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Electrostatic models of charged hydrogenic chains in a strong magnetic field

A. Escobar
Instituto de Ciencias Nucleares, Universidad Nacional Autónoma de México,
Circuito Exterior s/n Ciudad Universitaria, México, D.F., 04510, México.

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Simple one-dimensional electrostatic models of one-(two) electron molecular systems H_2^+, H_3^{2+}, H_4^{3+} and H_2, H_3^+, H_4^{2+} in a strong magnetic field are proposed to estimate the binding-(ionization) energy of the corresponding ground states. The study is carried out in the range of magnetic fieds $B = 10^2 - 10^6$ a.u. The models are inspired (and based) on the quasi one-dimensional form of the ground state electronic distribution function which is obtained by precise variational calculations in the Born-Oppenheimer approximation in a non-relativistic framework. It is shown that the models give, for all magnetic fields considered, a very good description of the binding-(ionization) energy of the one-electron molecular systems H_2^+, H_3^{2+}, H_4^{3+}, being accurate in 2.5%, 5% and 5% respectively, and 15% for the two-electron systems H_3^+, H_4^{2+} (30% for H_2) as compared with the corresponding variational calculations.

Keywords: Hydrogenic chains; strong magnetic field; electrostatic models.

Modelos electrostáticos unidimensionales simples de los sistemas moleculares de 1-(2) electrones H_2^+, H_3^{2+}, H_4^{3+} y H_2, H_3^+, H_4^{2+} en campos magnéticos intensos son propuestos para estimar la energía de amarre-(ionización) del correspondiente estado base. El estudio se lleva a cabo en el rango de campos magnéticos $B = 10^2 - 10^6$ a.u. Los modelos están inspirados (y basados) en la forma cuasi-unidimensional de la función de distribución electrónica, del estado base, que se obtiene mediante cálculos variacionales muy precisos realizados en la aproximación de Born-Oppenheimer en un tratamiento no relativista. Se muestra que los modelos brindan, para los campos magnéticos considerados, una muy buena aproximación a la energía de amarre-(ionización) de los sistemas moleculares de un electrón H_2^+, H_3^{2+} y H_4^{3+}, con una precisión relativa del 2.5%, 5% y 5% respectivamente, y con una precisión relativa del 15% para los sistemas moleculares de 2 electrones H_3^+, H_4^{2+} (30% para H_2) comparadas con los cálculos variacionales correspondientes.

Descriptores: Cadenas hidrogenoides; campos magnéticos intensos; modelos electrostáticos.

PACS: 31.15.Pf; 31.10.+z; 97.10.Ld

1. Introduction

Strong magnetic fields are present in the surfaces of neutron stars, where typically magnetic field varies in $B{\approx}10^{12}{-}10^{13}$ G, and can reach extraordinary values of $B \approx 10^{14} - 10^{16}$ G in the surface of the recently discovered magnetars^{i}. Since the discovery of the existence of strong magnetic fields several questions arose about the stability and structure of atoms and molecules exposed to such extreme magnetic fields [1,2].

First investigations about the structure of matter in strong magnetic fields [1,2] gave qualitative indications that due to the large quadrupole moment of the elongated electronic density cloud, new molecular systems, in the form of linear chains, could exist in an aligned configuration parallel to the magnetic field direction.

An accurate description of atomic and molecular systems in strong magnetic fields (even the most simple ones) has required the development of non-perturbative techniques which can give reliable results. An important step in the search for new exotic molecules in magnetic fields was achieved in 1999 with the theoretical discovery of the molecular ion H_3^{2+} [3] which can exist as a bound state for magnetic fields $B \gtrsim 10^{11}$ G. Later, it was shown that starting at different thresholds in the domain of magnetic fields $B \in [0, 10^{16}]$ G new chains of one and two electron systems composed of hydrogen and helium can exist in linear geometry (for a list of specific compounds and a review see [4] and also [6]).

In particular, the fact that the electronic cloud in a strong magnetic field acquires a cigarette-like form has suggested to use quasi-one dimensional approaches to solve the Schroedinger equation [7,8]. It is known that the one-dimensional Coulomb problem [9-11] describes a quantum system with many uses in atomic, molecular and condensed matter physics despite its apparent simplicity. For example, in the theory of a Mott exciton in a strong magnetic field [12] or in describing the problem of electrons over a pool of liquid helium. In this last case, given the charge and its image is hence clear that the electron is acted by a Coulomb interaction [13]. Additionally, an essentially two-dimentional set of electrons trapped in the levels of the one-dimentional Coulomb problem has been suggested as a possible realization of a quantum computing device [14].

Recently, some heuristic one-dimensional electrostatic models for one-electron molecular systems in a strong magnetic field have been introduced in Ref. 4. Altough very simple, their accuracy is enough to gain a certain qualitative insight about the structure of molecules in magnetic fields. For example, a model for a one-electron diatomic molecular ion (Z, Z, e) like H_2^+ (Z=1) in a strong magnetic field is described in Ref. 4; guided by the evolution of the electronic distribution of H_2^+ as the magnetic field is increased, *i.e.* evolving from a two peak configuration, for small magnetic fields, to a one (centered) peak configuration^{ii}, at strong magnetic fields, this model assumes that at equilibrium the electronic cloud can be mimicked by a point-like charge situated exactly in the middle between the charged centers. All three charges (two heavy centers of charge Z and one electron) are confined by the magnetic field inside a narrow cylindrical channel whose radius is limited to a domain defined by the Larmor radius. The electrostatic Coulomb energy E_{coul} (in a.u.) of such linear configuration of point charges is easily calculated, being

$$E_{\text{coul}} = -\frac{Z(4-Z)}{R_{\text{eq}}}, \tag{1}$$

where R_{eq} is the equilibrium distance between protons. E_{coul} is negative for $Z < 4$ predicting that the system can be bound even for $Z = 3$, the case of Li_2^{5+} which actually is predicted to exist for magnetic fields $B \gtrsim 10^4$ a.u. [15].

We should mention that the model presented, as all electrostatic models, assumes that point charges are fixed for each value of the magnetic field, then a configuration is called equilibrium configuration due to the fact that accurate variational results for the equilibrium distance(s) R_{eq} and the corresponding binding energies were used to develop the model^{iii}.

Of course, the validity of this model relies on the phenomenological assumption that the binding energy can be well approximated by the Coulomb electrostatic energy of such linear configuration of point charges^{iv}. There might exist a domain of magnetic field strength where this picture makes sense. This is, indeed, the case for very strong magnetic fields. For example, for $Z = 1$ (hydrogen molecular ion) the binding energy obtained from the above relation (1) is slightly overestimated being larger in 10% for a magnetic field $B = 10^4$ a.u. while it is larger in 5% for $B = 10^6$ a.u. (see [4]). It indicates that the accuracy of the model increases as a magnetic field grows. In any case, the approximate results given by this simple model are very surprising. Models of pointlike charges were proposed in Ref. 4 also for one-electron systems with 3 and 4 charged centers. Similar models have been also used for two-electron systems in a magnetic field [5].

Our goal in the present paper, is to develop further the above mentioned simple electrostatic models of the ground state of the one-electron hydrogenic chains H_2^+, H_3^{2+}, H_4^{3+} and the two-electron molecular systems H_2, H_3^+, H_4^{2+} in a strong magnetic field. The development consists of incorporating into the models the information contained in the electronic distribution which is obtained by precise variational calculations. Atomic units $m_e = -e = \hbar = a_0 = 1$ are used throughout although the energy is given in Rydbergs.

