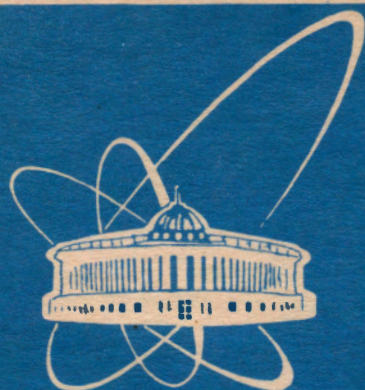


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ОБЪЕДИНЕННЫЙ
ИНСТИТУТ
ЯДЕРНЫХ
ИССЛЕДОВАНИЙ

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ZEEMAN EFFECT
IN THE OSCILLATOR REPRESENTATION

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1 Introduction

There are many quantum mechanical systems that are described by axially symmetrical potentials. Such a system as atoms in a constant magnetic field, the Zeeman effect, was one of the earliest problems studied in quantum mechanics [1]. Although many numerical and analytical investigations of this system have been reported in the literature [2], there is still today considerable interest in its detailed properties, especially in strong magnetic fields. The main motivation comes from astrophysics [3], where very strong magnetic fields are needed to understand the physics of neutron star surfaces and white dwarf stars.

The energies and eigenfunctions of deformed nuclei [4] and the electronic shell structure effects in metallic clusters [5] are described by the Schrödinger equation with axially symmetrical potentials.

Most quantum systems described by the Schrödinger equation with an axially symmetrical potential cannot be solved analytically. Thus, the solution of the Schrödinger equation with sufficiently arbitrary potentials of this type represents the main mathematical problem. Many approximate analytical and numerical methods have been worked out. Great progress in the development of computer techniques and effective algorithms for a numerical solution of differential equations enables us to obtain numerical solutions for the energy spectrum and wave functions with quite a high accuracy although practical calculations are usually very laborious and require powerful computers. The main purpose of these investigations is in the majority the construction of highly accurate numerical solutions of the Schrödinger equation for the hydrogen atom in a uniform magnetic field as well as the energies and eigenfunctions of deformed nuclei and the electronic shell structure effects in metallic clusters.

Nevertheless, the development of analytical methods is very important because only analytical methods permit us to investigate qualitative features of quantum physical systems and indicate effective ways for improvement of numerical algorithms.

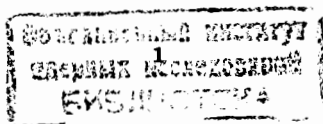
In this paper, the method of oscillator representation [6] will be extended to calculate the energies of the ground and excited states of the hydrogen atom in a uniform magnetic field of arbitrary strength. We shall see that this method gives very good results in the lowest approximation for the whole region of the magnetic field.

This paper is organized as follows. In section 2, the method of oscillator representation for the axially symmetric potential is formulated. In section 3, the energies of the ground and excited states of the hydrogen atom in a uniform magnetic field are calculated.

2 The Oscillator Representation for the axially symmetrical potentials

Formulation of the problem. Let us consider the Hamiltonian with an axially symmetrical potential

$$H = \frac{p^2}{2M} + V(r, \cos \theta) \quad (2.1)$$



The Schrödinger equation looks like:

$$\left[-\frac{1}{2M} \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) + V(r, \cos \theta) \right] \Psi(\vec{r}) = E \Psi(\vec{r}). \quad (2.2)$$

Taking into account the azimuthal symmetry of the problem we introduce the magnetic quantum number m so that the wave function can be represented

$$\Psi(\vec{r}) = \frac{e^{im\phi}}{\sqrt{2\pi}} \Psi_m(r, \cos \theta).$$

Eq.(2.2) gets the form

$$\left\{ -\frac{1}{2M} \left[\left(\frac{d^2}{dr^2} + \frac{2}{r} \frac{d}{dr} \right) + \frac{1}{r^2} \left(\frac{d^2}{d\theta^2} + \cot \theta \frac{d}{d\theta} - \frac{m^2}{\sin^2 \theta} \right) \right] + V(r, \cos \theta) \right\} \Psi_m(r, \cos \theta) = E_m \Psi_m(r, \cos \theta). \quad (2.3)$$

Our aim is to calculate the energy spectrum E_m and to find the wave functions $\Psi_m(r, \cos \theta)$ by using the oscillator representation method.

The wave function $\Psi_m(r, \cos \theta)$ depends on two variables: the radius $r = \sqrt{r^2}$ and the angle θ . We consider these variables r and θ in equation (2.3) as independent variables. In order to get the hermitian Hamiltonian in (2.3) over the variable θ let us multiply the equation by $\sin^2 \theta$ and introduce the new variable

$$u = \ln \left(\tan \frac{\theta}{2} \right)$$

so that one gets

$$\sin^2 \theta \left[\frac{d^2}{d\theta^2} + \cot \theta \frac{d}{d\theta} \right] = \left(\sin \theta \frac{d}{d\theta} \right)^2 = \frac{d^2}{du^2}.$$

