One-electron Coulomb Systems in Strong Magnetic Fields

Classification

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$\mathcal{F}$enomec $\mathcal{M}$ini-$\mathcal{W}$orkhsop on

$\mathcal{H}$igh $\mathcal{M}$agnetic $\mathcal{F}$ields and $\mathcal{N}$eutron $\mathcal{S}$tar $\mathcal{S}$urface

Outline

- Motivations
- Problem
- Method and basic assumptions
- One-electron atomic-molecular systems $(p \ldots \alpha \ldots ; e)$
  - H-like
  - Molecular ions “Diatomic ”$\mathrm{H}_2^+, \mathrm{He}_2^{3+}, (\mathrm{HeH})^{2+}$
  - “Triatomic ”$\mathrm{H}_3^{2+}, (\mathrm{H}-\mathrm{He}-\mathrm{H})^{3+}, (\mathrm{He}-\mathrm{H}-\mathrm{He})^{4+}$
  - “Polyatomic ”H_4^{3+}
- Classification
- Conclusion

A. Turbiner and JCLV, Physics Reports, 424 (2006)

Part I

Motivations

How does

ATOMIC-MOLECULAR PHYSICS IN A STRONG MAGNETIC FIELD

look like?

In strong magnetic fields

NEW CHEMICAL COMPOUNDS CAN APPEAR

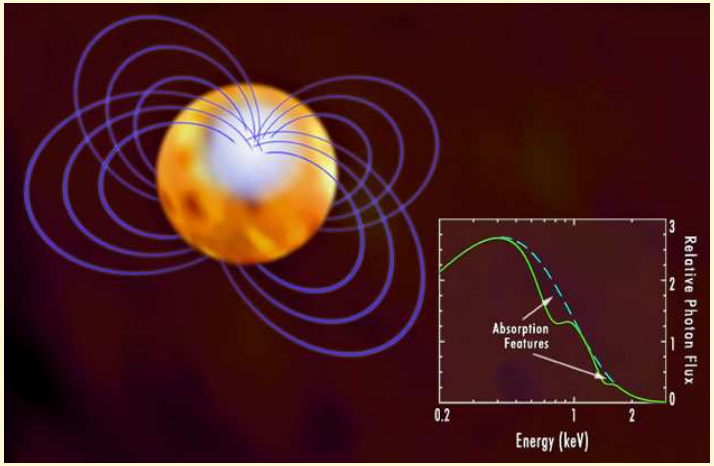
Neutron Stars
Possible scenario

- $R \sim 10\,$Km, $M \sim 1.4 M\odot$
- Atmosphere $(\sim 10cm)$
- $B_{surf} \sim 10^{12} - 10^{13}\,G$
- $T_{surf} \sim 10 - 100\,eV \quad (10^5 - 10^6)$ K
- E_{bind}(H-atom) $\sim 160 - 300\,eV$

Motivations

First Observational Discoveries
Chandra and *XMM-Newton* X-ray observatory
2002

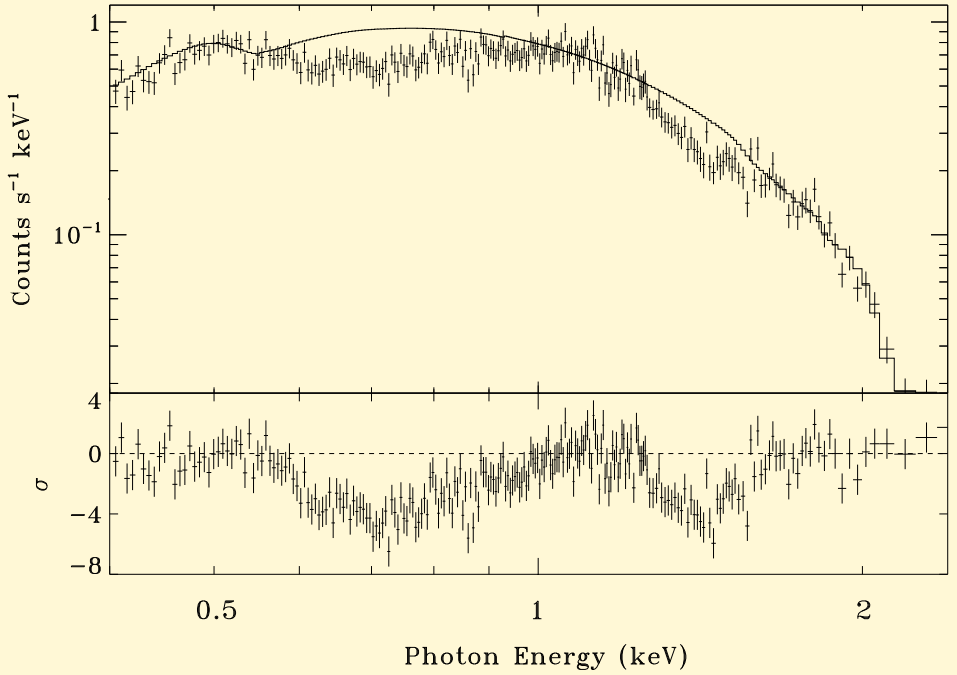
- Two absorption features at 0.7 keV and 1.4 keV in the X-ray spectrum of the isolated neutron star 1E1207.4-5209
- Possible atomic *or even* molecular content of the atmosphere



Chandra X-ray observatory, '02, Sanwal *et al.*

XMM-Newton X-ray observatory, '02, Mereghetti *et al.*

Motivations



D. Sanwal, G.G. Pavlov, V.E. Zavlin and M.E. Teter, Apj 574, L61 (2002)

Motivations

More Absorption features:

- RX J1308.6+2127 ($\sim$ 0.3KeV) '03 Haberl et al.
- RX J0720.4-3125 ($\sim$ 0.27 KeV) '04 Haberl et al.
- RX J1605.3+3249, ($\sim$ 0.45 KeV), '04 Van Kerkwijk et al.

