Toroidal configuration of the orbit of the electron of the hydrogen atom under strong external magnetic fields

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Abstract

In this paper we overview some results on the hydrogen atom in external static uniform magnetic fields. We focus on the case of very strong magnetic field, $B \gg B_0 = 2.3 \cdot 10^9$ Gauss, use various approximate models and, particularly, in the adiabatic approximation have calculated exactly the integral defining the effective potential. This potential appears to be finite at $z = 0$. Our consideration of the problem of highly magnetized atoms and molecules is motivated by the recently developed MagneGas technology by Santilli (http://www.magnegas.com). The ground state electron charge distribution of the hydrogen atom in an intense magnetic field is of a toroidal form, in agreement with that studied by Santilli. This physical picture is at the foundation of the new chemical species of magnecules proposed by Santilli.

1 Introduction

Weak external static uniform magnetic field B causes anomalous Zeeman splitting of the energy levels of the hydrogen atom, with ignorably small effect on the charge distribution of the electron. In the case of a more intense magnetic field which is strong enough to cause decoupling of a spin-orbital interaction (in atoms), $e\hbar B/2mc > \Delta E_{jj'} \simeq 10^{-3}$ eV, i.e. $B \simeq 10^5$ Gauss, a normal Zeeman effect is observed, again with ignorably small deformation of the electron orbits.

In the case of *weak* external magnetic field B, one can ignore the quadratic term in the field B because its contribution is small in comparison with that of the other terms in Schrödinger equation so that the *linear* approximation in the field B can be used. In such a linear approximation, the wave function of electron remains unperturbed, with the only effect being the well known Zeeman splitting of the energy levels of the hydrogen atom. In both Zeeman effects, the energy of interaction of electron with the magnetic field is assumed to be much smaller than the binding energy of the hydrogen atom, $e\hbar B/2mc \ll me^4/2\hbar^2 = 13.6$ eV, i.e. the intensity of the magnetic field is much smaller than some characteristic value, $B \ll B_0 = 2.4 \cdot 10^9$ Gauss $=$ 240000 Tesla (1 Tesla $= 10^4$ Gauss). Thus, the action of a weak magnetic field can be treated as a small perturbation of the hydrogen atom.

In the case of *very strong* magnetic field, $B \gg B_0$, the quadratic term in the field B makes a great contribution and can not be ignored. Calculations show that a considerable deformation of the electron charge distribution in the hydrogen atom occurs. Namely, under the influence of a very strong external magnetic field a magnetic confinement takes place, i.e. in the plane perpendicular to the direction of magnetic field the electron dynamics is determined mainly by the action of the magnetic field, while the Coulomb interaction of the electron with the nucleus can be viewed as a small perturbation. This adiabatic approximation allows one to separate variables in Schrödinger equation [1]. At the same time, in the direction along the direction of the magnetic field the motion of electron is governed both by the magnetic field effects and the Coulomb interaction of the electron with the nucleus.

In this paper we briefly review some results on the hydrogen atom in very strong external static uniform magnetic fields, focusing on the basic physical picture derived from the Schrödinger equation. Our consideration of the

problem of atoms and molecules exposed to strong external magnetic field is related to MagneGas technology and PlasmaArcFlow hadronic molecular reactors recently developed by Santilli [2].

The highest intensities maintained macroscopically at large distances in modern magnet laboratories are of the order of $10^5...10^6$ Gauss (~ 50 Tesla), i.e. much below $B_0 = 2.4 \cdot 10^9$ Gauss ($\sim 10^5$ Tesla). An extremely intense external magnetic field, $B \geq B_S = B_0/\alpha^2 = 4.4 \cdot 10^{13}$ Gauss, corresponds to the interaction energy of the order of mass of electron, $mc^2 = 0.5$ MeV; $\alpha = e^2/\hbar c$ is the fine structure constant. In this case, despite the fact that the extremely strong magnetic field does not make vacuum unstable in respect to creation of electron-positron pairs, one should account for relativistic and quantum electrodynamics (QED) effects, and invoke Dirac or Bethe-Salpeter equation. Such intensities are not currently available in laboratories. However, these are of interest in astrophysics, for example in studying an atmosphere of neutron stars and white dwarfs which is characterized by $B \simeq 10^9 \dots 10^{13}$ Gauss.

In this paper, we shall not consider intensities as high as Schwinger value B_S, and restrict our review by the intensities $2.4 \cdot 10^{10} \leq B \leq 2.4 \cdot 10^{11}$ Gauss ($10B_0 \dots 100B_0$), at which (nonrelativistic) Schrödinger equation can be used to a very good accuracy, and the adiabatic approximation can be made.

Relativistic and QED effects (loop contributions), as well as the effects such as those related to the finite mass, size, and magnetic moment of the nucleus, and the finite electromagnetic radius of electron, reveal themselves even at low magnetic field intensities, and can be accounted for as very small perturbations. These are beyond the scope of the present paper, while being of much importance in the high precision studies, such as those on stringent tests of the Lamb shift.

It should be noted that a locally high-intensity magnetic field may arise in the plasma as the result of nonlinear effects, which can lead to creation of stable self-confined structures having a nontrivial topology with knots [3]. Particularly, Faddeev and Niemi [3] recently argued that the static equilibrium configurations within the plasma are topologically stable solitons, that describe knotted and linked fluxtubes of helical magnetic fields. In the region close to such fluxtubes, we suppose the magnetic field intensity may be as high as B_0. In view of this, study of the action of strong magnetic field and the fluxtubes of magnetic fields on atoms and molecules becomes of much

interest in theoretical and applicational *plasmachemistry*.

Possible applications are in MagneGas technology, theoretical foundations and exciting implications of which are developed by Santilli [2]. We refer the reader to Ref. [2] for the recent studies, description, and applications of MagneGas technology and PlasmaArcFlow reactors. Remarkable experimental results, including Gas-Chromatographic Mass-Spectroscopic and InfraRed spectrum data of Santilli's magnegas, clearly indicates the presence of unconventional chemical species of *magnecules*, which have not been identified as conventional molecules, and are supposed to be due to the specific bonding of a magnetic origin. The basic physical picture of the magnecules proposed by Santilli [2] is related to the toroidal orbitals of the electrons of atoms exposed to a very strong magnetic field. The results of the present paper demonstrate this physical picture on the basis of the Schrödinger equation.

As the result of the action of very strong magnetic field, atoms attain great binding energy as compared to the case of zero magnetic field. Even at intermediate $B \simeq B_0$, the binding energy of atoms greatly deviates from that of zero-field case, and even lower field intensities may essentially affect chemical properties of molecules of heavy atoms. This enables creation of various other bound states in molecules, clusters and bulk matter [1, 2, 4].

The paper by Lai [4], who focused on very strong magnetic fields, $B \gg B_0$, motivated by the astrophysical applications, gives a good survey of the early and recent studies in this field, including those on the intermediate range, $B \simeq B_0$, multi-electron atoms, and H_2 molecule. Much number of papers using variational/numerical and/or analytical approaches to the problem of light and heavy atoms, ions, and H_2 molecule in strong magnetic field, have been published within the last six years (see, e.g., references in [4]). However, highly magnetized molecules of heavy atoms have not been systematically investigated. One of the surprising implications is that for some diatomic molecules of heavy atoms, the molecular binding energy is predicted to be several times bigger than the ground state energy of individual atoms. [5]

2 Landau levels of a single electron

To estimate intensity of the magnetic field which causes a considerable deformation of the ground state electron orbit of the hydrogen atom, one can

formally compare the Bohr radius of the hydrogen atom in the ground state, in zero external magnetic field, $a_0 = \hbar^2/me^2 \simeq 0.53 \cdot 10^{-8}$ cm = 1 a.u., with the radius of orbit of a single electron moving in the external static uniform magnetic field $\vec{B}$. Below, we give a brief summary of the latter issue.

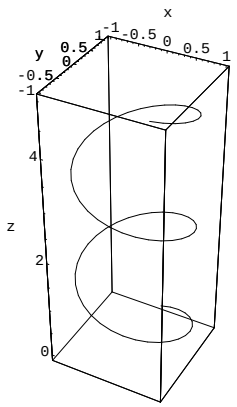

Figure 1: Classical orbit of the electron in an external static uniform magnetic field $\vec{B} = (0, 0, B)$ pointed along the z axis. The electron experiences a circular motion in the x, y plane and a linear motion in the z direction (a helical curve).

The mean radius of the orbital of a single electron moving in a static uniform magnetic field can be calculated exactly using Schrödinger equation, and is given by

$$R_n = \sqrt{\frac{n + 1/2}{\gamma}}, \tag{2.1}$$

where we have denoted

$$\gamma = \frac{eH}{2\hbar c}, \tag{2.2}$$

B is the intensity of the magnetic field pointed along the z axis, $\vec{B} = (0, 0, B)$, $\vec{r} = (r, \varphi, z)$ in cylindrical coordinates, and $n = 0, 1, \ldots$ is the principal quantum number. Thus, the radius of the orbit takes *discrete* set of values (2.1), and is referred to as Landau radius. This is in contrast to the well known *classical* motion of electron in the external magnetic field (a helical

curve is shown in Fig. 1), with the radius of the orbit being of a continuous set of values. The classical approach evidently can not be applied to study dynamics of the electron at atomic distances.

Corresponding energy levels E_n of a single electron moving in the external magnetic field are referred to as Landau energy levels,

$$E_n = E_n^{\perp} + E_{k_z}^{\parallel} = \hbar\Omega(n + \frac{1}{2}) + \frac{\hbar^2 k_z^2}{2m}, \tag{2.3}$$

where

$$\Omega = \frac{eH}{mc} \tag{2.4}$$

is so called cyclotron frequency, and $\hbar k_z$ is a projection of the electron's momentum $\hbar\vec{k}$ on the direction of the magnetic field, $-\infty < k_z < \infty$, m is the mass of electron, and $-e$ is the charge of electron.