The hermitian representation for the Schrödinger equation (2.3) has the form

$$\left\{ -\frac{1}{2 \cosh^2 u} \left(\frac{d^2}{dr^2} + \frac{2}{r} \frac{d}{dr} \right) - \frac{1}{2r^2} \left(\frac{d^2}{du^2} - m^2 \right) + \frac{M}{\cosh^2 u} (V(r, \tanh u) - E_m) \right\} \Psi_m(r, \tanh u) = 0$$

or

$$\left\{ -\frac{1}{2 \cosh^2 u} \left(\frac{d^2}{dr^2} + \frac{2}{r} \frac{d}{dr} - \frac{\nu(\nu+1)}{r^2} \right) - \frac{1}{2r^2} \left(\frac{d^2}{du^2} - m^2 + \frac{\nu(\nu+1)}{\cosh^2 u} \right) + \frac{M}{\cosh^2 u} (V(r, \tanh(u)) - E_m) \right\} \Psi_m(r, \tanh u) = 0 \quad (2.4)$$

where a new parameter ν is introduced.

The next step is to modify the variable r in equation (2.4) and the wave function $\Psi_m(r, \tanh u)$ so as to get a modified Schrödinger equation having the solution with the Gaussian asymptotic behaviour (see the details in refs. ([6], [7])). These substitutions are

$$r = Q^\rho, \quad \Psi_m(r, \tanh u) = Q^{\rho\nu} \cdot \Phi_m(Q, u),$$

where the parameters ρ and ν can be connected with the behaviour of the wave function at large and short distances to approximate the Gaussian asymptotics. The Schrödinger equation takes the form

$$\left[-\frac{1}{2 \cosh^2 u} \left(\frac{d^2}{dQ^2} + \frac{d-1}{Q} \cdot \frac{d}{dQ} \right) - \frac{\rho^2}{2Q^2} \left(\frac{d^2}{du^2} - m^2 + \frac{\nu(\nu+1)}{\cosh^2 u} \right) + W(Q, u, E_m) \right] \Phi_m(Q, u) = 0, \quad (2.5)$$

$$d = 2 + \rho(1 + 2\nu),$$

where the potential $W(Q, u, E)$ equals

$$W(Q, u, E) = \frac{M\rho^2 Q^{2\rho-2}}{\cosh^2 u} \cdot [V(Q, \tanh u) - E_m]. \quad (2.6)$$

The operator

$$\left(\frac{d^2}{dQ^2} + \frac{d-1}{Q} \cdot \frac{d}{dQ} \right) = \Delta_d$$

can be identified with the radial part of the Laplacian Δ_d in the space \mathbf{R}^d so that we can introduce Q_j as a vector in this space and look for the solution $\Phi_m(Q, u)$ of the Schrödinger equation (2.5) depending on Q^2 only, i.e. for the ground state in the space \mathbf{R}^d . Thus, the Hamiltonian can be written as

$$\mathbf{H} = \frac{1}{2 \cosh^2 u} P_Q^2 + \frac{\rho^2}{2Q^2} \left(P_u^2 + m^2 - \frac{\nu(\nu+1)}{\cosh^2 u} \right) + W(Q, u, E_m). \quad (2.7)$$

where $Q \in \mathbf{R}^d$ and $u \in \mathbf{R}^1$.

Our problem is formulated in the following way. We have the Hamiltonian $\mathbf{H} = \mathbf{H}(E_m)$, and we have to solve the Schrödinger equation

$$\mathbf{H}(E_m) \Phi_m(Q, u) = \varepsilon(E_m) \Phi_m(Q, u), \quad (2.8)$$

i.e. we have to find the ground state energy $\varepsilon(E_m)$. According to (2.4), the desired energy E_m is determined by the equation

$$\varepsilon(E_m) = 0. \quad (2.9)$$

Hamiltonians in the correct form. The correct form of a Hamiltonian is defined as follows. Let the Hamiltonian H be given and the Schrödinger equation

$$H\Psi = \varepsilon\Psi$$

can not be solved analytically. Let us introduce an auxiliary Hamiltonian $H(\xi)$ depending on a set of parameters ξ . This Hamiltonian should be chosen in such a way that, first, it could be close as much as possible to the initial Hamiltonian H and, second, the Schrödinger equation

$$H(\xi)\Psi(\xi) = \varepsilon(\xi)\Psi(\xi) \quad (2.10)$$

could be solved analytically, i.e. the wave function $\Psi(\xi)$ could be found in an explicit form. Now let us do the variational estimation of the initial total Hamiltonian over the wave function $\Psi(\xi)$

$$\varepsilon_0 = \min_{\xi} (\Psi(\xi)H\Psi(\xi)). \quad (2.11)$$

This minimization gives us the energy ε_0 in the lowest approximation, the values of parameters $\xi = \xi_0$ and the wave function in the zeroth approximation $\Psi_0 = \Psi(\xi_0)$. Let us represent the initial Hamiltonian in the form

$$\begin{aligned} H &= \mathbf{H}_0 + \mathbf{H}_I + \varepsilon_0, \\ \mathbf{H}_0 &= H(\xi_0) - \varepsilon(\xi_0) =: H(\xi_0) :, \\ \mathbf{H}_I &= H - H(\xi_0) + \varepsilon(\xi_0) - \varepsilon_0 =: H - H(\xi_0) :, \end{aligned} \quad (2.12)$$

where

$$\mathbf{H}_0\Psi_0 = 0,$$

and the normal product of an operator F with respect to the Hamiltonian \mathbf{H}_0 is defined as

$$: F := F - \langle \Psi_0 F \Psi_0 \rangle. \quad (2.13)$$

In what follows we shall call the representation (2.12) *the correct form* of the Hamiltonian H with respect to the Hamiltonian \mathbf{H}_0 .

