

$H_3^{(2+)}$ molecular ion in a strong magnetic field: a triangular configuration

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The bound state in the system of three protons and an electron (*pppe*) under a homogeneous strong magnetic field where the protons are situated at the vertices of an equilateral triangle perpendicular to the magnetic field lines is found. It is shown that for magnetic fields $B = 10^{11} - 4.414 \times 10^{13}$ G the potential energy curves as a function of the internuclear distance R have an explicit minimum. For all magnetic fields studied, the binding energy of the triangular configuration is less than the binding energy of the linear parallel configuration [A. Turbinder *et al. JETP Lett.* **69** (1999) 844]. As opposed to the linear case, the binding energy decreases with increasing magnetic field, while the equilibrium internuclear distance slowly increases.

Keywords: Strong magnetic field; molecules; exotic systems

En este trabajo se encontró el estado ligado en el sistema de tres protones y un electrón (*pppe*) bajo un campo magnético homogéneo intenso en donde los protones están situados en los vértices de un triángulo equilátero perpendicular a las líneas del campo magnético. Se demuestra que para campos magnéticos $B = 10^{11} - 4.414 \times 10^{13}$ G las curvas de energía potencial como función de la distancia internuclear R tienen un mínimo explícito. Para todos los campos magnéticos estudiados, la energía de amarre de la configuración triangular es menor que la energía de amarre de la configuración lineal paralela [A. Turbinder *et al. JETP Lett.* **69** (1999) 844]. Al contrario del caso lineal, la energía de amarre decrece con un aumento del campo magnético, mientras que la distancia de equilibrio internuclear decrece lentamente.

Descriptores: Campos magnéticos intensos; moléculas; sistemas exóticos

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1. Introduction

Recently a quantitative study of the system of three protons and an electron (*pppe*) in a strong magnetic field gave theoretical evidence of the existence of a bound state for magnetic fields $B > 10^{11}$ G [1]. The existence of such a state implies the existence of the exotic molecular ion $H_3^{(2+)}$. Many years ago Kadomtsev and Kudryavtsev [3], and Ruderman [4] pointed out the possible existence of linear exotic molecular systems in the presence of a strong magnetic field. Due to the enormous Lorentz force acting on the electronic cloud, it shrinks in the direction transverse to the magnetic field lines, leading to an effective quasi-one-dimensionality of the systems studied. This makes the electron-nuclei attraction more effective in compensating for the Coulombic repulsion of the nuclei. Such a fact suggests the possibility of the existence of exotic systems which do not exist without a magnetic field. It was shown some time ago that a strong magnetic field can lead to the formation of linear hydrogenic chains H_n , $n > 2$ situated along magnetic field lines [4–7]. More recently the first quantitative study of the possible existence of an exotic bound state in the system of three protons and an electron (*pppe*) in a strong magnetic field was carried out [1] and it confirmed existence of the $H_3^{(2+)}$ ion.

Although the linear parallel configuration (where protons are situated on a line parallel to the magnetic field line) for the system (*pppe*) seems to be optimal for very strong magnetic

fields, other possible configurations have to be considered in order to have a better understanding of the properties of such systems.

In this article we explore the possibility of the existence^(a) of the molecular ion $H_3^{(2+)}$ where the protons are situated at the vertices of an equilateral triangle perpendicular to a homogeneous magnetic field. Our present investigation is limited to magnetic fields $B = 10^{11} - 4.414 \times 10^{13}$ G for which a non-relativistic approach seems to be valid (for a general discussion of effects of relativistic corrections of molecular type systems in a strong magnetic field see Ref. 7). An attempt to make a detailed relativistic study of the hydrogen atom was carried out by Goldman *et al.* (see for example Ref. 8 and references therein). Our study is restricted to the ground state in the Born-Oppenheimer approximation.

