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Hydrogen atom H and $H_2{}^+$ molecule in strong magnetic fields

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The finite-elements method is used to solve, to the given degree of accuracy, bound states of the H atom and the molecular ion $H_2{}^+$ of hydrogen in a strong magnetic field, $10^9 < H < 10^{13}$ gauss, and stronger. In the case of the hydrogen atom, the results are in agreement (within a factor of $\sim 10^{-4}$) with results of the best variational calculations in the area of field changes, while in the case of the molecular hydrogen ion and for the $0 < H < 10^{11}$ gauss field they are far better than all calculations known to date. The opinion presented here is that the finite-elements method used in this paper—i.e., the method of direct solution of the particular problem on a plane—can also be successfully used in many other physics problems which are reduced to partial differential equations on a plane, and when perturbation theory or some other similar method of solution is not applicable.

The problem of the bound states of atoms and the molecular hydrogen ion (H and $H_2{}^+$) in strong magnetic fields, appears in astrophysics in its treatment of neutron stars.[1] This field reaches an intensity of 10^{13} G. In laboratory conditions an analogous problem takes place in semiconductors. In this case, excitons represent hydrogen "quasiatoms" with a small effective mass and large dielectric constant.[2] The appropriate dimensionless parameter, which determines the strength of the field, is equal to $\gamma = \mu_B H/R_\infty$, where μ_B is the Bohr magneton, H the field strength (measured in gauss), and R_∞ the rydberg (Ry) or effective rydberg in the case of atoms and in the case of excitons, respectively.

Various methods are usually used in treating areas of small, average, and large γ. As such, limits to their use are not fixed sharply enough and results for the bond energy of the H and $H_2{}^+$ system which are subsequently obtained, differ sometimes even in the first significant digit.

In the paper[3] a first attempt was made at spectra calculation of H and $H_2{}^+$ within the framework of the same approach in the whole area of γ change. However, for $\gamma = 0$ in the case of $H_2{}^+$ this method yields a value of 15.1 eV for the ground-state energy, instead of the exact value of 16.39 eV. In this way the problem of calculating to the given degree of exactness the binding energy of hydrogen H and the molecular hydrogen ion $H_2{}^+$ as a function of γ in the whole region $0 < \gamma < 10^4$ of γ change and greater, remains unresolved to this day.

In this paper we propose a general method for calculating, to the given degree of exactness, the bound states H and $H_2{}^+$ in fields which change in the interval $0 < \gamma < 10^4$ and greater.

The Hamiltonian of the hydrogen atom in a homogeneous magnetic field H directed along the z axis has the following form:

$$H_a = -\nabla_r^2 - (2/r) + \gamma l_z + \tfrac{1}{2}\gamma^2 r^2 \sin^2\theta \, ,$$

where l_z is the z component of the angular momentum operator $\vec{l} = -i[\vec{r} \times \nabla_{\vec{r}}]$, and r and θ are the spherical coordinates of the vector $\vec{r} = \{r, \theta, \varphi\}$.

The Hamiltonian of the hydrogen molecular ion in a homogeneous field H whose direction coincides with the direction of the vector $\vec{R}_{ab}$, which connects nuclei a and b (protons) in the Born-Oppenheimer approximation, has the following form:

$$H_I = -\nabla_{\vec{r}}^2 + \gamma l_z + \tfrac{1}{2}\gamma^2 r^2 \sin^2\theta - \frac{2}{r_a} - \frac{2}{r_b} + \frac{2}{R_{ab}} \, ,$$

where $\vec{r}_a = |\vec{r} - \frac{1}{2}\vec{R}_{ab}|$, $r_b = |\vec{r} + \frac{1}{2}\vec{R}_{ab}|$, $R_{ab} = |\vec{R}_{ab}|$, and r is the electron position vector with respect to the center of the R_{ab} segment. The Hamiltonian H_I is most naturally written in the spheroidal coordinates $\xi = (r_a + r_b)/R_{ab}$, $\eta = (r_a - r_b)/R_{ab}$, and φ, in which the variables are separated in the absence of a magnetic field ($\gamma = 0$).[4]

The projection l_z of the orbital moment l on the z axis (in the case of $H_2{}^+$ the z axis has the direction of the vector $\vec{R}_{ab}$), is conserved in the case of H just as it is in the case of $H_2{}^+$, $l_z = m$, and the angle dependence of the wave function has the form $(2\pi)^{-1/2} e^{im\varphi}$. After separation of azimuthal dependence, the problem of finding the bound states of the H and $H_2{}^+$ system with Hamiltonians H_a and H_I reduces to solving a typical partial differential equation problem on surfaces r, θ and ξ, η, respectively:

TABLE I. The ground-state energy E_a (Ry) and $E(R_0)$ (Ry) of the hydrogen atom and molecular ion in a magnetic field (remaining characteristics are described in the text).

