2D H^- when the magnetic field increases: e.g., when $\gamma = 0.0$, the energy level ordering is ^{1}S, ^{3}P, ^{1}P, ^{1}D, ^{3}D, ^{3}S, and when $\gamma = 0.1 \times 10^{-3}$Ry, it is ^{1}S, ^{3}P, ^{1}D, ^{1}P, ^{3}D, ^{3}S, i.e. the level crossing occurs between the ^{1}P and ^{1}D states. The physical origin of level crossing is the result of a competition between the Coulomb interaction, the term $2\gamma L_z$, and kinetic energy.

From Table 1, we also find that the energy values of the L+S=even states are lower than those of the adjacent L+S=odd states. Our present results are qualitatively in good agreement with those of Ref.[23] in 3D space which were studied under magnetic fields. This feature is a consequence of quantum mechanics symmetry. It has been discussed in previous publications[16] and will not be repeated here.

Table 1. Energies in units of Ry of both singlet and triplet S, P and D states of H^- in 2D space.

$\gamma(10^{-3}\mathrm{Ry})$	^{1}S	^{3}S	^{1}P	^{3}P	^{1}D	^{3}D
0.00	–2.6268500	–0.7973930	–1.1603070	–1.3889127	–1.1294698	–0.7973930
0.01	–2.6268424	–0.7972782	–1.1647095	–1.3933564	–1.1383010	–0.8061906
0.02	–2.6268198	–0.7968938	–1.1690044	–1.3977349	–1.1469700	–0.8147186
0.03	–2.6267882	–0.7962401	–1.1731921	–1.4020485	–1.1554770	–0.8229772
0.04	–2.6267291	–0.7953199	–1.1772727	–1.4062970	–1.1638224	–0.8309693
0.05	–2.6266610	–0.7941343	–1.1812463	–1.4104806	–1.1720067	–0.8386962
0.06	–2.6265779	–0.7926861	–1.1851134	–1.4145992	–1.1800308	–0.8461604
0.07	–2.6264796	–0.7909794	–1.1888743	–1.4186532	–1.1878953	–0.8533660
0.08	–2.6263663	–0.7890163	–1.1925295	–1.4226425	–1.1956012	–0.8603153
0.09	–2.6262378	–0.7860237	–1.1960794	–1.4265674	–1.2031498	–0.8670137
0.10	–2.6260943	–0.7843410	–1.1995248	–1.4304278	–1.2105422	–0.8734647

In order to understand the feature of the ground and low-excited states of a 2D hydrogen negative ion, it is useful to study the magnetic field effect. The dependence of the energy spectrum of both singlet and triplet S, P and D states of H^- on γ is plotted in Fig.1. It is readily seen that for S states the energies increase monotonically as the magnetic field strength increases because the term $2\gamma L_z$ is zero. The energy of the ^{3}S state is pushed higher and higher when the magnetic field increases and the increase of energy value with increasing γ is much larger than those of the other states studied here. This is due to the fact that for the ^{3}S state there exists the inherent nodal line in the wavefunction which results from quantum mechanics symmetry[13] and the failure to minimize the interaction energy;[24] hence, as the magnetic field increases, the motion of the electrons will be furious (the furiousness of an internal excitation is measured by the number of nodal lines contained in the wavefunction). On the other hand, for P and D states, at the beginning, the energy values decrease as the magnetic field strength increases, then the energy reaches a minimum at some state which is L-dependent and σ-dependent; after that, as γ increases further, the energy begins to increase. This can be interpreted as follows. When the magnetic field increases, the orbit radii of the electrons will decrease and the electron–electron repulsive interacting energy increases. If the enhance of the electron–electron repulsive interaction with the increase of γ is compensated by the decrease of the term $2\gamma L_z$, the energy will decrease; but if the enhance of the interaction with increasing γ is not counteracted by the decrease of $2\gamma L_z$, the energy will increase. Finally, we also find that when $\gamma > 1.0 \times 10^{-3}$Ry the energy values of ^{1}D and ^{3}P states are very much closer together and the energy difference of ^{3}D and ^{1}P states is almost identical with increasing γ.

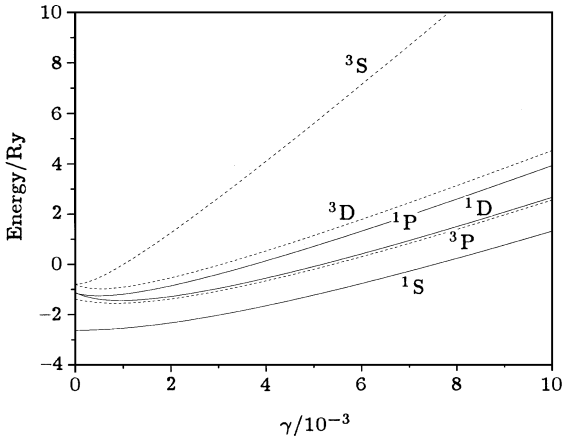


Fig.1. The energy spectrum of both singlet and triplet S, P and D states of a hydrogen negative ion H^- in a 2D space as a function of the magnetic field strength γ, solid curves for $S = 0$ and dashed curves for $S = 1$. The levels are labelled by ^{2S+1}L.

Although, to our knowledge, no experimental results involving a 2D H^- under magnetic fields have been reported, we hope that our results might be useful in the interpretation of future experimental data.

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