2. One-electron molecular systems in a strong magnetic field: electrostatic model for the ground state

For the non-relativistic description of the groud state $1\sigma_g$ of the one-electron molecular systems in a strong magnetic field B (parallel configuration^v), we can develop an electrostatic model as follows: In the first instance, we consider that the electronic charge distribution can be modeled by a linear density of charge $\lambda(z)$ situated along the magnetic field direction (z-direction), where $\lambda(z)$ is defined through the z-profile of the ground state electronic distribution Ψ_{var} obtained by variational calculations [4] being

$$\lambda(z) = e\frac{\int |\Psi_{\text{var}}(\rho,\phi,z)|^2 \rho\, d\rho d\phi}{\int |\Psi_{\text{var}}(\rho,\phi,z)|^2\, \rho\, d\rho d\phi dz}\,, \tag{2}$$

where (ρ, ϕ, z) are the cylindrical coordinates of the position vector of the electron, and ($e = -1$ in atomic units) is the electron charge. In a second step, the linear charge distribution (2) is approximated by a linear superposition of a finite number of standard Gaussian functions situated symmetrically with respect to the center of the molecular axis. Afterwards, each Gaussian curve is replaced by a point charge, located at the center of the Gaussian and whose value is equal to the corresponding linear coefficient amplitude (see Figs. 1 to 3). The number of Gaussian functions used in the model depends on the shape of the profile $\lambda(z)$. Roughly, for each local maximum of the profile a Gaussian function is introduced. However, this number is rather arbitrary. For example, for the system H_2^+ whose profile in the range of magnetic field considered presents a single maximum, three Gaussian functions were used (although, considering only one Gaussian function placed in the mid point between the line connecting the protons, does not alter the results significantly in this case). Let us take, for example, such configuration of three point charges used to construct a model for the molecular ion H_2^+ (see Fig. 1)

$$\begin{aligned}\lambda(z) = {}& \frac{q_1}{\sqrt{2\pi\sigma_1^2}}\, e^{-\frac{z^2}{2\sigma_1^2}} \\ & + \frac{q_2}{\sqrt{2\pi\sigma_2^2}}\left(e^{-\frac{(z-z_2)^2}{2\sigma_2^2}} + e^{-\frac{(z+z_2)^2}{2\sigma_2^2}}\right),\end{aligned} \tag{3}$$

where q_i, σ_i, z_i ($i = 1, 2$) are interpolation parameters. Such parameters are not all independent. In addition to the normalization condition, which allows us to write q_2 in terms of q_1, we can impose the condition

$$E_{\text{coul}} = E_b\,, \tag{4}$$

E_b being the variational binding energy and E_{coul} the electrostatic Coulomb energy. The Coulomb energy E_{coul} (in Rydbergs) is obtained after the replacement of these Gaussians by point charges (Fig. 1) and is given by^{vi}

$$E_{\text{coul}}(B){=}2\left(\frac{1}{R_{\text{eq}}}+\frac{4q_1}{R_{\text{eq}}}+\frac{2q_2}{|\frac{R_{\text{eq}}}{2}-z_2|}+\frac{2q_2}{|\frac{R_{\text{eq}}}{2}+z_2|}\right), \tag{5}$$

where the values of the equilibrium interproton distance $R_{\text{eq}}(B)$ as a function of the magnetic field strength B are taken from the variational calculations [4], which then allows us to express one parameter among q_i, σ_i, z_i ($i = 1, 2$) in terms of the others (for example $q_1{=}q_1(E_b, R_{\text{eq}}; z_1, q_2, z_2)$).

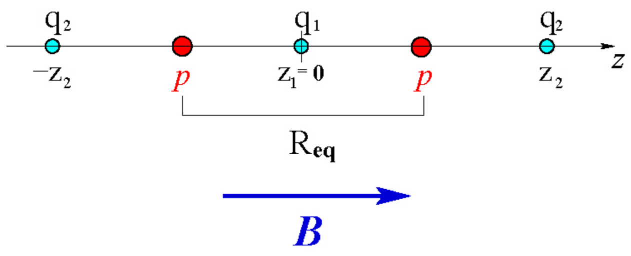

FIGURE 1. Electrostatic model for the ground state $1\sigma_g$ of the one-electron molecular ion H_2^+ in parallel configuration with a uniform and constant strong magnetic field $\mathbf{B} = (0, 0, B)$. The electronic cloud is replaced by three point like charges with fractional charge q_2, q_1, q_2 at the positions $-z_2, 0, z_2$ respectively.

The condition (4) is not as strong as it migth seem. Making use only of the normalization condition the relative difference between $E_{\rm coul}$ and E_b is less than 15% for all one electron systems and for all magnetic fields considered. On the other hand, imposing only (4) the resulting linear density of charge $\lambda(z)$ breaks the normalization condition, but in less than 2% for all systems and for all magnetic fields considered.

Condition (4) can be or not satisfied, but normalization condition must hold anyway. Then, according to this physical requirement we impose (4) and afterwards the normalization on $\lambda(z)$ is restored multiplying by an overall factor on $\lambda(z)$.

Suitable interpolation functions of the parameters $R_{\rm eq}$, q_i, z_i $(i = 1, 2)$ as functions of the magnetic field B were found, which allows us to write the Coulomb energy $E_{\rm coul}{=}E_{\rm coul}(B)$ as an explicit analytical approximation as function of the magnetic field B.

2.1. Calculations

In this section we show, for each one-electron system (H_2^+, H_3^{2+}, H_4^{3+}), the interpolating functions of the parameters $R_{\rm eq}$, q_i and z_i $(i = 1, 2, 3)$ as a function of the magnetic field strength B. Hereafter, magnetic field is defined in dimensionless units (a.u.) as B/B_0, where $B_0 = 2.35 \times 10^9$ G, which we continue to denote as B.

2.2. Ion H_2^+

The study is carried out in the range of magnetic fields $4255 \leq B \leq 10^5$ a.u. For this system a superposition of three Gaussian functions as in (3) was used to model the linear charge density $\lambda(z)$ (see 2). This charge density is defined by the z-profile of the corresponding ground state electronic distribution $\Psi_{\rm var}$ taken from [4]. The parameters of the model (3) which approximate $\lambda(z)$ for each magnetic field studied are summarized in the Table I.

The equilibrium interproton distance $R_{\rm eq}(B)$ as a function of the magnetic field strength B is taken from the variational calculations [4] and fitted by the formula given by

$$R_{\rm eq}(B){=}\frac{1.7288}{1{+}1.1365\log\{1{+}(0.0232B)^2{+}(0.0018B)^4\}}, \quad (6)$$

TABLE I. H_2^+ state $1\sigma_g$. Parameters which approximate the electronic charge density $\lambda(z)$ given as the sum of three (normalized) Gaussian functions. The electrostatic model is obtained replacing each Gaussian curve by a point charge, located at the center of the Gaussian and whose value is equal to the corresponding linear coefficient amplitude (see Fig. 1).

B (a.u.)	q_1 (a.u.)	q_2 (a.u.)	z_2 (a.u.)
4255	-0.89403	-0.05298	0.28201
10000	-0.92383	-0.03808	0.26209
18782	-0.95033	-0.02483	0.24239
42553	-0.95773	-0.02113	0.22279
100000	-0.95988	-0.02005	0.20276

The functional form of the dependence of $R_{\rm eq}(B)$ on the magnetic field, as well as for the interpolation for $z_2(B)$ (see below), is taken from the physics-inspired approximations based on the assumption that the dynamics of the one-electron Coulomb system in a strong magnetic field is governed by the ratio of transverse to longitudinal size of the electronic cloud (for details see [16]). The protons of the system H_2^+ are thus located at $z = \pm(R_{\rm eq}/2)$ with respect to the origin situated in the mid point on the line connecting protons.

As a function of the magnetic field B, the interpolating formula for the point charge q_1 located in the center ($z = 0$) is given by

$$q_1(B) = -\frac{0.0059 + 22.0211\,\sqrt{B} + B}{9.7408 + 31.9754\,\sqrt{B} + B}. \qquad (7)$$

This formula describes the approximated dependence of $q_1(B)$ on the magnetic field B. Notice that for $B \to \infty$, $q_1(B) \to$ -1 implying that as the magnetic fields increases, the electrostatic model is reduced to that with a one single point charge situated in the middle between the two protons of the molecule H_2^+ as it was proposed in Ref 4. The charge conservation condition $q_1 + 2q_2 = -1$ gives the interpolation for the two symmetric point charges $q_2(B)$ (see Fig. 1). Finally, the interpolation for the position of these two charges z_2 is given by

$$z_2{=}\frac{2.1117}{1{+}0.2523\log\{1{+}(1.0075\,B)^2{+}(0.1090\,B)^4\}}\,, \qquad (8)$$

where z_2, as $R_{\rm eq}$, is given in atomic units of distance ($a_0{=}1$ a.u.).

