One-electron Systems in Strong Magnetic Fields

Alexander Turbiner

(together with J.C. López V.)

Instituto de Ciencias Nucleares, UNAM, México

- Astrophysical Interest
  Neutron Stars Atmosphere (∼$10cm$) at $r \sim 5\,Km$
  $B_{surf} \sim 10^{12} - 10^{13}\,G$
  $T_{surf} \sim 10 - 100\,eV$

- Prediction: Formation of exotic *linear* molecular systems
  (Kadomtsev-Kudryavtsev '71, Ruderman '71)

  $\Rightarrow H_3,\ H_4, \ldots$ can exist in strong magnetic fields
  (Lai et. al. '92)

  $\Rightarrow H_3^{(2+)}$, $H_4^{(3+)}$ can exist in strong magnetic fields $B > 10^{11}\,G$ and $B > 10^{13}\,G$, respectively

  (A. Turbiner, J.C. López and U. Solís, '99)
  (J.C. López. and A. Turbiner '99)

Strong Magnetic Field

What does it mean 'strong' ?

Two natural *scales*:

- Magnetic fields for which μB is of order of magnitude or larger than the total energy of atoms and molecules
  (of the order of $Ry \equiv m_e e^4/2\hbar^2$)

$$B \gtrsim B_0 \equiv \frac{m_e^2 e^3 c}{\hbar^3} = 2.3505 \times 10^9\, G$$

- Magnetic fields for which the cyclotron energy of the electron is comparable with the electron mass

$$B \gtrsim B_{rel} = \frac{m_e^2 c^3}{\hbar e} = 4.414 \times 10^{13}\, G$$

relativistic effects can be essential

$\boxed{\textbf{Goal}}$

- Study of the bound state(s) in systems with one electron and a certain number of protons under a strong magnetic field:

$$(pe), \quad (ppe), \quad (pppe), \quad (ppppe)$$

and an existence of the corresponding chemical systems:

$$H, \quad H_2^+, \quad H_3^{(2+)}, \quad H_4^{(3+)}$$

- Linear configurations (linear chains) and non-linear configurations of the charged centers

$\boxed{\textbf{Method}}$

- Variational Calculation
- *Simple* and *unique* trial functions applicable for the whole range of accessible magnetic fields $(0 - 10^{13} G)$ which yield a high accuracy in energy

$\boxed{\textbf{Assumptions}}$

- Non-relativistic treatment – up to $B \simeq 4.414 \times 10^{13}\,G$
  (we neglect relativistic effects assuming that $\lesssim 10\%$ in E_{bind},
  by estimates of E. Salpeter *et al.*
  however, qualitative analysis gives $10^{-3}\%$ for H atom at
  $B = 10^{13}$G)

- Born-Oppenheimer approximation
  (infinitely heavy protons)

- Study of the ground state in general

- Mostly, parallel linear configuration (optimal)
  (all protons situated on a line parallel to the magnetic field line)

- Non-linear configuration $\Rightarrow$ Rotations around z axis $\Rightarrow$ energy grows

- We neglect a contribution stemming from spin degrees of freedom
  (change of reference point)

$\boxed{\boxed{\text{How to choose trial functions } \psi_{trial}?}}$

(A. Turbiner '80)

Given ψ_{trial}:

Potential

$$V_{trial} = \frac{\nabla^2 \psi_{trial}}{\psi_{trial}}$$

should reproduce:

- Coulomb singularities
- Asymptotic behavior at large distances — Harmonic Oscillator for $|x|, |y| \to \infty$

Hamiltonian

$$H_{trial} = -\nabla^2 + V_{trial}$$

Symmetries

Charged identical centers $\Rightarrow$

$$\psi_{trial} \quad \text{is (anti) symmetric under permutation of centers}$$

Ground State

$$\psi_{trial} \quad \text{has no nodes}$$

Variational energy calculation

We know the Hamiltonian for which ψ_{trial} is eigenfunction

$$H_{trial}\ \psi_{trial} = [p^2 + V_{trial}]\ \psi_{trial} = 0$$

then

$$\begin{aligned} E_{var} &= \int \psi^*_{trial}\ H\ \psi_{trial} \\ &= \int \psi^*_{trial}\ \underbrace{H_{trial}\ \psi_{trial}}_{=0} + \int \psi^*_{trial}\, (H - H_{trial})\, \psi_{trial} \\ &= 0 + \int \psi^*_{trial}\, (V - V_{trial})\, \psi_{trial}\ \text{``}+\ldots\text{''} \end{aligned}$$

- The variational energy is a sum of the first two terms of a certain perturbative series with perturbation $(V - V_{trial})$.
- Choosing different ψ_{trial} we can control the convergence of the series (if it exists) as well as the rate of convergence

In practice, Ψ_{trial} is taken to be *real* and

$$E_{var} = \frac{\int \Psi_{trial}\, (V - V_{trial})\, \Psi_{trial}}{\int \Psi^2_{trial}}$$

Technical Aspects

✤ The calculation involves two steps:

Numerical Multidimensional Integration and Minimization

- Different approaches (and routines) for the integration

  1. 1-d Gaussian integration CERN-LIB (multiple)
  2. Multidimensional Gaussian integration CERN-LIB
  3. Multidimensional MC integration CERN-LIB, NAG-LIB
  4. *Adaptive multidimensional integration NAG-LIB – final selection*

- Integration strategy

  1. Integration domain splits manually into subdomains to reproduce the integrand profile in optimal way
     (automatic adaptive integration fails)
  2. Convergence and rate of convergence estimation

- Different approaches (and routines) for minimization

  1. Genetic Algorithm
  2. Simulated Annealing
  3. *MINUIT CERN-LIB (Gradient, MC, Simplex, ...) – final selection*

✤ Computational resources:
IBM PC Pentium Pro 200 MHz

PART I

One-electron Systems. Linear Configuration

$$(pe), \quad (ppe), \quad (pppe), \quad (ppppe)$$

$$H, \quad H_2^+, \quad H_3^{(2+)}, \quad H_4^{(3+)}$$

Instructive Example
(A. Turbiner '82)

$$\boxed{\boxed{\text{Hydrogen in a magnetic field}}}$$

$$V = -\frac{2}{r} + \frac{B^2}{4}\rho^2, \qquad \rho^2 = x^2 + y^2.$$

Ground State

$$\psi_0 = \exp\left(-\alpha r - \beta B \rho^2/2\right)$$

α, β variational parameters

with

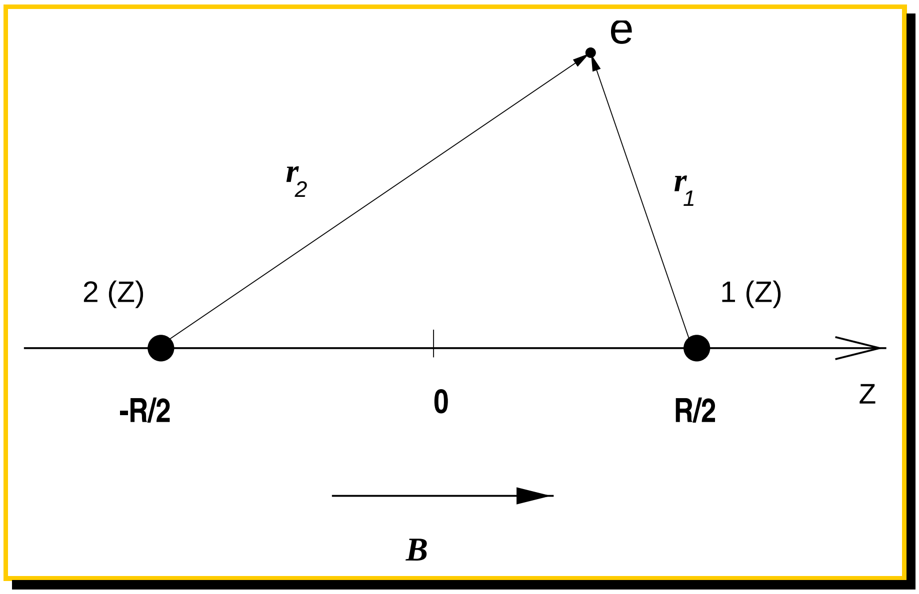
$$V_0 = \frac{\Delta\psi_0}{\psi_0} = -\frac{2\alpha}{r} + \frac{\beta^2 B^2}{4}\rho^2 + \underbrace{\frac{\alpha\beta B}{2}\frac{\rho^2}{r}}_{V-V_0}, \quad E_0 = -\alpha^2 + \beta B$$

Accuracy $\sim 10^{-4}$ **respect to the most accurate calculation:**

B(Gauss)	10^{11}	10^{12}	10^{13}
E_{var} (a.u.)	36.956	413.94	4232.6
E (Lai et al. '92)	36.929	413.57	4231.6

