One-Two Electrons Molecular Systems in a Strong Magnetic Field

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A particular overview of one-two electron Coulomb systems made out of several protons and/or α-particles which might exist in a strong magnetic field

$$B \leq 4.414 \times 10^{13}\ G$$

Characteristic field

$$B_0 = 2.35 \times 10^{13}\ G$$

(in collaboration with J.C. Lopez Vieyra & N. Guevara)

$1e$:

$H, \ H_2^+ , \quad \underline{H_3^{2+}} , \ |H_4^{3+}$

$(HeH)^{2+} , \ |(H - He - H)^{3+} , \ (He - H - He)^{4+}$

$He^+ , \quad \underline{He_2^{3+}}$

$\left[Li^{2+} , \quad Li_2^{5+} \ldots \right]$

(the list is complete for $B \le 4.414 \times 10^{13}$ G,
see *Physics Reports 424 (2006) 309-396*)

$2e$:

$H^- , \ H_2 , \ H_3^+ , \quad H_4^{2+}, \ H_5^{3+}, \ldots$

$(HeH)^+, \ (H - He - H)^{2+} , \ (He - H - He)^{3+} \ldots$

$He , \quad He_2^{2+}, \ He_3^{4+}, \ldots$

$\left[Li^+ , \quad Li_2^{4+} , \quad Li_3^{7+} \ldots \right]$

H-atom is stable but has a highest total energy among $1e - 2e$ systems

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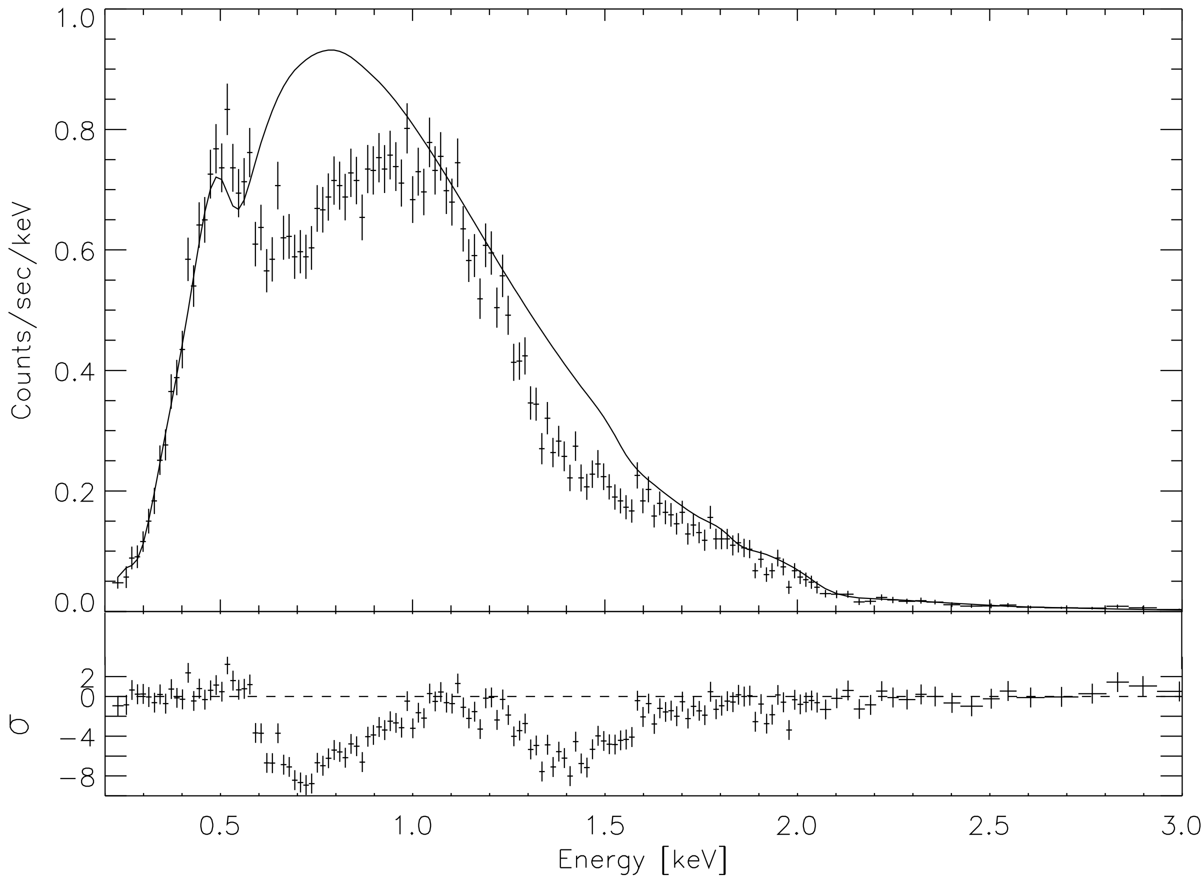
D. Sanwal, G.G. Pavlov, V.E. Zavlin and M.A. Teter (2002)
(First observation of absorption features)



Chandra + XMM-Newton data
(from Hailey & Mori, 2003)

Two absorption features:

$$E_1 = 730 \pm 100 \text{ eV} \qquad [53.7 \pm 7.4 Ry]$$

$$E_2 = 1400 \pm 130 \text{ eV} \qquad [102.9 \pm 9.6 Ry]$$

Why the problem is so difficult ?

- Highly-non-uniform asymptotics of potential at large distances
- A problem of several centers
- Weakly-bound states

$$E_{binding} << E_{total}$$

(e.g. for H_2^+ at $B = 10^{13}$ G the ratio is $\lesssim 10^{-2}$)

Method

❖ Variational Calculus

How to choose trial functions?