2. Method

The present calculations are carried out in the framework of a variational method. Trial functions are chosen in accordance with the following criterion (see Refs. 10–15): (i) the trial function $\Psi_t(x)$ should include all symmetry properties of the problem in hand; (ii) the trial function for the ground state should not vanish inside the domain where the problem is defined; (iii) the potential $V_t(x) = \nabla^2 \Psi_t / \Psi_t$, for which the trial function is an exact eigenfunction, should reproduce the original potential behavior near singularities as well as its

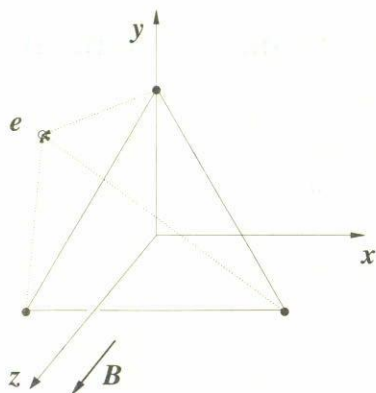


FIGURE 1. Triangular configuration for the $(pppe)$ system in a magnetic field \vec{B} directed along the z axis. The protons are situated in the (x, y) -plane and their positions are marked by black circles.

asymptotic behavior. This prescription has been successfully applied to the study of the H_2^+ ion in strong magnetic fields, giving the most accurate results for $B > 0$ [9], as well as to the study of the linear parallel configuration of the $H_3^{(2+)}$ and $H_4^{(3+)}$ ions in a strong magnetic field [1, 2].

We consider a system of one electron and three identical infinitely-heavy centers of unit charge situated at the vertices of an equilateral triangle with internuclear distance R (which is the length of the side of the triangle) lying in a plane perpendicular to the magnetic field of strength B directed along the z axis, $\vec{B} = (0, 0, B)$.

The potential corresponding to the system we study is given by

$$V = \frac{6}{R} - \frac{2}{r_1} - \frac{2}{r_2} - \frac{2}{r_3} + \frac{B^2 \rho^2}{4} + B \hat{\ell}_z, \quad (1)$$

where the quantity $\rho = \sqrt{x^2 + y^2}$ is the distance from the

electron position to the z -axis, $r_{1,2,3}$ are the distances from the electron to the first, second and third centers, respectively, R is the distance between centers (see Fig. 1 for notation) and $\hat{\ell}_z$ is the z -component of the angular momentum operator. The linear Zeeman effect term in the potential ($B \hat{\ell}_z$) can be dropped since we use real trial functions^(b) (see below). Spin Zeeman effects are neglected. Through the paper the Rydberg is used as the energy unit. For the other quantities standard atomic units are used.

3. Trial wave functions

The trial functions we are going to use for the present problem are similar to those that were exploited in Ref. 1 for the study of the linear parallel configuration. These functions were constructed according to the criterion described in Refs. 10–15. They contain the basic features of Coulomb systems in a magnetic field, as well as the symmetry property under permutation of the three charged centers. In particular, this implies that the potentials corresponding to those functions reproduce Coulomb-like behavior near the centers and two-dimensional oscillator behavior in the (x, y) plane at large distances (see below).

The simplest of these functions is a function of the Heitler-London type multiplied by the lowest Landau orbital:

$$\Psi_1 = e^{-\alpha_1(r_1+r_2+r_3)-\beta_1 B \rho^2/4}, \quad (2)$$

[cf. Eq. (2) in Ref. 1], where α_1 and β_1 are variational parameters. Since we consider the distance between centers as an extra variational parameter, the function has a total of three variational parameters. This function gives an adequate description of the covalent coupling of the system near equilibrium. As an illustration we show the potential corresponding to this function:

$$V_1 = \frac{\nabla^2 \Psi_1}{\Psi_1} = 3\alpha_1^2 - \beta_1 B - 2\alpha_1 \sum_{i=1}^3 \frac{1}{r_i} + 2\alpha_1^2 \sum_{i<j} (\hat{n}_i \cdot \hat{n}_j) + \alpha_1 \beta_1 B \sum_{i=1}^3 \frac{\rho^2 - (xx_i + yy_i)}{r_i} + \frac{\beta_1^2 B^2 \rho^2}{4}, \quad (3)$$

$$\hat{n}_i \cdot \hat{n}_j = \frac{1}{r_i r_j} [(x - x_i)(x - x_j) + (y - y_i)(y - y_j) + (z - z_i)(z - z_j)],$$

where \hat{n}_i ($i = 1, 2, 3$) is the unit vector in the direction of the vector pointing from the position of the i -th center to the position of the electron.