Domain of Magnetic Fields

$$2.35 \times 10^9\,\mathrm{G} \lesssim B \lesssim 4.414 \times 10^{13}\,\mathrm{G}$$

$$E_{cycl} = \hbar\omega_c \sim \frac{e^2}{a_0} \qquad E_{cycl} = \hbar\omega_c \sim m_e c^2$$

$$B_0 \equiv 1\mathrm{a.u.} = 2.35 \times 10^9\,\mathrm{G}$$

Domain of Magnetic Fields

$$2.35 \times 10^9\,\mathrm{G} \lesssim B \lesssim 4.414 \times 10^{13}\,\mathrm{G}$$

Strong(Non-perturbative) Non-relativistic

$$B_0 \equiv 1\mathrm{a.u.} = 2.35 \times 10^9\,\mathrm{G}$$

First Predictions

In a strong magnetic field
atomic systems acquire a *needle-like form*

- Prediction: polymer type neutral linear molecular chains

  Ruderman ’71 (Astrophysics)
  Kadomtsev-Kudryavtsev ’71 (Plasma Physics),

- (Salpeter et al ’92)
  $H_3,\ H_4, \ldots$

Goal

- Study of the *low-lying states* for one-electron Coulomb systems in a strong magnetic field

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

$$(\alpha e), \quad (p\alpha e), \quad (\alpha\alpha e), \quad (p\alpha pe)\ldots$$

  - Existence of the corresponding chemical compounds:

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

$$\mathrm{He}^+, \quad (\mathrm{HHe})^{(2+)}, \quad \mathrm{He}_2^{(3+)}, \quad (\mathrm{HHeH})^{(3+)}, \ldots$$

- Molecular Ions mostly in linear parallel configuration (optimal)

Problem

Why is it a difficult problem?

Weakly bound states

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

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

Method

- Variational Calculations
- *Simple and Adequate* trial functions which can give high accuracy in the total energy

Recipe for choosing ψ_{trial}:

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

should reproduce main features of original potential

encoding as many physical properties as possible into ψ_{trial}

(A. Turbiner '80)

Assumptions

- Non-relativistic ($\lesssim 10\%$ in E_{bind}, E. Salpeter *et al.*)
- **Born-Oppenheimer** approximation (zeroth order)

(fixed, infinitely heavy nuclei)

Technical Aspects

- Calculations involve two steps
  - Multidimensional Numerical Integration (NAGLIB)
  - Minimization (CERNLIB)

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◇ Integration Strategy:

Manual partitioning of the integration domain into subdomains following the integrand profile in an optimal way

Control of the convergence and rate of convergence

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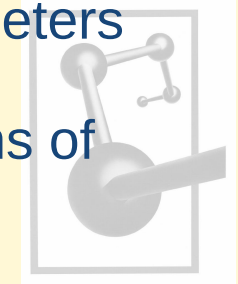
◇ Minimization Strategy:

Guide: Physical interpretation of the variational parameters

Smooth behavior of variational parameters as functions of the magnetic field



One-electron Coulomb Systems

Hydrogen Atom in a Magnetic Field

Potential (ground state)

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

- Several hundred articles since 1926
- Quadrupole moment was calculated until 2001 by A. Potekhin and A. Turbiner
- H-atom is stable but has the highest total energy among $1e$ systems

- **Ground State (A. Turbiner '80)**

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

α, β variational parameters

-

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

$(pe)-$system

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

Precision $\sim 10^{-4}$ respect to more accurate results:

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

REMARK: (A. Potekhin and A. Turbiner, '01)

$$\psi_0 = \exp -\sqrt{\alpha^2 r^2 + (\gamma_1 r^3 + \gamma_2 r^2\rho + \gamma_3 r\rho^2 + \gamma_4\rho^3) + \beta_1 B^2\rho^4/16 + \beta_2 B^2\rho^2 r^2/16}$$

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

He^+ atomic ion

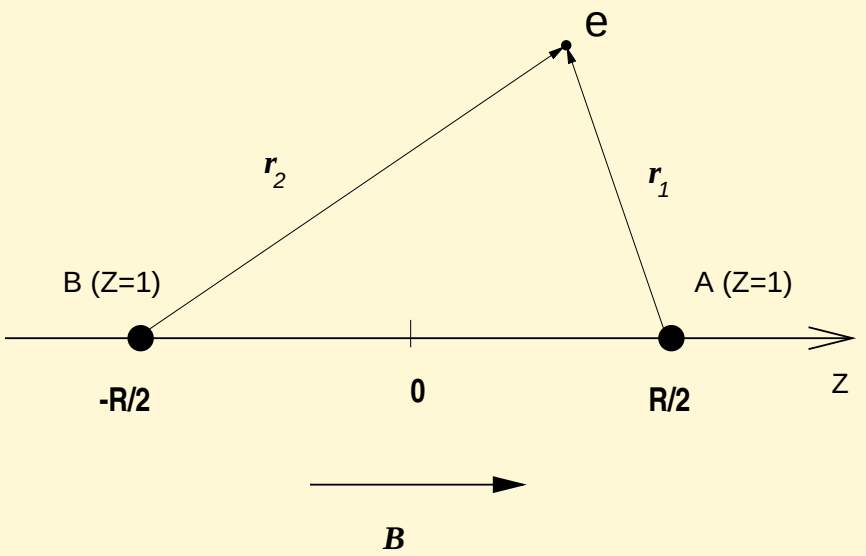
- Similar treatment as for H-atom
- Scaling relation for Hydrogen-like ions (in Born Oppenheimer approximation)

$$E_T(Z, BZ^2) = Z^2 E_T(Z = 1, B)$$

H_2^+ molecular ion (Parallel Configuration)