❖ Physical relevance (as many as possible physics properties should be encoded)

❖ Mathematical (computational) simplicity must **NOT** be a guiding principle

❖ Resulting perturbation theory should be convergent (see below)

Variational calculation

For chosen Ψ_{trial} a trial Potential

$$V_{trial} = \frac{\nabla^2 \Psi_{trial}}{\Psi_{trial}} \;,\; E_{trial} = 0$$

hence, we know the Hamiltonian for which the normalized Ψ_{trial} is eigenfunction

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

then

$$\begin{aligned} E_{var} &= \int \Psi^*_{trial}\ H\ \Psi_{trial} \\ &= \int \psi^*_{trial}\ \underbrace{H_{trial}\ \Psi_{trial}}_{=0} + \int \Psi^*_{trial}\,(H - H_{trial})\,\Psi_{trial} \\ &= 0 + \int \Psi^*_{trial}\,(V - V_{trial})\,\Psi_{trial}\ \text{``} + \ldots \text{''} \\ &\equiv E_0 + E_1 \text{``} + \ldots \text{''} \end{aligned}$$

- The variational energy is a sum of the first two terms of a certain perturbative series (PT) with perturbation $(V - V_{trial})$, $\Rightarrow$ smaller E_{var} does not guarantee faster convergence of PT

- How to calculate E_2 *in practice*? - in general, unsolved yet

HOW TO MEASURE DISTANCE $E_{var} - E_{exact}$?
still open question....

INSTRUCTIVE EXAMPLE

Hydrogen in a magnetic field (ground state)

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

$$\psi_0 = \exp\left(-\alpha r - \beta B \rho^2/4\right)$$

α, β variational parameters, where

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

Relative accuracy $\sim 10^{-4}$ *in total energy comparing to an accurate calculation.*

REMARK (AT '07):

$$\psi_0 = \exp\left(-\frac{ar + br^2 + c\rho^2 + dr\rho^2}{\sqrt{1 + \alpha r^2 + \beta \rho^2}}\right)$$

gives relative accuracy $\sim 10^{-7}$ in total energy for magnetic fields $0 < B < 4.414 \times 10^{13}$ G.

$$H: \quad E_b(10000\,a.u.) = 27.95\,Ry$$

$$He^+: \quad E_b(10000\,a.u.) = 78.43\,Ry$$

- Hydrogen atom in a magnetic field (ground state)

Howard-Hasegawa ('61) found leading term in asymptotics

$$E_{binding} \;=\; log^2 B + \dots \quad , \quad B \to \infty$$

at the Schwinger limit $B = B_{Schwinger} (\approx 2 \times 10^4 \, a.u.)$ the ratio

$$\frac{E^{exact}_{binding}}{log^2 B} \approx 1/3$$

asymptotics is delayed ...

There exists a striking relation between the *binding energies of the most bound one-electron systems made from $\alpha-$particles and made from protons:*

$$E_b^{He^+,\ He_2^{(3+)}} \approx 2\ E_b^{H_2^+,\ H_3^{2+}}$$

for $10^{11}\,G < B < 10^{14}\,G$

- For $B < 10^{12}\,G$ in l.h.s. E_b of He^+, otherwise E_b of the exotic He_2^{3+}
- For $B < 10^{13}\,G$ in r.h.s. E_b of H_2^+, otherwise E_b of the exotic H_3^{2+}

