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Hydrogen molecular ion in a strong parallel magnetic field

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The hydrogen molecular ion in a strong external magnetic field parallel to the molecular axis is investigated using a semianalytical method based on the presentation of the wave function in the form of a double power series in nonseparable space variables. The solution is determined from the requirement for the coefficients of the series to obey linear relations imposed by the Schrödinger equation. For the ground state, the method provides accuracy 10^{-8} hartree and higher for magnetic fields from 0 up to 10^4 T; the applicability of the technique to excited states is limited to lower field strengths. [S1050-2947(97)01604-1]

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I. INTRODUCTION

The existence of strong magnetic fields discovered on pulsars and white dwarf stars has given rise to a significant interest in the behavior of atoms and molecules in the presence of such fields [1]. Particular attention is drawn to superstrong magnetic fields existing on the surface of neutron stars ($\approx 10^8$ T) and to the region of fields which exist in the atmospheres of white dwarfs ($\approx 10^2 - 10^4$ T).

The presence of a strong magnetic field produces appreciable effects on the electronic structure of atoms, and on chemical bonds in molecules. Already the simplest molecule, the hydrogen molecular ion $H_2{}^+$, allows us to observe some of these effects, such as the contraction of the bond length and the growth of dissociation energy and vibrational energies with the increase of the field strength. The theoretical study of $H_2{}^+$ is facilitated by the absence of exchange and correlation effects, because we deal with a single electron moving in the field of two nuclei. As a consequence, this simple molecule has attracted a great deal of attention and is the subject of many investigations published in the literature.

The problem of the hydrogen molecular ion in the absence of external fields was basically solved already in [2], and subsequent work on the subject resulted in publishing extensive exact tables of energy levels [3–5]. Solution of the field-free problem is greatly facilitated by the fact that the two-center Schrödinger equation is separable in spheroidal coordinates. This is not a surprising fact, because in the classical limit the motion of a charged particle in the field of two Coulomb centers can be solved by separation of variables. The separability of the Schrödinger equation makes it possible to obtain exact solutions for $H_2{}^+$ and for similar systems, of which the most physically interesting is the HeH^{2+} ion [6].

The presence of an external magnetic field makes the situation much more complicated. If the field is oriented at an arbitrary angle to the molecular axis, none of the variables can be separated, and one deals with a complete three-dimensional problem. In the present work we consider only the situation when the magnetic field is parallel to the molecular axis. Under this condition it is possible to separate the dependence of the wave function on the angular variable φ, which is described by the usual multiplier $\exp(im\varphi)$, and obtain a nonseparable differential equation in two remaining space variables.

If the applied magnetic field is strong enough, the problem can be treated in the adiabatic approximation. In this approximation, the wave function is presented as the product of a Landau orbital by an unknown z-dependent function. The latter may be found either by a variational method [7] or by a fully numerical procedure like finite differences in [8] or numerical integration in [9]. Accuracy of this method can be substantially improved by taking a combination of several Landau orbitals, each multiplied by a separate unknown function of z, and solving the resulting set of Hartree-Fock-like differential equations for these functions [10]. The adiabatic approximation works best when the strength of the magnetic field is much larger than 1 a.u. and provides low accuracy for fields below 10^5 T.

To achieve good accuracy in low fields, one has to ensure the correct behavior of the wave function in the field-free limit, which was done in variational calculations with simple trial functions reported in [11,12]. The trial function used in [12] included a Gaussian-like term, and was suitable for description of the high-field region as well. Calculations with a single trial function were also performed for the nonparallel field orientation [13].

Significant attention was devoted to the traditional finite basis set methods, which were used to describe both parallel [14,15] and nonparallel configurations [16–18]. The basis set used in [15,18] is particularly promising because it is not restricted to the parallel configuration like the basis set in [14], or to the two-center problem as the set used in [16,17].

Other methods of solution include the finite-element method [19] and Monte Carlo calculations [20]. The method used in [21] is based on the assumption that in spheroidal coordinates variables can be approximately separated in analogy to the field-free case. The solution is presented as a product of two functions, and coupled differential equations for these functions are solved numerically to obtain approximate energy eigenvalues.

In the present work, we demonstrate that the nonseparable equation in two variables describing the ion in the applied parallel magnetic field can be solved to a very high degree of accuracy by a method very similar to the technique used for the solution of the field-free problem: we present the solution in the form of a double power series, obtain linear relations for the coefficients of the series, and require the resulting system of linear equations to have a nonsingular solution. This technique allows us to obtain nonrelativistic energy eigenvalues in the Born-Oppenheimer approximation with precision 10^{-8} hartree and higher, depending on the size of the series expansion, the quantum state, and the magnetic field strength. The method is best suited for fields below 10^4 T, its application for the high-field regime is hindered by the slow convergence of the solution. We present basic molecular parameters of the states $1\sigma_g$ and $1\pi_u$, calculated with precision exceeding the accuracy of corresponding results published in the literature so far.

The paper is organized as follows. In Sec. II, we derive the basic formulas, obtain a system of linear equations for coefficients of the double series, and discuss the technique of solution. In Sec. III, we investigate the convergence of solution and limits of its applicability. Calculated results and discussion of the method are presented in Sec. IV.

II. METHOD

The Schrödinger equation for the one-electron diatomic molecule in an external magnetic field is

$$\frac{1}{2m_e}\left(-i\hbar\boldsymbol{\nabla}+\frac{e}{c}\mathbf{A}\right)^2\Psi-e^2\left(\frac{Z_a}{r_a}+\frac{Z_b}{r_b}\right)\Psi=E\Psi, \qquad (1)$$

where $\mathbf{A}$ is the vector potential, Z_a and Z_b are nuclear charges, m_e is the electron mass, and r_a and r_b are the distances from the two nuclei. We consider homogeneous magnetic field $\mathbf{H}$ directed along the molecular axis and introduce the spheroidal coordinates

$$\xi=\frac{r_a+r_b}{R}, \qquad \eta=\frac{r_a-r_b}{R}, \qquad \varphi, \qquad (2)$$

R being the distance between the nuclei. We choose the gauge of the vector potential in the form

$$\mathbf{A}=(0,0,\tfrac{1}{2}Hr_\perp), \qquad (3)$$

where $r_\perp=(R/2)\sqrt{(\xi^2-1)(1-\eta^2)}$ is the distance from the molecular axis. Since $\mathrm{div}\mathbf{A}=0$, vector $\mathbf{A}$ commutes with $\boldsymbol{\nabla}$, and the Schrödinger equation takes the form

$$-\frac{\hbar^2}{2m_e}\Delta\Psi-\frac{ie\hbar}{2m_ec}H\frac{\partial\Psi}{\partial\varphi}+\frac{e^2}{2m_ec^2}\frac{H^2}{4}r_\perp^2\Psi$$
$$-e^2\left(\frac{Z_a}{r_a}+\frac{Z_b}{r_b}\right)\Psi=E\Psi. \qquad (4)$$