$\boxed{H_2^+ \text{ molecular ion (Parallel Configuration)}}$

(J.C.López, P. Hess and A. Turbiner '97)



$$V = -\frac{2}{r_1} - \frac{2}{r_2} + \frac{2}{R} + \frac{B^2\rho^2}{4}, \quad \text{(Ground State)}$$

$$\rho^2 = x^2 + y^2, \qquad l_z = 0$$

Bound States:

- $\boxed{1\sigma_g \texttt{ parity +}}$ (Ground State)
- $\boxed{1\sigma_u \texttt{ parity -}}$

$\boxed{\text{Trial Functions for } H_2^+}$

$\boxed{\text{I}}$

$$\psi_1 = \underbrace{e^{-\alpha_1(r_1+r_2)}}_{\text{Heitler-London}} \quad \underbrace{e^{-\beta_1 B\rho^2/4}}_{\text{Landau}}$$

α_1, β_1, R variational parameters

$$\begin{aligned} V_{trial}^{(1)} &= -2\alpha_1\left(\frac{1}{r_1}+\frac{1}{r_2}\right)+{\beta_1}^2\frac{B^2\rho^2}{4}+2{\alpha_1}^2-\beta_1 B \\ &\quad \underbrace{+\,2{\alpha_1}^2\vec{n_1}\cdot\vec{n_2}+\alpha_1\beta_1 B\rho^2\left(\frac{1}{r_1}+\frac{1}{r_2}\right)}_{V-V_{trial}} \end{aligned}$$

- ❖ $\alpha_1 = \beta_1 = 1$

  Coulomb singularities and Harmonic Oscillator behavior are reproduced exactly

- ❖ $\alpha_1, \beta_1 \neq 1$

  (anti) screening of the nuclear charges and of the magnetic field respectively

- ❖ We assume that the Heitler-London approximation can give a significant contribution for internuclear distances near equilibrium. Covalent coupling of the system to be verified *a posteriori*

$\boxed{\text{II}}$

$$\psi_2 = \underbrace{\left(e^{-\alpha_2 r_1} + \sigma e^{-\alpha_2 r_1}\right)}_{\text{Hund-Mulliken}} \; e^{-\beta_2 B\rho^2/4}$$

- α_2, β_2, R are variational parameters.
- We assume that this function can give a significant contribution for large internuclear distances
- Ionic coupling $H + p$ (to be verified *a posteriori*).

In order to describe both domains $R \simeq R_{eq}$ and $R \gg R_{eq}$:
we use *interpolations*

$\boxed{\text{III-1}}$ Non-linear Interpolation (most simple)

$$\psi_{3_1} = \underbrace{\left(e^{-\alpha_3 r_1 - \alpha_4 r_2} + \sigma e^{-\alpha_3 r_2 - \alpha_4 r_1}\right)}_{\text{Guillemin-Zener}} \; e^{-\beta_3 B\rho^2/4}$$

- If $\alpha_3 = \alpha_4$ then $\psi_{3_1} \to \psi_1$
- If $\alpha_4 = 0$ then $\psi_{3_1} \to \psi_2$
- Ionic $\leftrightarrow$ covalent coupling interpolation (verified *a posteriori*).
- $\alpha_3, \alpha_4, \beta_3, R$ are variational parameters

$\boxed{\text{III-2}}$ Linear Interpolation

$$\psi_{3_2} = A_1\psi_1 + A_2\psi_2$$

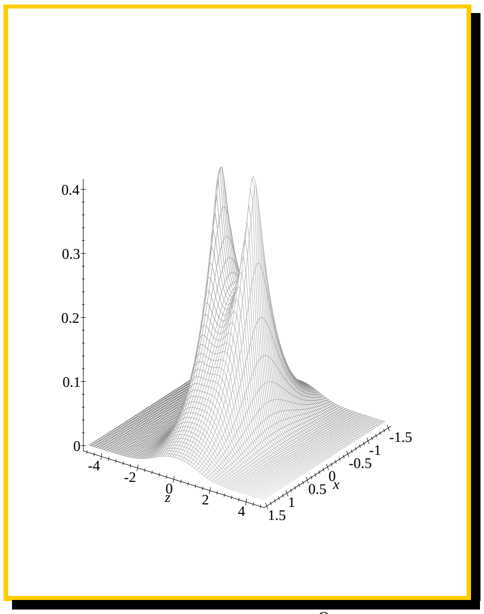
$\boxed{\text{IV}}$ Superposition of the two kinds of interpolation

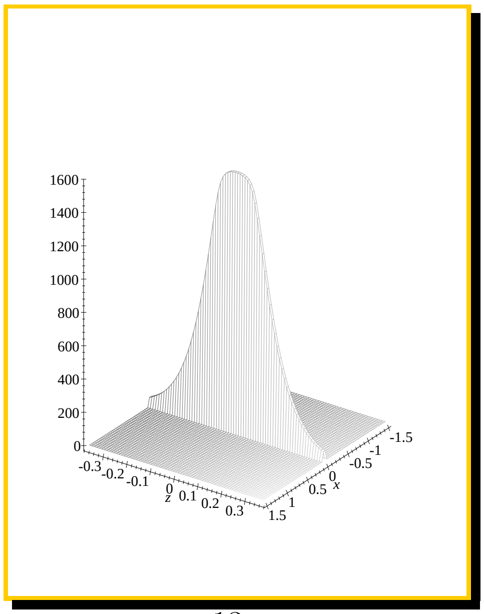
$$\psi_4 = A_{3_1}\psi_{3_1} + A_{3_2}\psi_{3_2}$$

- This single function describes the system in the range of magnetic fields up to $B = 4.414 \times 10^{13}\,G$
- 10 variational parameters
- ψ_4 gives the **lowest** total energies for the ground state compared with previous calculations (~ 50 calculations) for $B > 0\,G$ up to $B = 4.414 \times 10^{13}\,G$,
- For $B = 0$: Relative accuracy $\sim 10^{-5}$ (respect to the most accurate calculation)

Physical Phenomenon:

For $B \sim 5 \times 10^{11} G$ the coupling changes from ionic type to covalent type





$B = 10^9$ G $\qquad$ $B = 10^{13}$ G

Electronic density $|\Psi|^2$ for H_2^+

Comparison of the ground state $1\sigma_g$ of H_2^+ with results from other calculations. Equilibrium distance R, total energy E and binding energy $E_{bind} = B - E$

B (Gauss)	R (a.u.)	E (Ry)	E_{bind} (Ry)	Source
$B = 0$	1.9971	-1.20525	—	López et al. '97
	2.0000	-1.20527	—	Teller '30
	1.997	-1.20527	—	Wille '88
	1.997	-1.20526	—	Peek–Katriel '80
	2.0000	-1.205268	—	Wind '65
$B = 10^9$ G	1.9233	-1.15072	1.57616	López et al. '97
	1.924	-1.15072	1.57616	Wille '88
	1.921	—	1.5757	Peek-Katriel '80
	1.90	—	1.5529	Lai–Suen '82
$B = 10^{10}$ G	1.2464	1.08979	3.1646	López et al. '97
	1.246	1.09031	3.1641	Wille '88
	1.159	—	3.0036	Peek–Katriel '80
	1.10	—	3.0411	Lai–Suen '82
$B = 10^{11}$ G	0.593	35.0362	7.5080	López et al. '97
	0.593	35.0428	7.5013	Wille '88
	0.62	—	7.35	Lai–Salpeter '96
$B = 10^{12}$ G	0.283	408.300	17.141	López et al. '97
	0.278	408.566	16.875	Wille '88
	0.28	—	17.06	Lai–Salpeter '96
$B = 10^{13}$ G	0.147	4218.7	35.752	López et al. '97
	0.15	—	35.74	Lai–Salpeter '96

CONCLUSION (for H_2^+)

When the magnetic field grows:

- the system becomes more and more compact ($R_{eq} \simeq 2\, a.u.$ for $B = 0$ and $R_{eq} \simeq 0.15\, a.u.$ for $B = 10^{13}\, G$)
- the binding energy grows drastically up to $\simeq 36\, Ry \simeq 500\, eV$

In spite of the fact that the surface of neutron stars is characterized by very high temperatures ($\sim 10 - 100\, eV$), the system H_2^+ can exist (e.g. $E_{bind} \simeq 500\, eV$ for $B \simeq 10^{13}\, G$).

Now we proceed to the central point of the talk ...

