

H_2^+ ion in strong magnetic field: A variational study

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Using a single trial function, we perform an accurate calculation of the ground state $1\sigma_g$ of the hydrogenic molecular ion H_2^+ in a constant uniform magnetic field ranging from 0 to 10^{13} G. We show that this trial function also makes it possible to study the negative parity ground state $1\sigma_u$. We show that, over the whole range of magnetic fields studied the calculated binding energies are in most cases larger than binding energies obtained previously by other authors using different methods. [S1050-2947(97)08311-X]

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I. INTRODUCTION

For a long time the behavior of atomic and molecular systems in a strong magnetic field of order $B \geq 10^9$ G has attracted considerable attention. The main interest comes from both astrophysics—studies of white dwarfs and neutron stars (see Refs. [1,2], and also, for example, Refs. [3,4], and review [5] and references therein), as well as from chemistry—formation of unusual chemical compounds whose existence is impossible without strong magnetic fields [6] (for a review, see, for example, Ref. [7] and references therein).

There are many studies of the hydrogen atom H—the simplest atomic system—in a strong magnetic field, while the hydrogen molecular ion H_2^+ —the simplest molecular system which is stable with respect to dissociation $\text{H}_2^+ \rightarrow \text{H} + p$ —is much less explored. One of the major drawbacks of many of these studies is a restricted domain of applicability: they are accurate in the weak-magnetic-field region but are inappropriate for the strong magnetic field region, and vice versa. The goal of the present paper is to carry out an accurate variational calculation of H_2^+ in magnetic fields ranging from 0 to 10^{13} G¹ using a *unique* simple trial function equally applicable for any value of the magnetic-field strength. We restrict our consideration to the case where the magnetic field is directed along the axis of the molecule, which is evidently the optimal configuration leading to the lowest energy. Our main perception is that the calculations should not be technically complicated, and also easily reproduced, while the trial function should be simple enough to allow further analytic and numerical investigations.

II. CHOICE OF TRIAL FUNCTIONS

A constructive criterion for an adequate choice of trial function was formulated in Ref. [8], and further development was presented in Refs. [9,10]. In the simplest form the criterion is the following. The trial function $\Psi_t(x)$ should contain all symmetry properties of the problem at hand. If the ground state is studied, the trial function should not vanish inside of the domain where the problem is defined. The potential $V_t(x) = \nabla^2 \Psi_t / \Psi_t$, for which the trial function is an eigenfunction, should reproduce the original potential near singularities, and also its asymptotic behavior. The use of this simplest possible recipe has led to a unique one-parameter trial function, which, in particular, made it possible to carry out the first qualitative study of the ground state of the hydrogen molecule H_2 in the region of both weak and strong magnetic fields [11]. Later a few-parameter trial function was proposed for a description of the hydrogen atom in an arbitrary magnetic field, which led, for low-excited states, to an accuracy comparable with the best calculations [10,12].

Now we wish to apply the above-mentioned recipe to the ion H_2^+ . We work in the Born-Oppenheimer approximation. Let us first introduce the notation (see Fig. 1). We consider two attractive centers of charge Z situated on the z axis at a distance $R/2$ symmetrically with respect to the origin. The magnetic field of the strength B is directed along the z axis, and $r_{1,2}$ are the distances from the electron to the first(second) center, respectively. The quantity ρ is the distance from the electron to the z axis. Through the paper Ry is used as the energy unit. For the other quantities, standard atomic

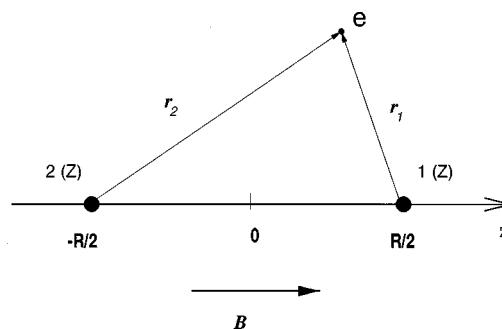


FIG. 1. H_2^+ in a magnetic field B . Explanation of the notations used.

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¹The relativistic corrections can still be neglected (see a discussion in Ref. [5], and references therein).