We introduce the atomic system of units; that is, we choose the Bohr radius $a_0=\hbar^2/m_ee^2=5.3\times10^{-9}$ cm as the unit of length, 1 hartree $E_0=2$ Ry$=m_ee^4/\hbar^2=27.2$ eV as the unit of energy, and the value $H_0=m_e^2e^3c/\hbar^3=2.35\times10^9$ G as the unit of magnetic intensity; the magnetic field is measured as $\gamma=H/H_0$. Eq. (4) becomes

$$\Delta\Psi+i\gamma\frac{\partial\Psi}{\partial\varphi}-\frac{\gamma^2}{4}r_\perp^2\Psi+2\left(\frac{Z_a}{r_a}+\frac{Z_b}{r_b}+E\right)\Psi=0. \qquad (5)$$

After performing differentiation in the spheroidal coordinates, we obtain the following equation:

$$(\xi^2-1)\Psi_{\xi\xi}+(1-\eta^2)\Psi_{\eta\eta}+2\xi\Psi_\xi-2\eta\Psi_\eta$$
$$+\frac{(\xi^2-\eta^2)}{(\xi^2-1)(1-\eta^2)}\Psi_{\varphi\varphi}+\frac{i\gamma R^2}{4}(\xi^2-\eta^2)\Psi_\varphi$$
$$-\frac{\gamma^2R^4}{64}(\xi^2-\eta^2)(\xi^2-1)(1-\eta^2)\Psi$$
$$+Z_+\xi\Psi+Z_-\eta\Psi+\frac{R^2E}{2}(\xi^2-\eta^2)\Psi=0. \qquad (6)$$

Here $Z_+=R(Z_a+Z_b)$, $Z_-=R(Z_b-Z_a)$, and subscripts ξ, η, and φ denote partial derivatives.

The dependence of the wave function on φ can be separated by introducing a new function $f(\xi,\eta)$ according to

$$\Psi(\xi,\eta,\varphi)=(\xi^2-1)^{|m|/2}(1-\eta^2)^{|m|/2}e^{im\varphi}f(\xi,\eta), \qquad (7)$$

where m is the magnetic quantum number. The equation for $f(\xi,\eta)$ is

$$(\xi^2-1)f_{\xi\xi}+(1-\eta^2)f_{\eta\eta}+2(|m|+1)(\xi f_\xi-\eta f_\eta)$$
$$+Z_+\xi f+Z_-\eta f+\frac{R^2}{2}\left(E-\frac{\gamma m}{2}\right)(\xi^2-\eta^2)f$$
$$-\frac{\gamma^2R^4}{64}(\xi^2-\eta^2)(\xi^2-1)(1-\eta^2)f=0. \qquad (8)$$

We introduce the binding energy defined as $E_b=(1+m+|m|)\gamma/2-E$ and separate the asymptote in the magnetic field by introducing a function $\psi(\xi,\eta)$:

$$f(\xi,\eta)=\exp\left[-\frac{\gamma R^2}{16}(\xi^2-1)(1-\eta^2)\right]\psi(\xi,\eta). \qquad (9)$$

The function ψ satisfies the following equation:

$$(\xi^2-1)\psi_{\xi\xi}+(1-\eta^2)\psi_{\eta\eta}+2(|m|+1)(\xi\psi_\xi-\eta\psi_\eta)$$
$$+Z_+\xi\psi+Z_-\eta\psi-p^2\xi^2\psi+p^2\eta^2\psi$$
$$-\Gamma(\xi^2-1)(1-\eta^2)(\xi\psi_\xi-\eta\psi_\eta)=0, \qquad (10)$$

where $\Gamma=\gamma R^2/4$ and $p^2=R^2E_b/2$. In the absence of magnetic field the behavior of the wave function at large ξ can be accounted for by the substitution [3]

$$\psi(\xi,\eta)=(\xi+1)^\sigma e^{-p\xi}\chi(\xi,\eta), \qquad (11)$$

where

$$\sigma=\frac{Z_+}{2p}-1-|m|. \qquad (12)$$

If $\eta=\pm1$ and $\xi\rightarrow\infty$, the net potential of the two nuclei becomes indistinguishable from that of a helium nucleus placed at $\xi=1$, $\eta=0$, and the wave function of $H_2{}^+$ must behave like the wave function of a singly ionized helium atom. Therefore, it must decay exponentially like $e^{-p\xi}$ [22]. Although the exact preexponential factor for He^+ will be different from that in Eq. (11), we nevertheless assume that $(\xi+1)^\sigma$ is a good choice, because it provides rapid convergence of solution in the field-free case. Substituting ψ in the form of Eq. (11) into Eq. (10), we obtain the following equation for χ:

$$\begin{aligned}
&(\xi^2-1)\chi_{\xi\xi}+(1-\eta^2)\chi_{\eta\eta}\\
&\quad+2[-p\xi^2+(\sigma+|m|+1)\xi-\sigma+p]\chi_\xi\\
&\quad-2(|m|+1)\eta\chi_\eta+\sigma\frac{(\sigma+2|m|)\xi-\sigma}{\xi+1}\chi\\
&\quad+[p^2\eta^2+Z_-\eta+(2p+1)\sigma-p^2]\chi\\
&\quad-\Gamma(\xi^2-1)(1-\eta^2)(\xi\chi_\xi-\eta\chi_\eta)\\
&\quad+\Gamma\xi(\xi-1)(1-\eta^2)(-\sigma+p+p\xi)\chi=0.
\end{aligned}\tag{13}$$

For the further analysis it is convenient to introduce an independent variable

$$t=\frac{\xi-1}{\xi+1}.\tag{14}$$

Equation (13) becomes

$$\begin{aligned}
&t(1-t)^2\chi_{tt}+(1-\eta^2)\chi_{\eta\eta}+t^2(1-2\sigma-|m|)\chi_t\\
&\quad+2t(\sigma-2p-1)\chi_t+(1+|m|)\chi_t\\
&\quad-2(|m|+1)\eta\chi_\eta+\sigma(\sigma+|m|)t\chi+p^2\eta^2\chi\\
&\quad+Z_-\eta\chi+[(2p+1+|m|)\sigma-p^2]\chi\\
&\quad-2\Gamma t\frac{1+t}{1-t}(1-\eta^2)\chi_t+\frac{4\Gamma t\eta}{(1-t)^2}(1-\eta^2)\chi_\eta\\
&\quad+\frac{2\Gamma t(1+t)}{(1-t)^3}(1-\eta^2)(2p-\sigma+\sigma t)\chi=0.
\end{aligned}\tag{15}$$