PART II

$H_3^{(2+)}$ molecular ion (Parallel Linear Configuration – Linear Configuration aligned with the magnetic field)

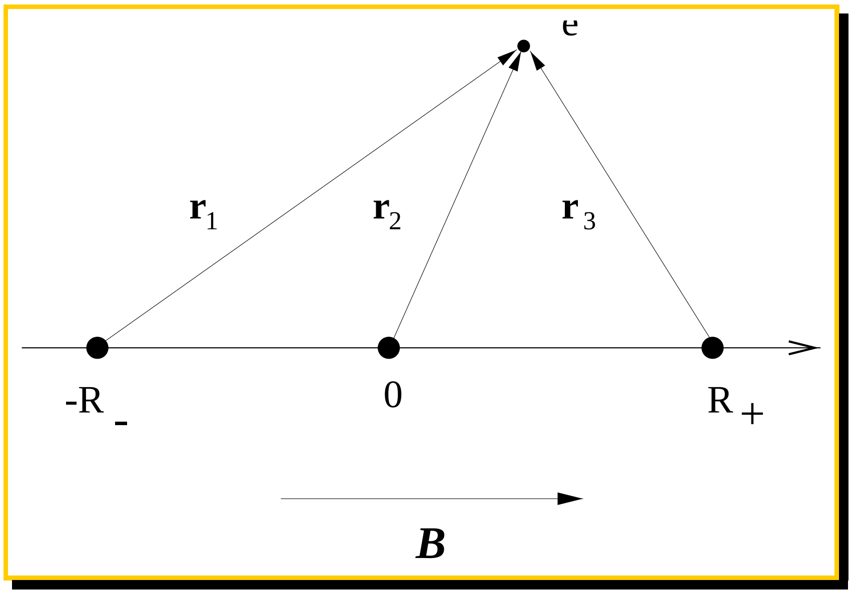
(First study of this system)

For $B \gtrsim 10^{11}\,G$ the system $(pppe)$ has a bound state which manifests existence of the exotic molecular ion $H_3^{(2+)}$

(A. Turbiner, J.C.López and U. Solis '99)

(*Without magnetic field* $H_3^{(2+)}$ *does NOT exist!*)

$H_3^{(2+)}$



$$V = \frac{2}{R_-} + \frac{2}{R_+} + \frac{2}{R_- + R_+} - \frac{2}{r_1} - \frac{2}{r_2} - \frac{2}{r_3} + \frac{B^2\rho^2}{4},$$

$$\rho^2 = x^2 + y^2, \qquad l_z = 0$$

$\boxed{\text{Trial functions for } H_3^{(2+)}}$

(An example)

$$\psi_1 = \underbrace{e^{-\alpha(r_1+r_2+r_3)}}_{\text{"Heitler-London"}} \quad \underbrace{e^{-\beta B\rho^2/4}}_{\text{Landau}}$$

❖ α, β, R variational parameters.

$$\begin{aligned} V^{(1)} &= \frac{\Delta\psi_1}{\psi_1} \\ &= 3\alpha^2 - B\beta - 2\alpha\left(\frac{1}{r_1} + \frac{1}{r_2} + \frac{1}{r_3}\right) + \frac{\beta^2 B^2 \rho^2}{4} \end{aligned}$$

$$+ 2\alpha^2\left[\frac{1}{r_1 r_2}\Big(\rho^2 + z(z+R_+)\Big) + \frac{1}{r_2 r_3}\Big(\rho^2 + z(z-R_-)\Big) + \right.$$

$$\left.\frac{1}{r_1 r_3}\Big(\rho^2 + (z-R_-)(z+R_+)\Big)\right] + \ \alpha\beta B\rho^2\left(\frac{1}{r_1} + \frac{1}{r_2} + \frac{1}{r_3}\right)$$

❖ Coulomb singularities and Harmonic Oscillator behavior for $\rho \to \infty$ are reproduced !

Trial Functions for $H_3^{(2+)}$

(collection)

$$\psi_1 = e^{-\alpha(r_1+r_2+r_3)}\ e^{-\beta B\rho^2/4}$$

$$\psi_2 = \left(e^{-\alpha_2 r_1} + e^{-\alpha_2 r_2} + e^{-\alpha_2 r_3}\right) e^{-\beta_2 B\rho^2/4}$$

$$\psi_3 = \left(e^{-\alpha_3(r_1+r_2)} + e^{-\alpha_3(r_1+r_3)} + e^{-\alpha_3(r_2+r_3)}\right) e^{-\beta_3 B\rho^2/4}$$

$$\psi_4 = \Big(e^{-\alpha_4 r_1-\alpha_5 r_2-\alpha_6 r_3} + e^{-\alpha_5 r_1-\alpha_4 r_2-\alpha_6 r_3}$$
$$+\, e^{-\alpha_4 r_1-\alpha_6 r_2-\alpha_5 r_3} + e^{-\alpha_6 r_1-\alpha_4 r_2-\alpha_5 r_3}$$
$$+\, e^{-\alpha_5 r_1-\alpha_6 r_2-\alpha_4 r_3} + e^{-\alpha_6 r_1-\alpha_5 r_2-\alpha_4 r_3}\Big) e^{-\beta_4 B\rho^2/4}$$

Superposition

$$\psi_{total} = A_1\psi_1 + A_2\psi_2 + A_3\psi_3 + A_4\psi_4$$

- ψ_1 corresponds to covalent coupling.
- ψ_2 corresponds to a coupling of the type $H + p + p$.
- ψ_3 corresponds to a coupling of the type $H_2^+ + p$.
- ψ_4 is a non-linear superposition of $\psi_{1,2,3}$

For $B < 10^{11} G$ the electronic total energy $E(R_+, R_-)$ has no minimum for finite values of R_+, R_-

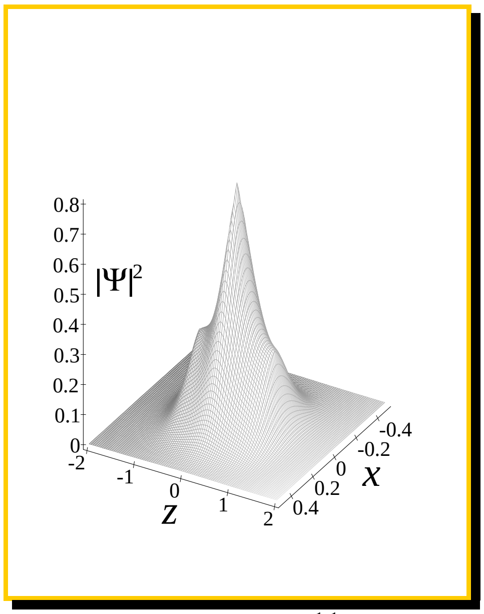
	$B=0$		$B=10^{11}$ G		$B=10^{12}$ G		$B=10^{13}$ G	
	E	R	E	R	E	R	E	R
H	-1.000	–	36.929	–	413.57	–	4231.6	–
H_2^+	-1.205	1.997	35.036	0.593	408.300	0.283	4218.662	0.147
$H_3^{(2+)}$	–	–	36.429	0.803	410.296	0.346	4220.090	0.165
Free e	–	–	42.544	–	425.441	–	4254.41	–

The results for the hydrogen atom are from Lai et al '92, for H_2^+ the results are from López et al. '97 and for $H_3^{(2+)}$ the results are from Turbiner et al. '99. The minimal total energy E and the equilibrium distance $R \equiv R_+ = R_-$ are in $a.u.$

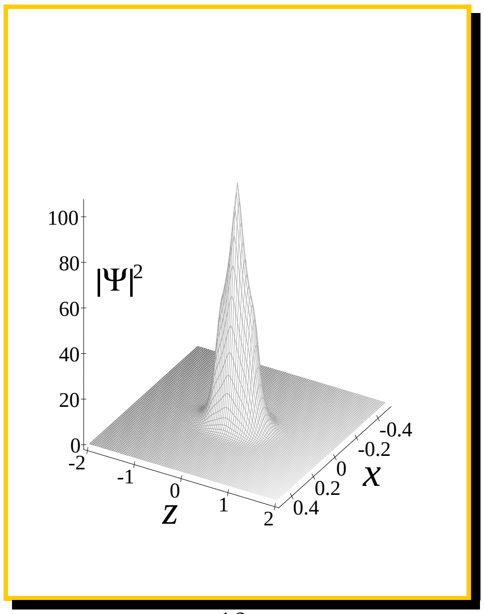
$$\boxed{H_3^{(2+)} \text{ can exist for } B \gtrsim 10^{11}\, G}$$