TABLE I. Ground-state energies and the equilibrium distances for the ground state $1\sigma_g$ of the ion H₂⁺ obtained using different trial wave functions as a function of the magnetic-field strength.

B		Ψ_1	Ψ_2	Ψ_{3-1}	Ψ_{3-2}	Ψ_4
0	E	-1.162 77	-1.172 99	-1.204 88	-1.204 88	-1.205 25
	R	1.846 78	2.003 49	1.997 99	1.998 10	1.997 06
10 ⁹ G	E	-1.117 60	-1.118 49	-1.150 07	-1.150 13	-1.150 71
	R	1.809 67	1.933 53	1.923 78	1.923 75	1.923 33
10 ¹⁰ G	E	1.118 35	1.157 13	1.100 98	1.100 95	1.089 93
	R	1.214 34	1.243 28	1.250 42	1.250 13	1.246 40
10 ¹¹ G	E	35.1065	35.2351	35.1016	35.0750	35.0374
	R	0.595 75	0.592 06	0.600 65	0.589 54	0.592 03
10 ¹² G	E	408.539	408.837	408.539	408.424	408.300
	R	0.289 28	0.283 72	0.289 27	0.284 22	0.283 33

TABLE II. Comparison of present calculations for the ground state $1\sigma_g$ of equilibrium distance R , energy E , and binding energy $BE=B-E$, with the results of other calculations [4,13–17].

B (G)	R (a.u.)	E (a.u.)	BE (a.u.)	Source
$B=0$	1.9971	-1.205 25		Present
	2.0000	-1.205 27		Teller [13]
	1.997	-1.205 27		Wille [14]
	1.997	-1.205 26		Peek-Katriel [15]
	2.0000	-1.205 268		Wind [16]
$B=10^9$ G	1.9233	1.150 72	1.576 16	Present
	1.924	1.150 72	1.576 16	Wille [14]
	1.921		1.5757	Peek-Katriel [15]
	1.90		1.5529	Lai-Suen [17]
$B=10^{10}$ G	1.2464	1.089 79	3.1646	Present
	1.246	1.090 31	3.1641	Wille [14]
	1.159		3.0036	Peek-Katriel [15]
	1.10		3.0411	Lai-Suen [17]
$B=10^{11}$ G	0.593	35.0362	7.5080	Present
	0.593	35.0428	7.5013	Wille [14]
	0.62		7.35	Lai-Salpeter [4]
$B=5\times 10^{11}$ G	0.351	199.238	13.483	Present
	0.350	199.315	13.406	Wille [14]
	0.35		13.38	Lai-Salpeter [4]
$B=10^{12}$ G	0.283	408.300	17.141	Present
	0.278	408.566	16.875	Wille [14]
	0.28		17.06	Lai-Salpeter [4]
$B=2\times 10^{12}$ G	0.230	829.274	21.609	Present
	0.23		21.54	Lai-Salpeter [4]
$B=5\times 10^{12}$ G	0.177	2098.3	28.954	Present
	0.18		28.90	Lai-Salpeter [4]
$B=10^{13}$ G	0.147	4218.7	35.752	Present
	0.15		35.74	Lai-Salpeter [4]