We look for the solution of Eq. (15) in the form

$$\chi(t,\eta)=\sum_{i=0}^{\infty}\sum_{j=0}^{\infty}a_{i,j}t^i\eta^j.\tag{16}$$

Substituting series (16) into Eq. (15), we obtain the following relation for coefficients $a_{i,j}$:

$$\begin{aligned}
&F_{i+1,j}a_{i+1,j}+\sum_{k=-3}^{0}\sum_{l=-2,-1,0,2}F_{i+k,j+l}a_{i+k,j+l}\\
&\quad+F_{i-4,j}a_{i-4,j}=0,
\end{aligned}\tag{17}$$

which is formally valid for all i and j if we assume that $a_{k,l}=0$ if $k<0$ or $l<0$. The coefficients F are

$$F_{i+1,j}=(i+1)(i+|m|+1),\tag{18}$$

$$F_{i,j-2}=p^2+2\Gamma i,$$

$$F_{i,j-1}=Z_-,$$

$$\begin{aligned}
F_{i,j}={}&i(-5i+2\sigma-4p-3|m|)-j(j+2|m|+1)\\
&+(2p+1+|m|)\sigma-p^2-2\Gamma i,
\end{aligned}$$

$$F_{i,j+2}=(j+1)(j+2),$$

$$F_{i-1,j-2}=-3p^2+2\Gamma(-i-2j+\sigma-2p+5),$$

$$F_{i-1,j-1}=-3Z_-,$$

$$\begin{aligned}
F_{i-1,j}={}&(i-1)(10i-8\sigma+12p+2|m|-10)\\
&+3j(j+2|m|+1)+(\sigma-6p-2|m|-3)\sigma\\
&+3p^2+2\Gamma(-i-2j+\sigma-2p+5),
\end{aligned}$$

$$F_{i-1,j+2}=-3(j+1)(j+2),$$

$$F_{i-2,j-2}=3p^2+2\Gamma(-i+2j-2p-2),$$

$$F_{i-2,j-1}=3Z_-,$$

$$\begin{aligned}
F_{i-2,j}={}&(i-2)(-10i+12\sigma-12p+2|m|+20)\\
&-3j(j+2|m|+1)+3(-\sigma+2p+1)\sigma\\
&-3p^2+2\Gamma(i-2j+2p-2),
\end{aligned}$$

$$F_{i-2,j+2}=3(j+1)(j+2),$$

$$F_{i-3,j-2}=-p^2+2\Gamma(i-\sigma-3),$$

$$F_{i-3,j-1}=-Z_-,$$

$$\begin{aligned}
F_{i-3,j}={}&(i-3)(5i-8\sigma+4p-3|m|-15)\\
&+j(j+2|m|+1)+(3\sigma-2p+2|m|-1)\sigma\\
&+p^2+2\Gamma(-i+\sigma+3),
\end{aligned}$$

$$F_{i-3,j+2}=-(j+1)(j+2),$$

$$F_{i-4,j}=(i-4)(-i+2\sigma+|m|+4)-\sigma(\sigma+|m|).$$

The recurrent relation (17) may be considered as an infinite set of homogeneous linear equations, and for Eq. (15) to have a solution the determinant of the coefficient matrix must be zero. In practice, series (16) has to be truncated to a finite number of terms. The most natural way to make such a truncation is to choose certain cutoff indices I and J and to set all $a_{i,j}$ for $i>I$ or $j>J$ to zero. Instead of the exact function χ we now deal with a truncated expansion

$$\chi^{I,J}(t,\eta)=\sum_{i=0}^{I}\sum_{j=0}^{J}a_{i,j}t^i\eta^j.\tag{19}$$

The coefficients $a_{i,j}$ are demanded to satisfy Eq. (17). The resulting set of homogeneous equations can be written in the form

$$\mathfrak{F}^{I,J}(p)A=0,\tag{20}$$

where A is a vector of length $L=(I+1)(J+1)$ with elements given by

$$A_{i+j(I+1)}=a_{i,j},\quad i=0,\ldots I,\quad j=0,\ldots,J,\tag{21}$$

and $\mathfrak{F}^{I,J}(p)$ is an $L\times L$ band matrix, whose nonzero elements are given by coefficients $F_{i+k,j+l}$ from Eq. (18),

$$\mathfrak{F}^{I,J}_{i+j(I+1),i+k+(j+l)(I+1)}=F_{i+k,j+l},$$

$$0\leqslant i+k\leqslant I,\quad 0\leqslant j+l\leqslant J. \qquad (22)$$

Solution of the problem in the taken I,J approximation is given by roots of the equation

$$\det[\mathfrak{F}^{I,J}(p)]=0. \qquad (23)$$

We shall denote corresponding approximate values of E_b as $(E_b)_{I,J}$. The principal question is the convergence of truncated solutions to the actual solution as the indices I and J go to infinity. This issue is addressed in Sec. III.

III. CONVERGENCE

As in the case of the field-free problem, we do not have a rigorous proof of the empirical fact that roots of Eq. (23) converge as indices I and J increase. The only way to justify this statement is to perform numerical analysis of convergence and to demonstrate that the numerical solution does converge when I and J independently increase. We performed such an analysis for the hydrogen atom in the magnetic field, for the field-free $H_2{}^+$ ion, and for H_2^+ in an applied magnetic field, and compared results obtained for the two former problems with the best benchmarks available to date [4,22]. To obtain the numerical solution of equation (23), we used a computer code based on the NAG (Numerical Algorithms Group) double precision library subroutine F01LBE, which performs LU decomposition of band matrices.

If we put the charge of one of the nuclei to zero (say, $Z_a=1$ and $Z_b=0$), we arrive at the problem of the hydrogen atom in an external magnetic field. Since the Schrödinger equation for this system in the nonrelativistic, infinite nuclear mass approximation has been recently exactly solved [22], and extensive tables of energy levels with precision up to 10^{-12} hartree are now available, we can use the hydrogen data for the preliminary check of our computational method and its rate of convergence.

TABLE I. Convergence of solution for the hydrogen atom in an external magnetic field in the nonrelativistic, infinite nuclear mass approximation . Ground state values of $(E_b)_{I,J}$ are calculated for different sets of I and J and for three fields strength $\gamma=0.01$, 0.1, and 1.0 a.u. The parameter R is 2.0 a.u. Exact values of E_b are taken from Ref. [22].

