Exotic Ion H_3^{++} in Strong Magnetic Fields: low-lying states

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Abstract

Main Results:

(1) The exotic system H_3^{++} (which does not exist without magnetic field) exists in strong magnetic fields:
(a) in triangular configuration for $B \approx 10^8 - 10^{11}$ G and (b) in linear configuration for $B > 10^{10}$ G
(2) In the linear configuration the positive z-parity states $1\sigma_g$, $1\pi_u$, $1\delta_g$ are bound states.
(3) In the linear configuration the negative z-parity states $1\sigma_u$, $1\pi_g$, $1\delta_u$ are repulsive states.

Possible application:
content of a neutron star atmosphere (about ~ 10 Km in radius and ~ 10 cm of atmosphere thickness) under a strong surface magnetic field $B = 10^{12} - 10^{13}$ G.

In 70's the first theoretical arguments were given indicating the physics of atoms and molecules in a strong magnetic field can exhibit a wealth of new and unexpected phenomena (Kadomtsev-Kudryatsev-Ruderman). In particular, the possibility of formation of unusual chemical compounds not existing without a magnetic field was emphasized. In practice, the atmosphere of neutron stars, which is characterized by enormous surface magnetic fields $\sim 10^{12} - 10^{13}$ G (up to 10^{15} G for magnetars), provides a valuable paradigm where this physics can be realized.

Recently the observational data (collected by the Chandra X-ray spatial observatory) of the soft X-ray spectrum of the isolated neutron star 1E1027.4-5209 revealed for the first time certain irregularities (Sanwal et al. '02). These irregularities might be interpreted as absorption features at ~ 0.7 KeV and ~ 1.4 KeV of a possible atomic-molecular nature assigned to the content of the neutron star atmosphere. In this context the study of the atomic and molecular, traditional and exotic systems in strong magnetic fields deserves a special attention.

The first already observed features for some atomic-molecular systems when the magnetic field increases are:

- The *total* and *binding* energies increase (The systems become more and more bound)
- Drastic decrease in the electron localization length in both directions, transverse and longitudinal, leading to a decrease in the equilibrium distance (The systems become more and more compact)
- The electronic cloud takes a needle-like form forming in most cases the quasi-one-dimensional systems with very unusual physical properties.

Goal

Study of molecular systems, traditional and exotic, in strong magnetic fields in the context of the variational method with simple and unique trial functions. These functions are modifications of the celebrated Heitler-London, Hund-Mulliken and Guillemin-Zener functions. Our goal is to find the domain of existence of the systems and then to obtain their description with sufficiently high accuracy in the whole range of magnetic fields where the non-relativistic approximation is valid: $B = 0 - 4.414\times10^{13}$G.

In particular, we have carried out a detailed study in the Born-Oppenheimer approximation of the ground state for the one-electron systems: (ppe)-system - the traditional molecular ion H_2^+ (the simplest molecular system) and for the systems ($pppe$) and ($ppppe$) giving rise to the exotic molecular ions H_3^{++} and H_4^{+++}, respectively, in linear configuration parallel to the magnetic field (Fig.1), and for different spatial configurations of the charged centers.

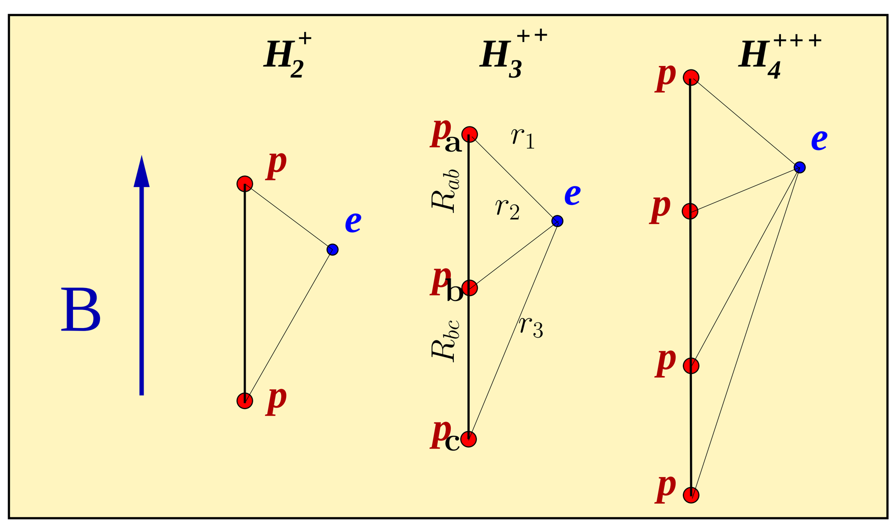


Fig. 1: One-electron molecular systems in a uniform magnetic field $\mathbf{B} = (0, 0, B)$: the traditional system H_2^+, and the exotic ions H_3^{++} and H_4^{++}.

