

“Molecular Properties” in Intense Magnetic Field

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The simple LCAO method has been used to find the effect of intense magnetic fields on the internuclear distance and the binding energy of the H_2^+ ion. The Spruch functions of the Hydrogen atom have been chosen as the basis. The results show that the magnetic pressure greatly affects the internuclear distance and the bonding energy. R_{eq} and E_{bind} as a function of α , the classical cyclotron radius of the electron, are given.

Introduction

Because strong magnetic fields are believed to exist in certain collapsed astronomical objects such as white dwarfs and neutron stars [1, 2] much attention has been directed in recent years to the energy levels of atoms under such conditions [3–14]. Spruch et al. [15] have proposed wave functions which could be used effectively to study the energy levels of atoms in magnetic fields of any strength. We report here on the effect of intense fields on the simplest molecule, i.e. the Hydrogen molecular ion.

Formulation and Results

In an external magnetic field, the Hamiltonian for the hydrogen molecular ion is

$$H = T - Z e^2/r_1 - Z e^2/r_2 + g_B + Z^2 e^2/R \quad (1)$$

with

$$g_B = - (i e \hbar B / 2 M c) \partial / \partial \varphi + (e^2 B^2 / 8 M c^2) \varrho^2 \quad (2)$$

where B is the applied uniform magnetic field and g_B is the magnetic interaction term defined in cylindrical coordinates. For convenience, the field has been taken along the molecular axis. The choice of the trial function depends on the BLP

model (Bohr-Landau-Pauli) of atoms in intense magnetic fields discussed in detail in [15]. The Spruch function for the ground state of the Hydrogen atom in the intense magnetic field is

$$\psi_{0m}(\varrho, r, \varphi) = N_m R_{0m}(\varrho) e^{-Z'r} \exp(i m \varphi) \quad (3)$$

in mixed spherical and cylindrical coordinates. The distance has been taken in atomic units.

The function $R_{0m}(\varrho)$ is the ground state Landau function [16] which is an eigen function of the free particle Hamiltonian $T + g_B$ and is given by

$$R_{0m}(\varrho) = (2/m!)^{1/2} \exp(-\varrho^2/2\alpha^2) \varrho^m / \alpha^{m+1}, \quad (4)$$

where α is the classical cyclotron radius of the electron and is given by $\alpha = (2c\hbar/eB)^{1/2}$. The ground state Landau energy, E_L , is degenerate in the magnetic quantum number, m , and is given by

$$E_L = \hbar^2 / M \alpha^2 = (a_0/\alpha)^2 e^2 / a_0. \quad (5)$$

The normalisation constant in (3) can be shown to be [15]

$$N_m^{-2} = 2\pi \alpha^2 Z' \gamma(m+2) U(m+2, 2, Z'^2 \alpha^2), \quad (6)$$

where $U(a, b, x)$ is the confluent Hypergeometric function of the second kind [18].

For the ground state of H_2^+ the simplest trial function could be assumed to be

$$\psi = C_1 \psi_{0m}(\varrho_1, r_1, \varphi_1) + C_2 \psi_{0m}(\varrho_2, r_2, \varphi_2). \quad (7)$$

Since the field has been taken along the molecular axis,

$$\varrho_1 = r_1 \sin \theta_1 = r_2 \sin \theta_2 = \varrho_2 \quad (8)$$

and

$$\psi = N_m R_{0m}(\varrho_1) e^{im\varphi_1} [C_1 e^{-Z'r_1} + C_2 e^{-Z'r_2}]. \quad (9)$$

The variation method leads to

$$E = E_L + E_H^m - (J + K)(1 + S) + Z^2/R, \quad (10)$$

where

$$S = N_m^2 \int R_{0m}^2(\varrho_1) e^{-Z'(r_1+r_2)} d\mathbf{r}, \quad (11)$$

$$J = Z N_m^2 \int R_{0m}^2(\varrho_1) e^{-2Z'r_1} / r_2 d\mathbf{r}, \quad (12)$$

$$K = Z N_m^2 \int R_{0m}^2(\varrho_1) e^{-Z'(r_1+r_2)} / r_2 d\mathbf{r}, \quad (13)$$

and E_H^m is the energy of the Hydrogen atom in the same field. Assuming that the Landau energy merely enters to define an energy reference level, the binding energy is

$$E_{bind} = - (J + K)(1 + S) + Z^2/R. \quad (14)$$

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After transforming to elliptical coordinates, with $m=0$, making the φ -integration and the following substitution,

$$y = R/\alpha; \quad x^2 = (y^2/4)(\mu^2 - 1) \quad (15)$$

the integrals (11)–(13) become

$$S = 2\pi N_0^2 y \alpha \int [I(x) X [2\mu^2/x + 1/x^3] - 1/x] \cdot X e^{-Z'y\alpha\mu} dx/\mu, \quad (16)$$

$$K = 8\pi Z N_0^2 \int \frac{I(x)}{x} e^{-Z'y\alpha\mu} dx, \quad (17)$$

and

$$J = aK + bL, \quad (18)$$

where

$$L = 8\pi Z N_0^2 \int \frac{I(x)}{x} e^{-Z'y\alpha\mu} dx/\mu, \quad (19)$$

$$a = \langle e^{-Z'y\alpha\mu} \rangle, \quad b = \langle \mu e^{-Z'y\alpha\mu} \rangle, \quad (20)$$

and

$$I(x) = x e^{-x^2} \int_0^x e^{t^2} dt$$

is Dawson's integral [17].