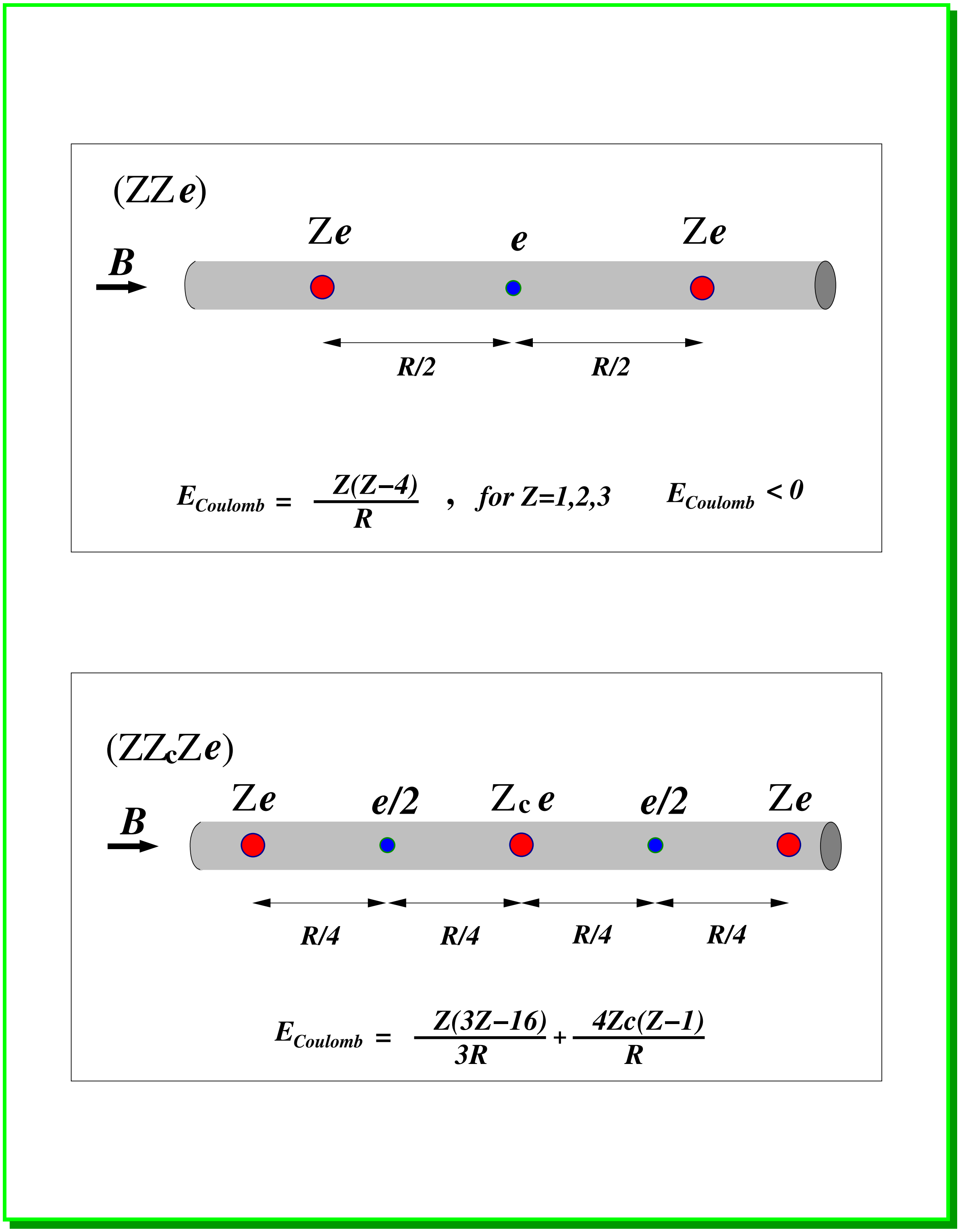
Summary

One-electron linear systems

Optimal configuration of linear H_2^+, H_3^{2+}, $H_4^{(3+)}$, $(HeH)^{2+}$ *and* $He_2^{(3+)}$ *is parallel, along magnetic field (when exist)*

when magnetic field grows:

- Binding energy of H, H_2^+, H_3^{2+}, H_4^{3+}, $(HeH)^{2+}$ and He_2^{3+} grows (when exist)
- Natural size of the systems $H_2^+, H_3^{2+}, (HeH)^{2+}$ and He_2^{3+} shrinks
- H_2^+ has the *lowest* E_{total} for $0 < B \lesssim 10^{13}\,G$ (made from protons)
- H_3^{2+} has the *lowest* E_{total} for $B \gtrsim 10^{13}\,G$ (made from protons)
- Possible existence of the system $H_5^{(4+)}$ for $B \gg 4.4 \times 10^{13}\,G$
- For $B \gtrsim 10^{12}\,G$ the exotic He_2^{3+} has the **lowest total energy** among systems made from protons and/or $\alpha-$particles
- **H_2^+ and linear H_3^{2+} binding energies $\equiv$ ionization energies at $B \sim 3 \times 10^{13}$ G coincide, both are $\sim 700\,$eV, while for He_2^{3+} and $(HeH)^{2+}$ it is $\sim 1400\,$eV**
- Something non-trial happens at the Schwinger limit $B \sim 4.414 \times 10^{13}$ G – many more exotic systems begin to exist


(ZZe)
Ze
e
Ze
B
R/2
R/2
E_Coulomb = Z(Z−4)/R , for Z=1,2,3   E_Coulomb < 0
(ZZcZe)
Ze
e/2
Zc e
e/2
Ze
B
R/4
R/4
R/4
R/4
E_Coulomb = Z(3Z−16)/3R + 4Zc(Z−1)/R

TWO ELECTRON SYSTEMS

The first step:

To study the Ground State $\Rrightarrow$ Existence

Phenomenon:

As magnetic field grows a change in quantum numbers of the ground state should occur (true level crossing)

The ground state sequence:

$$\begin{array}{ccccc} {}^1\Sigma_g & \rightarrow & {}^3\Sigma_u & \rightarrow & {}^3\Pi_u \\ m_l = 0 & & m_l = 0 & & m_l = -1 \\ m_s = 0 & & m_s = -1 & & m_s = -1 \end{array}$$

Typical for atomic systems a domain of ${}^3\Sigma_u$ ground state is absent

$B = 0$

Born-Oppenheimer ground state energies

H_2

$E_{BO} = -2.3469$ Ry (James and Coolidge, 15 parameters)

$E_{BO} = -2.3478$ Ry (Heidelberg group, $>$ 200 Gaussian orbitals)

$E_{BO} = -2.3484$ Ry *(A.T., N.Guevara, 14 parameters)* *

$E_{BO} = -2.3489$ Ry (**record calculations**, $\gtrsim$ 7000 J-C type functions)

H_3^+

(Lowest Linear Spin-Triplet State)