Notice that the lateral charges q_2 are situated outside of the equilibrium distance for all values of the magnetic field considered and that for $B \to \infty$ the lateral charges decrease their relative importance.

Table II shows, as a function of the magnetic field B, the values of the Coulomb energy $E_{\rm coul}$ of the electrostatic model of point charges and the corresponding variational binding

TABLE II. H_2^+ state $1\sigma_g$. Comparison of $E_{\rm coul}$ vs E_b. The relative difference $\Delta E = (|E_{\rm coul} - |E_b||/|E_b|)$ is less than 2.5% for all the range of magnetic fields considered.

$B(a.u.)$	$E_{\rm coul}(Ry)$	$E_b(Ry)$	$\Delta E(\%)$
4255	-36.5454	-35.7538	2.2
10000	-46.8141	-45.7970	2.2
18782	-55.8387	-54.5016	2.4
42553	-68.7737	-67.5826	1.7
100000	-82.7359	-83.5814	1.0

TABLE III. H_3^{2+} state $1\sigma_g$. Parameters which approximate the electronic charge density $\lambda(z)$ given as the sum of four (normalized) Gaussian functions situated symmetrically with respect to the center of the molecular axis.

$B\,(a.u.)$	$q_2\,(a.u.)$	$z_2\,(a.u.)$	$q_3\,(a.u.)$	$z_3\,(a.u.)$
425	-0.04188	0.04429	-0.45811	0.19696
1000	-0.03950	0.03061	-0.46049	0.15537
4255	-0.02081	0.00931	-0.47918	0.09948
10000	-0.01390	0.00443	-0.48609	0.07793
18782	-0.01042	0.00258	-0.48957	0.06562

energy E_b, where it is shown that the relative difference varies ΔE varies from 1 to 2.5 in all the range of magnetic fields studied.

2.3. Ion H_3^{2+}

The study is carried out in the range of magnetic fields $425 \leq B \leq 18782$ a.u. For this system a superposition of four Gaussian functions were used to fit the z-profile of the electronic distribution, *i.e.* $\lambda(z)$ (see Fig. 2). The parameters of the model which approximate $\lambda(z)$ for each magnetic field studied are summarized in the Table III.

The Coulomb energy $E_{\rm coul}$ (in Rydbergs) of such configuration of point charges is given by

$$E_{\rm coul}(B) = 2\Bigg(\frac{5}{R_{\rm eq}} + \frac{2q_2}{|\frac{R_{\rm eq}}{2} - z_2|} + \frac{2q_2}{|\frac{R_{\rm eq}}{2} + z_2|} + \frac{2q_3}{|\frac{R_{\rm eq}}{2} - z_3|} + \frac{2q_3}{|\frac{R_{\rm eq}}{2} + z_3|} + \frac{2q_2}{z_2} + \frac{2q_3}{z_3}\Bigg), \qquad (9)$$

where the equilibrium distance $R_{\rm eq}(B)$ as a function of the magnetic field strength B is taken from the variational calculations [4] and fitted by the formula

$$R_{\rm eq}(B) = \frac{0.8761}{1{+}0.3308\log\{1{+}(0.0026B)^2{+}(0.00047B)^4\}}, \qquad (10)$$

The protons of the system H_3^{2+} are thus located at $z{=}0, \pm(R_{\rm eq}/2)$ with the origin situated in the mid point on the line connecting protons.

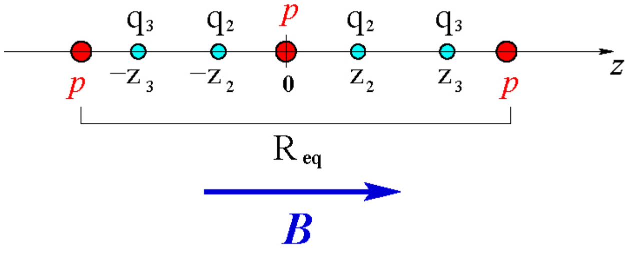

FIGURE 2. H_3^{2+} state $1\sigma_g$: Electrostatic model for the ground state $1\sigma_g$ of the one-electron molecular ion H_3^{2+} in parallel configuration with a uniform and constant strong magnetic field $\mathbf{B}{=}(0, 0, B)$. The electronic cloud is replaced by four point like charges with fractional charge q_3, q_2, q_2, q_3 located at the positions $-z_3, -z_2, z_2, z_3$ respectively.

As a function of the magnetic field B, the interpolating formula for the point charge q_3 located at $z = \pm z_3$ is given by

$$q_3(B) = -\frac{1.1634 + 0.00044\,B}{2.57928 + 0.00089\,B}. \qquad (11)$$

This formula describes the approximated dependence of $q_3(B)$ on the magnetic field B. Notice that for $B{\to}\infty$, $q_3(B) \to -0.494$ implying that as the magnetic fields increases, the electrostatic model is reduced to (almost) that with a two negative point charges situated at $\pm z_3, z_3{<}(R_{\rm eq}/2)\forall B$. The charge conservation condition $2q_1 + 2q_2 = -1$ gives the interpolation for the two symmetric point charges $q_2(B)$ (see Fig. 2). The interpolation for the position z_i $(i = 2, 3)$ of the two point charge q_i is given by

$$z_2(B) = \frac{7.1659}{1 + 3.0835\log\{1 + (0.00024\,B)^2\}} \times \left(\frac{1 + 0.00405\,B}{1 + B}\right), \qquad (12)$$

$$z_3(B){=}\frac{1.6333}{1{+}1.3342\log\{1{+}(0.0345B)^2{+}(0.004B)^4\}}. \qquad (13)$$

Notice that $z_2 < z_3$ for all values of the magnetic field B.

Table IV shows, as a function of the magnetic field B, the values of the Coulomb energy E_{coul} of the electrostatic model of point charges and the corresponding variational binding energy E_b.

TABLE IV. H_3^{2+} state $1\sigma_g$. Comparison of $E_{\rm coul}$ vs E_b. In general, the relative difference $\Delta E = (|E_{\rm coul} - |E_b||/|E_b|)$ is less than 5% for all the range of magnetic fields considered.

$B(a.u.)$	$E_{coul}(Ry)$	$E_b(Ry)$	$\Delta E(\%)$
425	-15.3869	-15.1580	1.5
1000	-20.5693	-20.7829	1.0
4255	-35.5729	-34.3905	3.4
10000	-47.7120	-45.4081	5.0
18782	-57.9764	-55.2311	4.9

TABLE V. H_4^{3+} state $1\sigma_g$. Parameters which approximate the electronic charge density $\lambda(z)$ given as the sum of four (normalized) Gaussian functions situated symmetrically with respect to the center of the molecular axis.

$B\,(a.u.)$	$q_2\,(a.u.)$	$z_2\,(a.u.)$	$q_3\,(a.u.)$	$z_3\,(a.u.)$
10^5	-0.04792	0.03037	-0.45207	0.05755
2×10^5	-0.03431	0.02583	-0.46568	0.04756
3×10^5	-0.03086	0.02370	-0.46913	0.04284
4×10^5	-0.02749	0.02242	-0.47250	0.03995
5×10^5	-0.02628	0.02113	-0.47371	0.03759
10^6	-0.02232	0.01849	-0.47767	0.03210

2.4. Ion H_4^{3+}

The study is carried out in the range of magnetic fields $1\times10^5 \le B \le 10^6$ a.u. For this system a superposition of four Gaussian functions were used to fit the z-profile of the electronic distribution, *i.e* $\lambda(z)$ (see 2). The parameters of the model which approximate $\lambda(z)$ for each magnetic field studied are summarized in the Table V.