$$H_3^{(2+)} \to H_2^+ + p$$

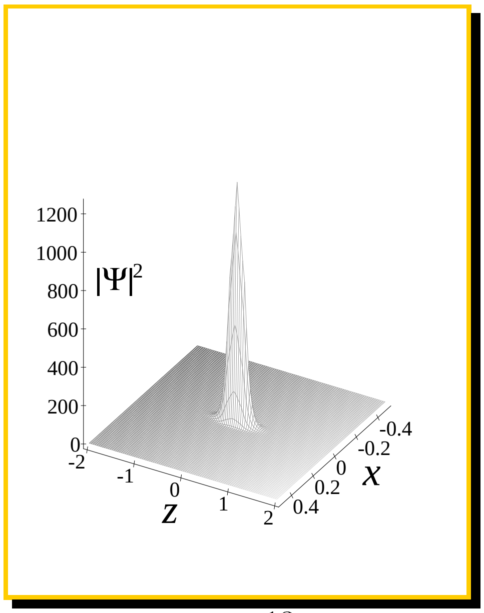
$$H_3^{(2+)} \nrightarrow H + p + p$$



$B = 10^{11}$ G

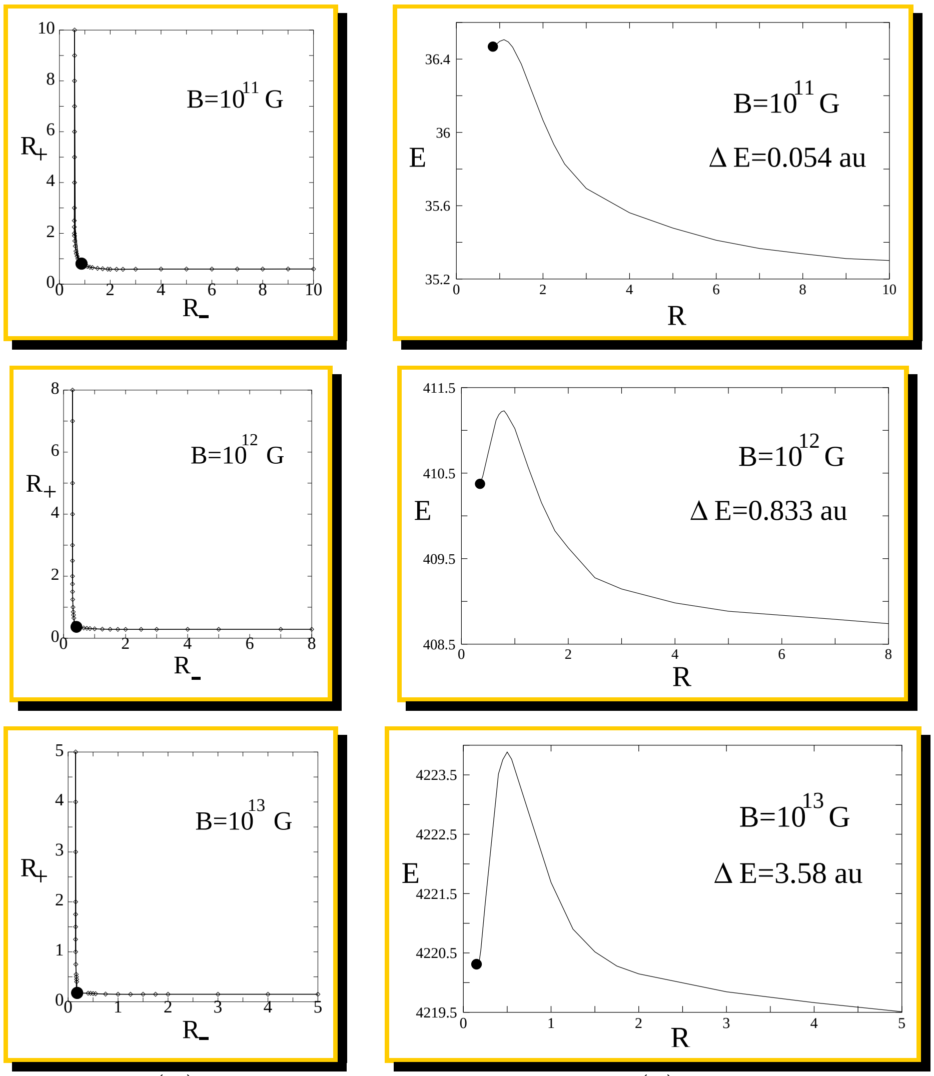


$B = 10^{12}$ G



$B = 10^{13}$ G

Dominant coupling for $H_3^{(2+)}$: covalent



(a) (b)

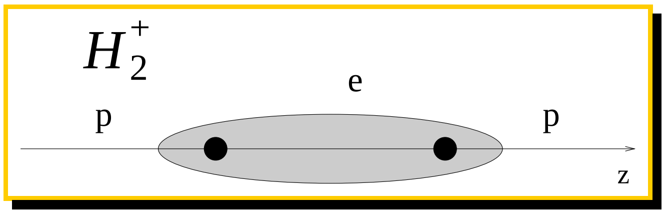
Valleys in the electronic potential energy surfaces (a) and their profiles (b) for magnetic fields $B = 10^{11}$ G, $B = 10^{12}$ G and $B = 10^{13}$ G. The minimum is indicated by a bullet.

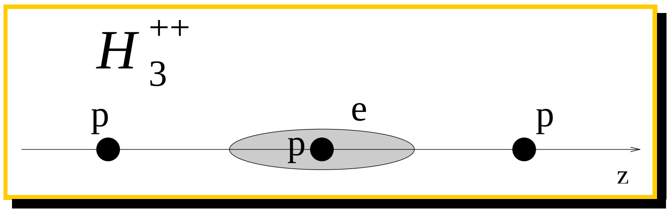
❖ Physical phenomenon:
In the contrary to the case of H_2^+, for $H_3^{(2+)}$ the expectation value of the longitudinal localization length of the electron is smaller than the "natural" size of the system

$$\boxed{\langle |z| \rangle < L}$$

where the "natural" size of the system L is defined as:

$$L = R \quad \text{for} \quad H_2^+ \ , \quad L = R_+ + R_- \quad \text{for} \quad H_3^{++}$$





B(Gauss)	H_2^+ $\langle\|z\|\rangle$	H_2^+ $L = R$	H_3^{++} $\langle\|z\|\rangle$	H_3^{++} $L = R_+ + R_-$
10^{11}	0.624	0.593	0.864	1.606
10^{12}	0.348	0.283	0.438	0.692
10^{13}	0.214	0.147	0.242	0.330

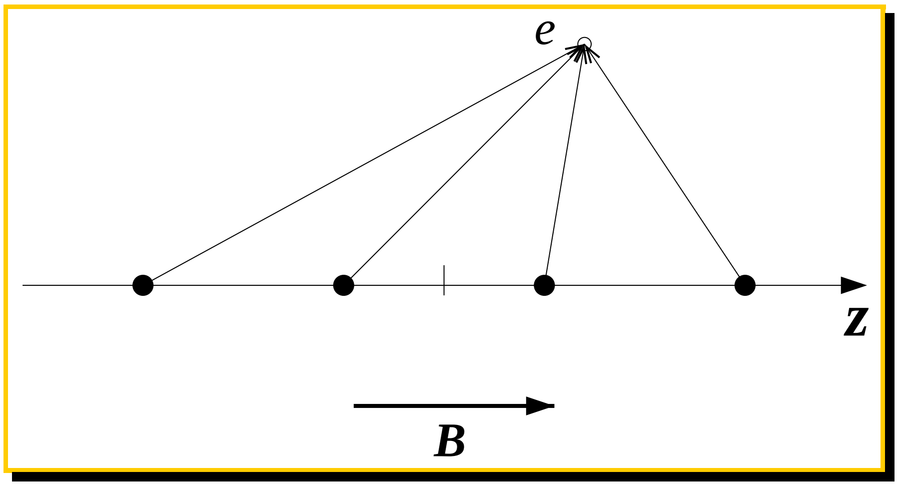
PART III

$\boxed{H_4^{(3+)} \text{ molecular ion (Parallel Configuration)}}$

(First study of this system)

For $B \gtrsim 10^{13}\,G$ the system $(ppppe)$ has a bound state manifesting the possible existence of the molecular ion $H_4^{(3+)}$

(J.C. López and A. Turbiner '99)



Trial functions

$\Psi_1 = e^{-\alpha_1 \left(\sum_{i=1}^{4} r_i\right) - \beta_1 B \rho^2/4}$ covalent coupling

$\Psi_2 = \left(\sum_{i=1}^{4} e^{-\alpha_2 r_i} \right) e^{-\beta_2 B \rho^2/4}$ ionic coupling $H + p + p + p$

$\Psi_3 = \left(\sum_{i<j} e^{-\alpha_3 (r_i + r_j)} \right) e^{-\beta_3 B \rho^2/4}$ ionic coupling $H_2^+ + p + p$

$\Psi_4 = \left(\sum_{i<j<k} e^{-\alpha_4 (r_i + r_j + r_k)} \right) e^{-\beta_4 B \rho^2/4}$ ionic coupling $H_3^{(2+)} + p$

