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Ion H_2^+ can dissociate in a strong magnetic field

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In framework of a variational method the molecular ion H_2^+ in a magnetic field is studied. An optimal form of the vector potential corresponding to a given magnetic field (gauge fixing) is chosen variationally. It is shown that for any magnetic field strength as well as for any orientation of the molecular axis the system (ppe) possesses a minimum in the potential energy. The stable configuration always corresponds to elongation along the magnetic line. However, for magnetic fields $B \gtrsim 5 \cdot 10^{11}$ G and some orientations the ion H_2^+ becomes unstable decaying to H-atom + p.

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Ion H_2^+ is the simplest one-electron molecular system, which is more stable than hydrogen atom. It appears to be one of the most studied problems in non-relativistic quantum mechanics. In particular, the wealth of physical phenomena displayed by this system when placed into a magnetic field becomes of a great importance in astrophysics, solid state and plasma physics. For instance, as the magnetic field grows the system becomes more and more strongly bound and compact. Such a behavior leads naturally to a guess that in spite of the huge temperatures on neutron star surfaces their atmosphere can still contain molecular objects [1, 2]. On the other hand, a shrinking of the equilibrium distance between protons with the growth of magnetic field, increases drastically the probability of nuclear fusion [3]. It is quite surprising that such a shrinking is also accompanied by a change from ionic to covalent character at $\sim 5 \cdot 10^{11}$ G [4] (see also [5]). The goal of this Letter is two-fold. Firstly, to show that the system (ppe) has always a minimum and correspondingly the molecular ion H_2^+ can exist for magnetic fields $\lesssim 4.414 \cdot 10^{13}$ G. Secondly, to demonstrate that for $B \gtrsim 5 \cdot 10^{11}$ G and for some orientations of the molecular axis the ion becomes unstable dissociating to H-atom + p. The variational method is used to study this problem.

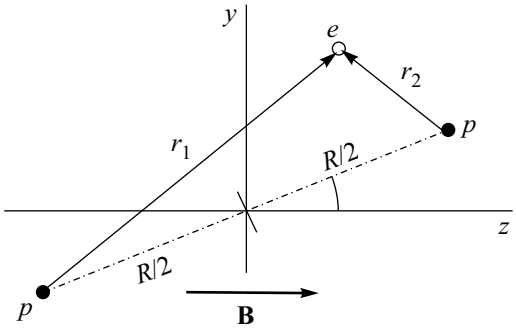

Fig.1. Geometrical setting for the H_2^+ ion in a magnetic field directed along the z-axis

The Hamiltonian which describes the H_2^+ molecular ion placed in a uniform constant magnetic field directed along the z-axis, $\mathcal{B} = (0, 0, B)$ (see, for example, [6]) is given by

$$\mathcal{H} = \hat{p}^2 + \frac{2}{R} - \frac{2}{r_1} - \frac{2}{r_2} + (\hat{p}\mathcal{A}) + \mathcal{A}^2, \qquad (1)$$

(see Fig.1), where $\hat{p} = -i\nabla$ is the momentum. $\mathcal{A}$ is a vector potential, which corresponds to the magnetic field $\mathcal{B}$.

The vector potential for given magnetic field is defined ambiguously, up to a gauge factor. Thus, the Hamiltonian is gauge-dependent but not the observables. Since we are going to use an approximate method for solving (1) our energies can be gauge-dependent (only the exact ones would be gauge-independent). Hence one can choose the form of the vector potential in an optimal

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way. Let us consider a certain one-parameter family of vector potentials corresponding to the constant magnetic field B (see for example [4])

$$\mathcal{A} = B(-(1-\xi)y, \xi x, 0), \tag{2}$$

where ξ is the parameter to be fixed in a certain optimal way. If $\xi = 1/2$ we get a gauge called symmetric or circular, while $\xi = 0$ corresponds to an asymmetric gauge (see [6]). By substituting (2) into (1) we arrive at the Hamiltonian

$$\mathcal{H} = -\nabla^2 + \frac{2}{R} - \frac{2}{r_1} - \frac{2}{r_2} + iB[-(1-\xi)y\partial_x + \xi x\partial_y] +$$

$$+B^2[\xi^2 x^2 + (1-\xi)^2 y^2]. \tag{3}$$

The idea of choosing an optimal gauge has widely been exploited in quantum field theoretical considerations. It has also been discussed in connection with the problem at hand (see for instance [7] and references therein). Perhaps, the first constructive (and remarkable) attempt to apply this idea was made by Larsen [4]. In his study of the ground state it was explicitly shown that gauge dependence of energy can be quite significant and even an oversimplified optimization procedure improves the numerical results.