Equation (18) may be justified by the fact that the value of "a" is found to be close to unity and that of "b" is small for the range of α and y studied.

The above integrals have been evaluated numerically by choosing the optimum values of Z' of the H-atom. The calculated R_{eq} and the corresponding E_{bind} are given in Table 1 and Figure 1.

Discussion and Conclusion

Even though the condensation of matter due to the presence of intense magnetic fields is known, the effect of such fields on the "molecular properties" such as the internuclear distance and the binding energy has been studied for the first time in a more quantitative manner. This was possible because of the effective choice of the trial function. The results clearly show that R_{eq} and E_{bind} depend sharply on the cyclotron radius of the electron α . A super strong magnetic field ties the electrons to the field lines so that their response to a Coulomb attraction

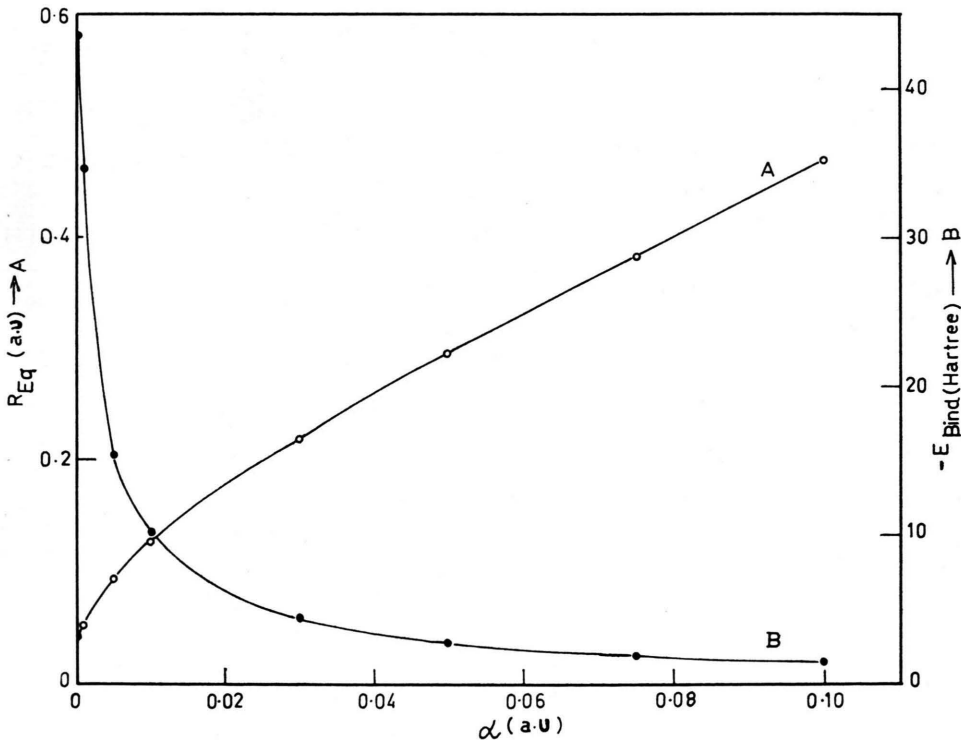


Fig. 1. The dependence of R_{eq} and E_{bind} on the cyclotron radius α .

Table 1. The calculated properties at various values of α .

α	Z'	S	Electronic Energy $-E_{el}$ (Hartree)	Binding Energy $-E_{bind}$ (Hartree)	Equilibrium Distance R_{eq} (au)
0.1	1.899	0.7120	9.2135	1.4831	0.469
0.075	2.190	0.7422	11.3684	1.9759	0.383
0.05	2.633	0.7776	15.0090	2.8882	0.295
0.03	3.239	0.8153	20.7686	4.4760	0.219
0.01	4.695	0.8694	38.3878	10.1655	0.128
0.005	5.695	0.8938	53.5252	15.3938	0.095
0.001	8.188	0.9293	103.8494	34.7252	0.052
0.0005	9.316	0.9389	129.4555	43.6235	0.042

is essentially restricted to a one dimensional motion parallel to the field. An immediate effect is a great increase in binding energy and a sharp decrease in the internuclear distance because the electron is much more likely to be found in between the two binding nuclei. Thus the calculation gives clear evidence for the formation of condensed state matter due to strong magnetic fields. The calculation can also be extended to magnetic chains of Hydrogen, which would throw more light on the stability of such chains.

Thus it appears that the Spruch functions are highly promising in exploring the properties of matter in intense magnetic fields.

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