H (gauss)	γ	R_0	$E(R_0)$	$W_0=2[E(R_0)+1/R_0]$	E_a	$E_B=W_0-E_a$	E_{osc}
10^9	$0.425\,502\,2$	1.9	−1.101 39	−1.150 15	−0.920 78	−0.229 37	
5×10^9	$0.212\,751\,1\times10$	1.7	−0.757 71	−0.338 94	0.049 46	−0.388 40	
10^{10}	$0.425\,501\,1\times10$	1.2	−0.286 99	1.092 69	1.640 34	−0.547 65	
5×10^{10}	$0.212\,751\,1\times10^2$	0.8	6.502 47	15.504 94	16.754 4	−1.249 3	
10^{11}	$0.425\,502\,2\times10^2$	0.6	15.870 09	35.673 52	36.847 89	−1.774 37	
5×10^{11}	$0.212\,751\,1\times10^3$	0.354	96.953 19	199.556 1	203.543 42	−3.987 32	
10^{12}	$0.425\,502\,2\times10^3$	0.287	201.189 3	409.347 3	416.431 25	−7.083 95	429.19
5×10^{12}	$0.212\,751\,1\times10^4$	0.181	1 049.031	2 109.111	2 151.766 9	−42.655	2 164.92
10^{13}	$0.425\,502\,2\times10^4$	0.15	2 115.95	4 245.234	4 323.205 5	−77.97	4 337.22
5×10^{13}	$0.212\,571\,1\times10^5$	0.104	10 678.75	21 376.72	21 928.05	−551.33	21 948.30
10^{14}	$0.425\,502\,2\times10^5$	0.086	21 402.58	42 828.41	45 396.85	−2568.44	45 404.33

$$H_a\psi_a(r,\theta)=-\left(\frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r}+\frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta}-\frac{m^2}{r^2\sin^2\theta}+\frac{2}{r}-\gamma m-\tfrac{1}{4}\gamma^2r^2\sin^2\theta\right)\psi_a(r,\theta)=E_a\psi_a(r,\theta)\,, \tag{1}$$

for $0\leqslant r<\infty$, $0\leqslant\theta<\pi$, with boundary conditions

$$\lim_{r\to0}r^2\frac{\partial\psi_a(r,\theta)}{\partial r}=0\,,\quad \lim_{\theta\to0\,\theta\to\pi}\frac{\partial\psi_a(r,\theta)}{\partial\theta}=0\,,\quad \lim_{r\to\infty}\psi_a(r,\theta)=0\,,$$

$$H_I\psi_I(\xi,\eta;R_{ab})=-\left[\frac{1}{2}\frac{4}{R_{ab}^2}\,\frac{1}{\xi^2-\eta^2}\left(\frac{\partial}{\partial\xi}(\xi^2-1)\frac{\partial}{\partial\xi}+\frac{\partial}{\partial\eta}(1-\eta^2)\frac{\partial}{\partial\eta}\right)+\frac{4}{R_{ab}}\,\frac{\xi}{\xi^2-\eta^2}-\frac{2}{R_{ab}^2}\,\frac{m^2}{(\xi^2-1)(1-\eta^2)}\right.$$
$$\left.-\gamma m-\frac{R_{ab}^2}{32}\gamma^2(1-\eta^2)(\xi^2-1)\right]\psi_I(\xi,\eta;R_{ab})=E_I(R_{ab})\psi_I(\xi,\eta;R_{ab})\,, \tag{2}$$

for $1\leqslant\xi<\infty$, $-1\leqslant\eta\leqslant1$, with boundary conditions

$$\lim_{\xi\to1+}(\xi^2-1)\frac{\partial\psi_I(\xi,\eta;R_{ab})}{\partial\xi}=0\,,$$

$$\lim_{\eta\to-1+1-}(1-\eta^2)\frac{\partial\psi_I(\xi,\eta;R_{ab})}{\partial\eta}=0\,,$$

$$\lim_{\xi\to\infty}\psi_I(\xi,\eta;R_{ab})=0\,.$$

These problems are solved by the finite-elements method,[5,6] which makes it possible to find eigenvalues for E_a, $E(R_{ab})$, and the eigenfunctions $\psi_a(r,\theta)$ and $\psi_I(\xi,\eta;R_{ab})$ to the given degree of exactness which in this paper amounts to 10^{-3}–10^{-4}. Having used the above-mentioned method, we present in Table I results of our calculations of the ground-state energy E_a of the atom and the molecular hydrogen ion $E_I(R_0)$ for certain values of the $0.425\leqslant\gamma\leqslant0.425\times10^5$ dimensionless parameter. These results correspond to $10^9\leqslant H\leqslant10^{14}$ G field strengths. {In point R_0 the total energy $W(R_{ab})=2[E_1(R_{ab})+R_{ab}^{-1}]$ of the hydrogen molecular ion is at a minimum.} In addition, Table I also presents values for the total energy $W_0=W(R_0)$ and energy of molecular hydrogen ion binding $E_B=W_0-E_a$, which is calculated in relation to the E_a energy of the hydrogen atom's ground state in a corresponding magnetic field.