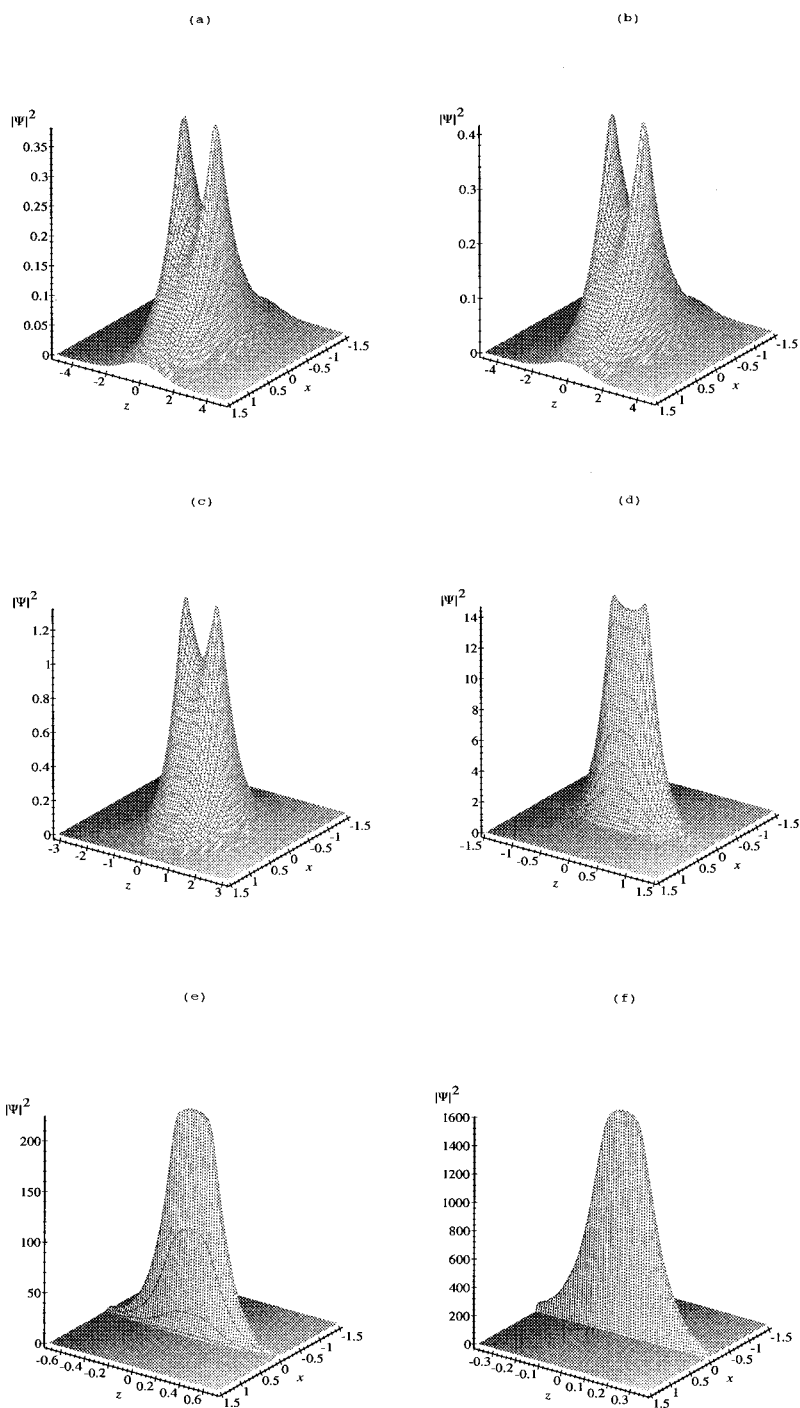


FIG. 2. The electronic probability density of the ground state $1\sigma_g$ at $y=0$ as a function of the magnetic-field strength. (a) $B=0$, (b) $B=10^9$ G, (c) $B=10^{10}$ G, (d) $B=10^{11}$ G, (e) $B=10^{12}$ G, and (f) $B=10^{13}$ G.

units are used. The potential corresponding to the problem we study is given by

$$V = \frac{2Z^2}{R} - \frac{2Z}{r_1} - \frac{2Z}{r_2} + \frac{B^2\rho^2}{4}, \quad (2.1)$$

where the first term has the meaning of the classical Coulomb energy of the interaction of two charged centers.

One of the simplest functions satisfying the above recipe is the Heitler-London function multiplied by the lowest Landau orbital:

$$\Psi_1 = e^{-\alpha_1 Z(r_1+r_2) - \beta_1 B\rho^2/4}, \quad (2.2)$$

where α_1 and β_1 are variational parameters. It has, in total, three variational parameters if we include the internuclear distance R in the search for the equilibrium distance. It is known that in the absence of a magnetic field a function of the Heitler-London type gives an adequate description of diatomic systems near their equilibrium position. The potential corresponding to this function is

TABLE III. Energy, binding energy, and equilibrium distance for the ground state of H₂⁺ of negative parity 1σ_u.