The equilibrium interproton distances R_1, R_2 (see Fig. 3) as a function of the magnetic field strength B are taken from the variational calculations [4] and fitted by the respective formula

$$R_1(B)=\frac{1.0919}{1+1.3482\log\{1+(0.0024B)^2+(0.00015B)^4\}}\times\left(\frac{1+1.0908\,B}{1+0.9593\,B}\right), \quad (14)$$

$$R_2(B)=\frac{1.1206}{1+1.2352\log\{1+(0.00105B)^2+(0.000096B)^4\}}\times\left(\frac{1+1.11996\,B}{1+0.9466\,B}\right). \quad (15)$$

The protons of the system H_4^{3+} are thus located at

$$z=\pm\frac{R_1}{2}, \quad \pm\frac{(R_1+2R_2)}{2}$$

with the origin situated in the mid point on the line connecting protons. Notice that $R_1 < R_2\,\forall\,B$.

As a function of the magnetic field B, the interpolating formula for the point charge q_3 located at $z=\pm z_3$ is given by

$$q_3(B)=-\frac{0.04144+0.7888\log\{1+(0.00004B)^2\}}{1.00636+1.60047\log\{1+(0.000034B)^2\}}, \quad (16)$$

This formula describes the approximated dependence of $q_3(B)$ on the magnetic field. Notice that for $B\to\infty$, $q_3(B)\to -0.492$ implying that as the magnetic fields increases, the electrostatic model is reduced to (almost) that with two negative point charges situated at

$$\pm z_3\,,\ \frac{R_1}{2} < z_3 < \frac{R_1+2R_2}{2}\,\forall\,B.$$

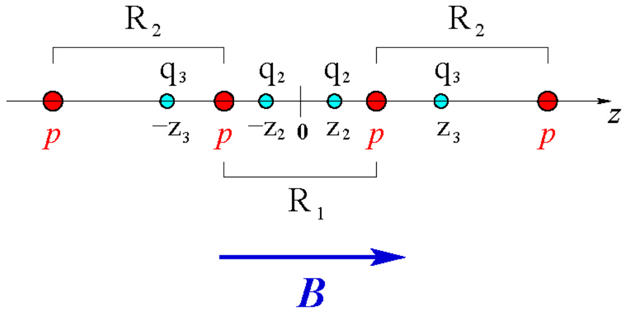

FIGURE 3. H_4^{3+} state $1\sigma_g$: Electrostatic model for the ground state $1\sigma_g$ of the one-electron molecular ion H_4^{3+} in parallel configuration with a uniform and constant strong magnetic field $\mathbf{B}=(0,0,B)$. The electronic cloud is replaced by four point like charges with fractional charge q_3, q_2, q_2, q_3 located at the positions $-z_3, -z_2, z_2, z_3$ respectively.

TABLE VI. H_4^{3+} state $1\sigma_g$. Comparison of $E_{\rm coul}$ vs E_b. In general, the relative difference $\Delta E = (|E_{\rm coul} - |E_b||/|E_b|)$ is less than 2.5% for all the range of magnetic fields considered.

$B(a.u.)$	$E_{\rm coul}(Ry)$	$E_b(Ry)$	$\Delta E\,(\%)$
1×10^5	-77.5705	-74.0368	4.7
2×10^5	-93.0368	-91.1208	2.1
3×10^5	-104.8920	-102.4702	2.3
4×10^5	-113.7690	-111.1897	2.3
5×10^5	-120.7930	-118.3093	2.0
10^6	-143.0300	-142.7426	0.2

The charge conservation condition $2q_1+2q_2=-1$ gives the interpolation for the two symmetric point charges $q_2(B)$ (see Fig. 3). The interpolation for the position z_i $(i=2,3)$ of the two point charge q_i is given by

$$z_2(B)=\frac{0.1781}{1+0.1897\log\{1+(0.000018\,B)^2\}}\times\left(\frac{1+0.3070\,B}{1+1.3992\,B}\right), \quad (17)$$

$$z_3(B)=\frac{0.3150}{1+0.2434\log\{1+(0.000017\,B)^2\}}\times\left(\frac{1+0.3369\,B}{1+1.3785\,B}\right). \quad (18)$$

Notice that $z_2 < (R_1/2)\,\forall\,B$.

Table VI shows the values of the Coulomb energy $E_{\rm coul}$ of the electrostatic model of point charges and the corresponding variational binding energy E_b.

2.5. Results

In the last sections simple one-dimensional electrostatic models of the one electron molecular systems H_2^+, H_3^{2+}, H_4^{3+} in a strong magnetic field were proposed to estimate the binding-

(ionization) energy of the corresponding ground states, giving the following main results:

- Compared with the binding energy obtained by precise variational calculation [4], the Coulomb energy E_{coul} has a relative error of less than 2.5%, 5% and 5% for the systems H_2^+, H_3^{2+}, H_4^{3+} respectively for any value of the magnetic field considered.

- The model predicts the existence of the system H_2^+ for any value of magnetic field in agreement with variational results. In the range $0 \leqslant B < \infty$, the corresponding Coulomb energy $E_{\text{coul}}(B)$ is a smooth, negative and monotonously decreasing function.

- For the system H_3^{2+} the electrostatic model predicts binding energies of -169.523 Ry at $B = 10^6$ a.u. and -262.108 Ry at $B = 10^7$ a.u. which implies a relative error (compared with variational calculations [4]) of less than 6%, 0.07% respectively even for these magnetic fields (two orders of magnitud larger that the values considered in the present study). For magnetic fields $B \gtrsim 200$ a.u. the Coulomb energy $E_{\text{coul}}(B)$ is a smooth, negative and decreasing function, for small values ($B < 30$) a.u. it becomes positive, which may be an indication that the system H_3^{2+} is not bound in this region of magnetic fields. According to variational results [4] H_3^{2+} has bound states from $B \gtrsim 10^2$ a.u.

- For the system H_4^{3+} and for magnetic fields $B \gtrsim 7\times 10^4$ a.u., the Coulomb energy $E_{\text{coul}}(B)$ is a negative, smooth and decreasing function. In the magnetic field interval $0 \leqslant B \leqslant 7 \times 10^4$ a.u., the energy $E_{\text{coul}}(B)$ is negative but not monotone. On the other side, using the variational method, it is found that the molecule H_4^{3+} is bound only for magnetic fields $B \gtrsim 10^4$ a.u., therefore extrapolation of the function $E_{coul}(B)$ for magnetic fields $0 \leqslant B \leqslant 10^4$ a.u. is not physical.

3. Two-electron molecular systems: electrostatic model of point charges and a charged cylinder

For the non-relativistic description of the ground state ${}^3\Pi_u$ (the notation used in Ref. 4 is adopted) of the two-electron molecular systems in a strong magnetic field B (parallel configuration^{vii}), we follow a treatment similar to that for the case of one-electron systems. In the first instance, we consider that the electronic total charge can be modeled by a linear density of charge $\Lambda(z)$ situated along the magnetic field direction (z-direction), where $\Lambda(z)$ is defined through the z-profile of the ground state electronic distribution Ψ_{var} obtained by variational calculations [6]

$$\Lambda(z) = 2e\frac{\int \Psi_{\text{var}}^* \Psi_{\text{var}} \rho_1 \rho_2 d\rho_1 dz_2 d\rho_2 d\varphi}{\int \Psi_{\text{var}}^* \Psi_{\text{var}} d\mathbf{r}_1 d\mathbf{r}_2};$$
$$z = z_1(z_2), \tag{19}$$

where (ρ_i, ϕ_i, z_i), $i = 1, 2$ are the cylindrical coordinates of the position vector $\mathbf{r}_i$ of the electron i, φ is the angle between $\mathbf{r}_1$ and $\mathbf{r}_2$ and e $(= -1$ in atomic units) is the electron charge.