Ground State $1\sigma_g$ $(m_\ell = 0, P_{AB} = +1)$

(JCLV, P. Hess and A. Turbiner '97; A. Turbiner and JCLV '03)



$$V = -\frac{2}{r_1} - \frac{2}{r_2} + \frac{2}{R} + B\, m_\ell + \frac{B^2\rho^2}{4},$$

$$\rho^2 = x^2 + y^2$$

Trial Functions for H_2^+

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

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

$$V_1^{trial} = -2\alpha_1\left(\frac{1}{r_1}+\frac{1}{r_2}\right) + \beta_1^2\frac{B^2\rho^2}{4} + 2\alpha_1^2 - \beta_1 B$$
$$+2\alpha_1^2\vec{n}_1\cdot\vec{n}_2 + \alpha_1\beta_1 B\rho^2\left(\frac{1}{r_1}+\frac{1}{r_2}\right)$$

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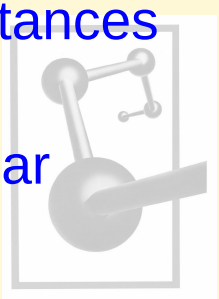
- Variational parameters: α_i, β_j
- $\alpha_i, \beta_j \neq 1$: screening (antiscreening) of the nuclear charges and of the magnetic field

- ψ_1 gives a significant contribution for internuclear distances near equilibrium (verified a posteriori)
- ψ_2 gives a significant contribution for large internuclear distances (verified a posteriori)



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Non-linear interpolation (simplest)

$$\psi_3 = \underbrace{\left(e^{-\alpha_3 r_1 - \alpha_4 r_2} + e^{-\alpha_3 r_2 - \alpha_4 r_1}\right)}_{\text{Guillemin-Zener}} e^{-\beta_3 B\rho^2/4}$$

- $\alpha_3 = \alpha_4 \rightarrow \psi_1$
- $\alpha_3(\alpha_4) = 0 \rightarrow \psi_2$

Superposition

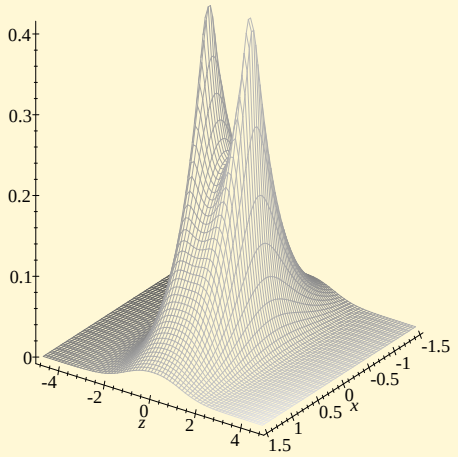
$$\Psi = A_1\psi_1 + A_2\psi_2 + A_3\psi_3$$

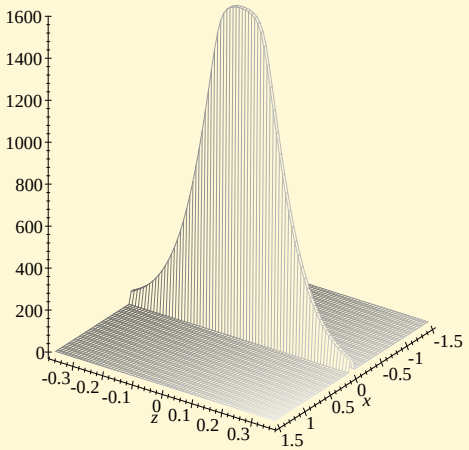
- 10 variational parameters
- Ψ leads to highly accurate results for the Total Energy of the ground state (in the whole domain of magnetic fields we studied)
  (among lowest E_T out of ~ 50 calculations)
- Relative accuracy $\sim 10^{-5}$ respect to the most accurate calculations of Vincke and Baye '06, and Guan *et al.* '03
- Excited states $1\sigma_u, 1\pi_{g,u}, 1\delta_{g,u}$ were studied in detail
  A. Turbiner and JCLV, 2004

M. Vincke and D. Baye, J. Phys. B 39, 2605 (2006)
X. Guan, B. Li and K.T. Taylor, J. Phys. B 36, 3569 (2003)

Physical Phenomenon:

For $B \sim 5 \times 10^{11} G$ type of *coupling* changes





$B = 10^9$ G

$B = 10^{13}$ G

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

JCLV, P. Hess and A. Turbiner *Phys. Rev. A* **56** 1997, 4496.

Comparison (Ground State)

B	E_T (Ry)	E_b (Ry)	R_{eq} (a.u.)	
$B = 0$	-1.20525	1.20525	1.997	Turbiner et al
	-1.20527	—	1.997	Wille '88
10^9 G	-1.15070	1.57623	1.923 ± 0.003	Turbiner et al. '04
	—	1.03	1.831	De Melo '76
	-1.15072	1.57625	1.924	Wille '88
	-1.15072	1.57625	1.9234	Guan et al. '04
1 a.u.	-0.94992	1.94992	1.752 ± 0.003	Turbiner et al
	—	1.9498	1.752	Larsen '82
	-0.94642	1.94642	1.76	Kappes et al. '95
	-0.94998	1.94998	1.752	Guan et al. '03

Comparison of the ground state $1\sigma_g$ of H_2^+ with results from other calculations.