Our aim is to study the ground state of (3). It is not difficult to see that there exists a certain gauge for which Hamiltonian (3) has a real ground state eigenfunction. This gauge will be here sought after and correspondingly deal with *real* trial functions in our variational calculations. In this case one can prove that the expectation value of the term $\sim B$ in (3) vanishes when it is taken over any real normalizable function. So, without loss of generality we can omit this term in the Hamiltonian. Finally, the recipe of our variational study can be formulated as follows: *Construct an adequate variational real trial function [8], which reproduces the original potential near Coulomb singularities and at large distances, where ξ should be included as a parameter. Perform a minimization of the energy functional by treating the trial function's free parameters and ξ on the same footing.* In particular, such an approach enables one to eventually find the *optimal* form of the Hamiltonian. The above recipe was successfully applied in a previous study of H_2^+ in magnetic field [5] and led to predict the existence of the exotic ion H_3^{++} at $B \gtrsim 10^{11}$ G [9].

One of the simplest trial functions satisfying the above-mentioned criterion is

$$\Psi_1 = \exp\{-\alpha_1(r_1 + r_2) - B[\beta_{1x}\xi x^2 + \beta_{1y}(1-\xi)y^2]\}, \tag{4}$$

(cf. [5]), where $\alpha_1, \beta_{1x,1y}$ are variational parameters. We here assume that $\xi \in [0,1]$ which is a restriction that will later be justified. Actually, this is a Heitler-London function multiplied by the lowest Landau orbital associated with the gauge (2). Presumably this function describes internuclear distances near the equilibrium and a covalent character. Another possible trial function is

$$\Psi_2 = \Big(\exp(-\alpha_2 r_1) + \exp(-\alpha_2 r_2)\Big) \times$$

$$\times \exp\{-B[\beta_{2x}\xi x^2 + \beta_{2y}(1-\xi)y^2]\}, \tag{5}$$

(cf. [5]), where $\alpha_2, \beta_{2x,2y}$ are variational parameters. This is a Hund-Mulliken function multiplied by the lowest Landau orbital. One can assume that for a sufficiently large internuclear distance R this function dominates, thus giving an essential contribution in this regime. Hence, it describes an interaction of a hydrogen atom and a proton (charged center), and can also describe a possible decay mode of H_2^+ onto them. There are two natural ways–linear and non-linear – to incorporate the behavior of the system both near equilibrium and at long distances in a single trial function. The non-linear interpolation is of the form

$$\Psi_{3-1} = \Big(\exp\{-\alpha_3 r_1 - \alpha_4 r_2\} + \exp\{-\alpha_3 r_2 - \alpha_4 r_1\}\Big) \times$$

$$\times \exp\{-B[\beta_{3x}\xi x^2 + \beta_{3y}(1-\xi)y^2]\} \tag{6}$$

(cf. [5]) where $\alpha_{3,4}, \beta_{3x,3y}$ are variational parameters. This is a Guillemin – Zener function multiplied by the

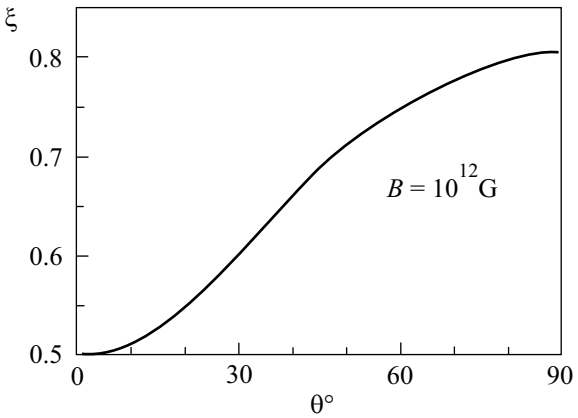

Fig.2. Gauge parameter as a function of the inclination angle for H_2^+. The magnetic field $B = 10^{12}$G was taken as an example. This dependence is found in the present study