If the Hamiltonian in the zeroth approximation equals the pure oscillator Hamiltonian in the space R^d , i.e.

$$\mathbf{H}_0 = \frac{1}{2} (P_Q^2 + \Omega^2 Q^2) - \frac{d}{2} \cdot \Omega = \Omega (a_j^\dagger a_j), \quad j = 1, \dots, d$$

then the correct form is equivalent to the *oscillator representation* (see [6]).

The ground state energy ε can be calculated by the perturbation method over the interaction Hamiltonian \mathbf{H}_I and turns out to be

$$\varepsilon = \varepsilon_0 + \varepsilon_1 + \varepsilon_2 + \dots = \varepsilon_0 - \left(\Psi_0 \mathbf{H}_I \frac{1}{\mathbf{H}_0} \mathbf{H}_I \Psi_0 \right) + \dots, \quad (2.14)$$

because

$$\mathbf{H}_0\Psi_0 = 0 \quad \text{and} \quad \varepsilon_1 = \langle \Psi_0 \mathbf{H}_I \Psi_0 \rangle = 0. \quad (2.15)$$

The accuracy of this approximation can be evaluated as

$$\delta \sim \left| \frac{\varepsilon_2}{\varepsilon_0} \right|. \quad (2.16)$$

The Hamiltonian (2.7) in the correct form. First of all we rewrite the Hamiltonian (2.7) in the form

$$\begin{aligned} \mathbf{H} &= \frac{1}{2\kappa_Q} (P_Q^2 + \Omega^2 Q^2 - d\Omega) + \frac{\rho^2}{2\kappa_u} \left(P_u^2 + m^2 - \frac{\nu(\nu+1)}{\cosh^2 u} \right) \\ &+ \left[W(Q, u, E_m) - \frac{\Omega^2}{2\kappa_Q} Q^2 + \frac{d}{2\kappa_Q} \Omega \right] \\ &+ \frac{1}{2} P_Q^2 \cdot \left(\frac{1}{\cosh^2 u} - \frac{1}{\kappa_Q} \right) + \frac{\rho^2}{2} \left(P_u^2 + m^2 - \frac{\nu(\nu+1)}{\cosh^2 u} \right) \cdot \left(\frac{1}{Q^2} - \frac{1}{\kappa_u} \right). \end{aligned} \quad (2.17)$$

This Hamiltonian contains five free parameters ν , ρ , Ω , κ_Q , and κ_u .

Let us choose

$$\mathbf{H}_0 = \frac{1}{2\kappa_Q} (P_Q^2 + \Omega^2 Q^2 - d\Omega) + \frac{\rho^2}{2\kappa_u} \left(P_u^2 + m^2 - \frac{\nu(\nu+1)}{\cosh^2 u} \right), \quad (2.18)$$

so that

$$\Psi_0 = \Phi_m(Q, u) = \frac{P_\nu^m(\tanh u)}{\sqrt{C_m(\nu)}} \cdot \left(\frac{\Omega}{\pi} \right)^{d/4} \cdot \exp \left\{ -\frac{1}{2} \Omega Q^2 \right\}, \quad (2.19)$$

$$C_m(\nu) = \int_{-\infty}^{\infty} du (P_\nu^m(\tanh u))^2 = \int_{-1}^1 dx \sqrt{1-x^2} \cdot (P_\nu^m(x))^2,$$

$$\langle \Psi_0, \Psi_0 \rangle = \int_{-\infty}^{\infty} du \int d^d Q \Phi_m(Q, u) \Phi_m(Q, u) = 1.$$

The oscillator canonical variables (P_Q, Q) can be written in the form

$$\begin{aligned} Q_j &= \frac{1}{\sqrt{2\Omega}} \cdot (a_j + a_j^\dagger), & P_{Q_j} &= \sqrt{\frac{\Omega}{2}} \cdot \frac{a_j - a_j^\dagger}{i}, \\ [a_i, a_j^\dagger] &= \delta_{ij}, & (i, j &= 1, 2, \dots, d). \end{aligned} \quad (2.20)$$

so that

$$\frac{1}{2\kappa_Q} (P_Q^2 + \Omega^2 Q^2 - d\Omega) = \frac{\Omega}{\kappa_Q} (a_j^\dagger a_j).$$

The operators a_j and a_j^\dagger are called the annihilation and creation operators. The ground or vacuum oscillator state

$$|0\rangle = \left(\frac{\Omega}{\pi} \right)^{d/4} \exp \left\{ -\frac{1}{2} \Omega Q^2 \right\}$$

satisfies the conditions

$$\langle 0|0\rangle = 1, \quad a_j|0\rangle = 0, \quad (j = 1, 2, \dots, d).$$

The function $P_\nu^m(z)$ is the solid spherical harmonic and it satisfies the equation

$$\left(\frac{d^2}{du^2} - m^2 + \frac{\nu(\nu+1)}{\cosh^2 u} \right) P_\nu^m(\tanh u) = 0, \quad (2.21)$$

where $m = 0, \pm 1, \pm 2, \dots$ are the azimuthal quantum numbers and ν is a parameter which can take any values. According to (2.11) the parameter ν can be determined by the minimization of the energy in the zeroth approximation. The basic properties of this function are given in the Appendix.