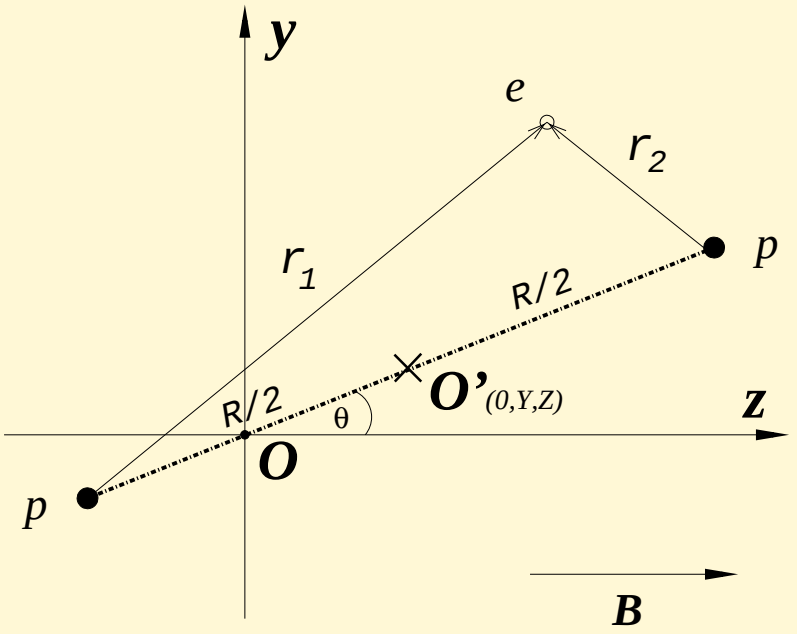
Comparison (Ground State)

B	E_T (Ry)	E_b (Ry)	R_{eq} (a.u.)	
10^{12} G	408.3896	17.1423	0.283 ± 0.001	Turbiner et al
	—	17.0588	0.28	Lai et al
	408.566	16.966	0.278	Wille
1000 a.u.	977.2213	22.7787	0.2197 ± 0.0005	Turbiner et al
	—	22.7069	0.221	Wunner et al
	—	22.67	0.222	Larsen
	977.21833	—	0.2198	Vincke and Baye '06
10^{13} G	4219.563	35.7559	0.1472 ± 0.0002	Turbiner et al
	4231.82	23.52	0.125	Wille
	—	35.74	0.15	Lai et al

Comparison of the ground state $1\sigma_g$ of H_2^+ with results from other calculations.

$(ppe)-$system (Inclined)

Molecular axis forming an angle θ with the magnetic field

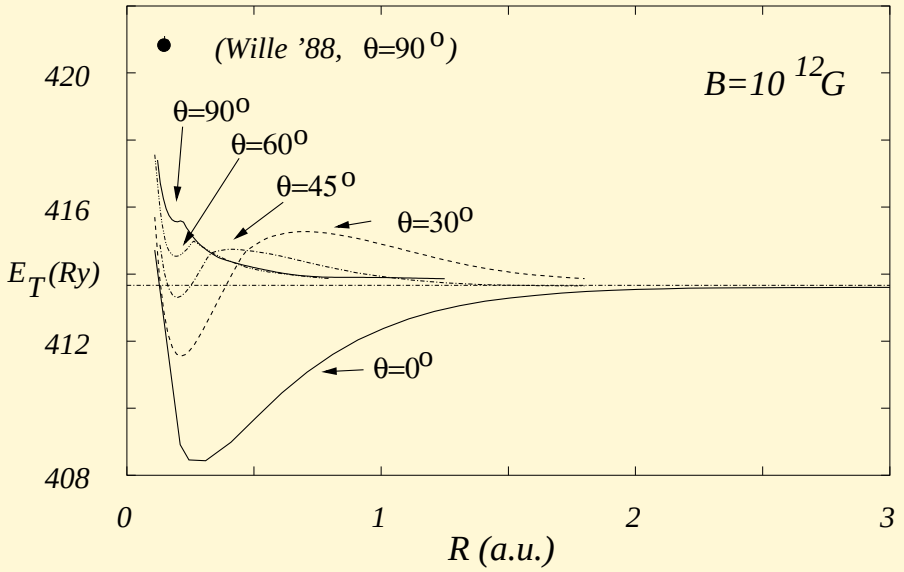


(Choice of an optimal gauge)

A. Turbiner and JCLV, 2003

$(ppe)-$system (Inclined)

Potential Energy Curves



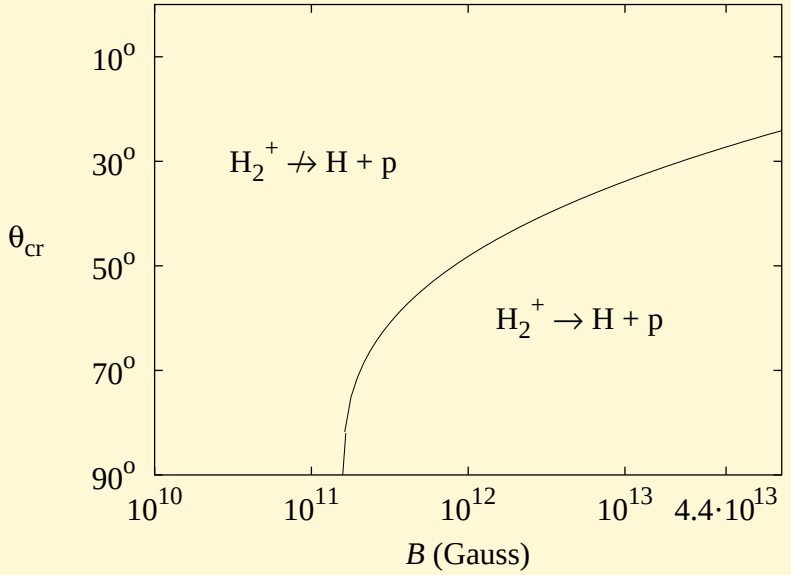
A. Turbiner and JCLV, 2003

Parallel Configuration is always optimal

H_2^+ is stable for all B and the most bound 1-e system made from protons for $B \lesssim 10^{13}$ G