I	$J=10$	$J=14$	$J=20$	$J=30$
	$\gamma=0.01$ (exact value is 0.504 975 002 759±10^{-12})			
10	0.504 843 164 768	0.504 843 195 147	0.504 843 195 148	0.504 843 195 148
20	0.504 969 383 395	0.504 969 413 880	0.504 969 413 881	0.504 969 413 881
30	0.504 974 574 005	0.504 974 604 438	0.504 974 604 439	0.504 974 604 439
40	0.504 974 931 984	0.504 974 962 419	0.504 974 962 420	0.504 974 962 420
50	0.504 974 967 068	0.504 974 997 508	0.504 974 997 509	0.504 974 997 509
60	0.504 974 971 492	0.504 975 001 934	0.504 975 001 935	0.504 975 001 935
70	0.504 974 972 166	0.504 975 002 608	0.504 975 002 609	0.504 975 002 609
80	0.504 974 972 285	0.504 975 002 728	0.504 975 002 729	0.504 975 002 729
90	0.504 974 972 309	0.504 975 002 751	0.504 975 002 752	0.504 975 002 752
100	0.504 974 972 314	0.504 975 002 757	0.504 975 002 758	0.504 975 002 758
	$\gamma=0.1$ (exact value is 0.547 526 480 401±10^{-12})			
10	0.545 877 600 859	0.545 877 497 140	0.545 877 497 200	0.545 877 497 201
20	0.547 401 018 482	0.547 401 261 422	0.547 401 260 867	0.547 401 260 867
30	0.547 510 274 894	0.547 510 810 989	0.547 510 812 189	0.547 510 812 189
40	0.547 523 536 342	0.547 523 855 071	0.547 523 861 551	0.547 523 861 552
50	0.547 525 979 430	0.547 525 940 412	0.547 525 949 508	0.547 525 949 506
60	0.547 526 683 78	0.547 526 350 52	0.547 526 356 64	0.547 526 356 63
70	0.547 526 977 44	0.547 526 449 5	0.547 526 448 3	0.547 526 448 28
80	0.547 527 125 8	0.547 526 481 9	0.547 526 471	0.547 526 471
90	0.547 527 206	0.547 526 497	0.547 526 478	0.547 526 477
100	0.547 527 251	0.547 526 506	0.547 526 49	0.547 526 49
	$\gamma=1.0$ (exact value is 0.831 168 896 733±10^{-12})			
10	0.823 315 789 589	0.823 886 586 134	0.823 877 944 836	0.823 877 944 366
20	0.827 225 148 646	0.830 547 700 02	0.830 880 754 783	0.830 881 495 01
30	0.838 021 927 3	0.828 904 472 9	0.831 157 560	0.831 153 652 9
40	0.857 749 50	0.829 056 78	0.831 416 83	0.831 167 9
50	0.875 854 19	0.836 392 3	0.832 483	0.831 169
60	0.889 605 03	0.850 22	0.834 461	0.831 172
70	0.899 753 5	0.866 29	0.836 1	0.831
80	0.907 26	0.881 4	0.834 5	0.832
90	0.912 63	0.894	0.825	0.82
100	0.916 17	0.904	Unstable	Unstable

Table I gives values of the ground-state binding energy of the hydrogen atom in a magnetic field for three different field strengths, $\gamma=0.01$, 0.1, and 1.0 a.u., computed at a fixed ''internuclear'' distance $R=2.0$ (the second nucleus is absent) for various combinations of I and J. As we see, for $\gamma=0.01$ the calculated values steadily converge to the exact solution, and for $I=100$ and $J=20$ our result differs from the true binding energy by only 10^{-12} hartree; for $I=30$ and $J=10$ the precision is better than 10^{-6} hartree. Convergence in J is very rapid; results for $J=14$ and 20 differ only in the 12th significant digit, and results for $J=20$ and 30 are, within our accuracy, identical. Convergence in I is asymptotically slower than in J, as demonstrated by the lower curve on Fig. 1, which shows the difference between pairs of E_b computed with I which differ from one another by ten, and with the same $J=10$. However, already $I=20$ gives five correct decimal digits of the result.

The situation is not as good for $\gamma=0.1$. The convergence in J is appreciably slower than for $\gamma=0.01$, and results for $J=20$ and 30 still differ in the 12th significant digit. Convergence in I is also much less rapid, as demonstrated by the middle curve on Fig. 1, and five correct digits are obtained only at $I=40$. In addition, for large I the computational algorithm becomes numerically unstable and rounding errors reduce the number of reliable digits which can be obtained using the present method. As a result, the maximum accuracy is achieved at a certain finite value of I, which is determined by the balance between the rate of convergence and numerical instabilities. For $\gamma=0.1$, we can obtain only eight decimal digits at $I=90$ and $J\geqslant 20$. If we increase the field up to $\gamma=1.0$, the method becomes so unstable that the best result achieved at $I=50$ and $J=30$ has only six correct digits; for higher fields, the instability renders the method practically useless.

The convergence properties of the magnetized H_2^+ problem are very similar to those observed for the hydrogen atom. This is demonstrated by Table II, which gives values of E_b for the state $1\sigma_g$ in the field-free case and for fields

TABLE II. Convergence of the solution for the ground state $1\sigma_g$ of the hydrogen molecular ion $H_2{}^+$. Calculations of $(E_b)_{I,J}$ are performed for the field-free ion ($\gamma=0$) and for three different field strengths $\gamma=0.01$, 0.1, and 1.0 a.u. at a fixed internuclear distance $R=2.0$. The exact value of E_b for $\gamma=0$ is taken from [4].

I	$J=10$	$J=14$	$J=20$	$J=30$
$\gamma=0.0$ (exact value is 1.102 634 214 494 9)				
6	1.102 634 128 816	1.102 634 214 092	1.102 634 214 102	1.102 634 214 102
8	1.102 634 129 197	1.102 634 214 472	1.102 634 214 483	1.102 634 214 483
10	1.102 634 129 209	1.102 634 214 484	1.102 634 214 494	1.102 634 214 494
12	1.102 634 129 209	1.102 634 214 485	1.102 634 214 495	1.102 634 214 495
14	1.102 634 129 209	1.102 634 214 485	1.102 634 214 495	1.102 634 214 495
$\gamma=0.01$				
10	1.107 573 777 781	1.107 573 850 145	1.107 573 850 153	1.107 573 850 153
20	1.107 617 314 016	1.107 617 386 414	1.107 617 386 422	1.107 617 386 422
30	1.107 618 072 051	1.107 618 144 448	1.107 618 144 456	1.107 618 144 456
40	1.107 618 097 971	1.107 618 170 368	1.107 618 170 375	1.107 618 170 375
50	1.107 618 099 355	1.107 618 171 752	1.107 618 171 759	1.107 618 171 759
60	1.107 618 099 457	1.107 618 171 853	1.107 618 171 861	1.107 618 171 861
70	1.107 618 099 466	1.107 618 171 863	1.107 618 171 870	1.107 618 171 870
80	1.107 618 099 467	1.107 618 171 864	1.107 618 171 871	1.107 618 171 871
90	1.107 618 099 467	1.107 618 171 864	1.107 618 171 871	1.107 618 171 871
$\gamma=0.1$				
10	1.150 405 200 262	1.150 405 220 941	1.150 405 220 946	1.150 405 220 946
20	1.151 012 103 477	1.151 012 138 532	1.151 012 138 515	1.151 012 138 515
30	1.151 033 414 683	1.151 033 452 810	1.151 033 452 823	1.151 033 452 823
40	1.151 034 869 761	1.151 034 900 220	1.151 034 900 286	1.151 034 900 286
50	1.151 035 018 578	1.151 035 044 739	1.151 035 044 787	1.151 035 044 787
60	1.151 035 038 76	1.151 035 063 47	1.151 035 063 469	1.151 035 063 47
70	1.151 035 042 0	1.151 035 066 4	1.151 035 066 39	1.151 035 066 38
80	1.151 035 042	1.151 035 067 1	1.151 035 066 86	1.151 035 066 8
90	1.151 035 04	1.151 035 067 7	1.151 035 067 2	1.151 035 067
100	1.151 035 0	1.151 035 064	1.151 035 07	1.151 035 06
$\gamma=1.0$				
10	1.464 878 255 204	1.465 006 079 242	1.465 004 788 905	1.465 004 788 835
20	1.470 624 782 772	1.470 303 906 582	1.470 342 076 43	1.470 342 134 29
30	1.473 251 707 1	1.470 521 039 7	1.470 530 754 7	1.470 529 580 0
40	1.475 793 69	1.471 049 369	1.470 550 89	1.470 539 31
50	1.477 537 17	1.472 071 8	1.470 558 3	1.470 540 3
60	1.478 555 0	1.473 32	1.470 500	1.470 54
70	1.479 11	1.474 53	1.470 2	1.470 4
80	1.479 40	1.475 6	1.470	1.472
90	1.479 55	1.476	1.47	1.48
100	1.479 58	1.48	Unstable	Unstable