Landau energy levels $E_n^{\perp}$ correspond to a discrete set of round orbits of electron which are projected to the transverse plane. The energy $E_{k_z}^{\parallel}$ corresponds to the free motion of electron in parallel to the magnetic field (*continuous* spectrum), with a conserved momentum $\hbar k_z$ along the magnetic field.

Regarding the above presented review of Landau's results, we remind that in the general case of *uniform* external magnetic field the coordinate and spin components of the total wave function of the electron can always be separated.

The corresponding coordinate component of the total wave function of the electron, obtained as an exact solution of Schrödinger equation for a single electron moving in the external magnetic field with vector-potential chosen as $A_r = A_z = 0$, $A_\varphi = rH/2$),

$$-\frac{\hbar^2}{2m}\left(\partial_r^2 + \frac{1}{r}\partial_r + \frac{1}{r^2}\partial_\varphi^2 + \partial_z^2 - \gamma^2 r^2 + 2i\gamma\partial_\varphi\right)\psi = E\psi, \tag{2.5}$$

is of the following form [1]:

$$\psi_{n,s,k_z}(r,\varphi,z) = \sqrt{2\gamma} I_{ns}(\gamma r^2)\frac{e^{il\varphi}}{\sqrt{2\pi}}\frac{e^{ik_z z}}{\sqrt{L}}, \tag{2.6}$$

where $I_{ns}(\rho)$ is Laguerre function,

$$I_{ns}(\rho) = \frac{1}{\sqrt{n!s!}} e^{-\rho/2}\rho^{(n-s)/2} Q_s^{n-s}(\rho); \tag{2.7}$$

Q_s^{n-s} is Laguerre polynomial, L is normalization constant, $l = 0, \pm 1, \pm 2, \ldots$ is azimuthal quantum number, $s = n - l$ is the radial quantum number, and we have denoted, for brevity,

$$\rho = \gamma r^2. \tag{2.8}$$

The wave function (2.6) depends on the angle φ as $\exp[il\varphi]$, and the energy (2.3) does not depend on the azimuthal quantum number l, so the system reveals a *rotational* symmetry in respect to the angle φ and all the Landau orbits are round.

Also, the energy (2.3) does not depend on the radial quantum number s. This means a degeneracy of the system in respect to the position of the center of the orbit, and corresponds to an "unfixed" position of the center. At $n - s > 0$, the origin of the coordinate system is inside the orbit while at $n - s < 0$ it is outside the orbit. The mean distance d between the origin of coordinate system and the center of orbit takes a discrete set of values, and is related to the quantum number s as follows:

$$d = \sqrt{\frac{s + 1/2}{\gamma}}. \tag{2.9}$$

Clearly, the energy (2.3) does not depend on this distance because of the homogeneity of the magnetic field, so it does not depend on s. However, it should be noted that the whole Landau orbit can not move on the (r, φ) plane continuously along the variation of the coordinate r. Instead, it can only "jump" to a certain distance, which depends on the intensity of the magnetic field, in accord to Eq. (2.9).

The spin components of the total wave function are trivially

$$\psi(\frac{1}{2}) = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad \psi(-\frac{1}{2}) = \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \tag{2.10}$$

with the corresponding energies

$$E_{spin} = \pm \mu_0 B, \tag{2.11}$$

to be added to the energy (2.3). Here,

$$\mu_0 = \frac{e\hbar}{2mc} \simeq 9.3 \cdot 10^{-21} \text{ erg} \cdot \text{Gauss}^{-1} = 5.8 \cdot 10^{-9} \text{ eV} \cdot \text{Gauss}^{-1} \tag{2.12}$$

is Bohr magneton. Below, we do not consider the energy (2.11) related to the interaction of the spin of electron with the external magnetic field because it decouples from the orbital motion and can be accounted for separately. As to the numerical estimation, at $B = B_0 = 2.4 \cdot 10^9$ Gauss, the energy $E_{spin} \simeq \pm 13.6$ eV.

For the *ground* level, i.e. at $n = 0$ and $s = 0$, and zero momentum of the electron in the z-direction, i.e. $\hbar k_z = 0$, we have from (2.3)

$$E_0^{\perp} = \frac{e\hbar B}{2mc}, \tag{2.13}$$

and due to Eq. (2.6) the corresponding normalized ground state wave function is

$$\psi_{000}(r, \varphi, z) = \psi_{000}(r) = \sqrt{\frac{\gamma}{\pi}}\, e^{-\gamma r^2/2}, \tag{2.14}$$

$\int_0^{\infty}\int_0^{2\pi} r dr d\varphi \; |\psi_{000}|^2 = 1$.

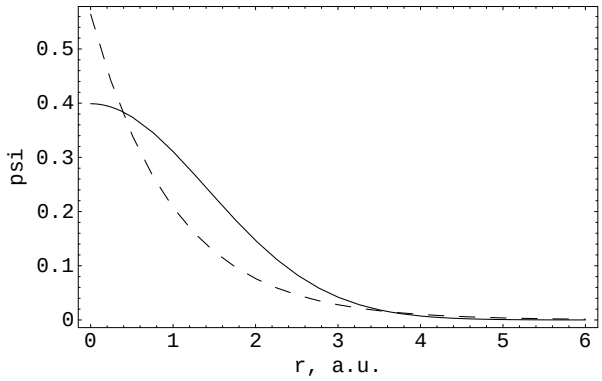

Figure 2: Landau ground state wave function of a single electron, ψ_{000} (solid curve), Eq. (2.14), in strong external magnetic field $B = B_0 = 2.4 \cdot 10^9$ Gauss, as a function of the distance r in cylindrical coordinates, and (for a comparison) the hydrogen ground state wave function (at *zero* external magnetic field), $(1/\sqrt{\pi})e^{-r/a_0}$ (dashed curve), as a function of the distance r in spherical coordinates. The associated probability densities are shown in Fig. 3; 1 a.u. $= a_0 = 0.53 \cdot 10^{-8}$ cm.

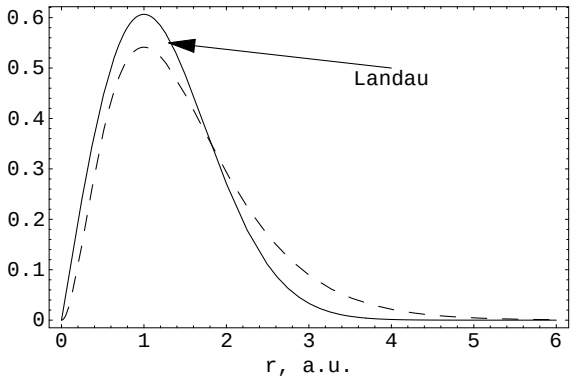

Figure 3: The probability density for the case of the Landau ground state of a single electron, $2\pi r|\psi_{000}|^2$ (solid curve), Eq. (2.14), in the strong external magnetic field $B = B_0 = 2.4 \cdot 10^9$ Gauss, as a function of the distance r in cylindrical coordinates, and (for a comparison) probability density of the hydrogen atom ground state (at *zero* external magnetic field), $4\pi r^2|(1/\sqrt{\pi})e^{-r/a_0}|^2$ (dashed curve), as a function of the distance r in spherical coordinates. The associated wave functions are shown in Fig. 2; 1 a.u. $= 0.53 \cdot 10^{-8}$ cm.

The corresponding (smallest) Landau radius of the orbit of electron is

$$R_0 = \sqrt{\frac{\hbar c}{eB}} \equiv \sqrt{\frac{1}{2\gamma}}, \tag{2.15}$$

in terms of which ψ_{000} reads

$$\psi_{000} = \sqrt{\frac{1}{2\pi R_0^2}}\; e^{-\frac{r^2}{4R_0^2}}. \tag{2.16}$$

Figure 2 depicts ground state wave function of a single electron, ψ_{000}, in strong external magnetic field $B = B_0 = 2.4 \cdot 10^9$ Gauss ($R_0 = 1$ a.u.), and (for a comparison) of the hydrogen ground state wave function, at *zero* external magnetic field, $(1/\sqrt{\pi})e^{-r/a_0}$. Figures 3 and 4 display the associated probability density of electron as a function of the distance r from the center of the orbit, the radius of which is about 1 a.u.

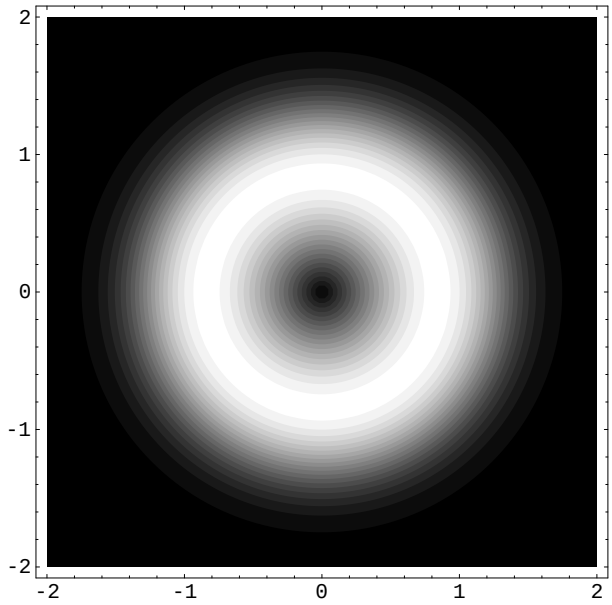

Figure 4: A contour plot of the (r, φ) probability density for the case of the Landau ground state of a single electron, $2\pi r|\psi_{000}|^2$, Eq. (2.14), in the strong external magnetic field $B = B_0 = 2.4 \cdot 10^9$ Gauss, as a function of the distance in a.u. (1 a.u. $= 0.53 \cdot 10^{-8}$ cm). Lighter area corresponds to higher probability to find electron. The set of maximal values of the probability density is referred to as an "orbit".