$(ppe)-$system (Inclined)

Domain of existence for H_2^+



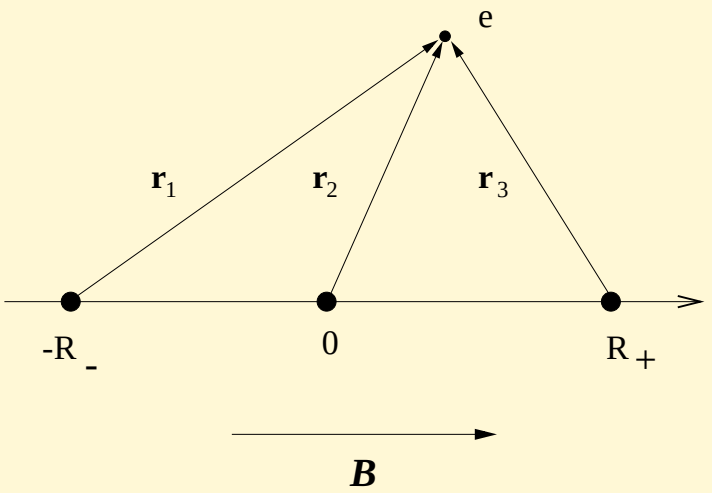
A. Turbiner and JCLV, 2003

Exotic Systems

Molecular Ion H_3^{++}: Linear Parallel Configuration

A. Turbiner, JCLV and U. Solis, (1999)

A. Turbiner, JCLV and N. Guevara, (2005)



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

$$\mathcal{H} = \hat{p}^2 + \frac{2}{R_+} + \frac{2}{R_-} + \frac{2}{R_+ + R_-} - \frac{2}{r_1} - \frac{2}{r_2} - \frac{2}{r_3} + (\hat{p}\mathcal{A} + \mathcal{A}\hat{p}) + \mathcal{A}^2$$

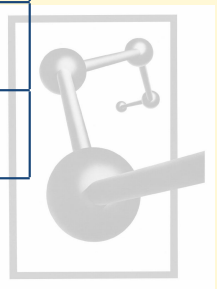
$\mathcal{A} = \frac{B}{2}(-y,\ x,\ 0)$ (symetric gauge)

Ground State $1\sigma_g$

For $B \gtrsim 10^{10}$G

- the total energy $E(R_+, R_-)$ exhibits a well pronounced minimum for finite values of R_+, R_-, $(R_+^{eq} = R_-^{eq} \equiv R_{eq})$
- H_3^{++} exists and is stable towards small deviations from linearity

B	E_T (Ry)	E_b (Ry)	R_{eq} (a.u.)
10^{10} G	1.8424	2.4129	2.072
10^{11} G	36.4297	6.1234	0.801
10^{12} G	410.3739	15.1580	0.345
10^{13} G	4220.9286	34.3905	0.166
4.414×10^{13} G	18727.7475	55.2312	0.110



$(pppe)-$system

- $\mathrm{H}_3^{(2+)}$ can exist in parallel linear configuration for $B \gtrsim 10^{10}$ G

$$\mathrm{H}_3^{(2+)} \rightarrow \mathrm{H}_2^{+}, \quad \mathrm{H}_3^{(2+)} \not\rightarrow \mathrm{H} + p + p$$

- Lowest excited states $1\pi_u, 1\delta_g$ exist for $B \gtrsim 10^{11}$ G

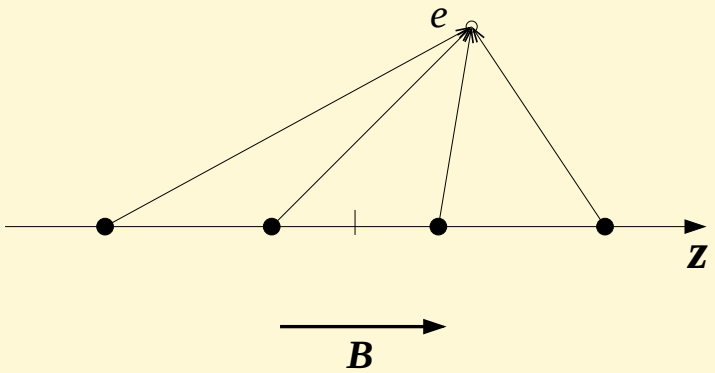
- For $B \gtrsim 10^{13}$ G: $E_T^{H_3^{++}} < E_T^{H_2^{+}}$!

$$\mathrm{H}_3^{(2+)} \not\rightarrow \mathrm{H}_2^{+}$$

Molecular Ion H_4^{+++}: Linear Parallel Configuration

A. Turbiner and JCLV (2000)

H.O. Pilon, 2006

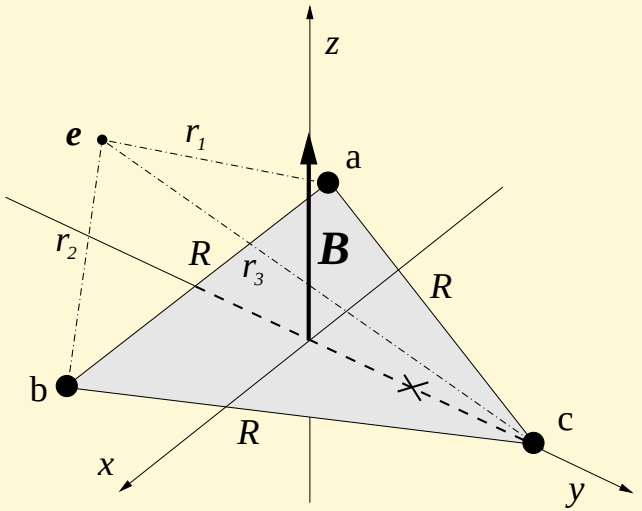


(H_4^{+++} *exists as a metastable bound state for magnetic fiels* $B \gtrsim 4.14 \times 10^{13}\, G\, !$)