A second trial function is a Hund-Mulliken type function multiplied by the lowest Landau orbital:

$$\Psi_2 = (e^{-\alpha_2 r_1} + e^{-\alpha_2 r_2} + e^{-\alpha_2 r_3}) e^{-\beta_2 B \rho^2/4}, \quad (4)$$

[cf. Eq. (4) in Ref. 1]. Here α_2 and β_2 are variational parameters. This function describes an ionic coupling of a hydrogen atom with two charged centers.

Another suitable trial function which describes an ionic coupling between an H_2^+ ion and a proton is given by

$$\Psi_3 = [e^{-\alpha_3(r_1+r_2)} + e^{-\alpha_3(r_1+r_3)} + e^{-\alpha_3(r_2+r_3)}] e^{-\beta_3 B \rho^2/4}, \quad (5)$$

[cf. Eq. (5) in Ref. 1] where α_3 and β_3 are variational parameters. Since the H_2^+ ion has the lowest total energy among the one-electron systems for $B \lesssim 10^{13}$ G [2], an important contribution coming from this trial function is expected.

In order to include in a single trial function the different physical behavior near equilibrium and at large distances, appropriate interpolations of the trial functions (2), (4) and (5) are done:

- i) A natural interpolation is given by a non-linear superposition of the form:

$$\Psi_{4-nls} = \left[\sum_{\{\alpha_4, \alpha_5, \alpha_6\}} e^{-\alpha_4 r_1 - \alpha_5 r_2 - \alpha_6 r_3} \right] e^{-\beta_4 B \rho^2 / 4}, \quad (6)$$

[cf. Eq. (6) in Ref. 1] where $\alpha_4, \alpha_5, \alpha_6$ and β_4 are variational parameters, and the sum is over all permutations of the parameters $\{\alpha_4, \alpha_5, \alpha_6\}$.

If all parameters coincide ($\alpha_4 = \alpha_5 = \alpha_6 = \alpha_1$), the function (6) reduces to the Heitler-London type function (2). Function (6) also reduces to the Hund-Mulliken type wave function (4) when only one parameter is non-zero say $\alpha_4 = \alpha_2$ and $\alpha_5 = \alpha_6 = 0$. If two parameters are non-zero, and equal, say, $\alpha_4 = \alpha_5 = \alpha_3$, and $\alpha_6 = 0$ it reduces to the trial function (5). When all parameters are different among themselves and different from zero, the function (6) provides us with a 3-center modification of a Guillemin-Zener type function. The function (6) has in total five variational parameters (including the internuclear distance R as one of the parameters).

- ii) Another more immediate interpolation is given by a linear superposition of the functions (2), (4) and (5):

$$\Psi_{5-ls} = A_1 \Psi_1 + A_2 \Psi_2 + A_3 \Psi_3, \quad (7)$$

where A_1, A_2, A_3 are taken as extra variational parameters. Since $\Psi_{1,2,3}$ are not orthogonal, the parameters $A_{1,2,3}$ do not have the usual meaning of weight factors.

For the present calculations we use a linear superposition of the above interpolations (6), (7) given by

$$\Psi_6 = A_1 \Psi_1 + A_2 \Psi_2 + A_3 \Psi_3 + A_4 \Psi_{4-nls}, \quad (8)$$

where A_1, A_2, A_3, A_4 are again considered as extra variational parameters with no meaning of weight factors. The function (8) combines in a single functional form a suitable description of the system for the different physical regimes (near equilibrium and large internuclear distances for strong and very strong magnetic fields). Therefore, we feel that it should provide a relevant approximation for the ground state of the system. This was indeed the case for the linear parallel configuration of H₃⁽²⁺⁾ (see Ref. 1). This function has in total fourteen variational parameters.