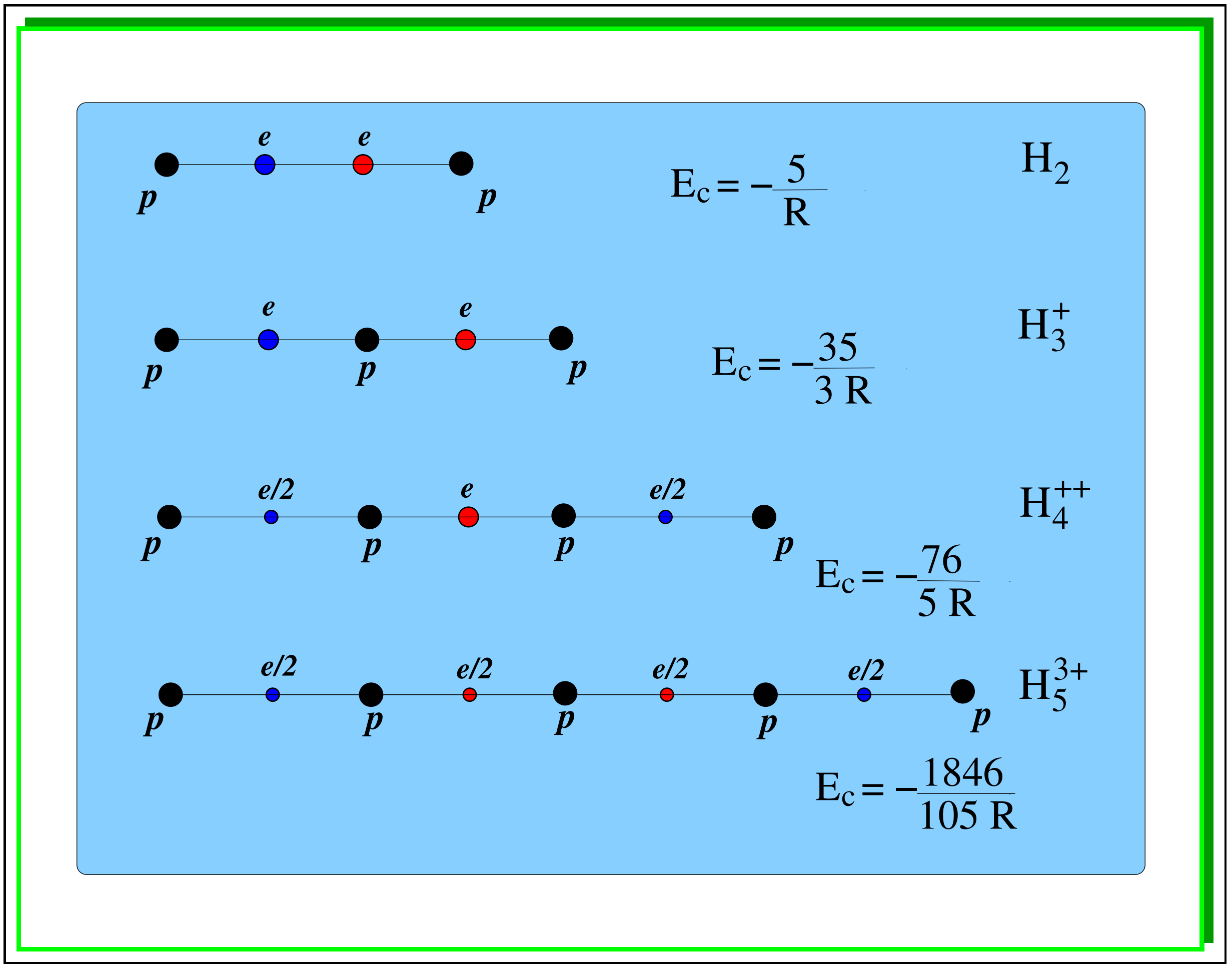
$E_{BO} = -2.2284$ Ry (Schaad et al, '74, CI)

$E_{BO} = -2.2298$ Ry *(A.T., J.C.Lopez V., N.Guevara, 22 parameters)* *

$E_{BO} = -2.2322$ (Clementi et al '91, CI + J-C type)

* Leading to the most accurate energy based on few-parametric trial functions.

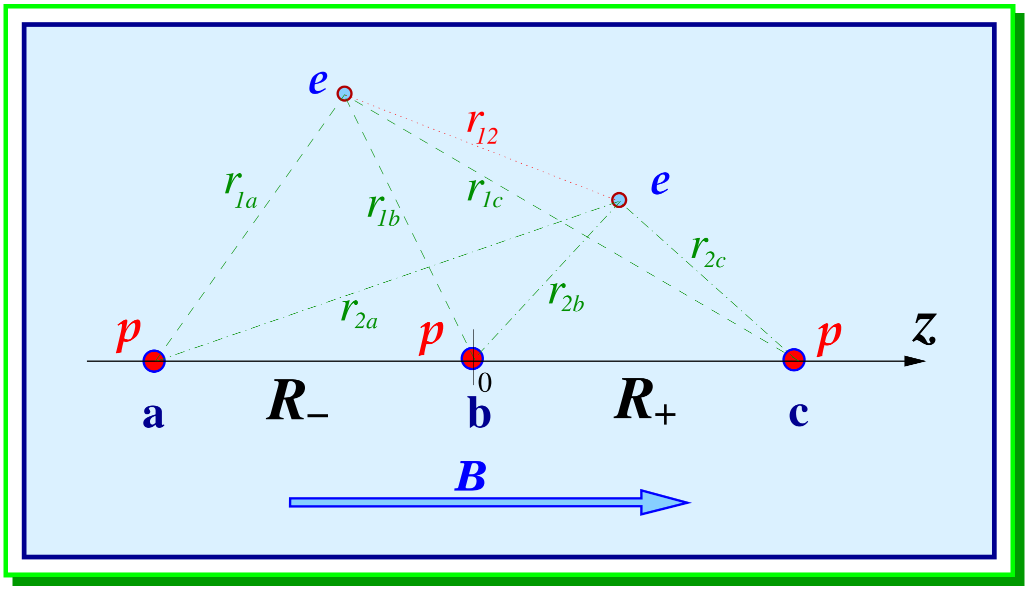
Electronic correlation appears in exponential form $exp(ar_{12})$ in our trial functions



p
e
e
p
$E_c = -\frac{5}{R}$
H_2
p
e
p
e
p
$E_c = -\frac{35}{3R}$
H_3^+
p
e/2
p
e
p
e/2
p
$E_c = -\frac{76}{5R}$
H_4^{++}
p
e/2
p
e/2
p
e/2
p
e/2
p
$E_c = -\frac{1846}{105R}$
H_5^{3+}