$1\pi_u$ excited state also exists

H_3^{++}: triangular configuration

JCLV (2000), JCLV and A. Turbiner (2002)



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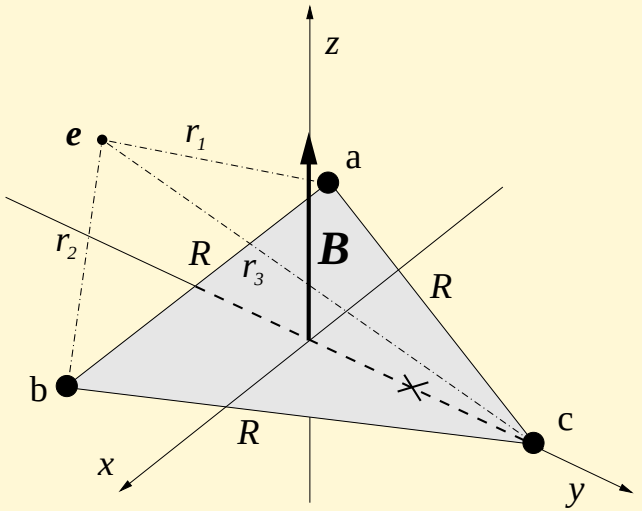


$$\mathcal{A} = B(-\xi(y-y_0),(1-\xi)(x-x_0),0)\ ,$$

optimal choice of gauge (variational)

- ξ, x_0, y_0 parameters
- *gauge center* $(\mathcal{A}(x,y)=0)$, is defined by $x=x_0, y=y_0$

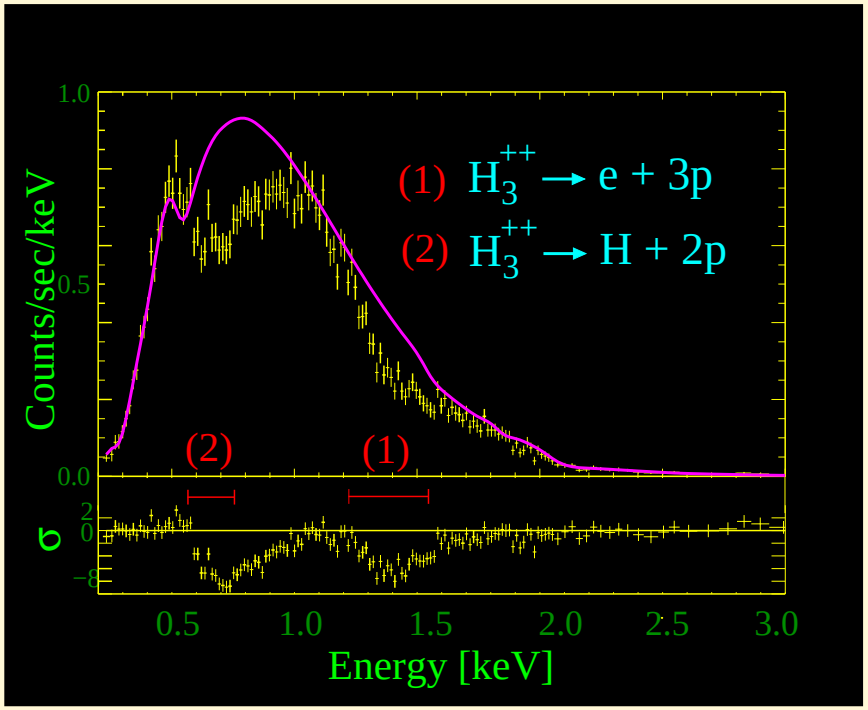
H_3^{++} Triangular

- The system $(pppe)$ with protons in a triangular equilateral configuration perpendicular to a magnetic field $\mathbf{B}$ exists as a metastable bound state for $10^8 \mathrm{G} \lesssim B \lesssim 10^{11}$ G

$$\mathrm{H}_3^{++} \rightarrow H + 2p$$

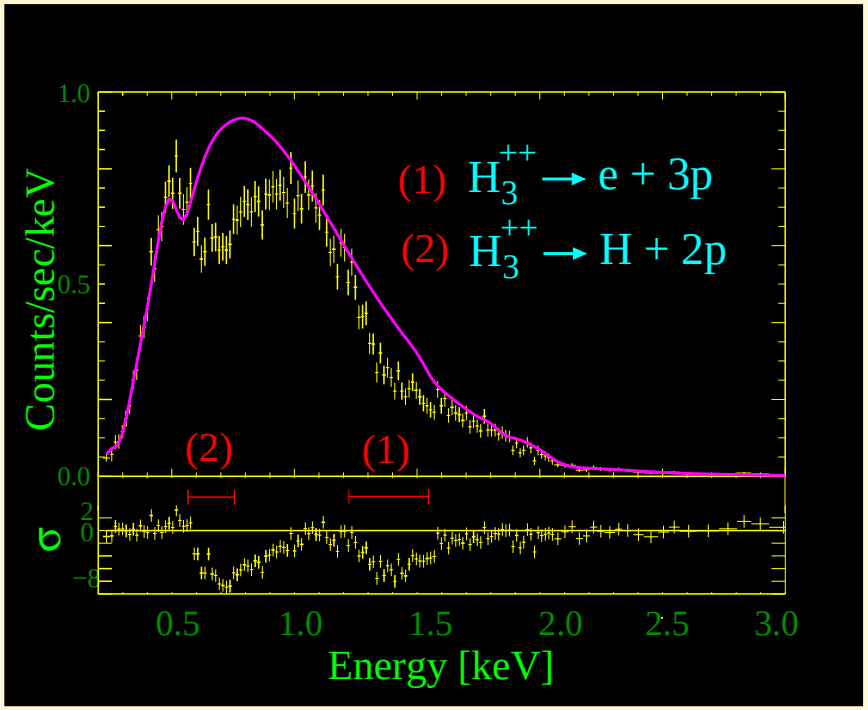
- precursor to linear configuration

1E1207.4-5209



X-Ray spectrum of the isolated neutron star 1E1207.4-5209
Absorption lines at 0.7 Kev and 1.4 KeV