The condition that the Landau radius R_0 is smaller than the Bohr radius, $R_0 < a_0$, which is adopted here as the condition of a considerable "deformation" of the electron orbit of the hydrogen atom, then implies

$$B > B_0 = \frac{m^2 ce^3}{\hbar^3} = 2.351 \cdot 10^9 \text{ Gauss}, \tag{2.17}$$

where m is mass of electron. Equivalently, this deformation condition corresponds to the case when the binding energy of the hydrogen atom, $|E_0^{Bohr}| = |-me^4/2\hbar^2| = 0.5$ a.u. $= 13.6$ eV, is smaller than the ground Landau energy $E_0^{\perp}$.

The above critical value of the magnetic field, B_0, is naturally taken as an *atomic unit* for the strength of the magnetic field, and corresponds to the

case when the pure Coulomb interaction energy of electron with nucleus is equal to the interaction energy of a single electron with the external magnetic field, $|E_0^{Bohr}| = E_0^{\perp} = 13.6$ eV, or equivalently, when the Bohr radius is equal to the Landau radius, $a_0 = R_0 = 0.53 \cdot 10^{-8}$ cm.

It should be stressed here that we take the characteristic parameters, Bohr energy $|E_0^{Bohr}|$ and Bohr radius a_0, of the hydrogen atom with a single purpose to establish criterium for the critical strength of the external magnetic field, for the hydrogen atom under consideration. For other atoms the critical value of the magnetic field may be evidently different.

3 Hydrogen atom in magnetic fields

After we have considered quantum dynamics of a single electron in the external magnetic field, we turn to consideration of the hydrogen atom in the external static uniform magnetic field.

We choose cylindrical coordinate system (r, φ, z), in which the external magnetic field is $\vec{B} = (0, 0, B)$, i.e., the magnetic field is directed along the z-axis. General Schrödinger equation for the electron moving around a fixed proton (Born-Oppenheimer approximation) in the presence of the external magnetic field is

$$-\frac{\hbar^2}{2m}\left(\partial_r^2 + \frac{1}{r}\partial_r + \frac{1}{r^2}\partial_\varphi^2 + \partial_z^2 + \frac{2me^2}{\hbar^2\sqrt{r^2+z^2}} - \gamma^2 r^2 + 2i\gamma\partial_\varphi\right)\psi = E\psi, \tag{3.1}$$

where $\gamma = eH/2\hbar c$. Note the presence of the term $2i\gamma\partial_\varphi$, which is *linear* in B, and of the term $-\gamma^2 r^2$, which is *quadratic* in B. The other terms do not depend on the magnetic field B.

The main problem in the nonrelativistic study of the hydrogen atom in the external magnetic field is to solve the above Schrödinger equation and find the energy spectrum.

In this equation, we can not directly separate *all* the variables, r, φ, and z, because of the presence of the Coulomb potential, $e^2/\sqrt{r^2+z^2}$, which does not allow us to make a direct separation in variables r and z.

Also, for the general case of an arbitrary intensity of the magnetic field, we can not ignore the term $\gamma^2 r^2$ in Eq. (3.1), which is quadratic in B, since this term is not small at *high* intensities of the magnetic field.

For example, at small intensities, $B \simeq 2.4 \cdot 10^4$ Gauss = 2.4 Tesla, the parameter $\gamma = eH/2\hbar c \simeq 1.7 \cdot 10^{11}$ cm^{-2} so that for $\langle r \rangle \simeq 0.5 \cdot 10^{-8}$ cm we get the estimation $\gamma^2 \langle r^2 \rangle \simeq 10^6$ cm^{-2} and Landau energy $\hbar\Omega/2$ is of the order of 10^{-4} eV, while at high intensities, $B \simeq B_0 = 2.4 \cdot 10^9$ Gauss $= 2.4 \cdot 10^5$ Tesla, the parameter $\gamma = \gamma_0 \simeq 1.7 \cdot 10^{16}$ cm^{-2} so that the estimations are: $\gamma^2 \langle r^2 \rangle \simeq 10^{16}$ cm^{-2} (greater by ten orders) and the ground Landau energy is about 13.6 eV (greater by five orders).

Below, we turn to approximate *ground state* solution of Eq. (3.1) for the case of *very strong* magnetic field.

3.1 Very strong magnetic field

Let us consider the approximation of a *very* strong magnetic field,

$$B \gg B_0 = 2.4 \cdot 10^9 \text{ Gauss}. \tag{3.2}$$

Under the above condition, in the transverse plane the Coulomb interaction of the electron with the nucleus is not important in comparison with the interaction of the electron with the external magnetic field. So, in accord to the exact solution (2.6) for a single electron, one can seek for an approximate ground state solution of Eq. (3.1) in the form (see, e.g. [1]) of factorized transverse and longitudinal parts,

$$\psi = e^{-\gamma r^2/2} \chi(z), \tag{3.3}$$

where we have used Landau wave function (2.14), $s = 0$, $l = 0$, and $\chi(z)$ denotes the longitudinal wave function to be found. This is so called *adiabatic approximation*. The charge distribution of the electron in the (r, φ) plane is thus characterized by the Landau wave function $\sim e^{-\gamma r^2/2}$, i.e. by the azimuthal symmetry.

In general, the adiabatic approximation corresponds to the case when the transverse motion of electron is totally determined by the intense magnetic field, which makes it "dance" at its cyclotron frequency. Specifically, the radius of the orbit is then *much smaller* than the Bohr radius, $R_0 \ll a_0$, or, equivalently, the Landau energy of electron is much bigger than the Bohr energy $E_0^{\perp} \gg |E_0^{Bohr}| = 13.6$ eV. In other words, this approximation means that the interaction of electron with the nucleus in the transverse plane is ignorably small (it is estimated to make about 2% correction at $B \simeq 10^{12}$

Gauss), and the energy spectrum in this plane is defined solely by the Landau levels. The remaining problem is thus to find the longitudinal energy spectrum, in the z direction.

Inserting wave function (3.3) into the Schrödinger equation (3.1), multiplying it by ψ^*, and integrating over variables r and φ in cylindrical coordinate system, we get the following equation characterizing the z dependence of the wave function:

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dz^2}+\frac{\hbar^2\gamma}{m}+C(z)\right)\chi(z)=E\chi(z), \tag{3.4}$$

where

$$C(z)=-\sqrt{\gamma}\,e^2\int_0^\infty\frac{e^{-\rho}}{\sqrt{\rho+\gamma z^2}}\,d\rho=-e^2\sqrt{\pi\gamma}\,e^{\gamma z^2}\mathrm{erfc}(\sqrt{\gamma}|\mathrm{z}|), \tag{3.5}$$

$\mathrm{erfc}(x)=1-\mathrm{erf}(x)$, and

$$\mathrm{erf(x)}=\frac{2}{\sqrt{\pi}}\int_0^{\mathrm{x}}\mathrm{e}^{-\mathrm{t}^2}\mathrm{dt} \tag{3.6}$$

is error function.

In Fig. 5, the exact potential $C(z)$ is plotted, at $B=2.4\cdot10^{11}$ Gauss $=100B_0$, for which case the lowest point of the potential is about $C(0)\simeq-337$ eV. In this case, in the (r,φ) plane, the hydrogen atom is characterized by the Landau energy $E_0^\perp=1360$ eV $\gg13.6$ eV, Landau radius $R_0=0.5\cdot10^{-9}$ cm $\ll0.5\cdot10^{-8}$ cm, and the cyclotron frequency is $\Omega=4\cdot10^{18}$ sec^{-1}. For a comparison, the Coulomb potential $-e^2/|z|$ is also shown. One can see that the Coulomb potential does not reproduce the effective potential $C(z)$ to a good accuracy at small z.

The arising effective potential $C(z)$ is of a nontrivial form, which does not allow us to solve Eq. (3.4) analytically. Below we approximate it by simple potentials, to make estimation on the ground state energy and wave function of the hydrogen atom.

3.1.1 The Coulomb potential approximation

At high intensity of the magnetic field, $\gamma\gg1$ so that under the condition $\gamma\langle z^2\rangle\gg1$ we can ignore ρ in the square root in the integrand in Eq. (3.5).

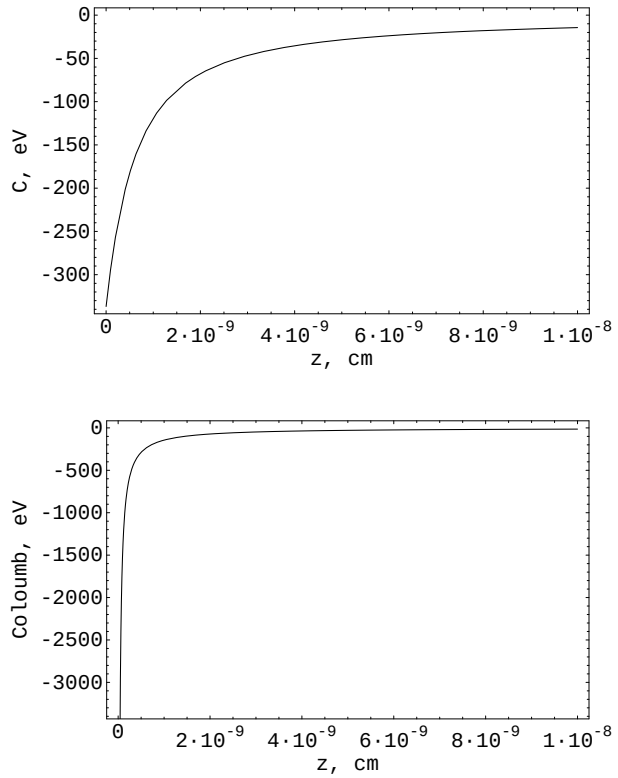

Figure 5: The exact effective potential $C(z)$ (top panel), at $B = 2.4 \cdot 10^{11}$ Gauss $= 100 B_0$, $C(0) = -337$ eV, and (for a comparison) Coulomb potential $-e^2/|z|$ (bottom panel).

