Hydrogen molecule in a strong magnetic field

A. V. Turbiner
Institute of Theoretical and Experimental Physics

(Submitted 10 October 1983)
Pis'ma Zh. Eksp. Teor. Fiz. **38**, No. 10, 510–514 (25 November 1983)

A quantitative study of the hydrogen molecule in an arbitrary constant magnetic field oriented along the axis of the molecule is performed for the first time. It is found that the molecule is stable in the entire range of fields studied (up to 10^{12} G). It is shown that at large distances, two ground-state hydrogen atoms repel each other in the presence of a field.

PACS numbers: 33.55. + c, 35.20.Gs

Giant magnetic fields (up to 10^{12}–10^{13} G) have recently been discovered on the surface of neutron stars.[1] It was already well known before that high fields 10^7–10^8 G exist on some white dwarfs (see, for example, Ref. 2). Under laboratory conditions, magnetic fields with high intensities effectively arise in semiconductors, where bound states of electrons with holes with small effective masses are present (see, for example, Refs. 2 and 3). All of this has given rise to the recently increased interest in the behavior of matter in strong magnetic fields. The problem was examined qualitatively in Ref. 4, where interesting physical phenomena were predicted. From the quantitative point of view, only hydrogen atoms have been reliably examined, although several attempts were made to study the H_2^+ ion.

In this paper we present the first quantitative calculation of a hydrogen molecule in a magnetic field of arbitrary intensity. The analysis was performed in the Born-Oppenheimer approximation and was restricted to the study of the state $^1\Sigma_g^+$ when the field is oriented along the axis of the molecule. The approach is based on using the "nonlinearization" procedure,[5] which permits examining the hydrogen atom, the molecular ion H_2^+ molecule in a unified manner. In addition, we shall show that at large distances atoms in the ground state repel each other.

The Hamiltonian describing the H_2 molecule in a constant magnetic field **B**, oriented along the axis of the molecule (z axis), has the following form in the Born-Oppenheimer approximation (the notation is explained in Fig. 1)

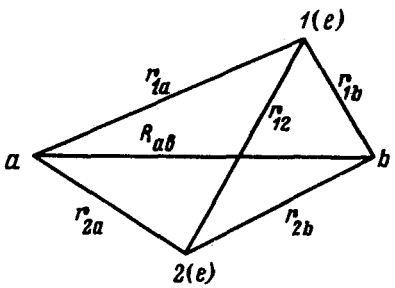

FIG. 1.

$$\mathcal{H}_{H_2} = -\frac{2}{r_{1a}} - \frac{2}{r_{1b}} - \frac{2}{r_{2a}} - \frac{2}{r_{2b}} + \frac{2}{r_{12}} + \frac{B^2}{4}(\rho_1^2 + \rho_2^2), \tag{1}$$

where $\rho_i^2 = x_i^2 + y_i^2$; the field B and the energy E are measured in atomic units $B_0 = 2.3505 \times 10^9$ G, $E_0 = \text{Ry} = 13.6$ eV). Equation (1) shows that we are examining the state $^1\Sigma_g^+$ and that the projections of the angular momenta on the z axis vanish. One of the simplest wave functions in a zeroth-order approximation, which is reasonable from the point of view of "Dyson's argument" (Ref. 6) (in application to quantum mechanics, see the discussion in Ref. 5), can be written in the following way:

$$\psi_0 = \exp\{-\alpha(r_{1a} + r_{1b} + r_{2a} + r_{2b}) + \beta r_{12} - \frac{B}{4}(\rho_1^2 + \rho_2^2)\}. \tag{2}$$