H_3^+ (A.T., N. Guevara, J.C. Lopez V. '06)

(linear, parallel configuration, the lowest states)



Basic trial function:

$$\psi^{(trial)} = (1+\sigma_e P_{12})$$
$$(1+\sigma_{_N} P_{ac})(1+\sigma_{_{N_a}} P_{ab}+\sigma_{_{N_a}} P_{bc})$$
$$\rho_1^{|m|} e^{im\phi_1}\ e^{\gamma r_{12}}\ \ e^{-\alpha_1 r_{1a}-\alpha_2 r_{1b}-\alpha_3 r_{1c}-\alpha_4 r_{2a}-\alpha_5 r_{2b}-\alpha_6 r_{2c}-B\beta_1\frac{\rho_1^2}{4}-B\beta_2\frac{\rho_2^2}{4}}$$

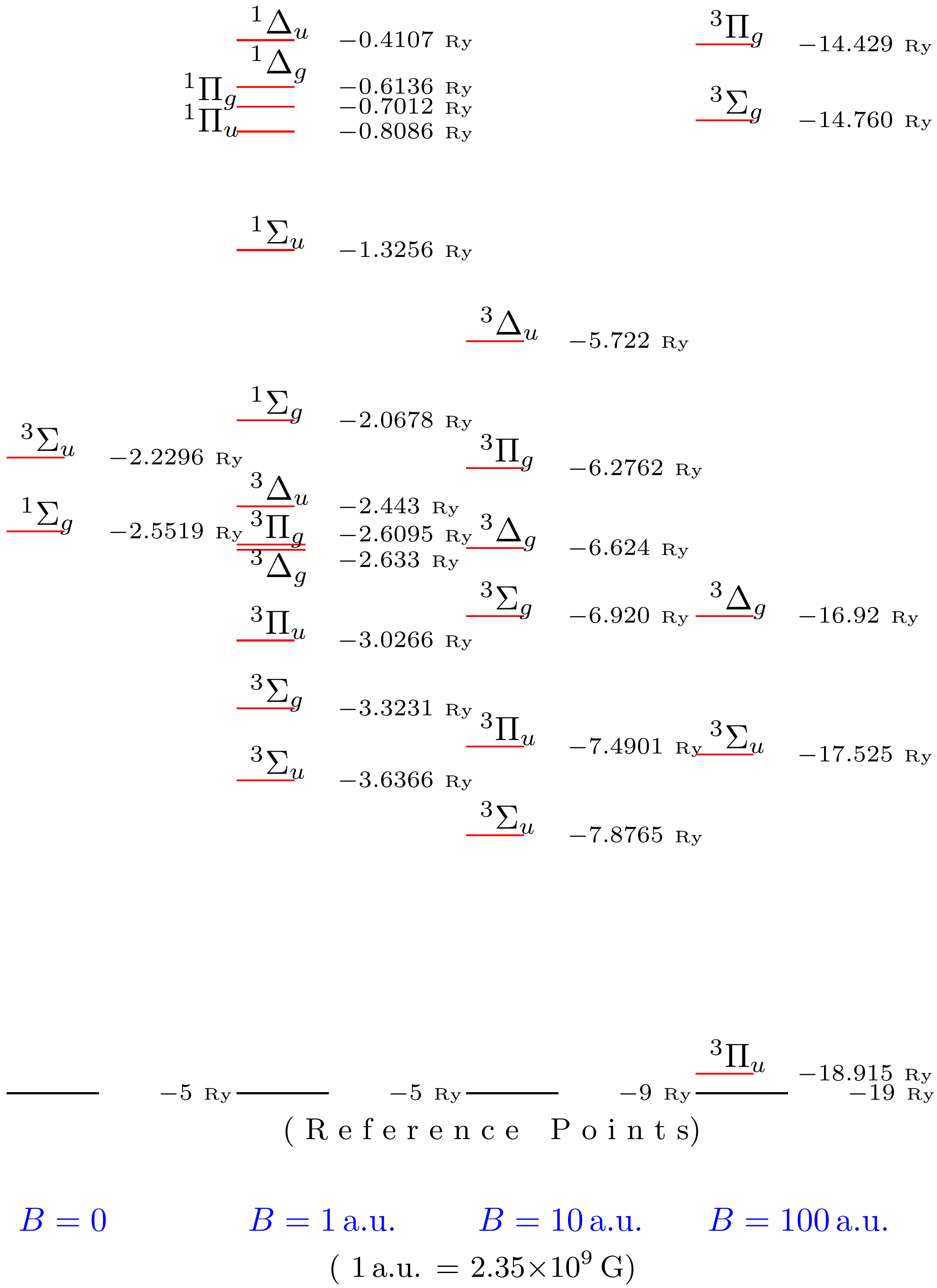
and its possible degenerations.