Then, one can perform the simplified integral and obtain the result

$$C(z) \simeq V(z) = -\frac{e^2}{|z|}, \quad \text{at } \gamma \langle z^2 \rangle \gg 1, \tag{3.7}$$

which appears to be a pure Coulomb interaction of electron with the nucleus, in the z direction. Therefore, Eq. (3.4) reduces to *one-dimensional* Schrödinger equation for Coulomb potential,

$$\left(\frac{\hbar^2}{2m} \frac{d^2}{dz^2} + \frac{e^2}{|z|} + \frac{\hbar^2 \gamma}{m} + E \right) \chi(z) = 0. \tag{3.8}$$

In atomic units ($e = \hbar = m = 1$), using the notation

$$E' = \frac{\hbar^2 \gamma}{m} + E, \quad n^2 = \frac{1}{-2E'}, \tag{3.9}$$

and introducing new variable

$$x = \frac{2z}{n}, \tag{3.10}$$

we rewrite the above equation in the following form:

$$\left[\frac{d}{dx^2} + \left(-\frac{1}{4} + \frac{n}{x}\right)\right] \chi(x) = 0, \tag{3.11}$$

where we assume, to simplify representation, $x > 0$. Introducing new function $v(x)$,

$$\chi(x) = x e^{-x/2} v(x), \tag{3.12}$$

we get the final form of the equation,

$$xv'' + (2 - x)v' - (1 - n)v = 0. \tag{3.13}$$

Note that this equation is identical to that obtained for the radial part of the three-dimensional Schrödinger equation for the hydrogen atom, at orbital quantum number zero. We note that it is a particular case of Cummer's equation,

$$xv'' + (b - x)v' - av = 0, \tag{3.14}$$

the general solution of which is given by

$$v(x) = C_1 \, {}_1F_1(a, b, x) + C_2 U(a, b, x) \tag{3.15}$$

where

$${}_1F_1(a, b, x) = \frac{\Gamma(b)}{\Gamma(b - a)\Gamma(a)} \int_0^1 e^{xt} t^{a-1} (1 - t)^{b-a-1} \, dt \tag{3.16}$$

and

$$U(a, b, x) = \frac{1}{\Gamma(a)} \int_0^\infty e^{-xt} t^{a-1} (1 + t)^{b-a-1} \, dt \tag{3.17}$$

are the confluent hypergeometric functions, and $C_{1,2}$ are constants. In our case, $a = 1 - n$ and $b = 2$.

For the wave function $\chi(x)$, we then have

$$\chi(x) = |x| e^{-|x|/2} \left[C_1^{\pm} {}_1F_1(1-n, 2, |x|) + C_2^{\pm} U(1-n, 2, |x|) \right], \qquad (3.18)$$

where x given by Eq. (3.10) is now allowed to have any real value, and the "$\pm$" sign in $C_{1,2}^{\pm}$ corresponds to the positive and negative values of x, respectively (the modulus sign is used for brevity).

Now we turn to the normalization issue.

The first hypergeometric function ${}_1F_1(1-n, 2, x)$ is finite at $x = 0$ for any n. At big x, it diverges exponentially, unless n is an integer number, $n = 1, 2, \ldots$, at which case it diverges polynomially.

The second hypergeometric function $U(1-n, 2, x)$ behaves differently, somewhat as a mirror image of the first one. In the limit $x \to 0$, it is finite for integer $n = 1, 2, 3, \ldots$, and diverges as $1/x$ for noninteger $n > 1$ and for $0 \leq n < 1$. In the limit $x \to \infty$, it diverges polynomially for integer n, tends to zero for noninteger $n > 1$ and for $n = 0$, and diverges for noninteger $0 < n < 1$. In Figs. 18 and 19 of Appendix, the hypergeometric functions ${}_1F_1(1-n, 2, x)$ and $U(1-n, 2, x)$ for $n = 0, 1/4, 1/2, 1, 3/2, 2, 5/2, 3$ are depicted (n may be taken, for example, $n = 0.133$ as well).

In general, because of the prefactor $xe^{-x/2}$ in the solution (3.18) which cancels some of the divergencies arising from the hypergeometric functions, we should take into account *both* of the two linearly independent solutions, to get the most general form of normalizable wave functions.

As a consequence, the eigenvalues may *differ* from those corresponding to $n = 1, 2, \ldots$ (which is an analogue of the principal quantum number in the ordinary hydrogen atom) so that n is allowed to take some *non-integer* values from 0 to ∞, provided that the wave function is normalizable.

We are interested in the ground state solution, which is an even state. For even states, in accord to the symmetry of the wave function under the inversion $z \to -z$, we have

$$C_1^+ = C_1^-, \quad C_2^+ = C_2^-, \quad \chi'(0) = 0. \qquad (3.19)$$

Also, since $n = 1$ gives $E' = -1/(2n^2) = -1/2$ a.u., we should seek a normalizable wave function for n in the interval $0 < n < 1$, in order to achieve the energy value, which is lower than $-1/2$ a.u. If it is successful, the value $n = 1$ indeed does not characterize the ground state. Instead, it may correspond to some excited state.

One can see that the problem is in a remarkable difference from the ordinary three-dimensional problem of the hydrogen atom, for which the principal quantum number n must be integer to get normalizable wave functions, and the value $n = 1$ corresponds to the lowest energy. The distinction is due to the fact that the additional factor x in the solution (3.18) does not cancel in the total wave function[1].

We restrict consideration by the even state so we can focus on the $x \geq 0$ domain, and drop the modulus sign,

$$\chi(x) = xe^{-x/2}\left[C_1^{\pm}\,{}_1F_1(1-n,2,x) + C_2^{\pm}U(1-n,2,x)\right]. \tag{3.20}$$

In summary, the problem is to identify a *minimal* value of n in the interval $0 < n \leq 1$, at which the wave function $\chi(x)$ represented by a combination of the *two* linearly independent solutions is normalizable and obeys the conditions (3.19).

The condition $\chi'(0) = 0$ implies

$$\begin{aligned}&\tfrac{1}{2}e^{-x/2}\left[C_1\left((2-x)\,{}_1F_1(1-n,2,x) + (1-n)x\,{}_1F_1(2-n,3,x)\right) + \right.\\ &\left. + C_2\left((2-x)U(1-n,2,x) - 2(1-n)xU(2-n,3,x)\right)\right]_{|x=0} = 0.\end{aligned} \tag{3.21}$$

The function ${}_1F_1(1-n,2,x)$ is well-defined at $x = 0$ for any n. The function $U(1-n,2,x)$ for small x behaves as $x^{-1}\Gamma^{-1}(1-n)$ so for $x = 0$ it appears to be infinite, unless $n = 1$. The function $U(2-n,3,x)$ for small x behaves as $x^{-2}\Gamma^{-1}(2-n)$ so for $x = 0$ it diverges ($\Gamma(a)$ is Euler gamma function). Therefore, there is no way to satisfy the above condition unless we put $C_2 = 0$, i.e. eliminate the second hypergeometric function, $U(1-n,2,x)$, as an unphysical solution. As the result, only the first hypergeometric function determines the wave function, at which case it is well-defined only for integer n.

For the first hypergeometric function as the remaining solution, the situation is well known,

$${}_1F_1(a,b,|x|)_{|x=0} = 1, \quad \frac{d}{dx}\,{}_1F_1(a,b,x)_{|x=0} = \frac{a}{b}. \tag{3.22}$$

[1]In the three-dimensional Coulomb problem it does cancel in the total wave function.

We take $n = 1$ as this value implies the lowest energy E' in this case. The energy for $n = 1$ is $E' = -1/2$ a.u., i.e.

$$E = -\frac{me^4}{2\hbar^2} - \frac{1}{2}\hbar\Omega, \tag{3.23}$$

where we have used $\hbar^2\gamma/m = \frac{1}{2}\hbar\Omega$ due to Eqs. (2.2) and (2.4).

Thus, the particular state $n = 1$ of the hydrogen atom is characterized by usual Bohr distance a_0 in the z direction, with the longitudinal wave function

$$\chi(z) \simeq |z| e^{-|z|/a_0}. \tag{3.24}$$

In addition, it is easy to check directly, without using the general hypergeometric function technique, that $\chi(z) = ze^{-z}$ satisfies the equation $(\frac{1}{2}d^2/dz^2 + 1/z + \epsilon)\chi(z) = 0$, for $\epsilon = -1/2$.

In the (r, φ) plane $(n = 0, s = 0)$ the orbit is characterized by the Landau radius $R_0 \ll a_0$, with the Landau wave function $\simeq e^{-r^2/4R_0^2}$, and the Landau energy $E_0^{\perp}$ given by the second term in Eq. (3.23). Thus, the $n = 1$ wave function in the Coulomb approximation is written as

$$\psi(r, \varphi, z) \simeq \sqrt{\frac{\gamma}{\pi}}\, ze^{-\gamma r^2/2 - |z|/a_0} = \sqrt{\frac{1}{2\pi R_0^2}}\; ze^{-\frac{r^2}{4R_0^2} - \frac{|z|}{a_0}}. \tag{3.25}$$

Also, spin of the electron for the ground state is aligned antiparallel to the magnetic field.