Formulation of the Problem

In the Born-Oppenheimer approximation of zero order (where protons are infinitely massive), the Schrödinger equation for a system of one-electron and a certain number of protons in a magnetic field $\mathbf{B}$ is

$$\left[(\mathbf{p}-\mathbf{A})^2 + V_c(r_1, r_2, \ldots)\right]\Psi(\mathbf{r}) = E\Psi(\mathbf{r}) \quad \text{(in a.u.)}$$

where $\mathbf{p} = -i\nabla$ is the *momentum of the electron*, $\mathbf{A}$ is a *vector potential* associated with the constant uniform magnetic field $\mathbf{B}$, and $V_c(r_1, r_2, \ldots)$ describes the *Coulomb interaction* between the charged particles. For the (ppe)-system, (see Figs.1,2):

$$V_c = \frac{2}{R_{ab}} + \frac{2}{R_{ac}} + \frac{2}{R_{bc}} - \frac{2}{r_1} - \frac{2}{r_2} - \frac{2}{r_3}.$$

In particular, for a uniform magnetic field in the z-direction, $\mathbf{B} = (0, 0, B)$ we can choose the vector potential in a *gauge*:

$$\mathbf{A} = B\big((\xi - 1)y,\ \xi x,\ 0\big),$$

where ξ is a gauge parameter. Observables are, of course, gauge invariant and do not depend on the value of ξ. In variational calculations for a fixed class of trial functions the variational energy (which is approximate) can depend on the gauge, there can exist an optimal value of ξ giving a minimal variational energy. Therefore one can consider ξ as a variational parameter.

H_3^{++} (triangular)

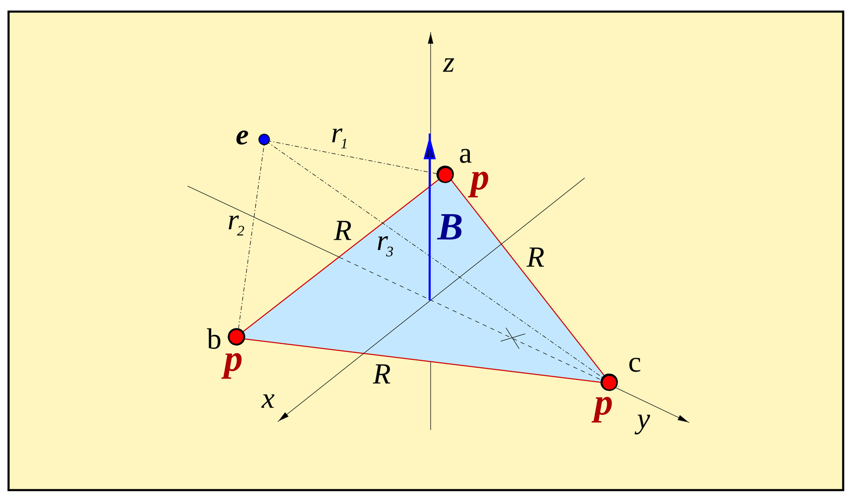
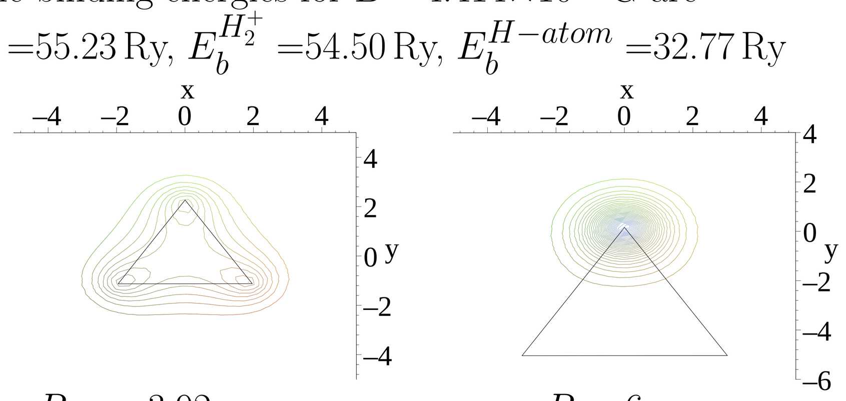


Fig.2: The H_3^{++} molecular ion in triangular (equilateral) configuration perpendicular to the magnetic field $\mathbf{B}$.

1. The system ($pppe$) in triangular equilateral configuration (See Fig.2) develops a well pronounced minimum for $10^8\,\text{G} < B < 10^{11}\,\text{G}$. Therefore the system H_3^{++} can exist for those magnetic fields
2. As the magnetic field increases the binding energy increases and the size of the triangle diminishes.

H_3^{++} (linear)

1. The system H_3^{++} in linear configuration exists for $B \geq 10^{11}$G.
2. As the magnetic field increases the binding energy increases and the internuclear distance decreases
3. For $B > 10^{13}$ G, H_3^{++} is the most stable one-electron system made from protons, in particular, $E_T^{H_3^{++}} < E_T^{H_2^+}$.
E.g. the binding energies for $B = 4.414\times10^{13}$ G are
$E_b^{H_3^{++}}$ =55.23 Ry, $E_b^{H_2^+}$ =54.50 Ry, E_b^{H-atom} =32.77 Ry



$R_{eq} = 3.92\,a.u.$ $R = 6\,a.u.$

Fig. 3: Evolution of the electronic distribution for the H_3^{++} ion in triangular configuration as function of the the size of the triangle (of side R) in a magnetic field $B = 10^9$G. Plots on the left describe the bound state and the plots in the right correspond to the situation when the dissociation $H_3^{++} \to H + p + p$ occurs.