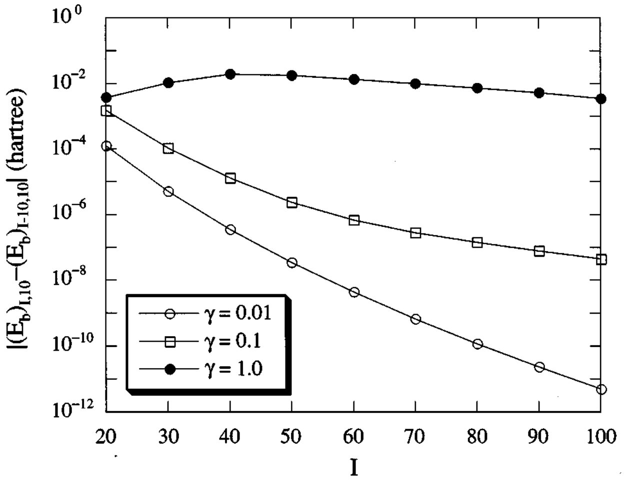

FIG. 1. The difference between $(E_b)_{I,10}$ and $(E_b)_{I-10,10}$ for the ground state of the hydrogen atom in a magnetic field as a function of the cutoff index I, computed at $R=2.0$ for three different values of the field strength.

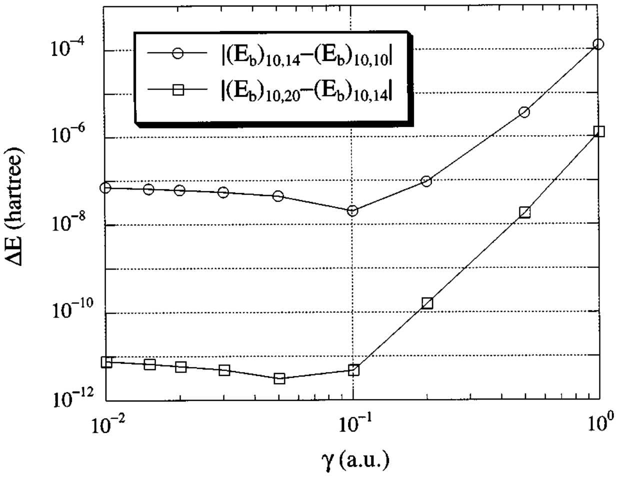

FIG. 2. Dependence of the rate of convergence over J for H_2^+ on the strength of the applied magnetic field. The convergence is measured by the difference between values $(E_b)_{10,10}$, $(E_b)_{10,14}$, and $(E_b)_{10,20}$.

$\gamma=0.01$, 0.1, and 1.0 a.u., computed with the same sets of I and J and at the same fixed internuclear distance $R=2.0$. In the absence of field, the convergence of E_b in I and J is very rapid: already $I=12$ and $J=20$ give 12 correct decimal digits of E. This conclusion agrees with the results reported in [4], where it was found that $I=16$ and $J=40$ (in our terms) provide precision better than 10^{-17} hartree.

Figure 2 shows how the strength of the applied magnetic field affects the rate of convergence in J. The latter is measured as the difference between subsequent values of E_b obtained with $I=10$ and $J=10$, 14, and 20. The magnetic field varies in the range $0.01\leqslant\gamma\leqslant1.0$. As we see, for $\gamma\leqslant0.1$ the convergence in J is still as good as in the absence of field (the difference between values for $J=20$ and 30 is less than 10^{-12} hartree), while for $\gamma>0.1$ the rate of convergence begins to slow down.

Convergence in I is substantially affected already by the field $\gamma=0.01$, and its rate rapidly decreases with the growth of the field strength. Figure 3 shows the dependence of the

TABLE III. Convergence of solution for the hydrogen molecular ion in the $1\pi_u$ state ($m=-1$). The internuclear distance is $R=8.0$ a.u. Calculations of $(E_b)_{I,J}$ were performed for the field-free ion ($\gamma=0$) and for fields $\gamma=0.01$ and 0.1. At $\gamma=1.0$, numerical stability was insufficient to provide reliable results.

I	$J=10$	$J=14$	$J=20$	$J=30$
	$\gamma=0.0$ (exact value is 0.259 510 631 269 1)			
4	0.259 509 674 909	0.259 510 630 254	0.259 510 631 284	0.259 510 631 284
6	0.259 509 674 894	0.259 510 630 239	0.259 510 631 269	0.259 510 631 269
8	0.259 509 674 894	0.259 510 630 239	0.259 510 631 269	0.259 510 631 269
	$\gamma=0.01$			
10	0.269 235 727 324	0.269 236 153 158	0.269 236 153 440	0.269 236 153 440
20	0.269 275 707 680	0.269 276 128 867	0.269 276 129 163	0.269 276 129 163
30	0.269 276 189 750	0.269 276 611 283	0.269 276 611 575	0.269 276 611 575
40	0.269 276 202 581	0.269 276 624 135	0.269 276 624 428	0.269 276 624 428
50	0.269 276 203 142	0.269 276 624 690	0.269 276 624 983	0.269 276 624 983
60	0.269 276 203 178	0.269 276 624 724	0.269 276 625 02	0.269 276 625 016
70	0.269 276 203 18	0.269 276 624 7	0.269 276 625 0	0.269 276 625 02
	$\gamma=0.1$			
10	0.337 702 541 088	0.337 695 300 732	0.337 695 303 112	0.337 695 303 450
20	0.338 603 907 15	0.338 655 551 122	0.338 656 124 43	0.338 656 125 443
30	0.338 657 841 8	0.338 671 245 4	0.338 680 089 1	0.338 680 158
40	0.338 696 326	0.338 671 45	0.338 681 32	0.338 681 00
50	0.338 716	0.338 677 1	0.338 681 8	0.338 678
60	0.338 7240	0.338 68	0.338 68	0.339
70	0.338 72	0.338 7	0.339	0.337