The variational procedure is carried out using the standard minimization package MINUIT from CERN-LIB. We use the integration routine D01FCF from NAG-LIB. All integrals are calculated with relative accuracy $> 10^{-8}$.

TABLE I. Variational results for the triangular configuration of the H₃⁽²⁺⁾ ion in a strong magnetic field. The total energy E_T and the binding energy $E_b = B - E_T$, are in Ry. The equilibrium internuclear distance R_{eq} and the expectation values of the longitudinal and transversal localization length of the electron $\langle |z| \rangle$ and $\langle |\rho| \rangle$ are in a.u.. The corresponding quantities for the H₃⁽²⁺⁾ ion in the linear parallel configuration were taken from Ref. 1. The energy of a free electron and its cyclotron radius $B^{-1/2}$ are also shown.

B (Gauss)	E_T	E_b	R_{eq}	$\langle z \rangle$	$\langle \rho \rangle$
Triangular Configuration					
10 ¹¹	40.5591	1.985	0.6237	0.561	0.192
10 ¹²	423.722	1.719	0.6414	0.595	0.061
10 ¹³	4252.724	1.690	0.6645	0.610	0.019
4.414 × 10 ¹³	18777.31	1.674	0.6757	0.622	0.009
Linear Configuration					
10 ¹¹	36.429	6.1151	0.803	0.864	0.186
10 ¹²	410.296	15.144	0.346	0.438	0.060
10 ¹³	4220.09	34.324	0.165	0.242	0.019
4.414 × 10 ¹³	18723.88	55.103	0.110	0.168	0.009
Free electron					
10 ¹¹	42.5441				0.153
10 ¹²	425.441				0.048
10 ¹³	4254.41				0.015
4.414 × 10 ¹³	18778.98				0.007

4. Results

The results of our calculations are presented in Table I. For all magnetic fields considered ($B = 10^{11} - 4.414 \times 10^{13}$ G) we found a minimum in the potential energy curve as a function of the internuclear distance R (see Fig. 2) indicating the formation of a bound state. For such magnetic fields the total energy of the triangular configuration is always larger than the total energy of the corresponding linear parallel configuration. Indeed this shows that for very strong magnetic fields the linear configuration is the most favored. However, a new, striking unexpected phenomenon appears when one considers a triangular configuration. While for the linear configuration the binding energy^(c) increases and the internuclear distance decreases as the magnetic field grows, the opposite is true for the triangular configuration. Namely, the binding energy slowly decreases and the internuclear distance slowly increases (!), both being almost constant. Similar behavior occurs with the longitudinal localization length of the electron $\langle |z| \rangle$ which also slowly increases in the triangular configuration with magnetic field increase, opposite to what happens in the linear configuration where it decreases rather sharply. The transverse size of the electronic cloud $\langle \rho \rangle$ is very close to the corresponding cyclotron radius $B^{-1/2}$ (a.u.) for both cases. We do not have a clear physical picture of this phenomenon and it needs further consideration.

TABLE II. Comparison of the total energy E_T for the triangular configuration of the system (*pppe*) for two arbitrary internuclear distances $R = 0.45$ and $R = 2.527$ obtained with trial functions $\Psi_{1,2,3,4}$, and with their linear superposition given by trial function Ψ_6 .