Optimal configuration:

linear, parallel, symmetric $R_+ = R_-(=R_{eq})$,

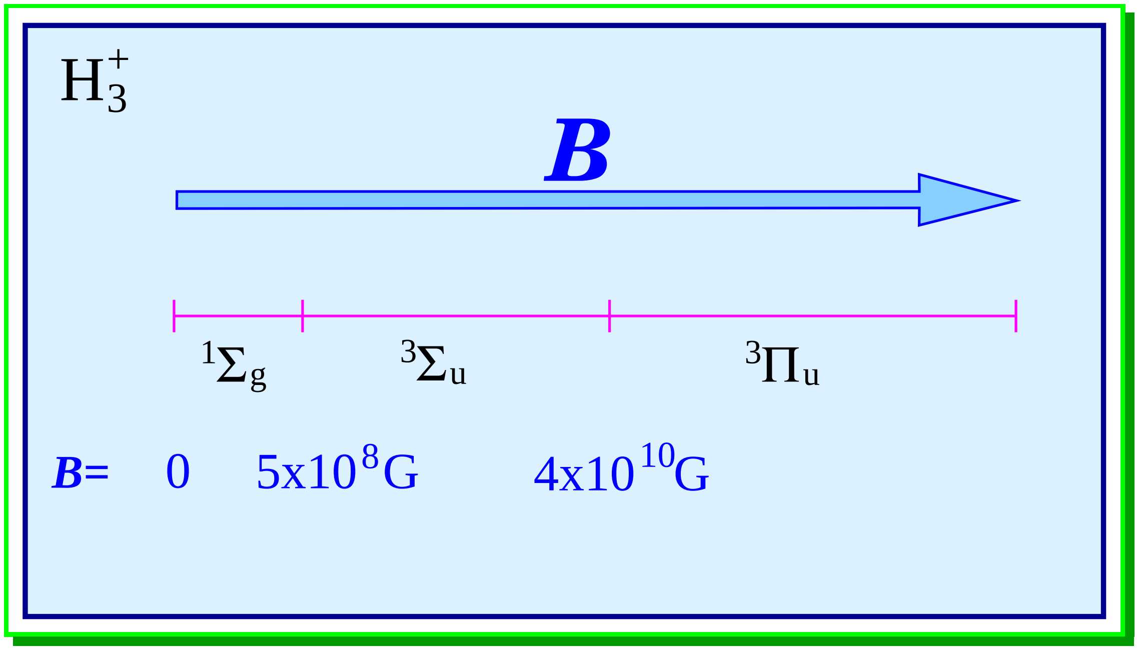
At $B \geq 0.1$ a.u. *it is stable towards all small deviations*

At $B \leq 0.1$ a.u. the ground state is of triangular geometry, linear configuration is unstable



Low-lying states of the H_3^+ in a magnetic field in parallel configuration

H_3^+:   *ground state*



At $B = 10000$ a.u.

$$E_T = -95.21\,Ry \qquad (R_{\pm}^{eq} = 0.093\,a.u.)$$

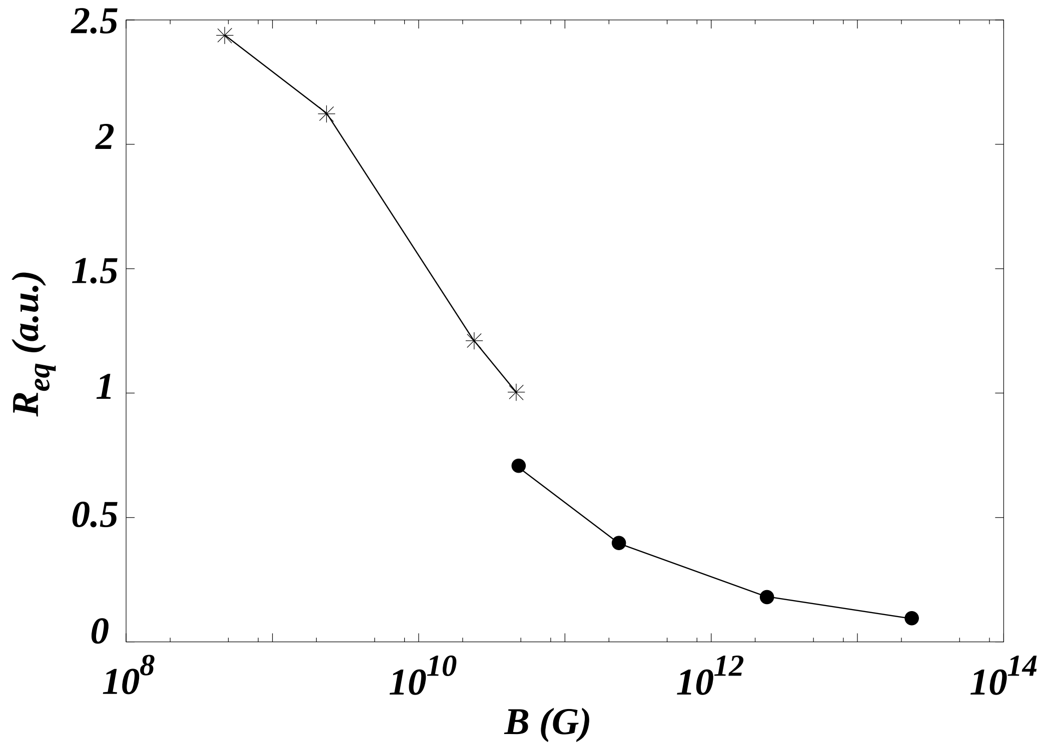
$$E_0^{vib} \;=\; 3.15\,Ry$$

$E_T(H_2(^3\Pi_u)) = -71.39\,Ry$, $E_T(H_2^+(1\pi_u){+}H(1s)) = -62.02\,Ry$

Dissociation energy: $H_3^+ \to H_2 + p$ is large, $23.82\,Ry$

Transition energy (from ground state to lowest excited state):