The associated probability density is evidently of a cylindrical (axial) symmetry and can be described as *two* Landau orbits of radius R_0 in different (r, φ) planes, one at the level $z = -a_0$, and the other at the level $z = +a_0$, with the nucleus at $z = 0$, as schematically depicted in Fig. 6. Presence of two Landau orbits occurs in accord to the wave function (3.25), which equals zero at $z = 0$ and is symmetrical with respect to the inversion, $z \to -z$. The electron moves simultaneously on these two orbits.

The above electron charge distribution supports the study made by Santilli [2] who proposed the polarized toroidal electron orbit in the hydrogen atom under the action of strong magnetic field, but the Coulomb approximation suggests the electron charge distribution in the form of *two* identical coaxial round orbits separated by relatively big vertical distance; see Fig. 6.

Note that the size of the hydrogen atom in the z direction is predicted to be about 10 times bigger than that in the transverse plane, i.e. $R_0 =$

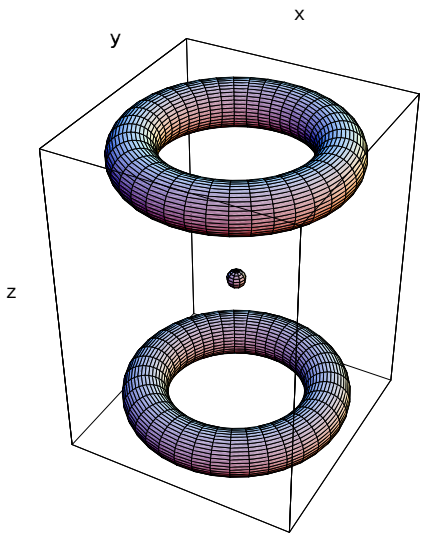

Figure 6: Schematic view on the hydrogen atom in the ground state, at very strong external magnetic field $\vec{B} = (0, 0, B)$, $B \gg B_0 = 2.4 \cdot 10^9$ Gauss, due to the Coulomb approximation approach, Eq. (3.25). One electron moves simultaneously on two Landau orbits of radius R_0 which are shown schematically as torii in the different $(x,\, y)$ planes, one torus at the level $z = -a_0$ and the other at the level $z = +a_0$, with the nucleus shown in the center at $z = 0$. Each torus represents the $(x,\, y)$ probability distribution as shown in Fig. 4 but with small Landau radius, $R_0 \ll a_0$. The spin of the electron is aligned antiparallel to the magnetic field.

$0.53 \cdot 10^{-9}$ cm $\simeq 0.1 a_0$; the hydrogen atom is thus highly elongated in the z direction (this ratio is *not* kept in Fig. 6). The cyclotron frequency (2.4) is of about $4 \cdot 10^{18}$ sec^{-1}. Classically, the linear velocity of the electron on such an orbit is $v = 2\pi R_0 \Omega$ and is estimated to be $v = 1.3 \cdot 10^{10}$ cm/sec $\simeq 0.4c$.

We should to note here that Landau radius R_0, at $B = 2.4 \cdot 10^{11}$ Gauss $= 100 B_0$, is about ten times bigger than Compton wavelength of electron, $\lambda_e / 2\pi \simeq 0.4 \cdot 10^{-10}$ cm, hence we can ignore quantum electrodynamics effects.

Finally, it should be noted that the above used Coulomb approximation is rather a crude one (see Fig. 5). Indeed, the energy in the z-direction does not depend on the magnetic field intensity while it is obvious that it should

depend on it. In the next Section, we approximate the effective potential $C(z)$ with a better accuracy.

3.1.2 The modified Coulomb potential approximation

We note that due to the exact result (3.5), the effective potential $C(z)$ tends to zero as $z \to \infty$ (not a surprise). However, a remarkable implication of the exact result is that $C(z)$ is *finite* at $z = 0$, namely,

$$C(0) = -\sqrt{\pi\gamma}\, e^2, \tag{3.26}$$

so that the effective potential $C(z)$ indeed can *not* be well approximated by the Coulomb potential, $-e^2/|z|$, at small z ($|z| < 10^{-8}$ cm) despite the fact that at big values of γ ($\gamma \gg \gamma_0 \simeq 1.7 \cdot 10^{16}$ cm^{-2}) the Coulomb potential reproduces $C(z)$ to a good accuracy at long and medium distances. Thus, the approximation considered in Sect. 3.1.1 appears to be not valid at (important) short distances.

Consequently, Eq. (3.4) with the *exactly* calculated $C(z)$ will yield the ground state of electron in the z direction which is drastically *different* from that with the Coulomb potential considered in Sect. 3.1.1. Thus, very intense magnetic field *essentially affects dynamics of electron not only in the* (r, φ) *plane but also in the* z *direction*. We expect that for the case of exact potential (3.5) the ground state is characterized by *much lower* energy in the z direction as compared to that of the one-dimensional Bohr state (3.23).

The exact potential $C(z)$ can be well approximated by the *modified* Coulomb potential,

$$C(z) \simeq V(z) = -\frac{e^2}{|z| + z_0}, \tag{3.27}$$

where z_0 is a parameter, $z_0 \neq 0$, which depends on the field intensity B due to

$$z_0 = -\frac{e^2}{C(0)} = \frac{1}{\sqrt{\pi\gamma}} = \sqrt{\frac{2\hbar c}{\pi e B}}. \tag{3.28}$$

The analytic advantage of this approximation is that $V(z)$ is *finite* at $z = 0$, being of Coulomb-type form.

Calculations for this approximate potential can be made in an essentially the same way as in the preceding Section, with $|x|$ being replaced by $|x| + x_0$,

where $x_0 > 0$ (we remind that $x = 2z/n$),

$$\chi(x) = (|x|+x_0)e^{-(|x|+x_0)/2}\left[C_1^{\pm}{}_1F_1(1-n,2,|x|+x_0) + C_2^{\pm}U(1-n,2,|x|+x_0)\right]. \tag{3.29}$$

An essential difference from the pure Coulomb potential case is that the potential (3.27) has no singularities. The $x \to 0$ asymptotic of the associated second hypergeometric function, $U(1-n,2,|x|+x_0)$ becomes well-defined for noninteger n. Thus, the condition $\chi'(x)_{|x=0} = 0$ does not lead to divergencies in the second solution for noninteger $n < 1$. It remains only to provide well-defined behavior of the wave function at $x \to \infty$.

Analysis shows that *normalizable* wave functions, as a combination of *two* linearly independent solutions, for the modified Coulomb potential *does exist* for various *non-integer*[2] n. We are interested in the ground state solution, so we consider the values of n from 0 to 1. Remind that $E' = -1/(2n)^2$ so that for $n < 1$ we obtain the energy lower than -0.5 a.u.

For $n < 1$, the first hypergeometric function is not suppressed by the prefactor $xe^{-x/2}$ in the solution (3.29) at large x so we are led to discard it as an unphysical solution by putting $C_1 = 0$. A normalizable ground state wave function for $n < 1$ is thus may be given by the second term in the solution (3.29). The condition $\chi'(x)_{|x=0} = 0$ implies

$$\begin{aligned}\tfrac{1}{2}e^{-(x+x_0)/2}C_2[(2-x-x_0)U(1-n,2,x+x_0)- \\ -2(1-n)(x+x_0)U(2-n,3,x+x_0))]_{|x=0} = 0.\end{aligned} \tag{3.30}$$

The l.h.s of this equation depends on n and x_0, so we can select some field intensity B, calculate associated value of the parameter $x_0 = x_0(B)$ and find the value of n, from which we obtain the ground state energy E'.

On the other hand, for the ground state this condition can be viewed, *vice versa*, as an equation to find x_0 for some given value of n [6]. Hereby we reverse the order of the derivation, to simplify numerical calculations.

For example, taking the noninteger value

$$n = 1/\sqrt{15.58} \simeq 0.253 < 1 \tag{3.31}$$

we find from Eq. (3.30) numerically

$$x_0 = 0.140841. \tag{3.32}$$

[2]This is the case when one obtains a kind of "fractional" quantum number n which does make sense.

This value is in confirmation with the result $x_0 = 0.141$ obtained by Heyl and Hernquist [6] (see Discussion). On the other hand, x_0 is related in accord to Eq. (3.28) to the intensity of the magnetic field,

$$x_0 = \frac{2z_0}{n} = \sqrt{\frac{8\hbar c}{\pi n^2 eB}}, \tag{3.33}$$

from which we obtain $B \simeq 4.7 \cdot 10^{12}$ Gauss. Hence, at this field intensity the ground state energy of the hydrogen atom is given by $E' = -1/(2n^2) = -15.58$ Rydberg.

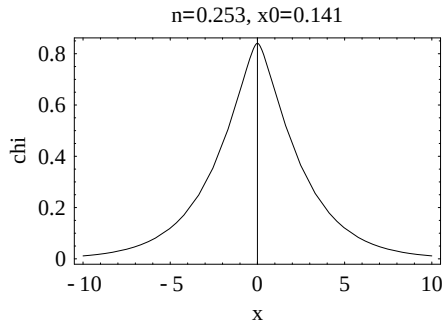

Figure 7: The longitudinal ground state wave function $\chi(x)$, Eq. (3.34), of the hydrogen atom in the magnetic field $B = 4.7 \cdot 10^{12}$ Gauss; $n = 1/\sqrt{-2E}$, $x = 2z/n$.

The longitudinal ground state wave function is given by

$$\chi(x) \simeq (|x| + x_0) e^{(|x|+x_0)/n} U(1-n, 2, |x| + x_0), \tag{3.34}$$

and is plotted in Fig. 7). The total wave function is

$$\chi(x) \simeq \sqrt{\frac{1}{2\pi R_0^2}} e^{-\frac{r^2}{4R_0^2}} (|x| + x_0) e^{(|x|+x_0)/n} U(1-n, 2, |x| + x_0), \tag{3.35}$$

and the associated three-dimensional probability density is schematically depicted in Fig. 8.