The positive parameters κ_Q and κ_u are defined by the condition that the interaction Hamiltonian does not contain the quadratic terms with P_Q^2 and P_u^2 . We have

$$\begin{aligned} \frac{1}{\cosh^2 u} &:= \frac{1}{\cosh^2 u} - \frac{1}{\kappa_Q}, & \frac{1}{\kappa_Q} &= \left(\Psi_0 \left| \frac{1}{\cosh^2 u} \right| \Psi_0 \right) = \frac{A_m^{(0)}(\nu)}{C_m(\nu)}, & (2.22) \\ A_m^{(n)}(\nu) &= \int_{-\infty}^{\infty} \frac{du}{\cosh^{2+n}(u)} (P_\nu^m(\tanh u))^2 = \int_{-1}^1 dx x^n (P_\nu^m(x))^2, \\ \frac{1}{Q^2} &:= \frac{1}{Q^2} - \frac{1}{\kappa_u}, & \frac{1}{\kappa_u} &= \left(\Psi_0 \left| \frac{1}{Q^2} \right| \Psi_0 \right) = \frac{\Omega}{d-2}, \end{aligned}$$

The representation of the functions $A_m^{(n)}(\nu)$ and $C_m(\nu)$ are given in the Appendix.

The parameters ν, ρ, Ω are determined by the condition

$$\begin{aligned} \varepsilon_0(E_m) &= \min_{\nu, \rho, \Omega} (\Psi_0 H \Psi_0) \\ &= \min_{\nu, \rho, \Omega} \left(\Psi_0 \left| \frac{M\rho^2 Q^{2\rho-2}}{\cosh^2(u)} [V(Q, \tanh u) - E_m] - \frac{\Omega^2}{2\kappa_Q} Q^2 + \frac{d}{2\kappa_Q} \Omega \right| \Psi_0 \right) & (2.23) \\ &= \min_{\nu, \rho, \Omega} \int_{-1}^1 \frac{dx}{C_m(\nu)} (P_\nu^m(x))^2 \left\{ M\rho^2 \left(\frac{\Omega}{\pi} \right)^{d/2} \int d^d Q Q^{2\rho-2} e^{-\Omega Q^2} [V(Q, x) - E_m] + \frac{d}{4} \Omega \right\} \\ &= \min_{\nu, \rho, \Omega} \int_{-1}^1 \frac{dx}{C_m(\nu)} (P_\nu^m(x))^2 \left\{ \frac{M\rho^2}{\Omega^{\rho-1}} \int_0^\infty dt \frac{t^{d/2+\rho-2} e^{-t}}{\Gamma(d/2)} \left[V \left(\sqrt{\frac{t}{\Omega}}, x \right) - E_m \right] + \frac{d}{4} \Omega \right\} \\ &= \min_{\nu, \rho, \Omega} [A(m, \nu, \rho, \Omega) - E_m B(m, \nu, \rho, \Omega)], \end{aligned}$$

where

$$\begin{aligned} A(m, \nu, \rho, \Omega) &= \int_{-1}^1 \frac{dx}{C_m(\nu)} (P_\nu^m(x))^2 \left\{ \frac{M\rho^2}{\Omega^{\rho-1}} \int_0^\infty dt \frac{t^{d/2+\rho-2} e^{-t}}{\Gamma(d/2)} V \left(\sqrt{\frac{t}{\Omega}}, x \right) + \frac{d}{4} \Omega \right\}; \\ B(m, \nu, \rho, \Omega) &= \int_{-1}^1 \frac{dx}{C_m(\nu)} (P_\nu^m(x))^2 \left\{ \frac{M\rho^2}{\Omega^{\rho-1}} \int_0^\infty dt \frac{t^{d/2+\rho-2} e^{-t}}{\Gamma(d/2)} \right\}. \end{aligned}$$

The energy E_m is determined by equation (2.9). Formulas (2.9) and (2.23) leads to

$$E_m = \min_{\nu, \rho, \Omega} \frac{A(m, \nu, \rho, \Omega)}{B(m, \nu, \rho, \Omega)}. \quad (2.24)$$

Really, the following chain of equalities are valid:

$$\begin{aligned} \varepsilon_0(E) &= \min_{\{\alpha\}} (A(\alpha) - EB(\alpha)), \\ \frac{\partial}{\partial \alpha_j} A(\alpha) - E \frac{\partial}{\partial \alpha_j} B(\alpha) &= 0, \\ A(\alpha) - EB(\alpha) &= 0, \\ \frac{\partial}{\partial \alpha_j} A(\alpha) - \frac{A(\alpha)}{B(\alpha)} \frac{\partial}{\partial \alpha_j} B(\alpha) &= 0, \\ \frac{\partial}{\partial \alpha_j} \frac{A(\alpha)}{B(\alpha)} &= 0, \\ E &= \min_{\{\alpha\}} \frac{A(\alpha)}{B(\alpha)}. \end{aligned}$$