$\Psi_{5-nls} = \left(\sum_{\{\alpha_1', \ldots \alpha_4'\}} e^{-\alpha_1' r_1 - \alpha_2' r_2 - \ldots - \alpha_4' r_4} \right) e^{-\beta' B \rho^2/4}$ Non-linear interpolation

Results for H (Lai et al. 96), H_2^+ (López et al. '97), $H_3^{(2+)}$ (Turbiner et al. '99) and $H_4^{(3+)}$ (López et al. '99): total energy E, longitudinal vibrational energy δE (measured from the bottom of the well) and the height of the barrier ΔE – all in Ry

B (Gauss)		H	H_2^+	$H_3^{(2+)}$	$H_4^{(3+)}$
	E	-1.000	-1.205	—	—
0	δE	—	0.0107	—	—
	ΔE	—	—	—	—
	E	36.996	35.036	36.429	—
10^{11}	δE	—	0.084	0.189	—
	ΔE	—	—	0.054	—
	E	413.94	408.30	410.296	—
10^{12}	δE	—	0.259	1.033	—
	ΔE	—	—	0.833	—
	E	4232.6	4218.665	4220.090	—
10^{13}	δE	—	0.714	2.406	—
	ΔE	—	—	3.58	—
	E	18747.4	18724.501	18723.88	18735.70
4.414×10^{13}	δE	—	1.233	4.27	—
	ΔE	—	—	6.5	0.4

$\boxed{\text{Vibrational longitudinal states for } H_3^{++}}$

(J.C.López and A. Turbiner '99)

- Study of the stability in the longitudinal direction
- Estimation of the lowest vibrational state position
- Harmonic approximation

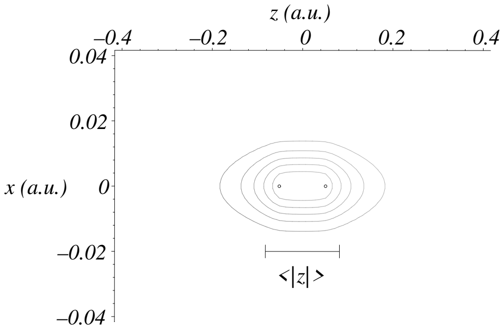
$$\delta E = \frac{1}{2}\hbar\omega_+ + \frac{1}{2}\hbar\omega_-$$

$\omega_\pm$ determined by curvatures around minimum of the well along the principal axes

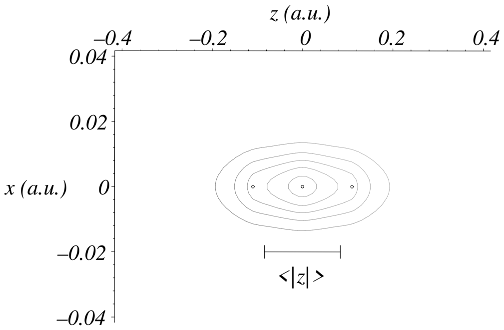
$$\mathcal{R}_+ = R_+ + R_- \ , \ \mathcal{R}_- = R_+ - R_-$$

For $B \gtrsim 10^{12}\, G$ the well is sufficiently deep to keep at least one longitudinal vibrational state

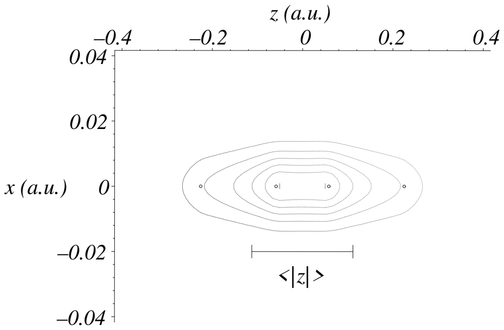
Electronic probability density $|\Psi|^2$ $(B = 4.414 \times 10^{13}\, G\ )$



(H_2^+)



$(H_3^{(2+)})$



$(H_4^{(3+)})$

Conclusion

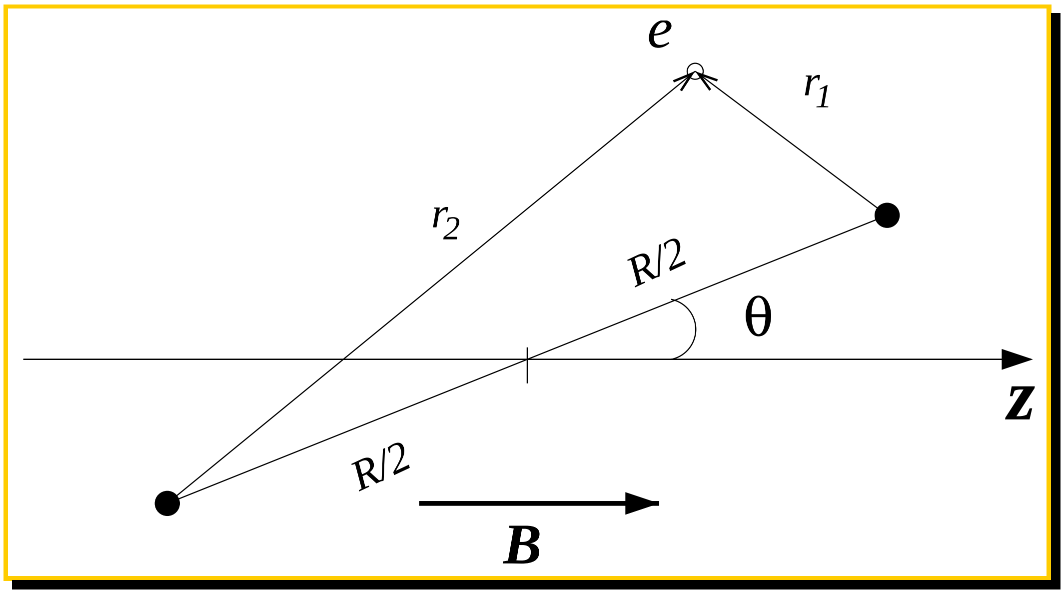
when B grows:

- Binding energy of $H,\ H_2^+,\ H_3^{(2+)}\ H_4^{(3+)}$ *grows*
- Natural size of the systems H_2^+ and $H_3^{(2+)}$ *decreases*
- H_2^+ has the *lowest* total energy E_{total} for $0 < B \lesssim 10^{13}\,G$
- $H_3^{(2+)}$ has the *lowest* E_{total} for $B \gtrsim 10^{13}\,G$
- Total energy E_{total} of $H_4^{(3+)}$ *larger* than E_{total} for H_2^+ and $H_3^{(2+)}$ but *less* than E_{total} for H
- Possible existence of the system $H_5^{(4+)}$ for $B > 10^{13}\,G$; but a reliable statement requires a consideration of relativistic corrections

PART IV

$\boxed{H_2^+\text{: inclined configuration}}$

(The molecular axis form an angle θ with magnetic field line)