The potential corresponding to it $V_0 - E_0 = \Delta\psi_0/\psi_0$ is

$$V_0 = [-2\alpha(\frac{1}{r_{1a}} + \frac{1}{r_{1b}} + \frac{1}{r_{2a}} + \frac{1}{r_{2b}}) + \frac{4\beta}{r_{12}} + \frac{B^2}{4}(\rho_1^2 + \rho_2^2)] + 2\alpha^2(\mathbf{n}_{1a}\mathbf{n}_{1b} + \mathbf{n}_{2a}\mathbf{n}_{2b})$$
$$- 2\alpha\beta[(\mathbf{n}_{1a} + \mathbf{n}_{1b})\mathbf{n}_{12} + (\mathbf{n}_{2a} + \mathbf{n}_{2b})\mathbf{n}_{21}] + \alpha B[\rho_1^2(\frac{1}{r_{1a}} + \frac{1}{r_{1b}}) + \rho_2^2(\frac{1}{r_{2a}} + \frac{1}{r_{2b}})]$$
$$- \beta B\frac{(\vec{\rho}_1 - \vec{\rho}_2)^2}{r_{12}}; \quad E_0 = -4\alpha^2 - 2\beta + 2B - \frac{2}{R_{ab}}. \tag{3}$$

The potential (3) contains many characteristic properties of the starting potential (1): for $\alpha = 1, \beta = 1/2$ it exactly reproduces the Coulomb poles, it has the correct asymptotic properties at large distances, and it has the correct symmetry properties relative to the exchange $1 \leftrightarrow 2, a \leftrightarrow b$. For this reason, we can hope that the perturbation theory with respect to the potential difference $V_1 = (V - V_0)$ will converge (see the discussion in Ref. 5). We shall limit ourselves in the perturbation series for the energy to a calculation of the first correction, which is equivalent to performing a variational calculation with the trial wave function (2). To increase the accuracy, we shall assume that the parameters α and β are free parameters and we shall perform the minimization with respect to them.

The wave function of the ground state of the hydrogen atom in a magnetic field[7]

$$\psi_0 = \exp(-\alpha r - \frac{B}{4}\rho^2) \tag{4}$$

and of the molecular ion H_2^+

$$\psi_0 = \exp\left(-\alpha(r_{1a} + r_{1b}) - \frac{B}{4}\rho_1^2\right) \tag{5}$$

can be written on the basis of analogous considerations and a variational calculation minimizing with respect to the parameter α can be performed.

The results of the calculations with different fields are presented in Table I. We note immediately that for large fields, the simplest trial functions (4) and (5), which contain a single free parameter, lead to accuracies of the order of several percent, while with high fields $\gtrsim 10^{11}$ G, they give essentially the best energy values. We emphasize the fact that a single function describes the region of low as well as high fields. This is a great advantage. The results concerning the hydrogen molecule can be compared only

TABLE I. Results of calculations of the energy and internuclear distance for the hydrogen atom, ion, and molecule.

B G	Atom	H_2^+ Ion		H_2^2 Molecule	
		R_{ab}	E	R_{ab}	E
0	−1	1.998	− 1.205	1.401 (1.4008)	− 2.2925 (− 2.3488)
10^9	− 0.904 (− 0.921)	1.907 (1.9)	− 1.146 (− 1.150)	1.337	− 2.1644
$5 \cdot 10^9$	0.125 (0.049)	1.489 (1.7)	− 0.331 (− 0.339)	1.203	− 0.3622
10^{10}	1.775 (1.640)	1.272 (1.2)	1.173 (1.093)	0.859	2.6651
$5 \cdot 10^{10}$	17.047 (16.754)	0.745 0.8	15.667 (15.505)	0.528	32.1192
10^{11}	37.136 (36.848)	0.607 (0.6)	35.338 (35.674)	0.463	71.520
$5 \cdot 10^{11}$	202.636 (203.543)	0.366 (0.354)	199.83 (199.56)	0.400	399.116
10^{12}	411.945 (416.431)	0.309 (0.287)	408.92 (409.35)	0.263	814.463

1) For the atom and the ion, the numbers in the parentheses correspond to the calculation performed in Ref. 8. For the molecule, they correspond to the experimental value (see, for example, Ref. 9). For the H_2^+ ion, a slightly more complicated approximation than (5) was used.

with calculations at $B = 0$ (see, for example, the table of different calculations in Ref. 9). We can see a difference from the experimental value at a level of 0.05 Ry and the wave function (2) is one of the best two-parameter functions, which has not been used previously. The sharp decrease in the internuclear distance with increasing magnitude of the magnetic field deserves special attention. I do not know of a simple physical explanation for this phenomenon, although when the field is perpendicular to the axis of the molecule, the trivial explanation is connected with the decrease in the transverse size of the electron cloud. We note that both the ionization energy and the energy of dissociation of the molecule into atoms[1)] increase monotonically with increasing field. There is a disagreement with the qualiltative analysis performed in Ref. 4: for fields 10^{11}–10^{12} G, the binding energy of the atom is approximately 2.7 times lower than that