The interaction Hamiltonian has the form

$$\begin{aligned} \mathbf{H}_I &= : \left[W(Q, u, E_m) - \frac{\Omega^2}{2\kappa_Q} Q^2 \right] : + \frac{1}{2} : \left(P_Q^2 + \frac{d\Omega}{2} \right) : \dots : \frac{1}{\cosh^2 u} : \\ &+ \frac{\rho^2}{2} : \left(P_u^2 + m^2 - \frac{\nu(\nu+1)}{\cosh^2 u} \right) : \dots : \frac{1}{Q^2} : \end{aligned} \quad (2.25)$$

where the normal product is defined by (2.13).

3 The Zeeman effect

The Schrödinger equation for an electron in combined Coulomb and magnetic fields makes the theoretical description of even such a simple system as a hydrogen atom in a uniform magnetic field quite difficult when the two field strengths are comparable. The investigation of the hydrogen atom in strong magnetic fields has wide applications in various domains of physics, such as astrophysics, plasma physics, surface physics and solid-state physics. In the past decade, a variety of methods has been proposed to calculate accurately the binding energies and eigenfunctions of the ground and excited state in the case when the magnetic field strengths are comparable or greater than the Coulomb field (see for example, [12]–[19]).

During the last years, several new approaches were worked out to treat the complete region changing of a magnetic field. The main purpose of these investigations consists, in the majority, in the construction of highly accurate numerical solutions of the Schrödinger equation for the hydrogen atom in a uniform magnetic field. Rösner *et al.* [12] tabulated the most extensive energies for the ground and low excited states by solving a group of coupled differential equations. They used up to 24 coupled orbitals in the transition

region between low and high fields. Similar tables of energies were also presented by Ivanov [13] by using the finite-difference method. A finite-element treatment was carried out by Kaschiev *et al.* [14] and Shertzer [15]. Rech and Gallas [16] investigated the ground-state energies by using the five-parameter variational method. Le-Guillou and Zinn-Justin [17] gave accurate energy values in low and transition regions for the ground state by using the weak-field expansion method. Chen and Goldman [18] obtained very accurate relativistic and nonrelativistic results by combining finite basis expansion and the variational method. Jinhua Xi *et al.* [19] tabulated the energies of the ground and low excited state of the hydrogen atom in a uniform magnetic field of arbitrary strengths. These results have been obtained by using B-spline basis sets.

In this section, the method of oscillator representation will be applied to calculate the energy values of the ground and excited states of the hydrogen atom in a uniform magnetic field of arbitrary strength.

The Hamiltonian of the hydrogen atom in an external magnetic field for spin down states is [1] (in the Rydberg atomic units):

$$H = \frac{1}{2}(\vec{P} - \vec{A})^2 - \frac{1}{r} + (\vec{B}\vec{S}) = \quad (3.1)$$

$$= \frac{1}{2}\vec{P}^2 - \frac{1}{r} + \frac{1}{8}B^2(x^2 + y^2) + \frac{1}{2}B(L_z - 1),$$

where the vector potential $\vec{A} = \frac{1}{2}[\vec{B}, \vec{r}]$ and the magnetic field \vec{B} has been oriented along the z-axis; L_z is the z-component of the orbital angular momentum operator and $S_z = 1/2$. The Schrödinger equation for the Hamiltonian (3.1) becomes

$$\left[\frac{1}{2}\vec{P}^2 - \frac{1}{r} + \frac{1}{2}r^2 \cdot \sin^2(\theta) \cdot \beta^2 + \beta(L_z - 1) \right] \Psi(\vec{r}) = E\Psi(\vec{r}), \quad (3.2)$$

where β is the strength parameter $\beta = \frac{1}{2}B$

Our problem is to calculate the energy values E_m of the ground and excited states of the hydrogen atom in a uniform magnetic field for arbitrary strength parameters β .

Taking into account (2.4-7) and after some transformations the modified Hamiltonian, according to (2.17), has the form

$$\mathbf{H} = \frac{1}{2\kappa_Q} (P_Q^2 + \Omega^2 \cdot Q^2 - d\Omega) + \frac{\rho^2}{2\kappa_u} \left(P_u^2 + m^2 - \frac{\nu(\nu+1)}{\cosh^2 u} \right) \quad (3.3)$$

$$+ \frac{1}{2}P_Q^2 \cdot \left(\frac{1}{\cosh^2 u} - \frac{1}{\kappa_Q} \right) + \frac{\rho^2}{2} \left(P_u^2 + m^2 - \frac{\nu(\nu+1)}{\cosh^2 u} \right) \cdot \left(\frac{1}{Q^2} - \frac{1}{\kappa_u} \right)$$

$$+ \left[\frac{\rho^2 Q^{2\rho-2}}{\cosh^2 u} \cdot \left(U - \frac{1}{Q^\rho} + \frac{1}{2} \frac{\beta^2 Q^{2\rho}}{\cosh^2 u} \right) - \frac{\Omega^2}{2\kappa_Q} \cdot Q^2 + \frac{d}{2\kappa_Q} \Omega \right],$$