In a second step, in analogy to the case of one-electron molecular systems, the linear charge distribution (17) is approximated by a linear superposition of a finite number of standard Gaussian functions situated symmetrically with respect to the center of the molecular axis. For simplicity, we assume equal contribution of each electron to this linear charge distribution $\Lambda(z)$

$$\Lambda(z) = \lambda_1(z) + \lambda_2(z)\,;\ \lambda_1 = \lambda_2 \tag{20}$$

where $\lambda_1(z)$ is the linear charge density associated with electron e_1 and similary for e_2. Both charge distribution $\lambda_i(z)$, $i = 1, 2$, normalized by construction to -1 (electron charge in a.u.), are given by the same linear superposition of Gaussian functions as $\Lambda(z)$, except that the linear coefficient amplitudes of the Gaussian curves are reduced by a factor of 2. However in a state ${}^3\Pi_u$ (a state with $M = 1$) we consider that one electron, let us say electron e_1, is in its ground state ($m_1 = 0$) and the other electron is in an excited state ($m_2 = 1$) where m_i ($i = 1, 2$) denotes the angular momentum projection of the i-electron on the magnetic field direction, and $M = m_1 + m_2$ represents the total magnetic quantum number.

This suggest reduce the linear charge distribution $\lambda_1(z)$, associated with e_1 ($m_1 = 0$), to a configuration of point charges replacing each Gaussian curve by a point charge located at the center of the Gaussian and whose value is equal to the corresponding linear coefficient amplitude, while $\lambda_2(z)$ associated with e_2 ($m_2 = 1$) is projected onto the surface of an infinite cylindrical shell of radius ρ_0, thus the electron 2 is described by a surface charge distribution $\sigma_2(z)$. We assume^{viii} $\rho_0 \approx \langle\rho\rangle$. The number of Gaussian functions used in the model depends on the shape of the profile $\Lambda(z)$. Roughly, for each local maximum of the z-profile a Gaussian function is introduced.

Explicitly the resulting surface charge distribution $\sigma_2(z)$ (normalized) has the form

$$\sigma_2(z) = \frac{\lambda_2(z)}{2\pi\rho}\ ;\ \int \sigma_2 dV = -1. \tag{21}$$

Is important to emphasize that the ground state ($m = 0$) wave function of an electron placed in a uniform and constant magnetic field $\mathbf{B} = (0, 0, B)$ has not nodes.

Using this electrostatic model^{ix}, we then obtain the Coulomb interaction energy

$$E_{\text{coul}} = E_{\text{coul}}(R, \rho_0; \{\sigma_i\}, \{q_i\}, \{z_i\}),$$

where R denotes the equilibrium internuclear distance(s) of the system. Normalization condition allows us to express one parameter among q_i, σ_i, z_i ($i = 1, 2$) in terms of the others.

However, unlike the previous case of one electron systems, the Coulomb energy E_{coul} can not be written in a closed form in terms of elementary functions.

Suitable interpolation functions of the parameters q_i, z_i, σ_i $(i = 1, 2, 3)$ as a functions of the magnetic field strength B where found, such functions allows us to write the Coulomb energy $E_{\text{coul}} = E_{\text{coul}}(B)$ as an explicit analytical approximation as function of the magnetic field B, with the distance (s) R and ρ_0 playing the roles of external parameters. If we use the values of R and ρ_0 obtained in variational calculations, we see that the electrostatic energy E_{coul} is not a good estimate for the variational energy -$E_I{}^x$. However we can find intervals $[\rho_{0-}, \rho_{0+}]$, $[R_-, R_+]$ for which the relative difference of ρ_0, R and E_{coul} from their variational counterparts $\langle\rho\rangle$, R_{eq} and -E_I respectively are less than 15% (30% for H_2).

3.1. Calculations

In this section we show, for each two-electron system **(H_2, H_3^+, H_4^{2+})**, the interpolating function of the parameters q_i, z_i and σ_i $(i = 1, 2, 3)$ as a function of the magnetic field strength B and the corresponding intervals $[\rho_{0-}, \rho_{0+}]$, $[R_-, R_+]$. Hereafter, magnetic field is defined in dimensionless units (a.u.) as B/B_0, where $B_0 = 2.35 \times 10^9$ G, which we continue to denote as B.

3.2. Molecule H_2

As a basic system, the molecule H_2 has been studied in presence of strong magnetic fields. It was found that the most stable configuration of the system is parallel to the magnetic field [6]. A relevant fact is that the state with the lowest total energy (ground state) depends on the magnetic field strength B. It evolves from spin-singlet $^1\Sigma_g$ state for small magnetic fields $0 \lesssim B \lesssim 0.18$ a.u. to spin-triplet $^3\Pi_u$ state for 12.3 a.u. $\lesssim B$ The molecule H_2 does not exist in the range of magnetic fields $0.18 \lesssim B \lesssim 12.3$ a.u., in which the lowest energy state corresponds to a repulsive (unbounded) $^3\Sigma_u$ state. The electrostatic study is carried out in the range of magnetic fields $100 \leq B \leq 10000$ a.u. For this system a superposition of three Gaussian functions was used to model the linear charge density $\Lambda(z)$ (see 17) defined by the z-profile of the corresponding ground state electronic distribution. The electrostatic model consists of (i) a set of point charges $\{q_i\}$ $(m_1 = 0)$ obtained replacing each Gaussian curve of $\lambda_1 (= \Lambda/2)$ by a point charge, located at the center of the Gaussian and whose value is equal to the corresponding linear coefficient amplitude and (ii) an infinite charged cylindrical shell $\sigma_2(z) = (\lambda_2)/(2\pi\rho)$ $(m_2 = 1)$ of radius ρ_0, (see Fig. 4). The parameters of the model which approximate $\Lambda(z)$ for each magnetic field studied are summarized in the Table VIII.

The Coulomb energy E_{coul} (in Rydbergs) is given by

$$E_{\text{coul}} = 2(E_{p-p} + E_{p-e_1,e_2} + E_{e_1-e_2})\,, \tag{22}$$

TABLE VIII. H_2 state $^3\Pi_u$. Parameters which approximate the electronic charge density $\Lambda(z)$ given as the sum of three Gaussian functions situated symmetrically with respect to the center of the molecular axis.

B (a.u.)	q_1 (a.u.)	σ_1 (a.u.)	q_2 (a.u.)	z_2 (a.u.)	σ_2 (a.u.)
100	0.63435	0.42474	0.18282	0.14724	0.15957
425	0.64121	0.31403	0.17939	0.10007	0.10580
1000	0.64873	0.26154	0.17563	0.07969	0.08446
4255	0.66495	0.19581	0.16752	0.05617	0.05912
10000	0.67017	0.16740	0.16491	0.04567	0.04930

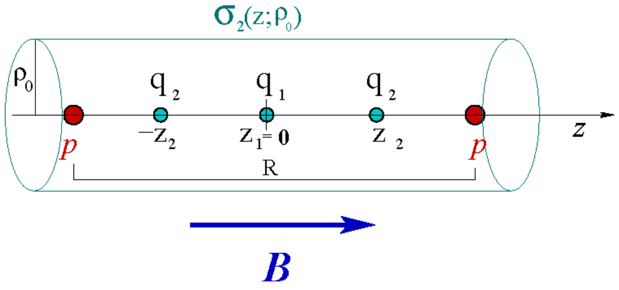

FIGURE 4. H_2 state $^3\Pi_u$: Electrostatic model for the ground state $^3\Pi_u$ of the two-electron molecular ion H_2 in parallel configuration with a uniform and constant strong magnetic field $\mathbf{B} = (0, 0, B)$. The electronic cloud is replaced by three point like charges with fractional charge q_2, q_1, q_2 $(m_1 = 0)$ located at the positions $-z_2, z_1, z_2$ respectively and an infinite charged cylindrical shell $(m_2 = 1)$ of radius ρ_0. The protons of the system H_2 are located at $z = \pm\,(R/2)$ with the origin situated in the mid point on the line connecting protons.