TABLE IV. The equilibrium internuclear distance R_{eq}, the total electronic energy $\varepsilon_T(R_{\mathrm{eq}})$, vibrational energy ω_R, and dissociation energy ε_D for the quantum state $1\sigma_g$ of $\mathrm{H}_2{}^+$ as functions of the applied magnetic field γ.

γ	R_{eq}	$\varepsilon_T(R_{\mathrm{eq}})$	ω_R	ε_D
0.00×10^{0}	1.997 19	−0.602 634 62	1.0591×10^{-2}	0.102 634 62
1.00×10^{-3}	1.997 19	−0.603 134 46	1.0591×10^{-2}	0.102 634 71
1.25×10^{-3}	1.997 19	−0.603 259 37	1.0591×10^{-2}	0.102 634 76
1.50×10^{-3}	1.997 19	−0.603 384 26	1.0591×10^{-2}	0.102 634 82
2.00×10^{-3}	1.997 19	−0.603 633 98	1.0591×10^{-2}	0.102 634 98
2.50×10^{-3}	1.997 19	−0.603 883 62	1.0591×10^{-2}	0.102 635 18
3.00×10^{-3}	1.997 19	−0.604 133 18	1.0591×10^{-2}	0.102 635 43
4.00×10^{-3}	1.997 19	−0.604 632 05	1.0591×10^{-2}	0.102 636 05
5.00×10^{-3}	1.997 18	−0.605 130 61	1.0591×10^{-2}	0.102 636 86
6.00×10^{-3}	1.997 18	−0.605 628 85	1.0591×10^{-2}	0.102 637 85
8.00×10^{-3}	1.997 16	−0.606 624 36	1.0591×10^{-2}	0.102 640 36
1.00×10^{-2}	1.997 14	−0.607 618 59	1.0591×10^{-2}	0.102 643 59
1.25×10^{-2}	1.997 11	−0.608 859 58	1.0591×10^{-2}	0.102 648 63
1.50×10^{-2}	1.997 08	−0.610 098 56	1.0592×10^{-2}	0.102 654 79
2.00×10^{-2}	1.996 99	−0.612 570 52	1.0593×10^{-2}	0.102 670 47
2.50×10^{-2}	1.996 88	−0.615 034 47	1.0594×10^{-2}	0.102 690 61
3.00×10^{-2}	1.996 74	−0.617 490 41	1.0596×10^{-2}	0.102 715 19
4.00×10^{-2}	1.996 39	−0.622 378 33	1.0601×10^{-2}	0.102 777 63
5.00×10^{-2}	1.995 93	−0.627 234 31	1.0606×10^{-2}	0.102 857 61
6.00×10^{-2}	1.995 38	−0.632 058 43	1.0613×10^{-2}	0.102 954 91
8.00×10^{-2}	1.993 99	−0.641 611 44	1.0631×10^{-2}	0.103 200 44
1.00×10^{-1}	1.992 21	−0.651 038 20	1.0653×10^{-2}	0.103 511 72

difference $|(E_b)_{I,10}-(E_b)_{I-10,10}|$ on I for $\gamma=0.01$, 0.1, and 1.0. For $\gamma=0.01$ the accuracy 10^{-12} hartree was achieved only at $I=80$; for stronger magnetic fields such a precision could not be achieved at all because of the loss of numerical stability. For $\gamma=1.0$ the precision of the most reliable values is only about 10^{-5} hartree.

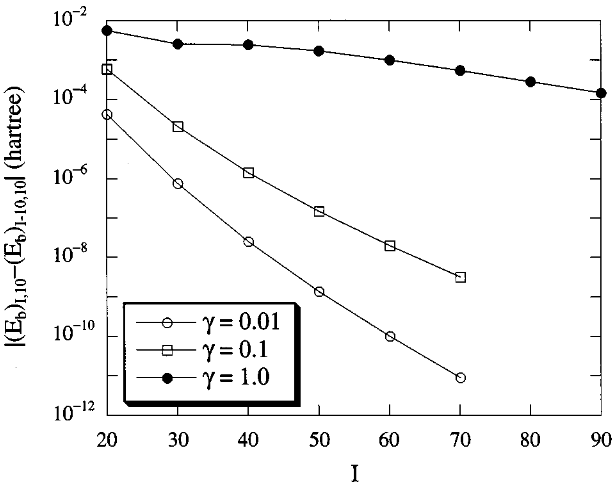

FIG. 3. The difference between $(E_b)_{I,10}$ and $(E_b)_{I-10,10}$, computed for $\mathrm{H}_2{}^+$ in the state $1\sigma_g$ at $R=2.0$, as a function of the cutoff index I for $\gamma=0.01$, 0.1, and 1.0 a.u.

Table III shows the convergence of E_b for the state $1\pi_u$ (the field-free $2p\pi_u$) with $m=-1$. While in the absence of field the convergence of results in I is even faster than in the previous case, in the presence of magnetic field the situation is worse than for $1\sigma_g$, and reliable results can be obtained only for $\gamma\lesssim0.01$; for $\gamma=1.0$ the method is completely unstable.

As we see, the method under consideration is applicable only for fields not exceeding 0.01–0.1 a.u., depending on the quantum state, and is practically useless for fields stronger than $\gamma=1.0$. It is interesting to compare our results with a semianalytical method for the hydrogen atom in a magnetic field reported in Ref. [23]. The authors of [23] represented the hydrogen wave function as a truncated double power series in the parabolic-cylindrical coordinate system and obtained a system of linear equations analogous to Eq. (20), which was required to have a nonsingular solution. They found that the convergence of results for $\gamma>0.5$ a.u. becomes slower, and for $\gamma=1$ the accuracy 10^{-6} hartree was obtained only when the degree of the truncated polynomial was about 50, which is quantitatively close to our observations.

To check if the rate of convergence depends on the exact form of the multiplier in substitution (11), we performed calculations with the function $\chi(\xi,\eta)$ defined as

$$\psi(\xi,\eta)=e^{-p\xi}\chi(\xi,\eta). \tag{24}$$

TABLE V. Values of R_{eq}, $\varepsilon_T(R_{\mathrm{eq}})$, ω_R, and ε_D for the hydrogen molecular ion in the quantum state $1\pi_u$ $(m=-1)$ calculated in the interval $0\leqslant\gamma\leqslant0.01$.