In contrast to the double Landau-type orbit implied by the Coulomb potential approximation, the modified Coulomb potential approach provides

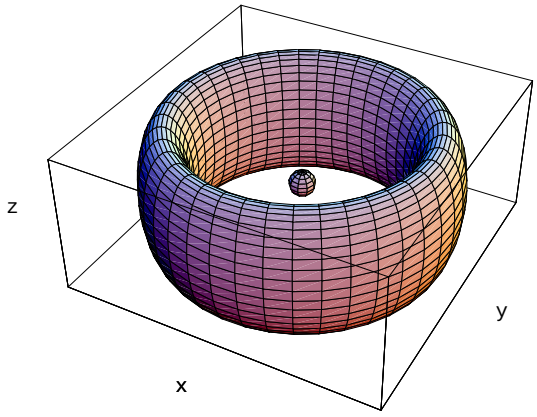

Figure 8: Schematic view of the hydrogen atom in the ground state, at very strong external magnetic field $\vec{B} = (0, 0, B)$, $B \gg B_0 = 2.4 \cdot 10^9$ Gauss, due to the *modified* Coulomb approximation approach. The electron moves on the Landau orbit of small radius $R_0 \ll 0.53 \cdot 10^{-8}$ cm, which is shown schematically as a torus. The vertical size of the atom is comparable to R_0. Spin of the electron is aligned antiparallel to the magnetic field.

qualitatively correct behavior and much better accuracy, and suggests a *single* Landau-type orbit shown in Fig. 8 for the *ground* state charge distribution of the hydrogen atom. This is in full agreement with Santilli's study [2] of the hydrogen atom in strong magnetic field.

Only excited states are characterized by the double Landau-type orbits depicted in Fig. 6. We shall not present calculations for the excited states in the present paper, and refer the reader to Discussion for some details on the results of the study made by Heyl and Hernquist [6].

3.1.3 Variational and numerical solutions

Review of approximate, variational, and numerical solutions can be found in the paper by Lai [4]. Accuracy of numerical solutions is about 3%, for the external magnetic field in the range from 10^{11} to 10^{15} Gauss. Figure 9 reproduces Fig. 1 of Ref. [4]. It represents the computed ionization energy Q_1 of the hydrogen atom and dissociation energy of H_2 molecule as functions

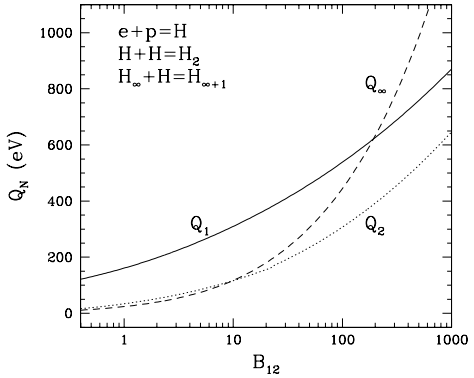

Figure 9: Ionization energies of the hydrogen atom and H_2 molecule exposed to very strong magnetic field; $B_{12} = B \cdot 10^{-12}$ Gauss (reproduction of Fig. 1 by Lai [4]).

of the intensity of the magnetic field; $B_{12} = B \cdot 10^{-12}$ Gauss, i.e. $B_{12} = 1$ means $B = 10^{12}$ Gauss.

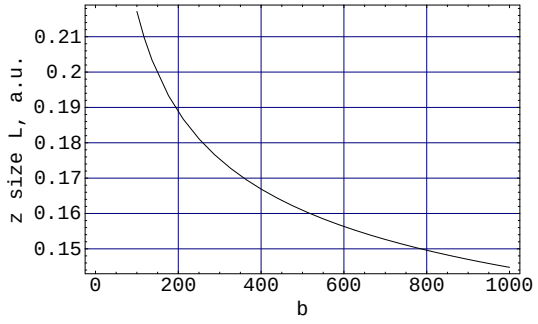

Figure 10: Longitudinal z-size of the hydrogen atom in the magnetic field, Eq. (3.36), as a function of the magnetic field intensity; $b = B/B_0$, $B_0 = 2.4 \cdot 10^9$ Gauss, 1 a.u. $= 0.53 \cdot 10^{-8}$ cm.

Due to the variational results [4], the z-size of the hydrogen atom in the

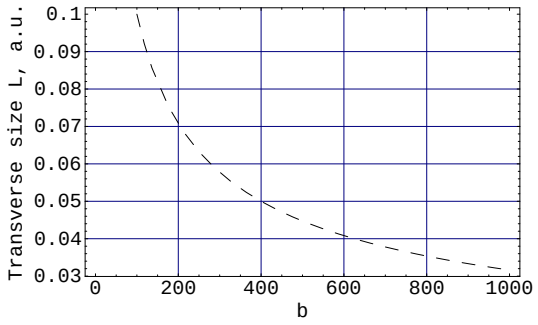

Figure 11: Transverse size of the hydrogen atom in the magnetic field, Eq. (3.37), as a function of the magnetic field intensity; $b = B/B_0$, $B_0 = 2.4 \cdot 10^9$ Gauss, 1 a.u. $= 0.53 \cdot 10^{-8}$ cm.

ground state is well approximated by the formula (Fig. 10)

$$L_z \simeq \frac{1}{\ln(B/B_0)} \text{ a.u.;} \tag{3.36}$$

the transverse (Landau) size is (Fig. 11)

$$L_\perp \simeq \frac{1}{\sqrt{B/B_0}} \text{ a.u.;} \tag{3.37}$$

and the ground state energy is (Fig. 12)

$$E \simeq -0.16[\ln(B/B_0)]^2 \text{ a.u.,} \tag{3.38}$$

with the accuracy of few percents, for $b \equiv B/B_0$ in the range from 10^2 to 10^6.

One can see for $B = 100B_0$, that the variational study predicts the ground state energy $E = -3.4$ a.u. $= -92.5$ eV (much lower than the value, -0.5 a.u., predicted by the $n = 1$ Coulomb approximation in Sect. 3.1.1), the transverse size $L_\perp$ of about 0.1 a.u. (the same as in the Coulomb approximation) and the z-size L_z of about 0.22 a.u. (much smaller than the value, 1 a.u., predicted by the Coulomb approximation). This confirms the result of the approximate analytic approach, in which $n < 1$ implies ground state energy much lower than -0.5 a.u.

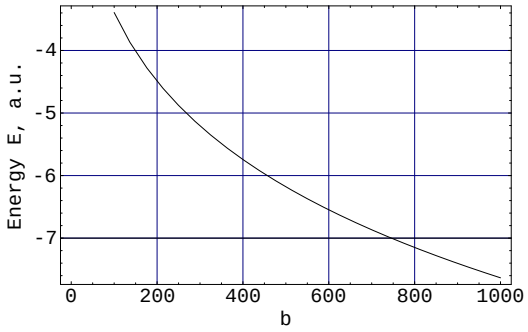

Figure 12: Variational ground state energy of the hydrogen atom in the magnetic field, Eq. (3.38), as a function of the magnetic field intensity; $b = B/B_0$, $B_0 = 2.4 \cdot 10^9$ Gauss, 1 a.u. = 27.2 eV.

4 Discussion

In a physical context, the used adiabatic approximation implies that the position of the nucleus is not "fixed" in the (r, φ) plane. Indeed, there is no reason for the nucleus to stay "exactly" at the center of the orbit when the Coulomb force in the transverse plane is totally ignored.

In contrast, in the z direction, we have more complicated situation, namely, the magnetic field leads to the effective interaction potential $C(z)$, which is finite at $z = 0$ and is Coulomb-like in the long-range asymptotic. Hence, the position of the nucleus remains to be fixed in the z direction relative to the orbit of the electron (bound state).

Due to the (crude) Coulomb approximation of Sect. 3.1.1, the electron probability density of the hydrogen atom under very intense magnetic field, at $n = 1$, appears to be of rather nontrivial form schematically depicted in Fig. 6.

More accurate approach may yield some different electron charge distributions but we expect that the symmetry requirements (namely, the axial symmetry and the (anti)symmetry under inversion $z \to -z$) would lead again to a toroidal orbit, which is *splitted into two* identical coaxial orbits (the torii are separated) similar to that shown in Fig. 6, or to an *unsplitted* one (the two torii are superimposed) as shown in Fig. 8.

Accurate analytic calculation of the ground and excited hydrogen wave

functions made by Heyl and Hernquist [6] in the adiabatic approximation leads to the longitudinal parts of the wave functions (the vertical z dependence) shown in Fig. 13, which reproduces the original Fig. 3 of their work; $\zeta = 2\pi\alpha z/\lambda_e$; $B = 4.7 \cdot 10^{12}$ Gauss. They used the modified Coulomb potential of the type (3.27), and the additional set of linearly independent solutions of the one-dimensional modified Coulomb problem in the form

$$(|x| + x_m)e^{-(|x|+x_m)/2}{}_1F_1(1-n, 2, |x| + x_m) \int^{|x|+x_m} \frac{e^t}{(t\,{}_1F_1(1-n, 2, t))^2}\, dt, \tag{4.1}$$

where $m = 0$ corresponds to the ground state. For the ground state with $n = 1/\sqrt{15.58}$, i.e. the binding energy is 15.58 Rydberg, they found $x_0 = 0.141$, which corresponds to $B = 4.7 \cdot 10^{12}$ Gauss. This result is in agreement with the study made in Sect. 3.1.2.