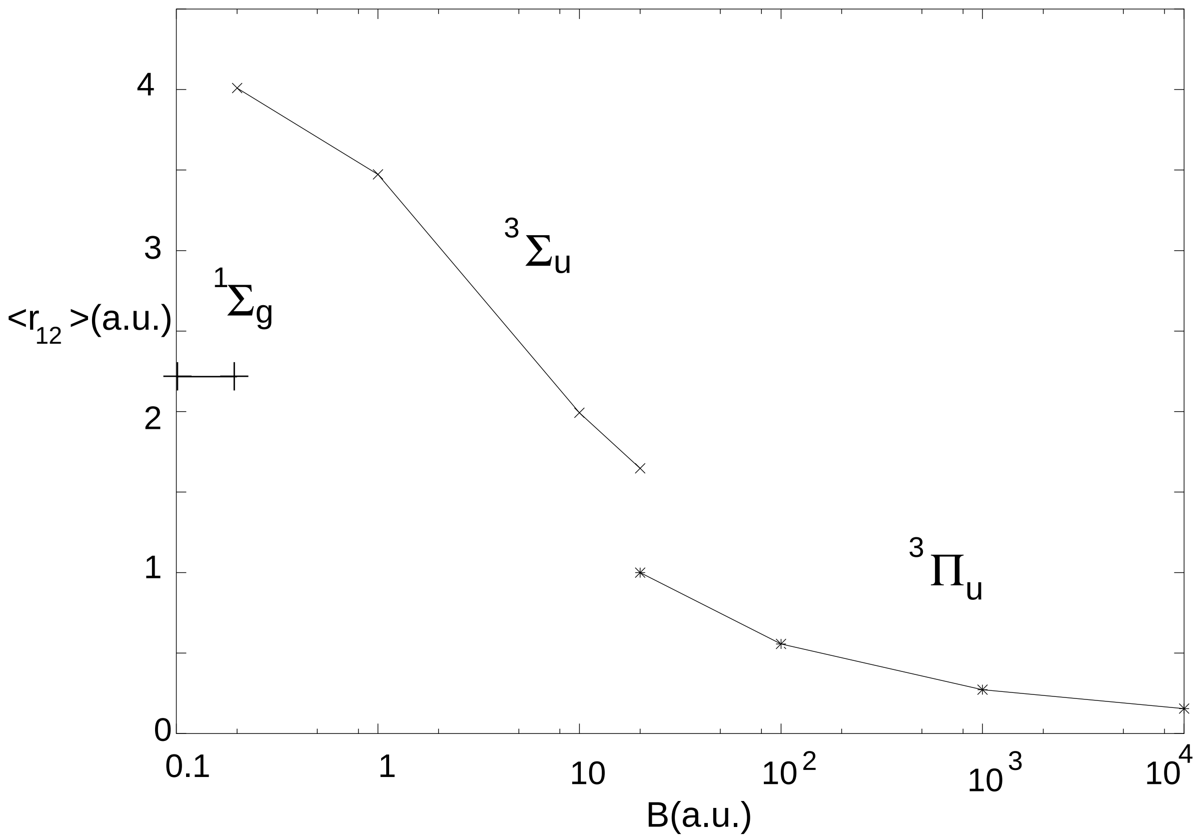
$$\Delta E(^3\Pi_u \to {}^3\Delta_g) = 7.76\,Ry$$



Equilibrium distance for the ground state: $^3\Sigma_u$ (stars) and $^3\Pi_u$ (bullets).

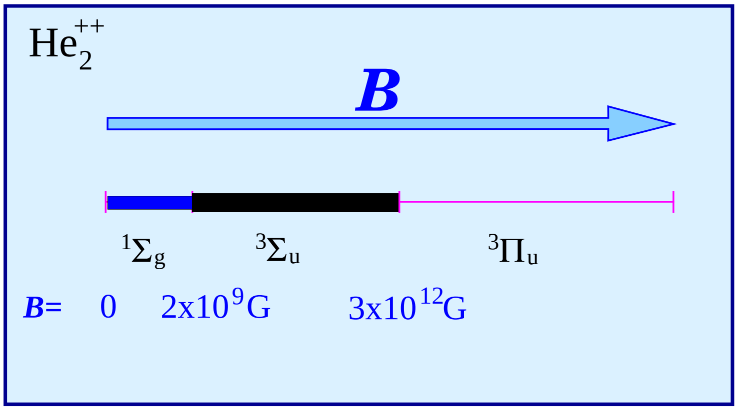
H_3^+ is the most stable $2e$-system among those made from protons for $0 \leq B \lesssim 2000\,\mathrm{a.u.}$

Stable - the lowest total energy, the highest energy is needed to dissociate (ionize) comparing to any other system



Pauli repulsion effects

He_2^{2+}: ground state
(A.T., N. Guevara '06, the first study)



Parallel configuration is optimal

metastable at $B < 0.85$ a.u. ($He_2^{2+} \to He^+ + He^+$)

stable at $B > 1100$ a.u., otherwise does not exist!
At $B = 10000$ a.u.

$$E_T = -174.51\,Ry \qquad (R_{eq} = 0.106\,a.u.)$$

$$E_0^{vib} \;=\; 1.16\,Ry$$

$$E_T(He^+ + He^+) = -156.85\,Ry\ (1s1s)\ ,\ = -137.26\,Ry\ (1s2p_{-1})$$

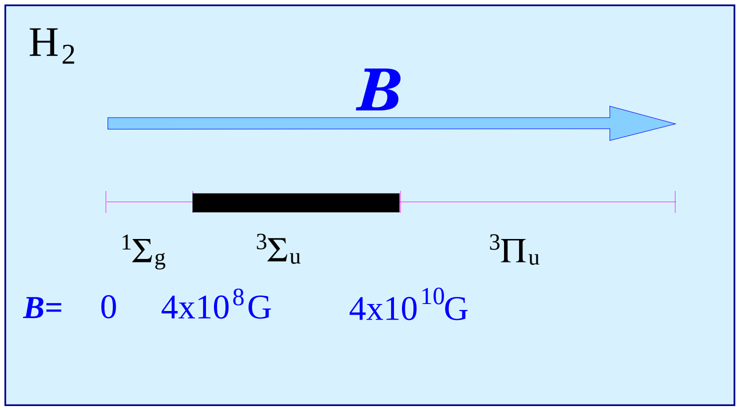
$$E_T(He_2^{3+}(1\sigma_g) + e) = -86.23\,Ry$$

Transition energy from the ground state $^3\Pi_u$ to the lowest excited state $^3\Delta_g$

$$\Delta E(^3\Pi_u \to {}^3\Delta_g) = 13.87\,Ry$$

H_2: *ground state*

(A.T. '83, ... Heidelberg group '90-'03, E. Salpeter et al '92-'96,...)