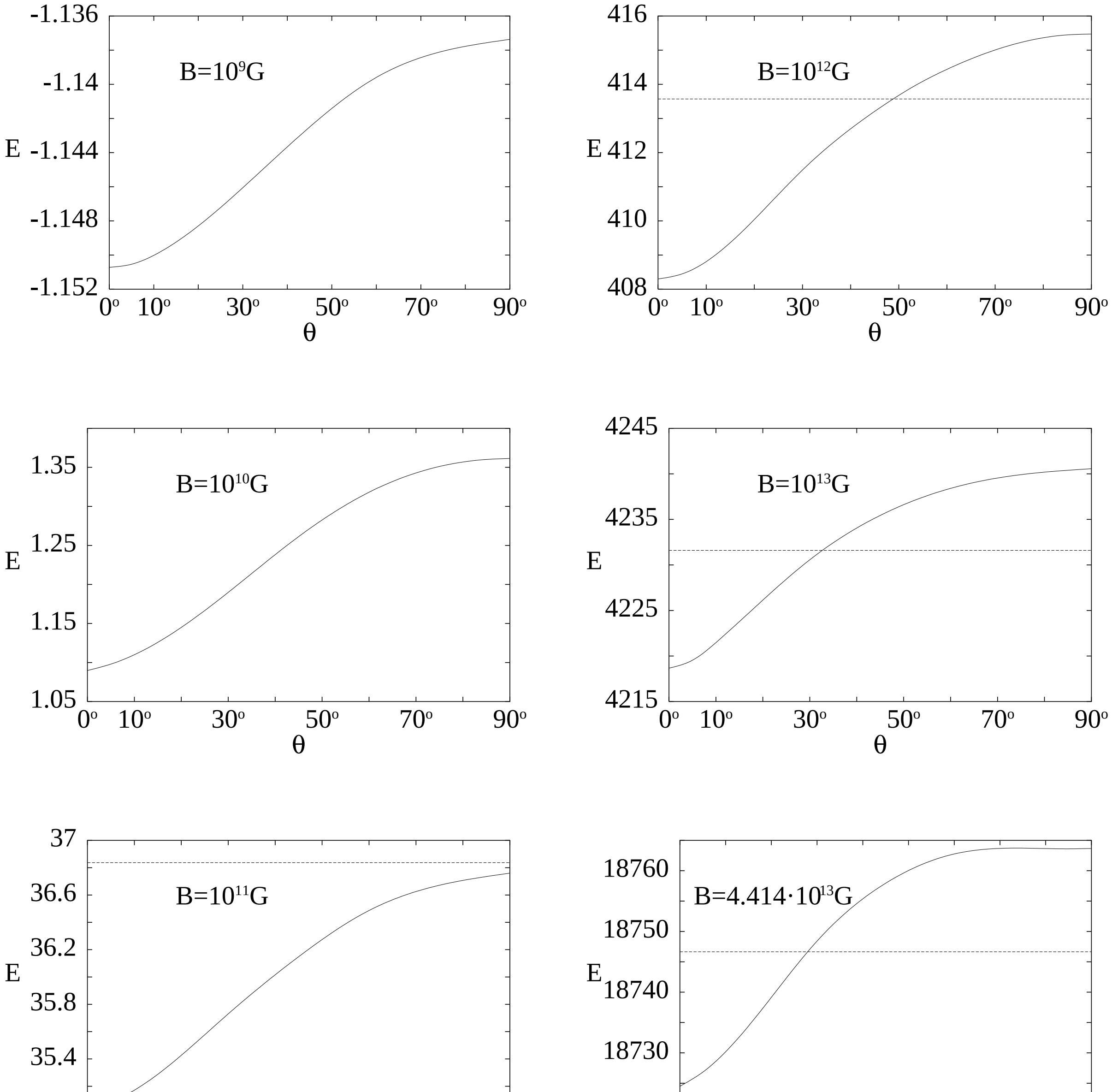
$$V = -\frac{2}{r_1} - \frac{2}{r_2} + \frac{2}{R} + \frac{B^2\rho^2}{4}, \quad \text{(Ground State)}$$

$$\rho^2 = x^2 + y^2, \qquad l_z = 0$$

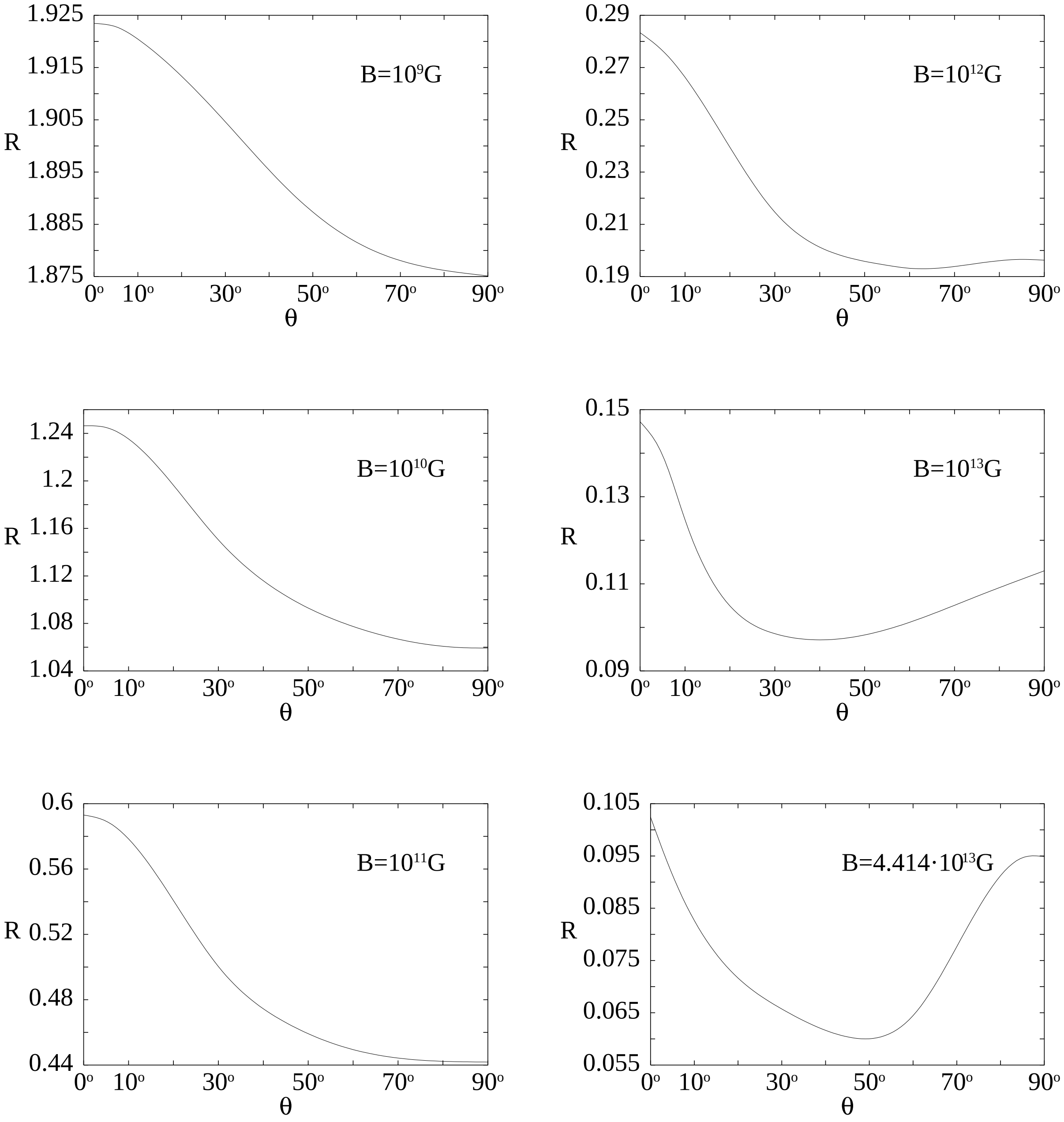
The same trial functions as for parallel configuration:

B	θ (deg)	E	E_b	R_{eq}	ζ
10^9G	0	-1.15072	1.5762	1.923	0.5
	(*)		1.5762	1.924	
	45	-1.14250	1.5679	1.891	0.5808
	90	-1.13737	1.5628	1.875	0.6380
	(*)		1.5638	1.879	
10^{10} G	0	1.08978	3.1646	1.246	0.5
	(*)		3.1641	1.246	
	45	1.26129	2.9931	1.103	0.5958
	90	1.36136	2.8931	1.059	0.6621
	(*)		2.8992	1.067	
10^{11} G	0	35.0362	7.5080	0.5931	0.5
	(*)		7.5013	0.593	
	45	36.1484	6.3957	0.4660	0.6237
	90	36.7600	5.7841	0.4418	0.7064
	(*)		5.6818	0.428	
10^{12}G	0	408.300	17.141	0.2833	0.5
	(*)		16.875	0.278	
	45	413.209	12.232	0.1980	0.6894
	90	415.472	9.9694	0.1963	0.8034
	(*)		4.5580	0.148	
10^{13} G	0	4218.67	35.749	0.1472	0.5
	45	4235.44	18.976	0.0974	0.8277
	90	4240.56	13.849	0.1130	0.9358
4.414×10^{13} G	0	18724.50	54.482	0.1024	0.5
	45	18757.94	21.040	0.0604	0.8160
	90	18763.67	15.318	0.0949	0.9797