1E1207.4-5209

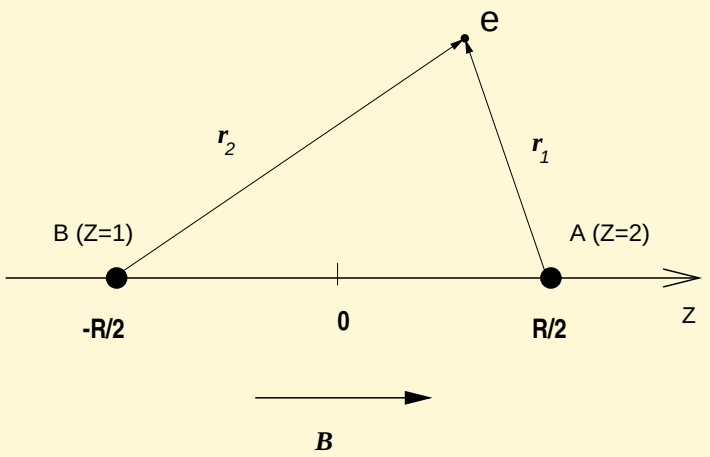


X-Ray spectrum of the isolated neutron star 1E1207.4-5209
Absorption lines at 0.7 Kev and 1.4 KeV

- Fotoionization $H_3^{++} \rightarrow e + 3p, \quad \mapsto$ line at 0.7 KeV
- Fotodissociation $H_3^{++} \rightarrow H_2^{+} + p, \quad \mapsto$ line at 1.4 KeV
- $B = (4 \pm 2) \times 10^{14}$ G

$(\alpha pe)-$system

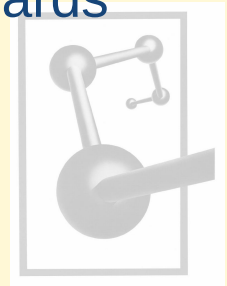
$(\mathrm{HeH})^{2+}$ molecular ion



- For $B \gtrsim 10^{12}$ G the system (αpe) has a bound state manisfesting the possible existence of the $(\mathrm{HeH})^{2+}$ molecular ion
- The excited states $1\pi, 1\delta$ also exist
- For $B \gtrsim 10^{13}$ G the ion $(\mathrm{HeH})^{2+}$ becomes stable towards the decay

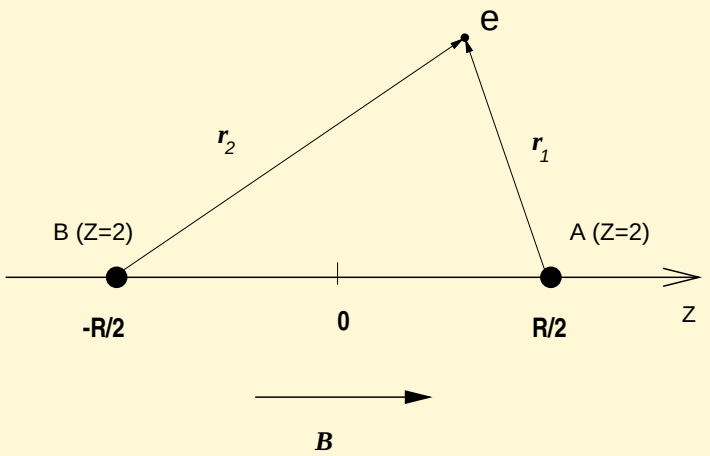
$$(\mathrm{HeH})^{2+} \not\to \mathrm{He}^{+} + p$$

- Parallel configuration is always optimal



$(\alpha\alpha e)-$system

He_2^{3+} molecular ion

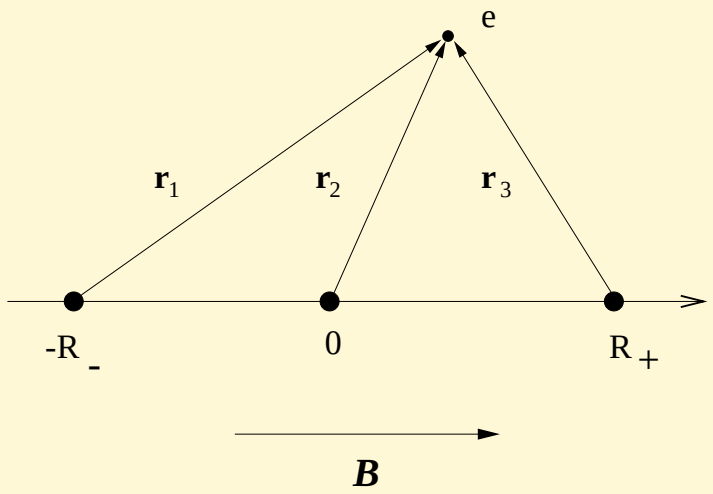


- For $B \gtrsim 2 \times 10^{11}$ G the system $(\alpha\alpha e)$ has a bound state manisfesting the possible existence of the He_2^{3+} molecular ion
- The excited states (of positive parity) $1\pi_u, 1\delta_g$ also exist
- For $B \gtrsim 10^{12}$ G the ion He_2^{3+} becomes stable towards the decay

$$\mathrm{He}_2^{3+} \not\to \mathrm{He}^+ + \alpha$$

- Parallel configuration is always optimal

$(p\alpha pe)$ and $(\alpha p\alpha e)-$systems



- For $B \gtrsim 3 \times 10^{13}$ G the systems $(p\alpha pe)$ and $(\alpha p\alpha e)$ have a bound state manisfesting the possible existence of the $(\mathrm{H}-\mathrm{He}-\mathrm{H})^{3+}$ and $(\mathrm{He}-\mathrm{H}-\mathrm{He})^{4+}$ molecular ions