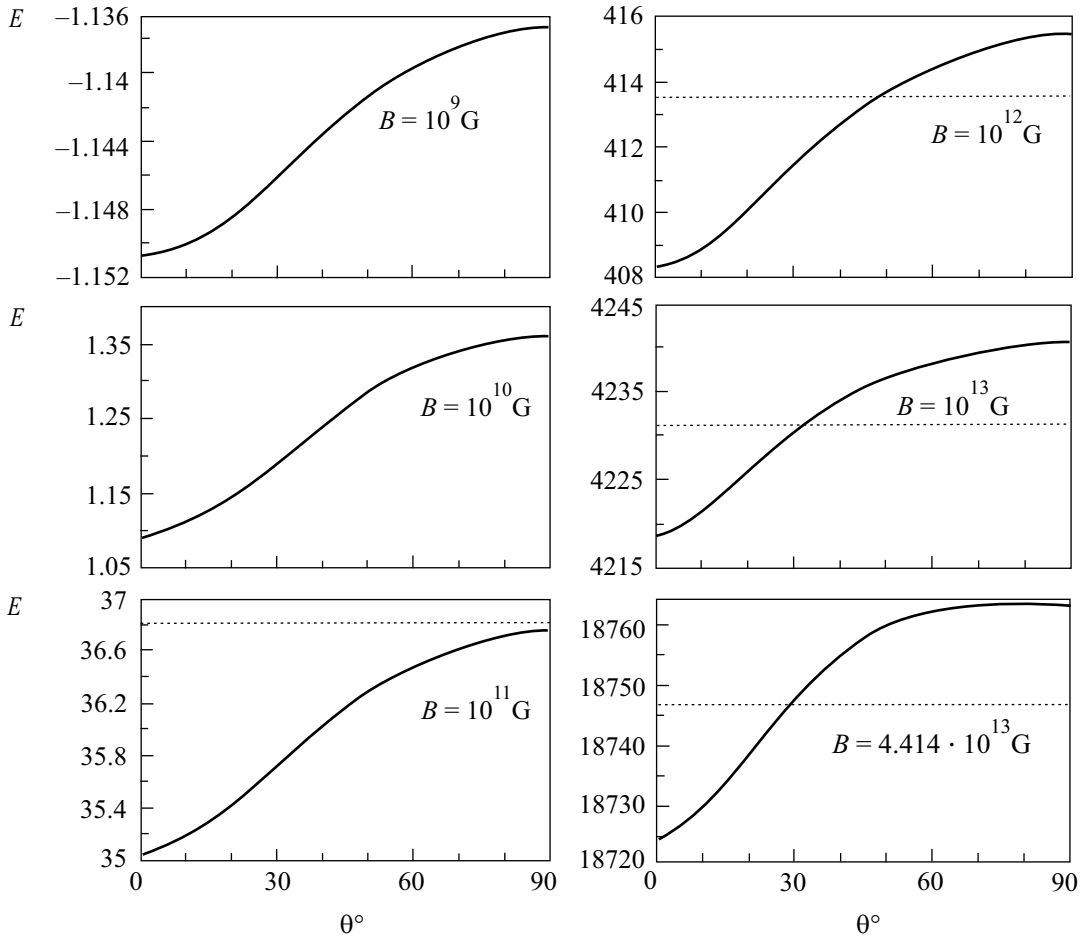

Fig.3. Total energy of the H_2^+ ion as a function of the inclination angle. The horizontal lines refer to the H ground state energy taken from Lai et al. [11]

lowest Landau orbital. The linear superposition is given by

$$\Psi_{3-2} = A_1\Psi_1 + A_2\Psi_2, \qquad (7)$$

where one of the parameters $A_{1,2}$ is kept fixed. The final form of the trial function is a linear superposition of functions (6) and (7)

$$\Psi_{trial} = A_1\Psi_1 + A_2\Psi_2 + A_{3-1}\Psi_{3-1}, \qquad (8)$$

where only two out of the three parameters A's are variationally treated. The total number of variational parameters in (8) is fourteen when ξ is included.