where

$$E_{(p-p)} = \frac{1}{R}\,, \tag{23}$$

$$E_{(p-e_1,e_2)} = \frac{4q_1}{R} + \frac{2q_2}{|\frac{R}{2} - z_2|} + \frac{2q_2}{|\frac{R}{2} + z_2|} + \Phi\left(-\frac{R}{2}\right) + \Phi\left(\frac{R}{2}\right)\,, \tag{24}$$

$$E_{(e_1-e_2)} = q_1\Phi(z_1) + q_2\Phi(-z_2) + q_2\Phi(z_2)\,, \tag{25}$$

where the subscripts p and e_1, e_2 denote the proton and electrons respectively (using this notation, $E_{(p-p)}$ is the repulsive interaction between protons, and similary for $E_{(p-e_1,e_2)}$ and $E_{(e_1-e_2)}$). As usual the electrostatic potential $\Phi(z;\rho_0)$, produced by the cylindrical shell $\sigma_2(z;\rho_0)$, is given by

$$\Phi(z;\rho_0) = \int \frac{\sigma_2(z';\rho_0)}{\sqrt{\rho_0^2 + (z - z')^2}} dz' d\rho' d\phi'\,, \tag{26}$$

As a function of the magnetic field B, the interpolating formula for the point charge q_1 located in the center $(z = 0)$ is given by

$$q_1 = -\frac{1.6757 + 0.001137\,B}{2.6531 + 0.001682\,B}\,, \tag{27}$$

TABLE VIII. H_2 state ${}^3\Pi_u$: Intervals $\Delta\rho_0 = [\rho_{0-}, \rho_{0+}]$ and $\Delta R = [R_-, R_+]$. The relative difference $\Delta E = (|E_{\rm coul} - |E_I||/|E_I|)$ is less than 30%.

B(a.u.)	ΔR (a.u.)	$\Delta\rho_0$ (a.u.)	$E_{\rm coul}$
100	[1.26$R_{\rm eq}$,1.3$R_{\rm eq}$]	[1.26$\langle\rho\rangle$,1.3$\langle\rho\rangle$]	[-1.296E_I,-1.238E_I]
425	[1.27$R_{\rm eq}$,1.3$R_{\rm eq}$]	[1.27$\langle\rho\rangle$,1.3$\langle\rho\rangle$]	[-1.293E_I,-1.246E_I]
1000	[1.27$R_{\rm eq}$,1.3$R_{\rm eq}$]	[1.27$\langle\rho\rangle$,1.3$\langle\rho\rangle$]	[-1.295E_I,-1.247E_I]
4255	[1.27$R_{\rm eq}$,1.3$R_{\rm eq}$]	[1.27$\langle\rho\rangle$,1.3$\langle\rho\rangle$]	[-1.285E_I,-1.236E_I]
10000	[1.29$R_{\rm eq}$,1.3$R_{\rm eq}$]	[1.29$\langle\rho\rangle$,1.3$\langle\rho\rangle$]	[-1.283E_I,-1.266E_I]

This formula describes the approximated dependence of $q_1(B)$ on the magnetic field B. Notice that for $B \to \infty$, $q_1(B) \to$ -0.67 . The charge conservation condition $q_1 + 2q_2 = -1$ gives the interpolation for the two symmetric point charges $q_2(B)$ (see Fig. 4).

The interpolation function for the position z_2 of the two charges q_2 is given by

$$z_2(B) = \frac{1.0152}{1+1.0553\log\{1+(0.16148B)^2+(0.01403B)^4\}}, \qquad (28)$$

For all the range of magnetic fields considered, $z_2 < (R_{\rm eq}/2)$ where $R_{\rm eq}$ is the equilibrium distance obtained with variational calculations [6].

Finally the corresponding variances σ_1, σ_2 are fitted by

$$\sigma_1(B) = \frac{2.68367}{1+0.62449\log\{1+(0.69290B)^2+(0.03944B)^4\}}, \qquad (29)$$

$$\sigma_2(B) = \frac{3.70302}{1+3.4712\log\{1+(0.24225B)^2+(0.02064B)^4\}}. \qquad (30)$$

Notice that $\sigma_1 > \sigma_2 \,\forall\, B$. In relative units ($R_{\rm eq} = 1$), in general both variances decrease as functions of the magnetic field B.

Table VIII shows the intervals $[\rho_{0-}, \rho_{0+}]$, $[R_-, R_+]$ for which the relative difference of ρ_0, R and $E_{\rm coul}$ from their variational counterparts $\langle\rho\rangle$, $R_{\rm eq}$ and -E_I respectively are less than 30%.

3.3. Ion H_3^+

The molecule H_3^+ has been studied in presence of strong magnetic fields [17]. It was found that the most stable configuration of the system is parallel to the field. A relevant fact is that the state with the lowest total energy (ground state) depends on the intensity of the field B. It evolves from spin-singlet ${}^1\Sigma_g$ state for small magnetic fields B <0.2 a.u. to weakly-bound spin-triplet ${}^3\Sigma_u$ state for intermediate fields 0.2 $\lesssim B \lesssim$ 20 a.u. and eventually to spin-triplet ${}^3\Pi_u$ state for $B > 20$ a.u. The electrostatic study is carried out in the range of magnetic fields $100 \leq B \leq 18782$ a.u. For this system a superposition of four Gaussian functions was used to model the linear charge density $\Lambda(z)$ (see 17) defined by the z-profile of the corresponding ground state electronic distribution. The parameters of the model which approximate $\Lambda(z)$ for each magnetic field studied are summarized in the Table X.

TABLE IX. H_3^+ state ${}^3\Pi_u$. Parameters which approximate the electronic charge density $\Lambda(z)$ given as the sum of four Gaussian functions situated symmetrically with respect to the center of the molecular axis.

B (a.u.)	q_3 (a.u.)	z_3 (a.u.)	σ_3 (a.u.)	q_2 (a.u.)	z_2 (a.u.)	σ_2 (a.u.)
100	0.32950	0.20773	0.29793	0.17049	0.19735	0.27051
1000	0.32376	0.10027	0.12499	0.17624	0.09147	0.26435
10000	0.28318	0.04655	0.05925	0.21682	0.04649	0.14583
18782	0.25980	0.04575	0.05794	0.24019	0.03901	0.13892

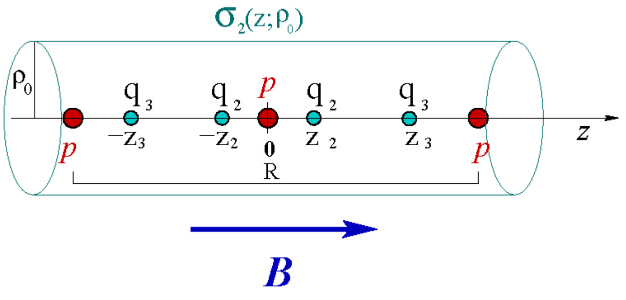

FIGURE 5. H_3^+ state ${}^3\Pi_u$: Electrostatic model for the ground state ${}^3\Pi_u$ of the two-electron molecular ion H_3^+ in parallel configuration with a uniform and constant strong magnetic field $\mathbf{B} = (0, 0, B)$.