$$d = 2 + \rho(2\nu + 1).$$

According to (2.23), the ground state energy of the Hamiltonian (3.3) in the zeroth approximations is

$$\epsilon_0(U_m) = \min_{\nu, \rho, \Omega} \int_{-1}^1 \frac{dx}{C_m(\nu)} (P_\nu^m(x))^2 \quad (3.4)$$

$$\left\{ \frac{\rho^2}{\Omega^{\rho-1}} \int_0^\infty dt \frac{t^{d/2+\rho-2} e^{-t}}{\Gamma(d/2)} \left[U - \left(\frac{\Omega}{t} \right)^{\rho/2} + \frac{\beta^2}{2} \cdot (1-x^2) \cdot \left(\frac{t}{\Omega} \right)^\rho \right] + \frac{d}{4} \Omega \right\}$$

$$= \min_{\nu, \rho, \Omega} \left\{ \frac{d}{4} \cdot \frac{A_m^{(0)}(\nu)}{C_m(\nu)} \cdot \Omega - \frac{\rho^2}{\Omega^{\rho/2-1}} \cdot \frac{A_m^{(0)}(\nu)}{C_m(\nu)} \cdot \frac{\Gamma(d/2 + \rho/2 - 1)}{\Gamma(d/2)} \right.$$

$$+ \frac{U \cdot \rho^2}{\Omega^{\rho-1}} \cdot \frac{\Gamma(d/2 + \rho - 1)}{\Gamma(d/2)} \cdot \frac{A_m^{(0)}(\nu)}{C_m(\nu)}$$

$$\left. + \frac{\rho^2 \beta^2}{2\Omega^{2\rho-1}} \left(\frac{A_m^{(0)}(\nu) - A_m^{(2)}(\nu)}{C_m(\nu)} \right) \cdot \frac{\Gamma(d/2 + 2\rho - 1)}{\Gamma(d/2)} \right\},$$

where the energy parameter

$$U_m = \beta(m-1) - E_m, \quad (3.5)$$

is introduced and m denotes the magnetic quantum number.

According to (2.9), the energy $\epsilon_0(U_m)$ equals zero so that the equation

$$\epsilon(U_m) = 0 \quad (3.6)$$

defines the parameter U_m as a function of the strength parameter β . Then, the energy of the hydrogen atom is determined by

$$E_m = \beta(m-1) - U_m. \quad (3.7)$$

After some simplifications of (3.4) we obtain

$$U_m(\beta) = \max_{\{\rho, \nu, \Omega\}} \left[\frac{A(m, \nu, \rho, \Omega)}{B(m, \nu, \rho, \Omega)} \right] = \max_{\{\rho, \nu, \Omega\}} \left\{ - \frac{\Omega^{\rho/2} \cdot \Gamma(d/2 + \rho/2 - 1)}{\Gamma(d/2 + \rho - 1)} \right. \quad (3.8)$$

$$+ \frac{\beta^2}{2\Omega^\rho} \cdot \left(1 - \frac{A_m^{(2)}(\nu)}{A_m^{(0)}(\nu)} \right) \cdot \frac{\Gamma(d/2 + 2\rho - 1)}{\Gamma(d/2 + \rho - 1)} + \frac{\Omega^{\rho/2}}{2\rho^2} \cdot \frac{\Gamma(d/2 + 1)}{\Gamma(d/2 + \rho - 1)} \left. \right\}$$

$$= \max_{\{\rho, \nu\}} \left[\frac{S}{2} \cdot \frac{\Gamma(\rho(1+\nu))}{\Gamma(\rho(1.5+\nu))} - \frac{\beta^2}{S^2} \cdot \left(1 - \frac{A_m^{(2)}(\nu)}{A_m^{(0)}(\nu)} \right) \cdot \frac{\Gamma(\rho(2.5+\nu))}{\Gamma(2+\rho(0.5+\nu))} \right],$$

where S is defined by the equation

$$S^4 - S^3 \cdot \rho^2 \frac{\Gamma(\rho(1+\nu))}{\Gamma(2+\rho(0.5+\nu))} - \rho^2 \beta^2 \cdot \left(1 - \frac{A_m^{(2)}(\nu)}{A_m^{(0)}(\nu)} \right) \cdot \frac{\Gamma(\rho(2.5+\nu))}{\Gamma(2+\rho(0.5+\nu))} = 0.$$

This equation (3.8) defines the energy parameter U_m as a function of the strength parameters β .

In this paper, we have calculated the numerical results only for the ground and low excited state, i.e. for the (1s) and (1p) with $m = 0$. The wave functions in the lowest approximation are defined by (2.19) and the reflection parity with respect to the x-y plane is carried by the function $P_\nu^m(\cos(\theta))$. In the Appendix, the basic relations for the

solid spherical harmonics $P_\nu^n(\cos(\theta))$ are given, and formula (A.4) shows that for fixed m and parity, in the lowest energy levels, the value $(-1)^\nu$ is equal to the parity of the state (see Table 1). The details of calculation of the functions $A_m^{(n)}(\nu)$ and $C_m(\nu)$ are given in the Appendix. The numerical results are shown in Tables 2 and 3.