B (Gauss)	R	Ψ_1	Ψ_2	Ψ_3	Ψ_4	Ψ_6
10^{11}	0.45	41.10121	41.12298	41.09077	41.09591	41.08986
	2.527	41.58129	41.58405	41.58146	41.58131	41.58122
10^{12}	0.45	423.9111	423.9195	423.9115	423.9111	423.9110
	2.527	424.4875	424.4877	424.4876	424.4876	424.4865
10^{13}	0.45	4252.956	4252.956	4252.956	4252.956	4252.956
	2.527	4253.461	4253.461	4253.461	4253.461	4253.460
4.414×10^{13}	0.45	18777.53	18777.53	18777.53	18777.53	18777.53
	2.527	18778.03	18778.03	18778.03	18778.03	18778.03

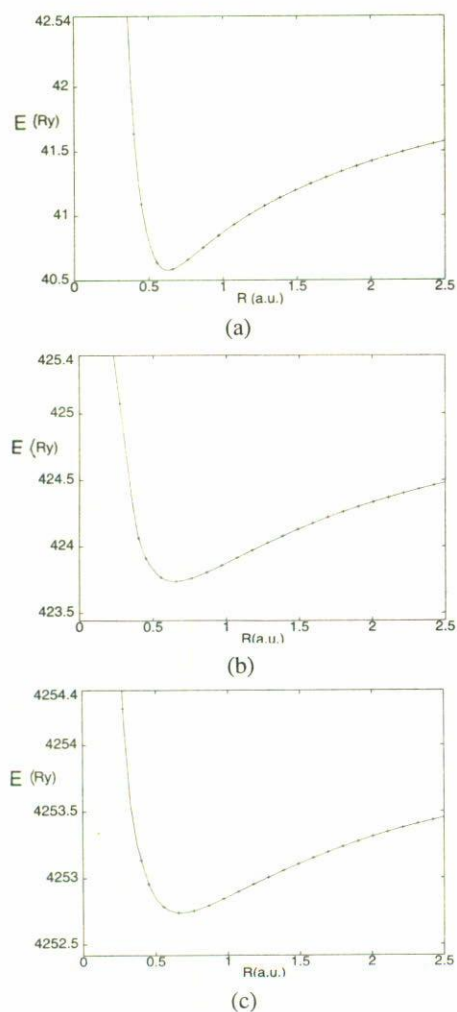


FIGURE 2. Potential energy curves as function of the internuclear distance R for the $H_3^{(2+)}$ molecular ion in the triangular configuration for magnetic field: (a) $B = 10^{11}$ G, (b) $B = 10^{12}$ G, (c) $B = 10^{13}$ G. The top of the energy scale corresponds to the value of the energy of a free electron $E_e = B$.

A surprising feature is revealed if we study different trial functions. In Table II the variational results for the total energy E_T for two quite arbitrarily chosen values of the internuclear distance, $R = 0.45$ and $R = 2.527$ are shown. For magnetic fields $10^{11} \lesssim B \lesssim 10^{12}$ G an adequate description of the system for internuclear distances $R \simeq 0.45$ is given by the trial function (5), modelling an ionic coupling, $H_2^+ + \text{proton}$. In this case, the single function (5) gives the lowest total energy among the trial functions $\Psi_{1,2,3,4}$. On the other hand, the trial function (2), modelling a covalent coupling gives the lowest total energy for $R \simeq 2.527$, giving a hint that a covalent coupling dominates when the internuclear distance is large compared to the equilibrium distance. Amazingly, for $B \gtrsim 10^{13}$ G the variational energy seems to be insensitive to the specific form of the trial function (!).

The electronic density distribution $|\Psi|^2$ in the plane $z = 0$ is shown in Fig. 3. For all magnetic fields $B = 10^{11} - 4.414 \times 10^{13}$ G the electronic density distribution $|\Psi|^2$ exhibits a single maximum located at the center of the triangle ($x = 0, y = 0$). As the magnetic field grows the electronic cloud becomes more concentrated around $x = 0, y = 0$, while its distance from the protons slowly increases.