γ	R_{eq}	$\varepsilon_T(R_{\mathrm{eq}})$	ω_R	ε_D
0.00×10^{0}	7.930 714	−0.134 513 816	$1.212\,46\times10^{-3}$	$9.513\,816\times10^{-3}$
1.00×10^{-4}	7.930 712	−0.134 613 792	$1.212\,46\times10^{-3}$	$9.513\,822\times10^{-3}$
1.25×10^{-4}	7.930 712	−0.134 638 779	$1.212\,46\times10^{-3}$	$9.513\,826\times10^{-3}$
1.50×10^{-4}	7.930 711	−0.134 663 763	$1.212\,46\times10^{-3}$	$9.513\,831\times10^{-3}$
2.00×10^{-4}	7.930 708	−0.134 713 723	$1.212\,46\times10^{-3}$	$9.513\,843\times10^{-3}$
2.50×10^{-4}	7.930 705	−0.134 763 670	$1.212\,46\times10^{-3}$	$9.513\,858\times10^{-3}$
3.00×10^{-4}	7.930 701	−0.134 813 606	$1.212\,47\times10^{-3}$	$9.513\,876\times10^{-3}$
4.00×10^{-4}	7.930 691	−0.134 913 443	$1.212\,47\times10^{-3}$	$9.513\,923\times10^{-3}$
5.00×10^{-4}	7.930 677	−0.135 013 233	$1.212\,47\times10^{-3}$	$9.513\,983\times10^{-3}$
6.00×10^{-4}	7.930 661	−0.135 112 977	$1.212\,48\times10^{-3}$	$9.514\,057\times10^{-3}$
8.00×10^{-4}	7.930 620	−0.135 312 325	$1.212\,50\times10^{-3}$	$9.514\,244\times10^{-3}$
1.00×10^{-3}	7.930 568	−0.135 511 486	$1.212\,52\times10^{-3}$	$9.514\,486\times10^{-3}$
1.25×10^{-3}	7.930 485	−0.135 760 175	$1.212\,55\times10^{-3}$	$9.514\,862\times10^{-3}$
1.50×10^{-3}	7.930 385	−0.136 008 573	$1.212\,59\times10^{-3}$	$9.515\,323\times10^{-3}$
2.00×10^{-3}	7.930 129	−0.136 504 496	$1.212\,68\times10^{-3}$	$9.516\,494\times10^{-3}$
2.50×10^{-3}	7.929 800	−0.136 999 255	$1.212\,81\times10^{-3}$	$9.518\,000\times10^{-3}$
3.00×10^{-3}	7.929 398	−0.137 492 849	$1.212\,96\times10^{-3}$	$9.519\,840\times10^{-3}$
4.00×10^{-3}	7.928 376	−0.138 476 547	$1.213\,35\times10^{-3}$	$9.524\,518\times10^{-3}$
5.00×10^{-3}	7.927 063	−0.139 455 595	$1.213\,85\times10^{-3}$	$9.530\,523\times10^{-3}$
6.00×10^{-3}	7.925 462	−0.140 429 998	$1.214\,47\times10^{-3}$	$9.537\,848\times10^{-3}$
8.00×10^{-3}	7.921 399	−0.142 364 896	$1.216\,02\times10^{-3}$	$9.556\,425\times10^{-3}$
1.00×10^{-2}	7.916 205	−0.144 281 310	$1.218\,01\times10^{-3}$	$9.580\,165\times10^{-3}$

In the field-free case the convergence in I was five times slower than with Eq. (11), and an accuracy within 10^{-12} hartree was achieved only at $I=60$. However, the convergence rate for $\gamma\geqslant0.01$ was practically the same as with definition (11). Therefore, although substitution (11) is the best known choice for a field-free hydrogen molecular ion, it does not offer appreciable advantages over Eq. (24) when the magnetic field is present.

IV. RESULTS AND CONCLUSIONS

We performed a calculation of basic molecular parameters for two quantum states of the hydrogen molecular ion in the magnetic field. The ground state $1\sigma_g$, which evolves from the field-free ground state $1s\sigma_g$, is studied in the field range $0\leqslant\gamma\leqslant0.1$. The state $1\pi_u$, which is the lowest state with $m=-1$, and which corresponds to the field-free state $2p\pi_u$, is studied in the range $0\leqslant\gamma\leqslant0.01$ a.u.

The calculated parameters include the equilibrium internuclear distance R_{eq}, the total electronic energy at the equilibrium distance $\varepsilon_T(R_{\mathrm{eq}})$, the energies of the small (harmonic) vibrations about the equilibrium position in the direction parallel to the magnetic field, and the dissociation energies ε_D of the process $\mathrm{H}_2{}^+\rightarrow\mathrm{H}+p^+$. The total electronic energy is measured with respect to the free electron energy $\gamma/2$ and is defined as $\varepsilon_T(R)=1/R-E_b(R)$; its absolute value is equal to the dissociation energy of the process $\mathrm{H}_2{}^+\rightarrow p^+ + p^+ + e^-$. To determine the energy of the dissociation into a neutral hydrogen atom and a free proton, we used values of E_b for the hydrogen atom from Ref. [22]. The vibrational energy ω_R is determined as

$$\omega_R=\left(\frac{1}{\mu}\,\frac{d^2\varepsilon_T}{dR^2}\right)^{1/2}\Bigg|_{R=R_{\mathrm{eq}}}, \tag{25}$$

where $\mu=m_p/2$ is the reduced mass of the system of two nuclei.

Molecular parameters of the ground state $1\sigma_g$ are given in Table IV. The total electronic energy is almost linear with respect to the magnetic field strength γ, the other quoted parameters are quadratic in γ. For $\gamma\leqslant0.1$ their dependencies on the field strength can be described by the following approximate formulas (all quantities are given in atomic units):

$$R_{\mathrm{eq}}^{1\sigma_g}(\gamma)=1.99719-0.5\gamma^2\pm10^{-5}, \tag{26a}$$

$$[\varepsilon_T^{1\sigma_g}(R_{\mathrm{eq}})](\gamma)=-0.602\,634\,62-0.5\gamma+0.16\gamma^2 \pm(10^{-8}+10^{-2}\gamma^3), \tag{26b}$$

$$\omega_R^{1\sigma_g}(\gamma)=0.010591+0.006284\gamma^2\pm10^{-6}. \tag{26c}$$

TABLE VI. Comparison of results obtained by the present method with previously reported calculations for the ground state of $H_2{}^+$ in magnetic field. Present results are given in the first line of each entry, B is the magnetic field strength, and other quantities are the same as in Table IV.