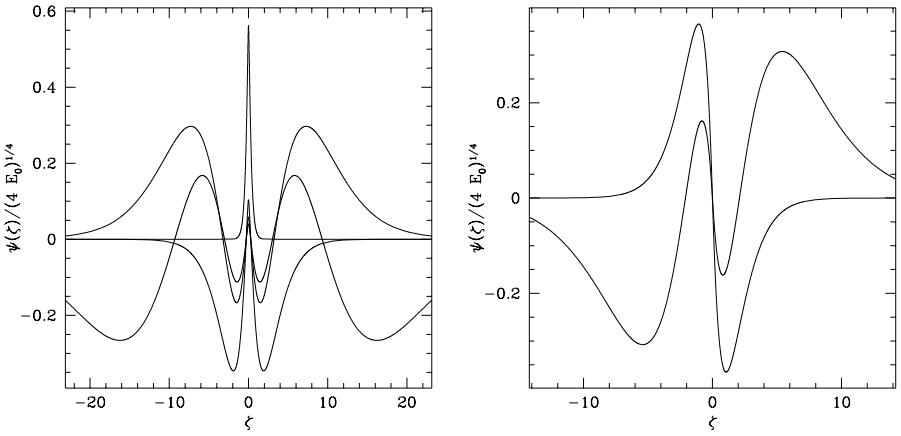

Figure 13: The axial wavefunctions of hydrogen in an intense magnetic field (analytic calculation) for $B = 4.7 \cdot 10^{12}$ Gauss. The first four even states with axial excitations, $|000\rangle$ (ground state), $|002\rangle$, $|004\rangle$, and $|006\rangle$ (left panel), and odd states $|001\rangle$ and $|003\rangle$ (right panel) are depicted. Here, $B = 4.7 \cdot 10^{12}$ Gauss, ground state energy is $E = -15.58$ Rydberg, $n = 1/\sqrt{15.58}$, $\zeta = 2z/n$ corresponds to x in our notation; z in a.u., 1 a.u. $= 0.53 \cdot 10^{-8}$ cm (reproduction of Figure 3 by Heyl and Hernquist [6]).

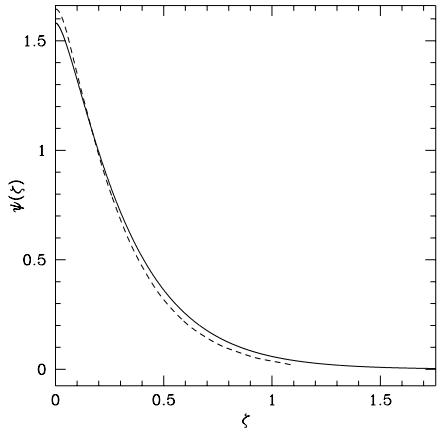

Figure 14: The axial ground state $|000\rangle$ wavefunction of hydrogen in an intense magnetic field, analytic calculation (solid curve) and numerical result (dashed line); $B = 4.7 \cdot 10^{12}$ Gauss, $E = -15.58$ Rydberg, $n = 1/\sqrt{15.58}$, $\zeta = 2z/n$ corresponds to x in our notation; z in a.u., 1 a.u. $= 0.53 \cdot 10^{-8}$ cm (reproduction of Figure 4 by Heyl and Hernquist [6]).

One can see from Fig. 13 that the peak of the ground state wave function $|000\rangle$ is at the point $z = 0$ (see also Fig. 14 for a close view) while the largest peaks of the excited wave functions are away from the point $z = 0$ (as it was expected to be). Consequently, the associated longitudinal probability distributions (square modules of the wave functions multiplied by the volume factor of the chosen coordinate system) are symmetric with respect to $z \to -z$, and their maxima are placed in the center $z = 0$ for the ground state, and away from the center for the excited states.

In contrast to the double toroidal orbit (Fig. 6) implied by the Coulomb approximation of Sect. 3.1.1, the modified Coulomb potential approach suggests a *single* toroidal orbit (Fig. 8) for the *ground* state charge distribution of the hydrogen atom. This confirms Santilli's study [2] of the hydrogen atom in strong magnetic field. The excited states $|00\nu\rangle$ are characterized by a double toroidal orbit schematically depicted in Fig. 6.

The computed ground state $|000\rangle$ binding energy of the hydrogen atom for different field intensities are [6]:

Magnetic field B (Gauss)	Binding energy, $\|000\rangle$ state (Rydberg)
4.7×10^{12}	15.58
9.4×10^{12}	18.80
23.5×10^{12}	23.81
4.7×10^{13}	28.22
9.4×10^{13}	33.21
23.5×10^{13}	40.75
4.7×10^{14}	47.20

They calculated first-order perturbative corrections to the above energies and obtained the values, which are in a good agreement with the results by Lai [4] (see Fig. 9) and Ruder *et al.* [1].

It is remarkable to note that in very strong magnetic field, the energy differences between the excited states and the ground state of the hydrogen atom are small in comparison to the absolute value of the ground state energy. The excited states are represented by the double torii configurations since the peaks of the associated wave functions spread far away from the center $z = 0$ in both $+z$ and $-z$ directions.

The above ground state electron charge distributions strongly support the study made by Santilli [2] who proposed the polarized toroidal electron orbit in the hydrogen atom under the action of strong magnetic field as a physical picture at the foundation of the new chemical species of magnecules. The only addition to this picture is that the the excited states are characterized by the double torii configuration.

Since zero field ground state case is characterized by perfect spherically symmetric electron charge distribution of the hydrogen atom, intermediate intensities of the magnetic field are naturally expected to imply a distorted spherical distribution. However, deeper analysis is required for the intermediate magnetic field intensities because the adiabatic approximation is not longer valid in this case. Namely, an interesting problem is to solve the Schrödinger equation (3.1) for the case when intensity of the magnetic field is not very strong, $B \leq B_0$, with the corresponding characteristic Landau ground state energy of about the Bohr energy. In this case, both the Coulomb and magnetic interactions should be taken at the same footing that leads to complications in its analytic study.

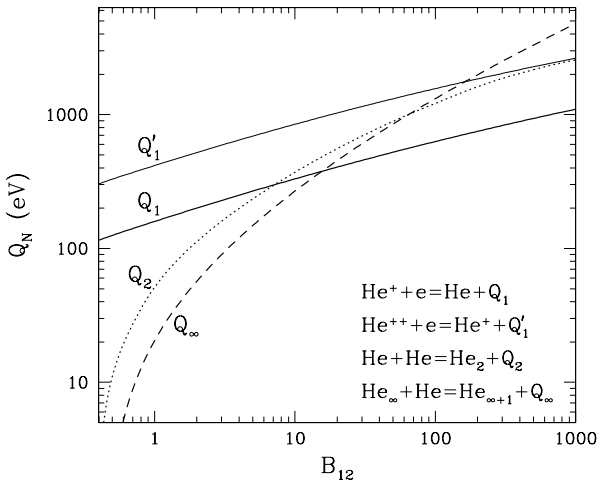

Figure 15: Ionization energies of He atom exposed to very strong magnetic field (numerical solutions); $B_{12} = B \cdot 10^{-12}$ Gauss (reproduction of Fig. 5 by Lai [4]).

As to the multi-electron atoms, an interesting problem is to study action of a very strong external magnetic field on He atom (see. e.g., Heyl and Hernquist [6] and Lai [4]; Fig. 15) and on the multi-electron heavy atoms, with outer electrons characterized by a *nonspherical* charge distribution, such as the p-electrons in Carbon atom, orbitals of which penetrate the orbitals of inner electrons. Very intense magnetic field would force such outer electrons to follow *small round* Landau orbits. In addition to the effect of a direct action of the magnetic field on the inner electrons, a series of essential rearrangements of the whole electron structure of the atom seems to be occur with a variation of the external magnetic field strength. Indeed, the magnetic field competes with both the Coulomb energy, which is different for different states of electrons, and the electron-electron interactions, including spin pairings. However, it is evident that at sufficiently strong fields, all the electron spins are aligned antiparallel to the magnetic field — fully spin polarized configuration — while at lower field intensities various partial spin polarized configurations are possible.

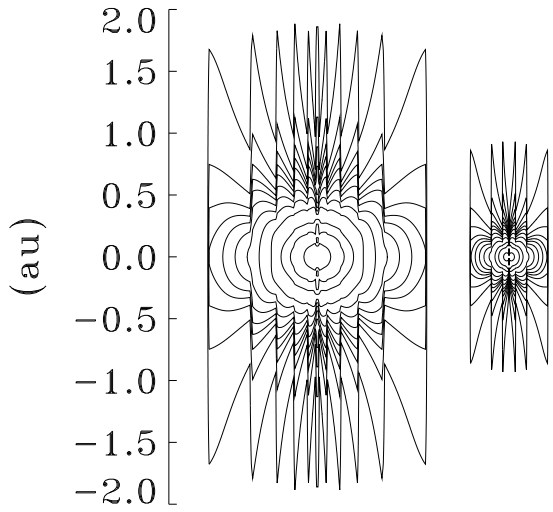

Figure 16: Contour plots of the (r, z) plane electron density of the iron atom according to density matrix theory at two different magnetic field strengths, 10^{11} Gauss (left) and 10^{12} Gauss (right). The outermost contour encloses 99% of the negative charge, the next 90%, then 80% etc., and the two innermost 5% and 1% respectively (reproduction of Fig. 5 by Johnsen and Yngvason [5]).

In accord to the numerical calculations based on the density matrix theory approach by Johnsen and Yngvason [5], which is in quite good agreement with the result of Hartree-Fock approach at very strong magnetic field intensities, the inner domain in the iron atom (26 electrons) is characterized by slightly distorted spherically symmetric distribution even at the intensities as high as $B = 100B_0 \ldots 1000B_0$. The outer domain appears to be of specific, highly elongated distribution along the direction of the magnetic field as shown in Fig. 16. The possible interpretation that the inner electrons remain to have spherical distribution while outer electrons undergo the squeeze seems to be not correct unless the spin state of the iron atom is verified to be partially polarized. So, we can conclude that all the electrons are in

highly magnetically polarized state (Landau state mixed a little by Coulomb interaction), and the electron structure is a kind of *Landau multi-electron cylindrical shell*, with spins of all the electrons being aligned antiparallel to the magnetic field (fully spin polarized configuration).