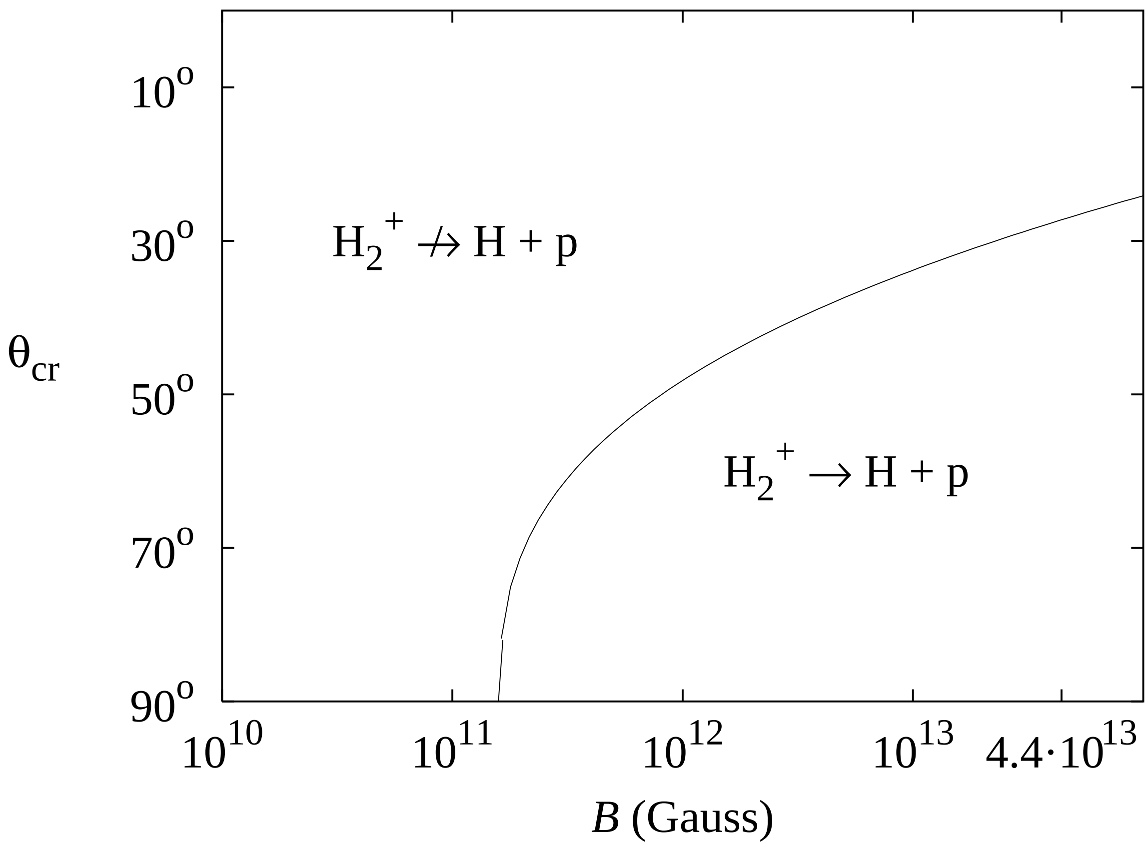
H_2^+ inclined configuration



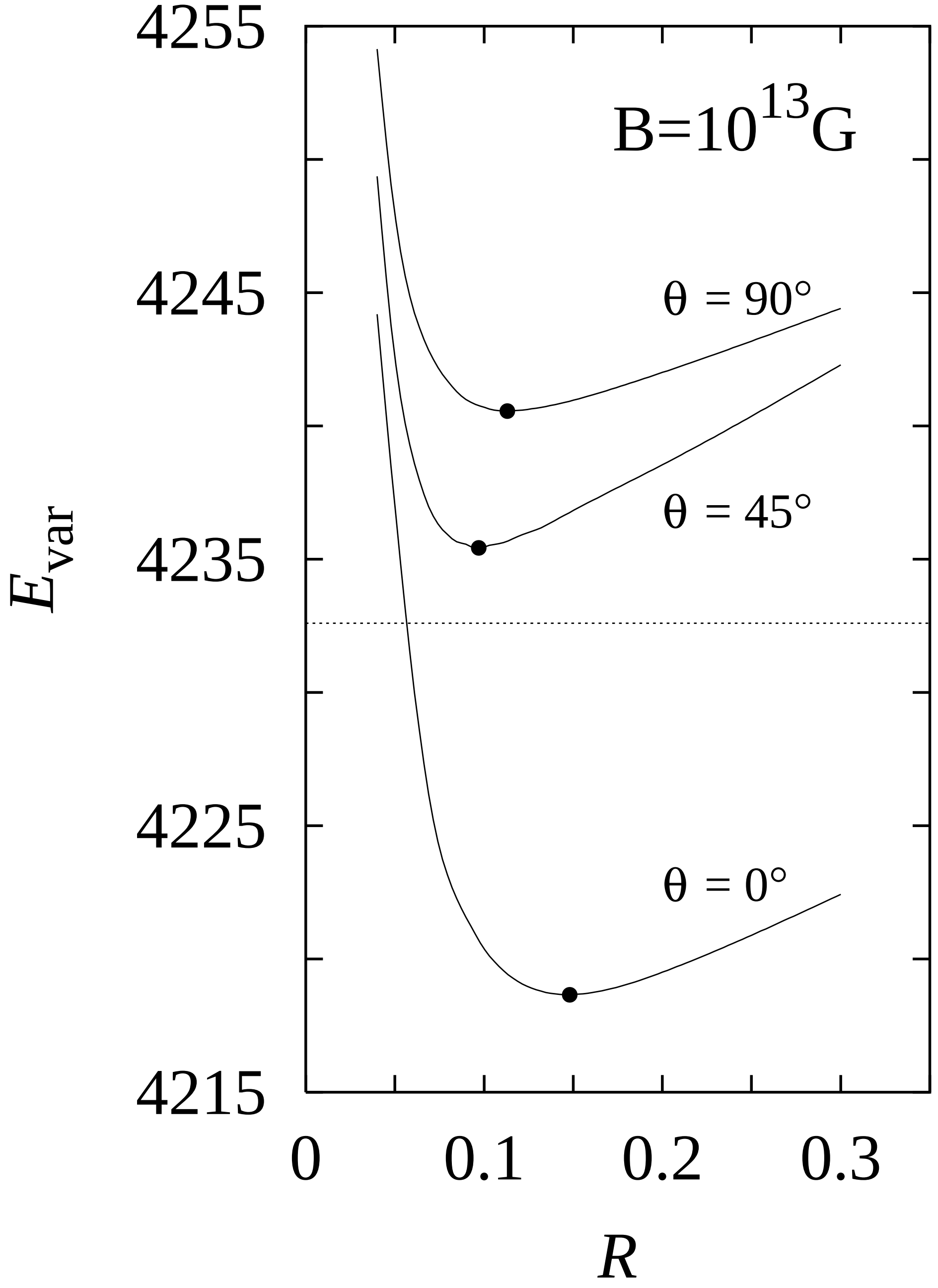
H_2^+ total energy as function of the inclination angle. Horizontal line is the total energy of H-atom



H_2^+ equilibrium distance as function of the inclination angle



H_2^+: domains of dissociation $\Leftrightarrow$ non-dissociation

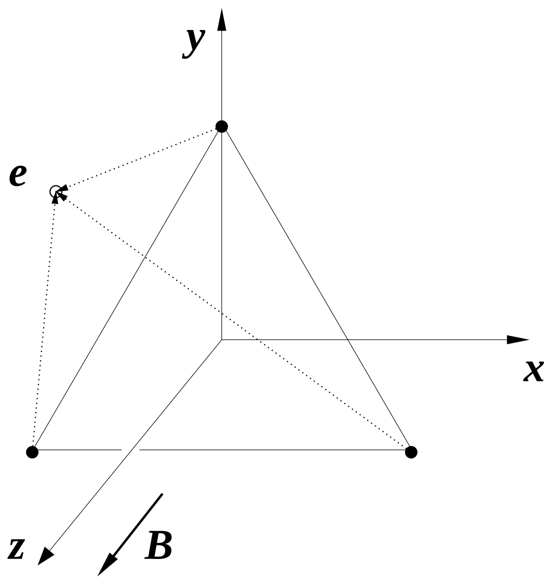


H_2^+ electronic curves for $B = 10^{13}$ G

PART V

H_3^{++} in a triangular configuration

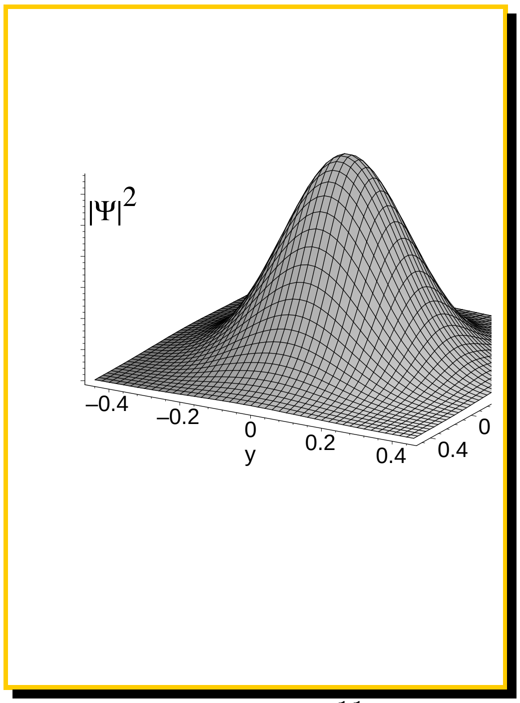
(The protons form an equilateral triangle perpendicular to the magnetic field line)