B,T	γ	R_{eq}	$\varepsilon_T(R_{\mathrm{eq}})$	ω_R	ε_D
0	0.0	1.997 19	−0.602 634 62	1.0591×10^{-2}	0.102 634 62
		1.997[a]		1.08×10^{-2} [a]	
10^3	$4.254\,38\times10^{-3}$	1.997 19	−0.604 758 91	1.0591×10^{-2}	0.102 636 24
		1.997[a]		1.08×10^{-2} [a]	
10^4	$4.254\,38\times10^{-2}$	1.996 28	−0.623 616 62	1.0602×10^{-2}	0.102 796 32
		1.996[a]		1.09×10^{-2} [a]	
		1.996[b]	−0.623 62 [b]		0.102 80[b]
2×10^4	$8.508\,76\times10^{-2}$	1.993 57	−0.644 021 36	1.0636×10^{-2}	0.103 273 50
		1.993[a]		1.09×10^{-2} [a]	

[a] Reference [16].

[b] Reference [21].

The corresponding data for the state $1\pi_u$ (the lowest quantum state with $m=-1$) are given in Table V. Approximate expressions for the molecular parameters which are valid in the range $0\leqslant\gamma\leqslant0.01$ are

$$R_{\mathrm{eq}}^{1\pi_u}(\gamma)=7.930714-146.1\gamma^2\pm(10^{-6}+10^4\gamma^4), \tag{27a}$$

$$[\varepsilon_T^{1\pi_u}(R_{\mathrm{eq}})](\gamma)=-0.134\,513\,816-\gamma+2.33\gamma^2 \pm(10^{-9}+100\gamma^4), \tag{27b}$$

$$\omega_R^{1\pi_u}(\gamma)=1.21246\times10^{-3}+0.0555\gamma^2\pm2\times10^{-8}. \tag{27c}$$

Table VI presents a comparison of results obtained by the present method with previously reported accurate calculations of $H_2{}^+$ in magnetic fields below 0.1 a.u. The comparison is restricted only to the ground state, since parameters of the state $1\pi_u$ are reported only for fields from 10^4 T and stronger [21], which exceeds the field range considered in our work. As we see, our results are in very good agreement with previous computations.

In the absence of magnetic field the potential energy curve of the state $1\pi_u$ exhibits a small hump which is located at $R\approx25.81$ a.u. and whose value in the maximum is equal to $-0.124\,856$ hartree. In the presence of a moderately strong magnetic field this qualitative picture of the energy curve behavior remains the same, although the curve is shifted down due to the increase of binding energy of the hydrogen atom in $2p_{-1}$ state.

Results of our work indicate that the employed semianalytical method of solution is best suited for weak and moderately strong magnetic fields ($\leqslant10^4$–10^5 T). This conclusion is in agreement with the results of Ref. [23], where it was found that a similar technique applied to the hydrogen atom in a magnetic field converges very well for $\gamma\leqslant0.5$, and exhibits slower convergence for stronger fields.

Although the onset of the numerical instability on the γ scale may be delayed to a some extent by performing calculations with quadruple precision, the convergence of the solution in the cutoff indices I and J becomes slower with the growth of γ, which means that a longer computational time will be required to find the determinant of the band matrix $\mathfrak{F}^{I,J}(p)$. This fact can, in turn, impose limitations on the range of γ for which the method is practically applicable and on quantum states which can be treated.

A substantial advantage of the applied method over the usual finite basis set and variational methods resides in its high accuracy, which is not affected by selection of basis functions or by choice of variational parameters, and which can be controlled in a straightforward manner by increasing the degrees of the expansion (19). This fact allows one to perform an accurate calculation of other important physical parameters which may depend on the exact distribution of the electron density (e.g., multipole moments). In addition, benchmark results obtained using the present method can be used to check the validity of alternative computational methods which may be applied to the magnetized hydrogen molecular ion.

It should be pointed out that the technique used in the present work is not restricted to the hydrogen molecular ion only. It is applicable without modifications for the treatment of other two-center one-electron problems, including that of HeH^{2+} in a parallel magnetic field.

ACKNOWLEDGMENTS

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[1] M. A. Liberman and B. Johansson, Usp. Fiz. Nauk **165**, 121 (1995) [Sov. Phys.—Usp. **38**, 117 (1995)].

[2] Ø. Burrau, K. Dan. Vidensk. Selsk. Mat. Fys. Medd. **7**, No. 14 (1927).

[3] D. R. Bates, K. Ledsham, and A. L. Stewart, Philos. Trans. Roy. Soc. London Ser. A **246**, 215 (1953).

[4] J. M. Peek, J. Chem. Phys. **43**, 3004 (1965).

[5] M. M. Madsen and J. M. Peek, At. Data. **2**, 171 (1971).

[6] T. G. Winter, M. D. Duncan, and N. F. Lane, J. Phys. B **10**, 285 (1977).

[7] C. P. de Melo, R. Ferreira, H. S. Brandi, and L. C. M. Miranda, Phys. Rev. Lett. **37**, 676 (1976).

[8] J. C. Le Guillou and J. Zinn-Justin, Ann. Phys. (N.Y.) **154**, 440 (1984).

[9] J. Ozaki and Y. Hayashi, J. Phys. Soc. Jpn. **58**, 3564 (1989); J. Ozaki, *ibid.* **62**, 1516 (1993).

[10] G. Wunner, H. Herold and H. Ruder, Phys. Lett. A **88**, 344 (1982).

[11] C. P. de Melo *et al.*, Phys. Rev. A **18**, 12 (1978).

[12] J. Ozaki and Y. Tomishima, Phys. Lett. A **82**, 449 (1981).

[13] D. M. Larsen, Phys. Rev. A **25**, 1295 (1982).

[14] M. Vincke and D. Baye, J. Phys. B **18**, 167 (1985).

[15] U. Kappes, P. Schmelcher, and T. Pacher, Phys. Rev. A **50**, 3775 (1994); U. Kappes and P. Schmelcher, *ibid.* **51**, 4542 (1995).

[16] U. Wille, J. Phys. B **20**, L417 (1987).

[17] U. Wille, Phys. Rev. A **38**, 3210 (1988).

[18] U. Kappes and P. Schmelcher, Phys. Rev. A **53**, 3869 (1996).

[19] M. S. Kaschiev, S. I. Vinitsky, and F. R. Vukajlović, Phys. Rev. A **22**, 557 (1980).

[20] J. Ozaki and Y. Tomishima, J. Phys. Soc. Jpn. **52**, 1142 (1983).

[21] J. M. Peek and J. Katriel, Phys. Rev. A **21**, 413 (1980).

[22] Yu. P. Kravchenko, M. A. Liberman, and B. Johansson, Phys. Rev. A **54**, 287 (1996).

[23] O. L. Silva Filho and A. L. A. Fonseca, Phys. Rev. A **50**, 4383 (1994).