The Coulomb interaction energy $E_{\rm coul}$ (in Rydbergs) is given by

$$E_{\rm coul} = 2(E_{p-p} + E_{p-e_1,e_2} + E_{e_1-e_2})\,, \qquad (31)$$

where

$$E_{p-p} = \frac{5}{R}\,, \qquad (32)$$

$$\begin{aligned} E_{p-e_1,e_2} &= \frac{2q_3}{|\frac{R}{2} - z_3|} + \frac{2q_3}{|\frac{R}{2} + z_3|} \\ &+ \frac{2q_2}{|\frac{R}{2} - z_2|} + \frac{2q_2}{|\frac{R}{2} + z_2|} + \frac{2q_3}{|z_3|} \\ &+ \frac{2q_2}{|z_2|} + \Phi\left(-\frac{R}{2}\right) + \Phi(0) + \Phi\left(\frac{R}{2}\right), \qquad (33) \\ E_{e_1-e_2} &= q_3\Phi(-z_3) \\ &+ q_3\Phi(z_3) + q_2\Phi(-z_2) + q_2\Phi(z_2). \qquad (34) \end{aligned}$$

As a function of the magnetic field B, the interpolating formula for the point charge q_3 located at $z = \pm z_3$ is given by

$$q_3(B) = \frac{1.88093 + 0.000179\,B}{5.66932 + 0.000728\,B}. \qquad (35)$$

This formula describes the approximated dependence of $q_3(B)$ on the magnetic field. Notice that for $B\to\infty$, $q_3(B)\to -0.24$, $z_2 < z_3 < (R/2)\,\forall\, B$. The charge conservation condition $2q_1 + 2q_2 = -1$ gives the interpolation for the two symmetric point charges $q_2(B)$ (see Fig. 5). The interpolation for the position z_i $(i = 2, 3)$ of the two point charges q_i is given by

$$z_3(B) = \frac{1.39441}{1 + 1.38206\log\{1 + (0.077667\,B)^2 + (0.009420\,B)^4\}}\,, \tag{36}$$

$$z_2(B) = \frac{0.19845}{1+0.20969\log\{1+(8.83244\times 10^{-5}B)^2+(0.004052B)^4\}}, \tag{37}$$

$z_3 > z_2\,\forall\, B$, finally the corresponding variances σ_3, σ_2 are fitted by

$$\sigma_3(B) = \frac{1.55132}{1 + 1.1988\log\{1 + (0.055867\,B)^2 + (0.010451\,B)^4\}}\,, \tag{38}$$

$$\sigma_2(B) = \frac{1}{1 + 0.95415\log\{1 + (0.019994\,B)^2\}}\left(\frac{1 + 1.76429\,B}{1 + B}\right). \tag{39}$$

TABLE X. H_3^+ state $^3\Pi_u$: Intervals $\Delta\rho_0 = [\rho_{0-}, \rho_{0+}]$ and $\Delta R = [R_-, R_+]$. The relative difference $\Delta E = (|E_{\text{coul}} - |E_I||)/(|E_I|)$ is less than 15% for all the range of magnetic fields considered.

$B(a.u.)$	$\Delta R\,(a.u.)$	$\Delta\rho_0\,(a.u.)$	$E_{\text{coul}}(Ry)$
100	[1.1R_{eq},1.15R_{eq}]	[1.1$\langle\rho\rangle$,1.15$\langle\rho\rangle$]	[-1.115E_I,-1.075E_I]
1000	[1.1R_{eq},1.15R_{eq}]	[1.1$\langle\rho\rangle$,1.15$\langle\rho\rangle$]	[-1.083E_I,-1.044E_I]
10000	[1.1R_{eq},1.15R_{eq}]	[1.1$\langle\rho\rangle$,1.15$\langle\rho\rangle$]	[-1.085E_I,-1.048E_I]
18782	[1.1R_{eq},1.15R_{eq}]	[1.1$\langle\rho\rangle$,1.15$\langle\rho\rangle$]	[-1.071E_I,-1.034E_I]

Table X shows the intervals $[\rho_{0-}, \rho_{0+}]$, $[R_-, R_+]$ for which the relative difference of ρ_0, R and E_{coul} from their variational counterparts $\langle\rho\rangle$, R_{eq} and -E_I respectively are less than 15%.

3.4. Ion H_4^{2+}

It is well known that in the absence of a magnetic field, the exotic molecular system H_4^{2+} does not exist. However, for $B \gtrsim 2000$ a.u. the system becomes bound in the linear configuration aligned along the magnetic line, the state with the lowest total energy (ground state) being realized by the spin-triplet $^3\Pi_u$ state [6]. For $\lesssim B \lesssim 2000$ a.u. the ground state corresponds to the repulsive spin-triplet $^3\Sigma_u$ state. As the molecule H_3^+, the electrostatic study is carried out in the range of magnetic fields $100 \leq B \leq 18782$ a.u. For this system a superposition of four Gaussian functions was used to model the linear charge density $\Lambda(z)$ (see 17) defined by the z-profile of the corresponding ground state electronic distribution. The parameters of the model which approximate $\Lambda(z)$ for each magnetic field studied are summarized in the Table XI.

The Coulomb energy E_{coul} (in Rydbergs) is given by

$$E_{\text{coul}} = 2(E_{p-p} + E_{p-e_1,e_2} + E_{e_1-e_2})\,, \tag{40}$$

where

$$E_{p-p} = \frac{1}{R_1} + \frac{2}{R_2} + \frac{2}{R_1 + R_2} + \frac{1}{R_1 + 2R_2}\,, \tag{41}$$

$$\begin{aligned} E_{p-e_1,e_2} = {} & \frac{2q_2}{|\frac{R_1}{2} + R_2 - z_2|} + \frac{2q_2}{|\frac{R_1}{2} + R_2 + z_2|} \\ & + \frac{2q_2}{|\frac{R_1}{2} - z_2|} + \frac{2q_2}{|\frac{R_1}{2} + z_2|} + \frac{2q_3}{|\frac{R_1}{2} + R_2 - z_3|} \\ & + \frac{2q_3}{|\frac{R_1}{2} + R_2 + z_3|} + \frac{2q_3}{|\frac{R_1}{2} - z_3|} + \frac{2q_3}{|\frac{R_1}{2} + z_3|} \\ & + \Phi\left(-\frac{R_1}{2}\right) + \Phi\left(-\frac{(R_1 + 2R_2)}{2}\right) + \Phi\left(\frac{R_1}{2}\right) \\ & + \Phi\left(\frac{(R_1 + 2R_2)}{2}\right), \end{aligned} \tag{42}$$

$$\begin{aligned} E_{e_1-e_2} = {} & q_2\Phi(-z_2) \\ & + q_2\Phi(z_2) + q_3\Phi(-z_3) + q_3\Phi(z_3). \end{aligned} \tag{43}$$

As a function of the magnetic field B, the interpolating formula for the point charge q_2 located at $z = \pm z_2$ is given by

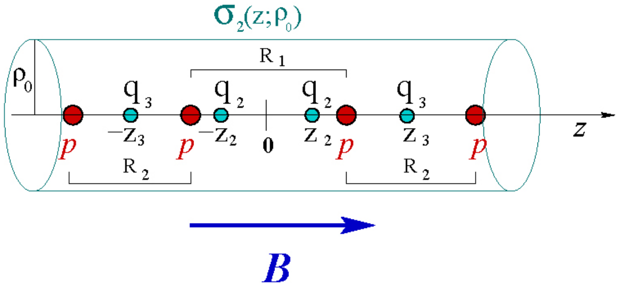

FIGURE 6. H_2^{2+} state $^3\Pi_u$: Electrostatic model for the ground state $^3\Pi_u$ of the two-electron molecular ion H_4^{2+} in parallel configuration with a uniform and constant strong magnetic field $\mathbf{B}=(0, 0, B)$.

TABLE XI. H_4^{2+} ground state. Parameters which approximate the electronic charge density $\Lambda(z)$ given as the sum of four Gaussian functions situated symmetrically with respect to the center of the molecular axis.