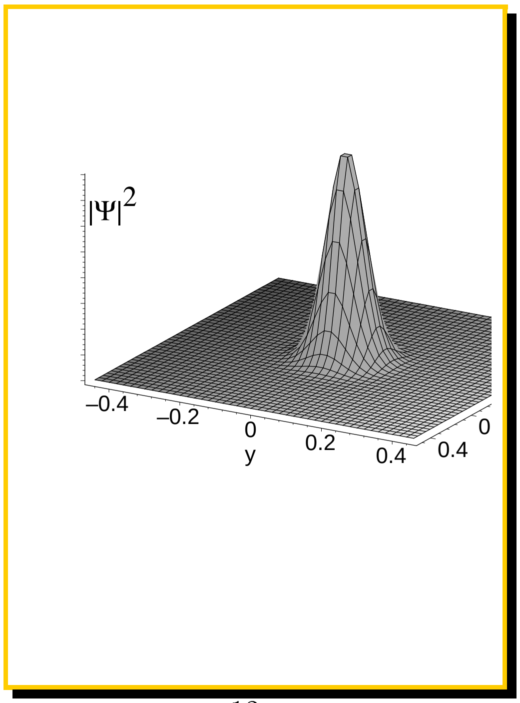
- There *exist* a minimum in $E(R)$ for $10^{11} \lesssim B \lesssim 4.414 \times 10^{13}\, G$, where R is the length of the triangle side
- Since the system ($pppe$) in a triangular configuration has a bound state this manifests existence of the $H_3^{(2+)}$ molecular ion in triangular configuration
- Internuclear distance $R \sim 0.6\, a.u.$ almost constant
- Binding Energy $E_{bind} \sim 2\, Ry$ almost constant
- $E_{bind}^{triangular} \; < \; E_{bind}^{lineal}$
- Triangular configuration unstable. Decay to linear configuration, etc...

B (Gauss)	E_{total}	E_{bind}	R_{eq}	$<\|z\|>$	$<\rho>$
		Triangular Configuration			
10^8	-0.8396	0.882	18.733		
10^9	-0.5249	0.950	3.1607		
10^{10}	2.7242	1.530	1.4010		
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

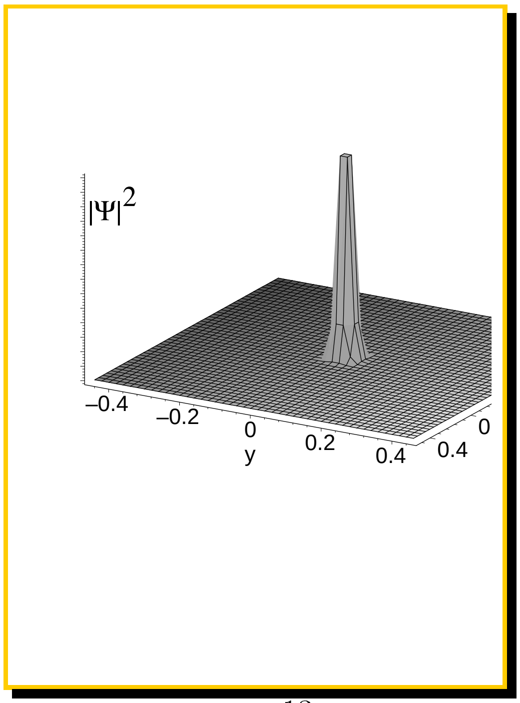
B (Gauss)	E_{total}	E_{bind}	R_{eq}	ζ
Triangular Configuration				
10^8	-0.8396	0.882	18.7325	0.5
10^9	-0.5249	0.9504	3.1607	0.5
10^{10}	2.7242	1.5302	1.40102	0.5016
10^{11}	40.5584	1.986	0.6235	0.5020
10^{12}	423.657	1.7845	0.6502	0.9452
10^{13}	4252.71	1.7055	0.75011	0.9973
4.414×10^{13}	18777.18	1.8033	0.6803	0.9987
Linear Configuration				
10^{10}	1.8464	2.4080	2.053	0.5
10^{11}	36.429	6.1151	0.803	0.5
10^{12}	410.296	15.144	0.346	0.5
10^{13}	4220.09	34.324	0.165	0.5
4.414×10^{13}	18723.88	55.103	0.110	0.5
Free Electron				
10^{11}	42.5441			
10^{12}	425.441			
10^{13}	4254.41			
4.414×10^{13}	18778.98			



$B = 10^{11}$ G

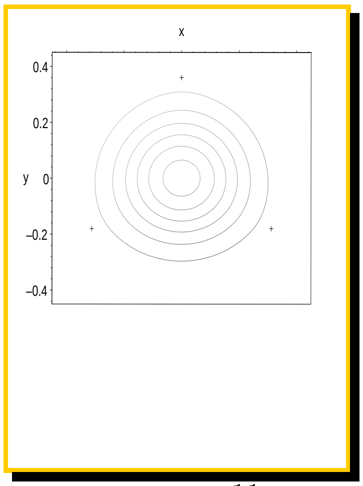


$B = 10^{12}$ G

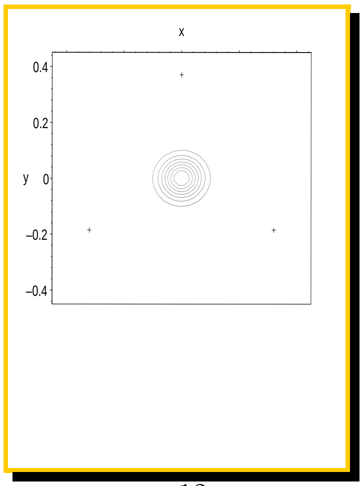


$B = 10^{13}$ G

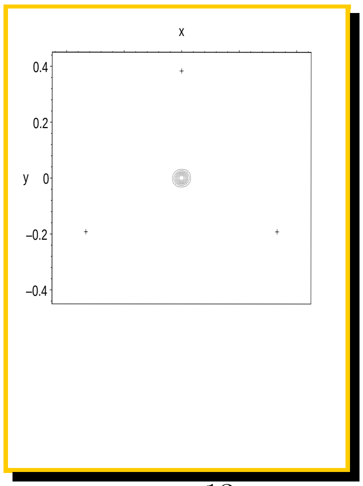
Dominant coupling for $H_3^{(2+)}$ in triangular configuration: covalent



$B = 10^{11}$ G



$B = 10^{12}$ G



$B = 10^{13}$ G

References

[1] M. Ruderman, in *Physics of Dense Matter*, edited by C.J.Hansen (Klumer, Dordrecht, 1974)

[2] V.K. Khersonskii, *Astrophys.Space Sci.* **98** 255 (1984); **117**, 47 (1985); *Sov. Astron.* **31**, 225 (1987)

[3] D. Lai, E. Salpeter, *Phys. Rev.* **A52**, 2611 (1995)

[4] D. Lai, E. Salpeter, *Phys. Rev.* **A53**, 152 (1995)

[5] M.A. Liberman, B. Johansson, *Soviet Phys. - Usp. Fiz. Nauk.* **165**, 121-142 (1995); *Sov. Phys. Uspekhi* **38**, 117-136 (1995) (English Translation).

[6] B.B. Kadomtsev, V.S. Kudryavtsev, *Soviet Phys. - Pis'ma ZhETF* **13**, 15, 61 (1971); *JETP Lett.* **13**, 9, 42 (1971) (English Translation)

[7] U. Kappes, P. Schmelcher, *Phys. Rev.* **A51** 4542 (1995)

[8] A. V. Turbiner, *Soviet Phys. - ZhETF* **79**, 1719-1745 (1980); *JETP* **52**, 868-876 (1980) (English Translation).

[9] A.V. Turbiner, *Soviet Phys. - Usp. Fiz. Nauk.* **144**, 35-78 (1984); *Sov. Phys. Uspekhi* **27**, 668-694 (1984) (English Translation).

[10] A.V. Turbiner, *Soviet Phys. - Yad. Fiz.* **46**, 204-218 (1987); *Sov. Journ. of Nucl. Phys.* **46**, 125-134 (1987) (English Translation).

[11] A.V. Turbiner, *Soviet Phys. - Pisma ZhETF* **38**, 510-515 (1983); *JETP Lett.* **38**, 618-622 (1983) (English Translation).

[12] A.V. Turbiner, Ph.D. Thesis, ITEP, Moscow, 1989

[13] E. Teller, *Zs. f Phys.* **61**, 458 (1930); E.A. Hylleraas, *Zs. f Phys.* **71**, 739 (1931)

[14] U. Wille, *Phys. Rev.* **A38**, 3210-3235 (1988)

[15] J.M. Peek and J. Katriel, *Phys. Rev.***A21**, 413 (1980).

[16] H. Wind, *J. Chem. Phys.***42**, 2371 (1965)

[17] C.S. Lai and B. Suen, *Canadian J. Phys.* **55**, 609 (1977).