It is easy to prove a general statement that if a system possesses axial rotational symmetry (in our case it appears if the molecular axis coincides with the magnetic line, $\theta = 0^o$, see Fig.1), the optimal gauge corresponds to $\xi = 1/2$ (symmetric or circular gauge). It is precisely the gauge which was used in most of previously performed H_2^+-studies. However, this is not the case if $\theta \neq 0^o$. As an example one can see in Fig.2 the behavior of ξ as a function of θ at $B = 10^{12}$ G. It is typical behavior for all studied magnetic fields both weak and strong, up to the non-relativistic limit, $B = 4.414 \cdot 10^{13}$ G. It justifies our above assumption with regard to the domain of gauge parameter, $\xi \in [0, 1]$.

We carried out extensive studies of the ground state $1\sigma_g$ of H_2^+ for magnetic fields $B = 0 - 4.414 \cdot 10^{13}$ G and orientations ranging from 0^o (parallel configuration) to 90° (perpendicular configuration). They turned out to be more accurate than any available results yet obtained except for a domain of small magnetic fields for the perpendicular configuration, where the results by Wille [10] appear to be slightly better[4)]. The detailed numerical analysis and comparison with available calculations will be published elsewhere.

[4)]These results were obtained using a basis set expansion including up to approximately 500 terms depending on the value of magnetic field.

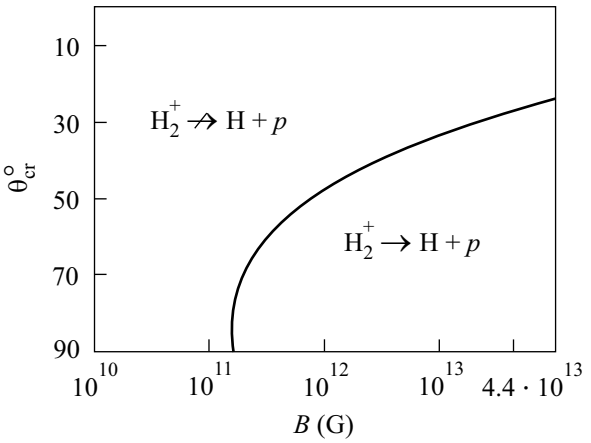

Fig.4. Critical angle for dissociation of H_2^+

As previously obtained by other authors [3, 10, 4] we confirm quantitatively a natural expectation that the parallel configuration is the most stable for all magnetic fields $B \lesssim 4.414 \cdot 10^{13}$ G, where non-relativisitic considerations are valid. The total energy of the molecular ion H_2^+ as a function of angle θ for different magnetic fields, is shown in Fig.3. For any magnetic field in the region $B = 0 - 4.414 \cdot 10^{13}$ G and any orientation a well-pronounced minimum in the total energy is attained at finite internuclear distances. This is in contradiction with a statement by Khersonsky [3] about the non-existence of a minimum for some values of the magnetic field and orientation. Perhaps, it it worth to emphasize that in that article the variational study was carried out using a trial function which is almost coincident with that of eq.(5). We can thus presume that the above statement is an artifact arising from insufficient accuracy of calculations. The horizontal line in Fig.3 presents the hydrogen atom total energy in the magnetic field (see [11]). For magnetic fields $B > 1.8 \cdot 10^{11}\, G$ the total energy of the atom becomes lower than that of H_2^+ for angles larger than some critical angle, θ_{cr}. It points to the possible dissociation channel $H_2^+ \to$ H-atom $+ p$. The dependence of the critical angle θ_{cr} on the magnetic field is shown in Fig. 4. It is quite striking that dissociation occurs for a wider and wider range of orientations as the magnetic field grows reaching $25^\circ \lesssim \theta \leqslant 90^\circ$ for $B = 4.414 \cdot 10^{13}$ G.

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