Table 1. The lowest energy levels for fixed m and parity. The designation is for the hydrogenic energy level appropriate in the limit of zero magnetic field.

m	Parity	ν	Designation
0	even	0	1s $m_\ell = 0$
0	odd	1	2p $m_\ell = 0$
± 1	odd	1	2p $m_\ell = \pm 1$
± 1	even	2	3d $m_\ell = \pm 1$
± 2	even	2	3d $m_\ell = \pm 2$
± 2	odd	3	4f $m_\ell = \pm 2$

Table 2. Binding energy (in a.u.) of the hydrogen ground state (1s) in a uniform magnetic field.

β	ρ	ν	S	$U^{(0)}$	$E_0^{(0)}$	Rosner[12]	Jinhua [19]
0.0	2.0	0.0	2.0	.5	.50	.5000	.5000
0.0001	2.0	0.0	2.0	.5	.5001	.5001	.5001
0.001	2.0	0.0	2.0	.5	.501	.501	.501
0.01	2.0	0.0	2.0004	.4999	.5099	.5099	.5099
0.1	2.0	-.0002	2.03815	.49038	.59038	.590380	.590381
0.5	1.952	-.01268	2.39839	.33111	.83111	.831169	.831169
1.0	1.870	-.0307	2.71097	.0222	1.0222	1.022214	1.0222138
5.0	1.5	-.0749	3.536811	-3.2523	1.7477	1.747797	1.7477969
10.0	1.42	-.09915	4.458418	-7.7846	2.2154	2.21539	2.21539
50.0	1.0	-.14036	6.55383	-46.2146	3.7854	3.78905	3.78985
100.0	1.0	-.15838	9.1584676	-95.27746	4.7254	4.72655	4.72656
200.0	1.0	-.1737	12.838846	-194.147	5.853	5.85115	5.85118
500.0	1.0	-.18984	20.13583	-492.338	7.662	7.66205	7.6645
1000.0	1.0	-.19926	28.3555	-990.6934	9.3066	9.30448	9.315

Table 3. Binding energy (in a.u.) of the hydrogen 2p ($m = 0$) state in a uniform magnetic field.

β	ρ	ν	S	$U^{(0)}$	$2E_0^{(0)}$	Liu and Starace[20]	Jinhua [19]
0.0	2.0	1.0	1.0	.25	.25		.25
0.0001	2.0	1.0	1.0	.25	.2502		.25019988
0.001	2.0	1.0	1.001	.249985	.251985		.251988
0.01	2.0	1.0	1.0047	.2488	.2688		.268812
0.05	2.0	1.0	1.0925	.2247	.3247	.3048	.32482
0.1	2.0	1.07	1.243	.17016	.37016		.370368
0.5	2.0	1.0816	2.20621	-.4800	.5200	.5114	.520013
1.0	1.986	1.09	2.9277	-1.405	0.5950	.5900	.5954219
5.0	1.9266	1.095	5.7384	-9.235	.765		.7652994
50.0	1.856	1.095	16.07247	-99.073	.927	.9274	.92723
100.0	1.67	1.0065	17.41846	-199.045	.955	.9548	.95305
200.0	1.56	.94566	21.132726	-399.03	.970		.97072
500.0	1.485	.90104	30.15155	-999.015	.985		.9840
1000.	1.400	.8403	38.063951	-1999.009	.991	.9912	.990

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Appendix

Let us consider equation (2.21)

$$\left(\frac{d^2}{du^2} - m^2 + \frac{\nu(\nu+1)}{\cosh^2 u} \right) P_\nu^m(\tanh u) = 0, \quad (\text{A.1})$$

which is defined in the interval $(-\infty < u < \infty)$. Let us introduce the new variable

$$x = \tanh(u),$$

and after some simplifications the equation (A.1) looks like

$$\left[(1-x^2) \frac{d^2}{dx^2} - 2 \frac{d}{dx} - \frac{m^2}{1-x^2} - \nu(\nu+1) \right] P_\nu^m(x) = 0. \quad (\text{A.2})$$

One can see that $P_\nu^m(x)$ is the solid spherical harmonic, $m = 0, \pm 1, \pm 2, \dots$ are the azimuthal quantum numbers and ν is a parameter which can take any values. The solid spherical harmonic satisfies the following recurrent relations [21]:

$$P_\nu^m(x) = (-1)^m (1-x^2)^{m/2} \frac{d^m}{dx^m} P_\nu(x), \quad (\text{A.3})$$

$$xP_\nu^m(x) = \frac{1}{2\nu+1} \cdot [(\nu-m+1)P_{\nu+1}^m(x) + (\nu+m)P_{\nu-1}^m(x)],$$

which are valid for $P_\nu^m = P_\nu^m$ or $P_\nu^m = Q_\nu^m$.