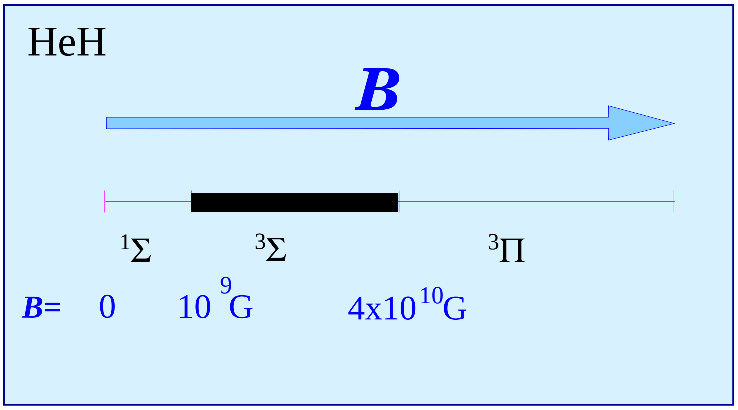
Parallel configuration is optimal,

stable, when exists, but always

$$E_T(H_3^+) \; < \; E_T(H_2)$$

$(HeH)^+$: *ground state*

(A.T., N. Guevara '07)



Parallel configuration is optimal

At $B = 10000\,\text{a.u.}$

$$E_T = -133.49\,Ry \qquad (R_{eq} = 0.104\,a.u.)$$

$E_T = -129.7\,\text{Ry}$ (Heyl & Hernquist, '98, first calculation)

$$E_0^{vib} \;=\; 1.41\,Ry$$

$$E_T(He^+ + H) = -86.79\,Ry\ (2p_{-1}1s)\ ,\ = -99.98\,Ry\ (1s2p_{-1})$$

$$E_T(He(1^3(-1)^+) + p) = -110.30\,Ry$$

Transition energy from the ground state $^3\Pi$ to the lowest excited state $^3\Delta$

$$\Delta E(^3\Pi \to {}^3\Delta) = 9.87\,Ry$$

Two-electron Charged Hydrogenic Chains

★ At $B \gtrsim 4 \times 10^8$ G

H_3^+ does exist and the most bound for $B \lesssim 4 \times 10^{12}$ G
(H_2 is the only competitor for $B \gtrsim 4 \times 10^{10}$ G)

★ At $B \gtrsim 4 \times 10^{12}$ G

H_4^{2+} does occur and becomes the most bound finite chain
at $B = 10000$ a.u

$$E_T = -100.00\,Ry \qquad (R_{eq} = 0.086\,a.u.)$$

$$E_T(H_4^{2+}) \;<\; E_T(H_3^+) \;<\; E_T(H_2)$$

★ At $B \gtrsim 10^{13}$ G

H_5^{3+} does occur but *always metastable*

For $B \gtrsim 4 \times 10^{10}$ G the H_2-molecule is stable but has the highest total energy among $2e$ molecular systems made from protons

Two-electron Charged Helium Chains

★ At $B \gtrsim 4 \times 10^{12}$ G

Two molecules He_2^{2+} and He_3^{4+} do exist with $^3\Pi_u$ ground state

He_2^{2+} is the most bound

He_3^{4+} decay to $He_2^{2+}(^3\Pi_u) + \alpha$

for He_3^{4+} at $B = 10000$ a.u

$$E_T = -163.9\, Ry \qquad (R_{eq} = 0.123\, a.u.)$$

Surprisingly, even the $Li_3^{(7+)}$-ion does display binding: at $B = 10000$ a.u

$$E_T = -180.3\, Ry \qquad (R_{eq} = 0.178\, a.u.)$$

CONCLUSION

- At $B > 10^8$ G for all studied 1-2e molecular systems the optimal geometry is linear parallel (heavy particles are situated along magnetic line)

- For all studied 2e systems a transition occurs at $B \sim 10^8$ Gauss:
  the spin-singlet ground state becomes the spin-triplet state of the lowest energy (bound or unbound)

- For many studied 2e proton contained molecular systems at $B \gtrsim 10^{11}$ Gauss the spin-triplet strongly bound ground state $^3\Pi_u$ appears
  $(m_l = m_s = -1)$ -
  the celebrated Ruderman state

- The ion H_4^{2+} exists at $B > 10^{11}$ Gauss (linear parallel configuration) with $^3\Pi_u$ as ground state. At first, H_4^{2+} decays to H_3^+ but for $B \gtrsim 5 \times 10^{12}$ Gauss the ion H_4^{2+} becomes stable(!):
  it is a short, charged, Ruderman chain
  In this domain the ion H_5^{3+} occurs being always metastable

- Practically, basic transition, dissociation and ionization energies

at $B \sim 10^{12} - 4.414 \times 10^{13}$ Gauss of two-electron systems

(found so far) are in the region 100-1000 eV