B (G)	R (a.u.)	E (a.u.)	BE (a.u.)	Source
$B=0$	12.746	-1.000 10	1.000 10	Present
	12.55	-1.000 12	1.000 12	Peek-Katriel [15]
$B=10^9$ G	11.039	-0.920 63	1.346 08	Present
	10.55	-0.917 134		Peek-Katriel [15]
$B=10^{10}$ G	6.4035	1.6585	2.595 92	Present
	4.18	2.1294		Peek-Katriel [15]
$B=10^{11}$ G	3.7391	36.945	5.599 01	Present
$B=10^{12}$ G	2.4329	413.92	11.519	Present
$B=10^{13}$ G	1.7532	4232.6	21.851	Present

$$\begin{aligned}
V_1 = & 2Z^2\alpha_1^2 - B\beta_1 - 2Z\alpha_1 \left(\frac{1}{r_1} + \frac{1}{r_2} \right) + \frac{\beta_1^2 B^2 \rho^2}{4} \\
& + 2Z^2 \frac{\alpha_1^2}{r_1 r_2} [\rho^2 + z^2 - R^2/4] \\
& + Z\alpha_1 B \beta_1 \rho^2 \left(\frac{1}{r_1} + \frac{1}{r_2} \right). \quad (2.3)
\end{aligned}$$

It is clear that this potential reproduces the original potential (2.1) near Coulomb singularities and, at large distances, $|x| \rightarrow \infty$.

The Hund-Mulliken function multiplied by the lowest Landau orbital is another possible trial function,

$$\Psi_2 = (e^{-\alpha_2 Z r_1} + e^{-\alpha_2 Z r_2}) e^{-\beta_2 B \rho^2/4}, \quad (2.4)$$

where α_2 and β_2 are variational parameters. It is well known that this function, in the absence of a magnetic field, describes the region of large internuclear distances. The calculations we performed show that this property remains valid for all magnetic fields up to 10^{13} G. Like Eq. (2.2), the trial function (2.4) is characterized by three variational parameters. In order to take into account both equilibrium and large distances, we should use an interpolation of Eqs. (2.2) and (2.4). There are two natural ways to interpolate.

(i) A nonlinear superposition

$$\Psi_{3-1} = (e^{-\alpha_3 Z r_1 - \alpha_4 Z r_2} + \sigma e^{-\alpha_4 Z r_1 - \alpha_3 Z r_2}) e^{-\beta_3 B \rho^2/4}, \quad (2.5)$$

where α_3 , α_4 , and β_3 are variational parameters. The parameter $\sigma = \pm 1$ depends on which positive parity 1σ_g or negative parity 1σ_u states we consider. Function (2.5) is a modification of the Guillemin-Zener function used for a description of the molecular ion H₂⁺. If $\alpha_3 = \alpha_4$, function (2.5) reduces to Eq. (2.2), and, if $\alpha_3 = 0$, it coincides with Eq. (2.4). In total, there are four variational parameters characterizing the trial function (2.5).

(ii) A linear superposition of Eqs. (2.2) and (2.4),

$$\Psi_{3-2} = A_1 \Psi_1 + A_2 \Psi_2, \quad (2.6)$$

where the relative weight of Eqs. (2.2) and (2.4) in Eq. (2.6) is taken as an extra variational parameter. It is a seven-parameter trial function.

Of course, as a natural continuation of the above interpolation procedure, one can take a linear superposition of all three functions: the modified Heitler-London, Hund-Mulliken, and Guillemin-Zener functions (2.2), (2.4), and (2.5)

$$\begin{aligned}
\Psi_4 = & A_{3-1} \Psi_{3-1} + A_{3-2} \Psi_{3-2} \\
= & A_{3-1} \Psi_{3-1} + A_1 \Psi_1 + A_2 \Psi_2, \quad (2.7)
\end{aligned}$$

where again, as in the case of the function (2.6) the relative weights of different components are variational parameters. In total, the trial function (2.7) is characterized by ten variational parameters. Most of our calculations will be carried out using this function. The minimization procedure was done using the standard minimization package MINUIT from CERN-LIB on a Pentium-Pro personal computer. All integrals were calculated numerically with relative accuracy $\leq 10^{-7}$.