For the calculations $A_m^{(n)}(\nu)$ and $C_m(\nu)$ we used the representation:

$$P_\nu^m(x) = \sum_{k=m}^{\infty} \frac{2k+1}{\nu+k+1} \cdot \frac{\sin(\pi(\nu-k))}{\pi(\nu-k)} \cdot \frac{\Gamma(\nu+m+1)}{\Gamma(\nu-m+1)} \cdot \frac{\Gamma(k-m+1)}{\Gamma(k+m+1)} \cdot P_k^m(x),$$

$$\int_{-1}^1 dx P_k^m(x) P_n^m(x) = \frac{2}{2n+1} \cdot \frac{\Gamma(n+m+1)}{\Gamma(n-m+1)} \cdot \delta_{nk}. \quad (\text{A.4})$$

We have

$$A_m^{(n)}(\nu) = \int_{-1}^{+1} dx \cdot \left(P_\nu^m(x) x^n P_\nu^m(x) \right) \quad (\text{A.5})$$

$$= \sum_{j,k=0}^{\infty} \frac{2k+1}{\nu+k+1} \cdot \frac{2j+1}{\nu+j+1} \cdot \frac{\sin(\pi(\nu-k))}{\pi(\nu-k)} \cdot \frac{\sin(\pi(\nu-j))}{\pi(\nu-j)}$$

$$\cdot \left(\frac{\Gamma(\nu+m+1)}{\Gamma(\nu-m+1)} \right)^2 \cdot \frac{\Gamma(k-m+1)}{\Gamma(k+m+1)} \cdot \frac{\Gamma(j-m+1)}{\Gamma(j+m+1)} \cdot \int_{-1}^1 dx P_k^m(x) x^n P_j^m(x).$$

Let us define the even and odd wave functions with respect to the x-y plane, with $m=0$:

$$EP_\nu^0(x) = \frac{\sin(\pi\nu)}{\pi\nu} \sum_{j=0}^{\infty} \left[\frac{\nu}{\nu-2j} - \frac{\nu}{\nu+2j+1} \right] \cdot P_{2j}(x) \quad (\text{A.6})$$

$|\nu| \geq 0;$

$$OP_\nu^0(x) = \frac{\sin(\pi\nu)}{\pi\nu} \sum_{j=1}^{\infty} \left[\frac{\nu}{\nu-2j+1} - \frac{\nu}{\nu+2j} \right] \cdot P_{2j-1}(x)$$

$|\nu| \geq 1.$

Taking into account these formulas, from (A.5) we get for $n=0$ and $n=2$

$$EA_0^{(0)}(\nu) = \left(\frac{\sin(\pi\nu)}{\pi\nu} \right)^2 \sum_{j=0}^{\infty} \left[\frac{\nu}{\nu-2j} - \frac{\nu}{\nu+2j+1} \right]^2 \cdot \frac{2}{4j+3} \quad (\text{A.7})$$

$$OA_0^{(0)}(\nu) = \left(\frac{\sin(\pi\nu)}{\pi\nu} \right)^2 \sum_{j=1}^{\infty} \left[\frac{\nu}{\nu-2j+1} - \frac{\nu}{\nu+2j} \right]^2 \cdot \frac{2}{4j-1}$$

$$EA_0^{(2)}(\nu) = \left(\frac{\sin(\pi\nu)}{\pi\nu} \right)^2 \sum_{j=0}^{\infty} \left[\frac{\nu}{\nu-2j} - \frac{\nu}{\nu+2j+1} \right]^2 \quad (\text{A.8})$$

$$\left\{ \frac{(2j+1)(2j+2)}{(4j+1)(4j+3)} \cdot \frac{2}{4j+5} \cdot \left(\frac{\nu}{\nu-2j-2} - \frac{\nu}{\nu+2j+3} \right) \right.$$

$$+ \left[\frac{(2j+1)^2}{(4j+1)(4j+3)} + \frac{4j^2}{(4j+1)(4j-1)} \right] \cdot \frac{2}{4j+1} \cdot \left(\frac{\nu}{\nu-2j} - \frac{\nu}{\nu+2j+1} \right)$$

$$\left. + \frac{2j(2j-1)}{(4j+1)(4j-1)} \cdot \frac{2}{4j-3} \cdot \left(\frac{\nu}{\nu-2j+2} - \frac{\nu}{\nu+2j-1} \right) \right\},$$

$$OA_0^{(2)}(\nu) = \left(\frac{\sin(\pi\nu)}{\pi\nu} \right)^2 \sum_{j=1}^{\infty} \left[\frac{\nu}{\nu-2j+1} - \frac{\nu}{\nu+2j} \right]^2 \quad (\text{A.9})$$

$$\left\{ \frac{2j(2j+1)}{(4j+1)(4j-1)} \cdot \frac{2}{4j+3} \cdot \left(\frac{\nu}{\nu-2j-1} - \frac{\nu}{\nu+2j+2} \right) \right.$$

$$+ \left[\frac{4j^2}{(4j+1)(4j-1)} + \frac{(2j-1)^2}{(4j-3)(4j-1)} \right] \cdot \frac{2}{4j-1} \cdot \left(\frac{\nu}{\nu-2j+1} - \frac{\nu}{\nu+2j} \right)$$

$$\left. + \frac{(2j-2)(2j-1)}{(4j-3)(4j-1)} \cdot \frac{2}{4j-5} \cdot \left(\frac{\nu}{\nu-2j+3} - \frac{\nu}{\nu+2j-2} \right) \right\}.$$

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