Another remark regarding Fig. 16 is that the contours indicating nearly spherical distribution will always appear since the Coulomb center (nucleus) is not totally eliminated from the consideration (non-adiabatic approximation), and it forces a spherical distribution to some degree, which evidently depends on the distance from the center (closer to the center, more sphericity). We note that Fig. 16 is in qualitative agreement with Fig. 6 in the sense that the predicted charge distribution reveals symmetry under the inversion $z \to -z$, with the characteristic z-elongated toroidal orbits.

An exciting problem is to study H_2 molecule under the action of strong external static uniform magnetic field using Schrödinger equation. Since the binding energy of H_2 molecule is of about 4.75 eV (much less than 13.6 eV of individual hydrogen atoms) and two interacting electrons of spin 1/2 participate dynamics we expect interesting physical predictions. For example, it is interesting to analyze the problem of bonding, in the presence of a strong magnetic field.

However, before studying H_2 molecule it would be very useful to investigate much simpler two-center system, H_2^+ ion, as it can give valuable information on the features of a two-center system under the action of a strong magnetic field. We refer the interested reader to Refs. [4, 6] for details of studies on H_2^+ ion and H_2 molecule in strong magnetic field. Figure 17 displays ground and first excited state wave functions of H_2^+ ion calculated by Heyl and Hernquist [6].

Finally, it should be noted that studies on the atomic and molecular systems in strong magnetic fields and related issues are becoming extensive last years. We refer the reader to a recent review by Lai [4] for an extensive list of references, and below present summary of some selected recent papers.

The work by Kravchenko *et al.* [8] uses an orthogonal approach and achieves very high precision by solving the general problem of the hydrogen atom in an arbitrarily strong magnetic field. This analytical work is of much importance as it provides solid ground to analyze few-electron and multi-electron atoms, and simple diatomic molecules.

A series of papers by Schmelcher *et al.* [9] is devoted to a systematic study of various simple atomic, ionic and molecular systems in strong magnetic

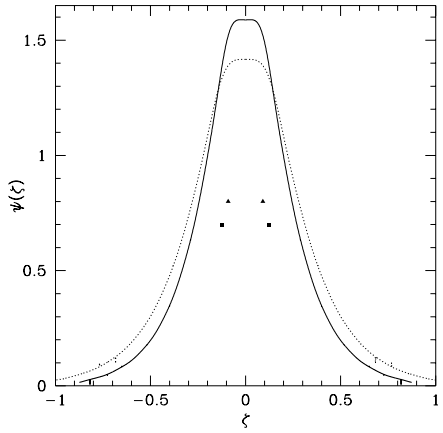

Figure 17: The ground and first-excited state of H_2^+ ion. The solid line traces $|000\rangle$, and the dashed line follows $|0\,\text{-}1\,0\rangle$. The triangles give the positions of the protons for the ground state and the squares for the excited state. Magnetic field $B = 4.7 \cdot 10^{12}$ Gauss is pointed along the internuclear axis; $\zeta = 2\pi\alpha z/\lambda_e$ denotes z in a.u.; 1 a.u. $= 0.53 \cdot 10^{-8}$ cm (reproduction of Figure 5 by Heyl and Hernquist [6]).

fields via Hartree-Fock method. One of the papers by Schmelcher *et al.* considers the carbon atom.

Analytical approximations have been constructed by Potekhin [10] for binding energies, quantum mechanical sizes and oscillator strengths of main radiative transitions of hydrogen atoms arbitrarily *moving* in magnetic fields $\simeq 10^{12} \ldots 10^{13}$ Gauss. This approach is of much importance in investigating an interaction of highly magnetized hydrogen atoms in a gaseous phase.

Computational finite element method for *time-dependent* Schrödinger equation has been developed by Watanabe and Tsukada [11] to study dynamics of electrons in a magnetic field that can be used effectively for mesoscopic systems, such as small clusters.

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Appendix

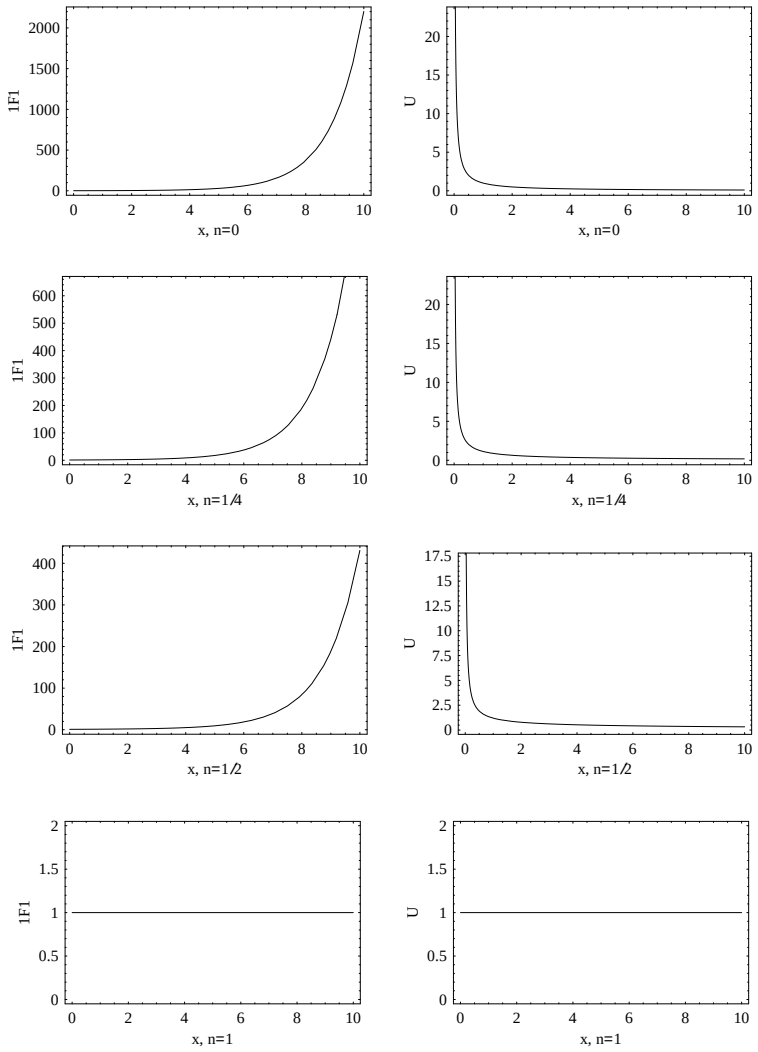

Figure 18: The confluent hypergeometric functions ${}_1F_1(1-n,2,x)$ and $U(1-n,2,x)$ for various n.

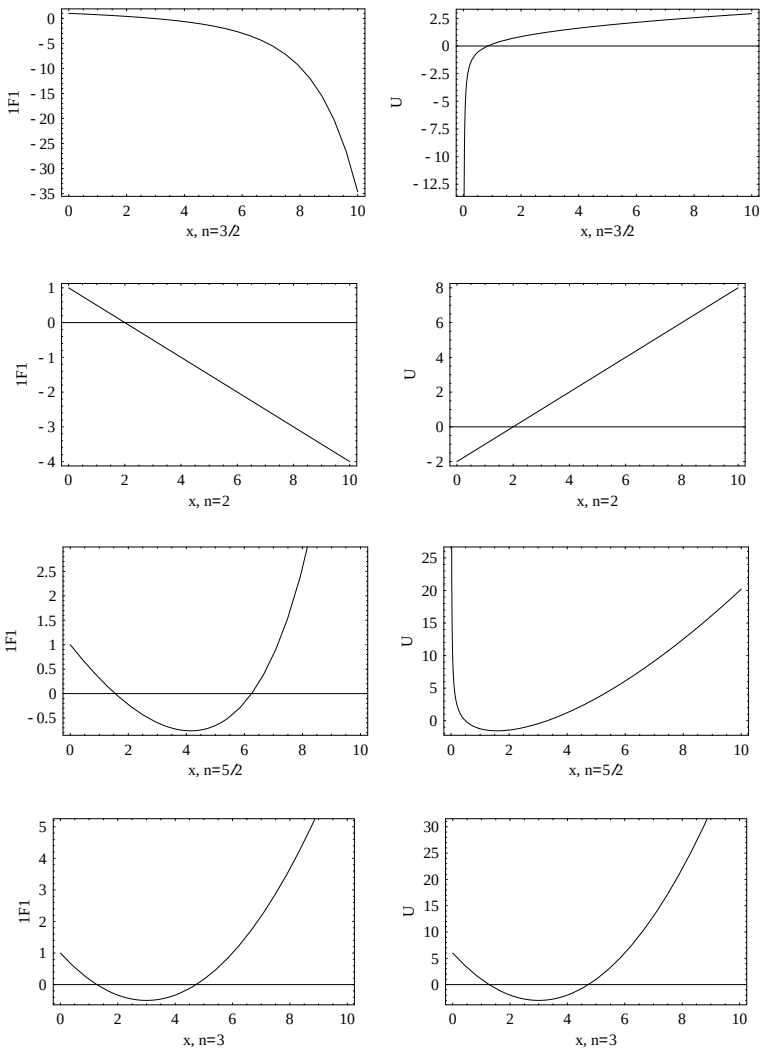

Figure 19: The confluent hypergeometric functions ${}_1F_1(1-n,2,x)$ and $U(1-n,2,x)$ for various n.

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