III. RESULTS

In order to present our results, we begin with the study of the dependence of our variational results on different trial functions (see Table I). It turned out that all variational parameters are of the order of one independently on the value of the magnetic-field strength. In Table II we give a comparison of our calculations with the best-known results. Since we are doing a variational study of the problem, the (binding) energies obtained represent (lower) upper bounds to the exact energies. No need to mention that many calculations were performed for the case of the H₂⁺ ion in absence of a magnetic field. Our results are in agreement with the best calculations within an absolute accuracy of 10^{-5} . For all studied values of the magnetic field ($\leq 10^{13}$ G), our results for binding energies exceed the best-known results at the present. Among all previously made calculations, we should emphasize that those performed by Wille [14] have the most extended domain of applicability. The accuracy of these results is almost as good as the accuracy of our results for magnetic fields $B \leq 10^{11}$ G. However, for larger magnetic fields the accuracy of his results decreases drastically.

Figure 2 shows the electronic density distribution as a function of magnetic field. For a small magnetic field the distribution has two clear maxima corresponding to the positions of the centers. The situation changes drastically for magnetic fields of the order of $B \approx 3 \times 10^{11}$ G, where the probability of finding the electron in any position between the two centers is practically the same. For larger magnetic fields the electron is preferably located between the two centers with the maximum in the middle, $z=0$ [see Figs. 2(e) and 2(f)]. Due to a loss of accuracy, this phenomenon was not observed in Ref. [14]. It is worth noticing that for all magnetic fields studied the region of large internuclear distances is dominated by the Hund-Mulliken function (4).

In Table III the results of the study of a ground state of negative parity ($1\sigma_u$) are presented. Let us note that in the absence of a magnetic field the electron is not bounded pos-

sessing a shallow minimum (see, for example, Refs. [13,15]). However, in a magnetic field the electron becomes bounded in agreement with general expectations [6] (see also Ref. [15]).

In conclusion, we want to emphasize that we present the most accurate calculations for the ground-state energies and equilibrium distances of the molecular ion H_2^+ in a magnetic field. Unlike the majority of other studies our calculations stem from a unique framework covering both weak- and strong-magnetic-field regimes.

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- [1] M. Ruderman, in *Physics of Dense Matter*, edited by C. J. Hansen (Kluwer, Dordrecht, 1974)
- [2] V. K. Khersonskii, *Astrophys. Space Sci.* **98**, 255 (1984); **117**, 47 (1985); *Sov. Astron.* **31**, 225 (1987).
- [3] D. Lai and E. Salpeter, *Phys. Rev. A* **52**, 2611 (1995).
- [4] D. Lai and E. Salpeter, *Phys. Rev. A* **53**, 152 (1996).
- [5] M. A. Liberman, B. Johansson, *Usp. Fiz. Nauk.* **165**, 121 (1995) [*Sov. Phys. Usp.* **38**, 117 (1995)].
- [6] B. B. Kadomtsev and V. S. Kudryavtsev, *Pis'ma Zh. Eksp. Teor. Fiz.* **13**, 15, 61 (1971) [*JETP Lett.* **13**, 9 (1971); **13**, 42 (1971)].
- [7] U. Kappes and P. Schmelcher, *Phys. Rev. A* **51**, 4542 (1995).
- [8] A. V. Turbiner, *Zh. Eksp. Teor. Fiz.* **79**, 1719 (1980) [*Sov. Phys. JETP* **52**, 868 (1980)].
- [9] A. V. Turbiner, *Usp. Fiz. Nauk* **144**, 35 (1984) [*Sov. Phys. Usp.* **27**, 668 (1984)].
- [10] A. V. Turbiner, *Yad. Fiz.* **46**, 204 (1987) [*Sov. J. Nucl. Phys.* **46**, 125 (1987)].
- [11] A. V. Turbiner, *Pis'ma Zh. Eksp. Teor. Fiz.* **38**, 510 (1983) [*JETP Lett.* **38**, 618 (1983)].
- [12] A.V. Turbiner, Ph.D. thesis, ITEP, Moscow, 1989.
- [13] E. Teller, *Z. Phys.* **61**, 458 (1930); E. A. Hylleraas, *ibid.* **71**, 739 (1931).
- [14] U. Wille, *Phys. Rev. A* **38**, 3210 (1988).
- [15] J. M. Peek and J. Katriel, *Phys. Rev. A* **21**, 413 (1980).
- [16] H. Wind, *J. Chem. Phys.* **42**, 2371 (1965).
- [17] C. S. Lai and B. Suen, *Can. J. Phys.* **55**, 609 (1977).