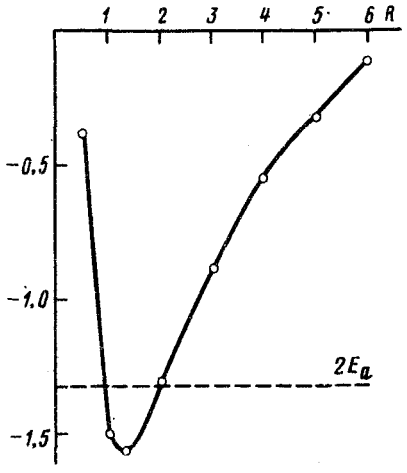

FIG. 2. Dependence of the energy of an H_2 molecule on the internuclear distance R_{ab}.

of the molecule, rather than four times lower as predicted in Ref. 4. This could be related to the delayed onset of the asymptotic regime.

The last problem, which we would like to discuss, is the interaction of atoms at large distances in the presence of a field. It is well known that atoms in S states at large distances are attracted according to the law $E(R) \sim -1/R^6$ (for example, Ref. 10) due to the dipole-dipole interaction of the induced dipoles. In the presence of a magnetic field, a second interaction mechanism arises. The point is that an atom in a magnetic field acquires a quadrupole moment proportional to $\mathscr{H}^2$.[4] For this reason, there is a quadrupole-quadrupole interaction in first-order perturbation theory, in addition to the dipole-dipole interaction in second-order perturbation theory. It is easy to show that the last mechanism dominates at large distances and that the interaction energy (when the field is parallel to the axis of the molecule) is given by

$$E(R) = \frac{3}{2}\frac{D^2}{R^5}. \tag{6}$$

This equation is valid for any angle between the field and the axis of the molecule. Only its coefficient changes the maximum value of the coefficient is 3/2, while its minimum value is 9/16 (when the field is perpendicular to the axis). Thus when the atoms are separated, repulsion at some point replaces attraction and the molecules dissociate into atoms. This qualitative analysis is illustrated by the quantitative calculation (see Fig. 2) performed in a field $B = 2.3505 \times 10^9$ G.

In conclusion, I want to thank K. G. Boreskov, B. B. Kadomtsev, V. S. Karakhtanov, and K. A. Ter-Martirosyan for their interest in the work and for useful discussions.

[1)]This phenomenon is important in the analysis of a plasma in strong fields.

[1]J. Trumper, W. Pietsch, C. Reppin *et al.*, Ann. New York Acad. Science **302**, 538 (1977).
[2]R. H. Garstang, Rept. Prog. Phys. **40**, 105 (1977).

[3]D. Cabib, E. Fabrio, and G. Fiorio, Nuovo Cim. **B10**, 185 (1972).
[4]B. B. Kadomtsev and V. S. Kudryavtsev, Pis'ma Zh. Eksp. Teor. Fiz. **13**, 15 (1971) [JETP Lett. **13**, 9 (1971)]; *ibid.* **13**, 9 (1971) [*ibid.* **13**, 42 (1971)].
[5]A. V. Turbiner, Zh. Eksp. Teor. Fiz. **79**, 1719 (1980) [Sov. Phys. JETP **52**, 868 (1980)]; J. Phys. **A14**, 164 (1981).
[6]F. Dyson, Phys. Rev. **85**, 631 (1952).
[7]A. V. Turbiner, Preprint ITEP-79, 1982; J. Phys. A (in print).
[8]M. S. Kaschiev, S. I. Vinitsky, and F. Vukajlovic, Phys. Rev. **A22**, 55 (1980).
[9]A. D. McLean, A. Weiss, and M. Yoshimine, Rev. Mod. Phys. **32**, 211 (1960).
[10]L. D. Landau and E. M. Lifshitz, Kvantovaya mekhanika (Quantum Mechanics), Nauka, Moscow, 1974.

Translated by M. Alferieff
Edited by S. J. Amoretty