5. Conclusions

From our results we can draw the conclusion that the exotic molecular ion $H_3^{(2+)}$ can exist in the presence of a strong magnetic field in a triangular configuration of the charged centers and is stable relative to a ground state hydrogen atom and two protons for the same magnetic field. In particular, in the present article we have shown that the molecular ion $H_3^{(2+)}$ can also exist in the equilateral (fixed nuclei) triangular configuration perpendicular to the magnetic field which is unstable with respect to a decay mode to the linear configuration. Furthermore, since the total energy of $H_3^{(2+)}$ lies above the corresponding total energy for the H_2^+ molecular ion for

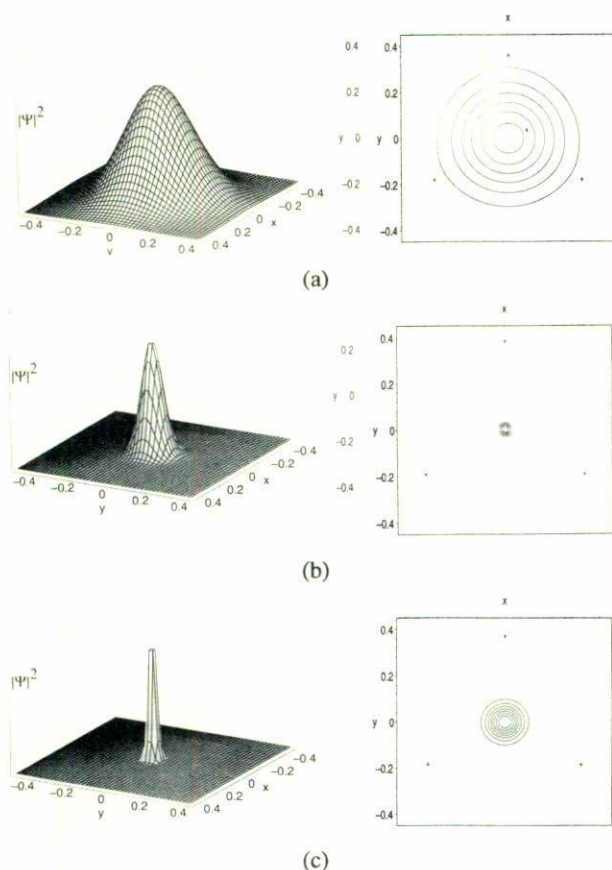


FIGURE 3. Electronic probability density $|\Psi|^2$ for the $H_3^{(2+)}$ molecular ion in the triangular configuration at $z = 0$ and its corresponding contours for (a) $B = 10^{11}$ G, (b) $B = 10^{12}$ G, (c) $B = 10^{13}$ G. The position of the charged centers is indicated by crosses. Normalization of $|\Psi|^2$ is not fixed.

all magnetic fields studied, there exists a dissociation channel $H_3^{(2+)} \rightarrow H_2^+ + p$. A study of the lifetime of $H_3^{(2+)}$ is beyond the scope of the present article and will be explored elsewhere.

The results of our variational study for the ground state show that, contrary to the case of the linear parallel configuration, the binding energy of the system decreases, and the internuclear distance increases as the magnetic field grows from $B = 10^{11}$ G to 4.414×10^{13} G. A more extended study of this, as well as other configurations, is needed in order to gain a better understanding of the properties of the exotic system $H_3^{(2+)}$. In particular, a proper contribution coming from the linear Zeeman effect term in (1) has to be taken into account. However, the fact that the linear Zeeman effect contribution vanishes in our consideration (which occurs when real trial functions are considered) looks relevant in the region of very strong magnetic fields $B = 10^{11} - 4.414 \times 10^{13}$ G where this term can be neglected in any case.

Although in general it is not clear so far (see discussion in Ref. 7) how an adiabatic separation of the electronic and the nuclear motion can be performed in the presence of a strong external magnetic field, our fixed-nuclei approach is a good starting point to study the exotic molecular ion $H_3^{(2+)}$.

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(a) In this context, the word ‘existence’ has the meaning of appearance of a minimum in the potential energy curves and thus the existence of bound states.
 (b) For a real trial function the expectation value of the z -component of the angular momentum $\langle \ell_z \rangle$ is equal to zero and leads to a vanishing contribution to the variational energy of the linear Zeeman effect term.
 (c) The binding energy is defined as the affinity to keep the electron bound, $E_b = B - E_T$. B is given in Ry and thus has the meaning of the energy of a free electron in a magnetic field.

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