One-electron systems in a magnetic field $B = 10^{12}$ G

(Molecular Ions in Linear Parallel Configuration)

	He_2^{3+}	$(HeH)^{++}$	H_2^+	H_3^{2+}	He^+	H
E_T	396.864		408.390	410.374		
E_b	28.668		17.1423	15.158	30.87	11.870
R_{eq}	0.420		0.283	0.345		
E^0_{vib}	0.100		0.266	0.338		
E^0_{rot}	0.778		1.093	0.762		
ΔE	1.024		—	0.267		

Energies are in Ry. Internuclear distances are in a.u.

A. Turbiner and JCLV, Physics Reports 424 (2006), IJMPA (in press)

A.Y. Potekhin and A. Turbiner, Phys. Rev. **A 63** (2001) for H-atom

One-electron systems in a magnetic field $B = 10^{13}$ G

(Molecular Ions in Linear Parallel Configuration)

	He_2^{3+}	$(HeH)^{++}$	H_2^+	H_3^{2+}	He^+	H
E_T	4190.182	4195.693	4219.563	4220.929		
E_b	65.137	59.626	35.756	34.3905	61.99	22.5
R_{eq}	0.193	0.185	0.147	0.166		
E^0_{vib}	0.366	0.41	0.714	1.088		
E^0_{rot}	3.617	—	4.875	3.613		
ΔE	7.328	1.197	—	1.895		

Energies are in Ry. Internuclear distances are in a.u.

A. Turbiner and JCLV, Physics Reports 424 (2006), IJMPA (in press)

A.Y. Potekhin and A. Turbiner, Phys. Rev. **A 63** (2001) for H-atom

One-electron systems in a magnetic field $B = 4.414 \times 10^{13}$ G

(Molecular Ions in Linear Parallel Configuration)

	He_2^{3+}	$(HeH)^{++}$	H_2^+	H_3^{2+}	He^+	H
E_T	18677.857	18690.398	18728.477	18727.7521		
E_b	105.121	92.858	54.502	55.2312	92.53	32.5
R_{eq}	0.126	0.120	0.102	0.110		
E^0_{vib}	0.738	0.880	1.248	2.078		
E^0_{rot}	9.208	13.153	12.065	9.310		
ΔE	17.19	4.22	—	4.815		

Energies are in Ry. Internuclear distances are in a.u.

A. Turbiner and JCLV, Physics Reports 424 (2006), IJMPA (in press)

A.Y. Potekhin and A. Turbiner, Phys. Rev. **A 63** (2001) for H-atom

One-electron Coulomb systems

	$B < 10^{11}$ G		$10^{11}\text{G} \lesssim B \lesssim 3\times 10^{13}$ G		$B \gtrsim 3\times 10^{13}$ G	
H	*2*	*3*	*3*	*6*	*4*	*9*
H_2^+	*1*	*2*	*1*	*4*	*2*	*5*
H_3^{++}			2	5	*1*	*4*
H_4^{3+}					3	8
He^+		*1*	*1*	*1*	*2*	*2*
$(HeH)^{++}$			3	3	3	3
He_2^{3+}			2	2	*1*	*1*
$(H\,He\,H)^{3+}$					4	6
$(He\,H\,He)^{4+}$					5	7

Conclusion

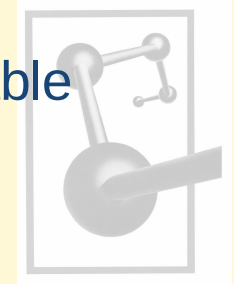
Conclusion

One-electron linear systems
(For more details see recent Physics Reports)

Optimal configuration of linear $\mathrm{H}_2^+, \mathrm{H}_3^{2+}, \mathrm{H}_4^{3+}, (\mathrm{HeH})^{2+}, \mathrm{He}_2^{3+}$ is parallel, along the magnetic field direction (when exist)

When magnetic field grows:

- Binding energy of $\mathrm{H}, \mathrm{H}_2^+, \mathrm{H}_3^{2+}, \mathrm{H}_4^{3+}, (\mathrm{HeH})^{2+}$ and He_2^{3+} grows (when exist)
- H_2^+ has the lowest E_{Total} for $0 < B \lesssim 10^{13}$ G (systems made of protons)
- H_3^{2+} has the lowest E_{Total} for $B \gtrsim 10^{13}$ G (systems made of protons)
- Possible existence of H_5^{4+} for $B \gtrsim 4.4^{13}$ G but a reliable consideration requires a consideration of relativistic corrections



Conclusion

- For $B \gtrsim 10^{12}$ G the exotic system He_2^{3+} has the lowest total energy among the systems made from protons and/or $\alpha-$particles
- H_2^+ and linear H_3^{++} binding energies (ionization energies) at $B \simeq 3 \times 10^{13}$ G coincide, both being $\sim 700eV$, while for He_2^{3+} it is $\simeq 1400eV$