$B\,(a.u.)$	$q_2\,(a.u.)$	$z_2\,(a.u.)$	$\sigma_2\,(a.u.)$	$q_3\,(a.u.)$	$z_3\,(a.u.)$	$\sigma_3\,(a.u.)$
100	0.470132	0.098422	0.412104	0.029867	0.448526	0.30471
1000	0.462995	0.043426	0.212223	0.037004	0.192696	0.16069
10000	0.362742	0.021508	0.109725	0.137257	0.094341	0.12014
18782	0.111161	0.018676	0.058242	0.388838	0.083406	0.08205

$$q_2(B)=\frac{0.46730}{1+2.85481\log\{1+(3.2607\times10^{-5}B)^2\}}. \tag{44}$$

This formula describes the approximated dependence of $q_2(B)$ on the magnetic field. The charge conservation condition $2q_1+2q_2=-1$ gives the interpolation for the two symmetric point charges $q_3(B)$ (see Fig. 6). The interpolation for the position z_i $(i=2,3)$ of the two point charges q_i is given by

$$z_2(B)=\frac{0.59035}{1+1.36931\log\{1+(0.060622\,B)^2+(0.009125\,B^4\}}\,, \tag{45}$$

$$z_3(B)=\frac{3.06313}{1+1.60496\log\{(1+0.059972\,B)^2+(0.009441\,B)^4)}\,, \tag{46}$$

$z_3>z_2\,\forall\,B$, finally the corresponding variances σ_3,σ_2 are fitted by

$$\sigma_2(B)=\frac{5.65161}{1+2.76837\log\{1+(5.01591\times10^{-6}\,B)^2+(0.010304\,B)^4\}}\,, \tag{47}$$

$$\sigma_3(B)=\frac{1.67862}{1+1.65664\log\{1+(0.098154\,B)^2\}}\left(\frac{1+1.56427\,B}{1+B}\right). \tag{48}$$

TABLE XII. H_4^{2+} state $^3\Pi_u$: Intervals $\Delta\rho_0=[\rho_{0-},\rho_{0+}]$ and $\Delta R=[R_-,R_+]$. The relative difference $\Delta E=(|E_{\rm coul}-|E_I||/|E_I|)$ is less than 15% for all the range of magnetic fields considered.

$B(a.u.)$	$\Delta R\,(a.u.)$	$\Delta\rho_0\,(a.u.)$	$E_{\rm coul}(Ry)$
100	$[R_{\rm eq},1.05R_{\rm eq}]$	$[\langle\rho\rangle,1.05\langle\rho\rangle]$	$[-1.038E_I,-1.126E_I]$
1000	$[R_{\rm eq},1.05R_{\rm eq}]$	$[\langle\rho\rangle,1.05\langle\rho\rangle]$	$[-1.064E_I,-0.974E_I]$
10000	$[1.1R_{\rm eq},1.15R_{\rm eq}]$	$[1.1\langle\rho\rangle,1.15\langle\rho\rangle]$	$[-1.115E_I,-1.060E_I]$
18782	$[1.1R_{\rm eq},1.15R_{\rm eq}]$	$[1.1\langle\rho\rangle,1.15\langle\rho\rangle]$	$[-1.081E_I,-1.053E_I]$

Table XII shows the intervals $[\rho_{0-},\rho_{0+}]$, $[R_-,R_+]$ for which the relative difference of ρ_0, R and $E_{\rm coul}$ from their variational counterparts $\langle\rho\rangle$, $R_{\rm eq}$ and -E_I respectively are less than 15%.

3.5. Results

In the last sections simple electrostatic models of two electron molecular systems H_2, H_3^+, H_4^{2+} in a strong magnetic field were proposed to estimate the double ionization energy of the corresponding ground states, giving the following main results:

- Two electron molecular systems H_2, H_3^+, H_4^{2+} in a strong magnetic field are described by a heuristic model (electrostatic model of point charges and a charged cylinder) inspired in precise variational calculations.

- Compared with the double ionization energy obtained by precise variational calculations [4], the Coulomb energy $E_{\rm coul}$ has a relative error of less than 30%, 15% and 15% for the systems H_2, H_3^+, H_4^{2+} respectively for any value of the magnetic field considered.

4. Conclusions

Simple one-dimensional electrostatic models of one-(two) electron molecular systems H_2^+, H_3^{2+}, H_4^{3+} and H_2, H_3^+, H_4^{2+} in a strong magnetic field are presented to estimate the binding-(ionization) energy of the corresponding ground states, being accurate for the systems H_2^+, H_3^{2+}, H_4^{3+} in 2.5%, 5% and 5% respectively, and 15% for the two-electron systems H_3^+, H_4^{2+} (30% for H_2) compared with the corresponding variational calculations.

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$i.$ The conversion factor 1 a.u. $= 2.35 \times 10^9$ G is used in the present work.

$ii.$ The electronic distribution of H_2^+ is symmetric with respect to the plane whose normal is parallel to the magnetic field direction. For strong magnetic field the peak is situated in the middle between the charged centers.

$iii.$ From a classical point of view and considering only electromagnetic interactions, a closed system of charged particles in the vacuum can not be in a stable equilibrium. However, in quantum mechanics such equilibrium configuration can be realized.

$iv.$ As some confusion may arise at this point, we must emphasize that the present approach is a pure electrostatic model and not an effective one-dimensional approximation of the Schroedinger equation. In particular we do not define an effective Coulomb interaction.

$v.$ The infinitely-heavy charged centers located on a line parallel to the magnetic field direction.

$vi.$ The interactions between the electronic point charges $\{q_i\}$ are not taken into account due to the fact that the electron does not interact with itself.

$vii.$ The infinitely-heavy charged centers located on a line parallel to the magnetic field direction.

$viii.$ Where $\langle\rho\rangle \equiv \frac{\int \rho_2 |\Psi_{var}|^2 d\mathbf{r}_1 d\mathbf{r}_2}{\int |\Psi_{var}|^2 \, d\mathbf{r}_1 d\mathbf{r}_2}$.

$ix.$ The interactions between the point charges $\{q_i\}$ are not taken into account due to the fact that the electron e_1 does not interact with itself, but the interaction between the point charges $\{q_i\}$ and the cylindrical surface charge distribution σ_2 (associated with e_2) is taken into account.

$x.$ E_I denotes the double ionization energy obtained by variational calculations [6].

1. B.B. Kadomtsev and V.S. Kudryavtsev, *Pis'ma ZhETF* **15** (1971) 61; *Sov. Phys. JETP Lett. 13*, **9** (1971) 42.
2. M. Ruderman, *Phys. Rev. Lett.* **27** (1971) 1306.
3. A. Turbiner, J.C. López, and U. Solis H., *Pis'ma v ZhETF* **69** (1999) 800; *JETP Lett.* **69** (1999) 844.
4. A.V. Turbiner and J.C. López Vieyra, *Phys. Repts.* **424** (2006) 309.
5. A.V. Turbiner, *Astrophysics and Space Science* **308** (2007) 267.
6. A.V. Turbiner, N.L. Guevara, and J.C. Lopez Vieyra, *Phys. Rev. A* **81** (2010) 042503.
7. R.D. Benguria, R. Brummelhuis, P. Duclos, and S. Perez-Oyarzun, *J. Phys. B* **37** (2004) 23112320.
8. L.D. Landau, and E.M. Lifshitz, *Quantum Mechanics (Non-relativistic theory)* 3^{rd} Ed. p. 462.
9. R.P. Martínez-y-Romero *et al.*, *Rev. Mex. Fis.* **35** (1989) 617.
10. Nuñez-Yépez *et al.*, *Phys. Rev. A.* **39** (1989) 4307.
11. L.J. Boya, M. Kmiecik, and A. Bohm, *Physical Review A* **37** (1988) 3567.
12. Elliot y Loudon, *J. Phys. Chem. Solids* **15** (1960) 196.
13. M.W. Cole and M.H. Cohen, *Phys. Rev. Lett.* **23** (1969) 1238.
14. P.M. Platzman and M.J. Dykman, *Science* **284** (1999) 1967.
15. H. Olivares-Pilón, D. Baye, A.V. Turbiner, and J.C. López Vieyra, *J. Phys. B: At. Mol. Opt. Phys.* **43** (2010) 065702.
16. A.V. Turbiner, A.B.Kaidalov, and J.C. López Vieyra, [arXiv:0506019v1] [physics.atom-ph] .
17. A.V. Turbiner, N.L. Guevara, and J.C. López Vieyra, *Astrophysics and Space Science* **308** (2007) 499.