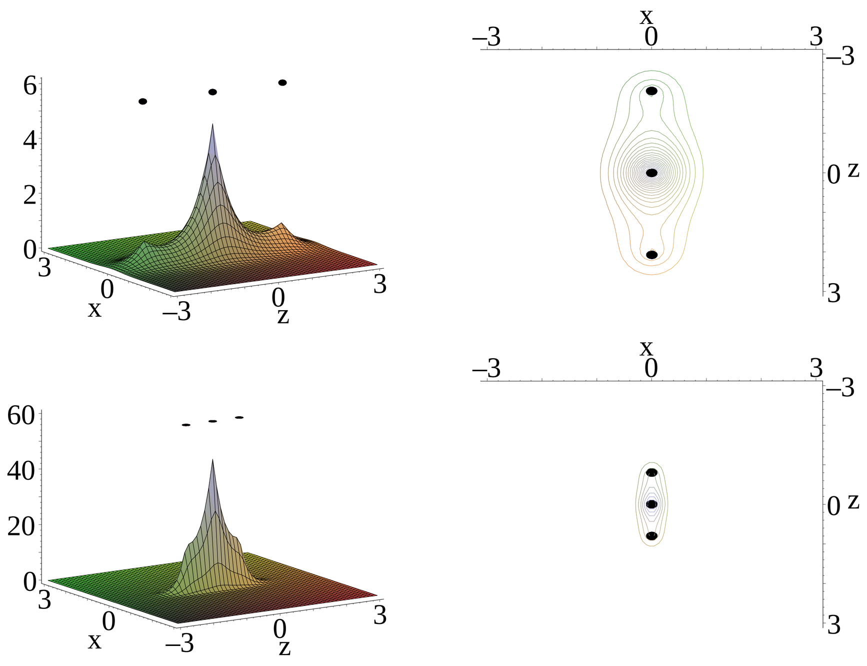


Fig. 4: Illustration of the evolution of the normalized electronic distribution $\psi^2(x, y = 0, z)/\int \psi^2(x, y, z)d\vec{r}$ for the ion H_3^{++} in linear configuration aligned with a magnetic field at (a) $B = 10^{11}$ G and (b) $B = 10^{12}$ G.

Excited states of H_3^{++}

For all magnetic fields $B \geq 10^{11}$ G:

1. Positive z-parity states $1\sigma_g$, $1\pi_u$, $1\delta_g$ are bound
2. Negative z-parity states $1\sigma_u$, $1\pi_g$, $1\delta_u$ are repulsive
3. The following hierarchy appears:

$$E_T^{1\sigma_g} < E_T^{1\pi_u} < E_T^{1\delta_g}, \qquad R_{eq}^{1\sigma_g} < R_{eq}^{1\pi_u} < R_{eq}^{1\delta_g}.$$

E.g. for $B = 10^{12}$ G:

$$E_b^{1\sigma_g} = 15.16\,\text{Ry}, E_b^{1\pi_u} = 10.17\,\text{Ry}, E_b^{1\delta_g} = 8.28\,\text{Ry}$$

$$R_{eq}^{1\sigma_g} = 0.345\,\text{a.u.}, R_{eq}^{1\pi_u} = 0.497\,\text{a.u.}, R_{eq}^{1\delta_g} = 0.601\,\text{a.u.}$$

The absorption features at ~ 700 eV and ~ 1400 eV discovered in radiation of the neutron star 1E1207.4-5209 by Chandra (Sanwal et al., 2002) and confirmed by XMM-Newton can be explained if one assumes that the main abundance in the atmosphere is H_3^{++} and the magnetic field strength is $(4 \pm 2) \times 10^{14}$ G. Photodissociation $H_3^{++} \to H + 2p$ corresponds to absorption feature at ~ 700 eV, and photoionization $H_3^{++} \to e + 3p$ contributes to absorption feature at ~ 1400 eV. Photodissociation $H_3^{++} \to H_2^+ + p$ corresponds to absorption feature at 80−150 eV, and it is not seen being beyond of Chandra detector acceptance.

Publications

1. *'One-electron molecular systems in a strong magnetic field'*, A. Turbiner and J.C. López Vieyra, *Physics Reports*, vol. 424, (March 2006) pp. 309-396
2. (a) *'H_3^{++} can exist in strong magnetic field'*, A. Turbiner, J.-C. Lopez and U. Solis H., *JETP Letters* **69**, 844-850 (1999)
(b) *'The exotic H_3^{++} ion in a strong magnetic field. Linear configuration'*, A.V. Turbiner, J.C. López Vieyra and N. L. Guevara, *Physical Review* **A72**, 023403, (2005)
3. *'H_3^{++} in a strong magnetic field: triangular configuration'*, J.C. Lopez V. and A. Turbiner, *Physical Review* **A66**, 023409 (2002)