In the case of $\gamma=0$, the problem of the bound states of H_2^+ is reduced to the problem of two Coulomb centers in quantum mechanics. This problem is solved to the high degree of exactness of $\sim10^{-12}$ (Ref. 4). Using the finite-elements method, the same problem is solved to an exactness of 10^{-4}–10^{-5} (Ref. 6). By way of comparison,

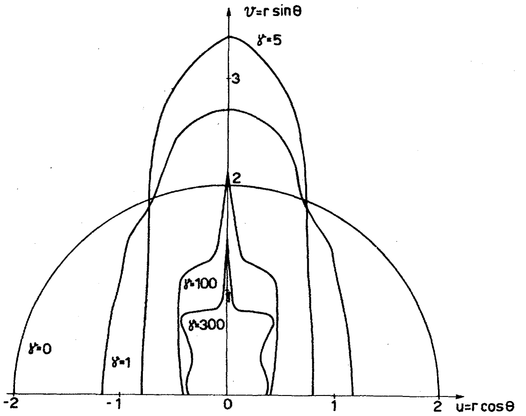

FIG. 1. Node lines of the wave function of the excited state of the hydrogen atom for different values of the $\gamma=\mu_BH/R_\infty$ parameter of the magnetic field, which for $\gamma=0$ goes into the node line of the $2S$ wave function of the isolated hydrogen atom.

TABLE II. The ground-state energy E_a (Ry) of the hydrogen atom in the magnetic field $H=\gamma R_\infty/\mu_B$.

γ	H. S. Brandi (Ref. 10)	D. Cabib (Ref. 2)	Dos Santos (Ref. 8)	R. K. Bhaduri (Ref. 3)	This work
0					−0.999 957
1	−0.523 86	−0.662 41	−0.633 08	−1	−0.662 28
2	0.091 90	−0.044 50	−0.027 59	−0.002 94	−0.044 43
3	0.809 11	0.670 87	0.684 02		0.671 19
4	1.579 8	1.438 4	1.450 2		1.438 72
5	2.384 2	2.239 2	2.251 0		2.239 6
20				15.683 83	15.592 7
100				92.74	92.522 3
300				289.868	290.362 2
1000				985.758	991.877 7

the last column in Table I presents energy E_{osc} values for the ground state of the anisotropic oscillator. As the intensity of the H field increases, the corresponding E_a values of the hydrogen atom's ground state gravitate toward these values. For example, then, for $H=10^{14}$ G, $E_{\text{osc}}-E_a\approx 7.5$ Ry, which represents $\approx 0.02\%$ of the corresponding value of the anisotropic oscillator energy. Let us note that up to the present time, all variational investigations of this problem of the molecular hydrogen ion in strong magnetic fields[3,7] give in the region $0<\gamma<5$, values for the binding energy E_B which are even 50% greater than the energy values given in this paper.

In Fig. 1, on the u, v plane, the node lines of wave functions of the excited state of the hydrogen atom are represented for various values of the parameter $\gamma=0$, 1, 5, 100, and 300. In the case of $\gamma=0$, this coincides with the node lines of the 2S state of the isolated hydrogen atom. With γ growth, node lines approach the v axis, and for all values of variables are symmetrical with respect to the direction of the field which has z-axis direction.

Using our method of calculation, Table II compares E_a values of the ground state of the hydrogen atom in a homogeneous magnetic field which changes in the interval $0<\gamma<1000$ with the results of other authors. In the whole $0<\gamma<1000$ region our findings coincide with the best variational calculations with an exactness of $\sim 10^{-4}$. Calculations are performed in several works[2,8,9] for the $0\leqslant\gamma\leqslant 5$ region but are only performed in one work[3] in the whole $0\leqslant\gamma\leqslant 1000$ region. For $\gamma>10^4$ values it is necessary to take relativistic effects into consideration.[10]

The algorithm[6] based on the finite-elements method[5] used in this paper makes it possible to solve, to the given degree of exactness, the problem of bound states of the H atom and the molecular ion H_2^+ of hydrogen in a homogeneous magnetic field and in a wide range of changes in the strength of the H magnetic field. It should be mentioned that in our approach it is neither necessary to introduce any kind of supplemental hypothesis, or, as is usually the case, to select special trial functions for different areas of H changes.[2,3,8,7,9] It is our opinion that this algorithm can also be very useful in solving other problems which are reduced to the direct solution of partial differential equations on a plane.

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