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H-LIKE AND He-LIKE SYSTEMS IN A SUPERSTRONG MAGNETIC FIELD: NUMERIC CALCULATION

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The structure of the quantum states for the H-like and He-like atomic systems in a static magnetic field (γ=0.01–10000; in units of $B_0 = m^2e^3c/h^3Z^3$) is studied. The energies of the high-field ground states for neutral hydrogen and helium atoms are calculated. An effective representation for the wave function Hamiltonian is used at the calculations, obtained on the basis of the numeric solution of the Schrödinger equation for an atom in magnetic field within the operator perturbation theory.

The electron structure of atomic systems in strong magnetic field can be drastically changed (e.g. white stars, pulsars etc.). The interest to the problem of hydrogen atom in a static magnetic field was also stimulated in the recent years by experimental observation of complicated spectra with narrow resonances coexisting with a broad one [1-10]. Hydrogen atom in static magnetic field has been considered as a prototype of the quantum chaotic system. Theoretical estimates of its spectrum were carried out on the basis of different approaches, in particular, the random natrix theory, the WKB approximation, two-dimensional mesh Hartree-Fock method, $1/Z$ expansion theory [1-8]. It has been shown that the predictions of the theory in the immediate vicinity of the ionization threshold are to be improved.

In this paper we consider and calculate the structure of the quantum states of H-like and He-like atomic systems in a static magnetic field ($\gamma=B/B_0$=0.01-10000; in the units of $B_0 = m^2e^3c/h^3Z^3$). We have constructed the effective representation for the wave function Hamiltonian. It is obtained on the basis of the numeric solution of the Schrödinger equation within the operator perturbation theory method and the well-known "distorted-wave" approximation in the scattering theory [1]. It is shown that the wave functions and the structure of the spectrum are intermediate between the regular and chaotic structure [1]. The estimates of the resonance widths are presented. We also calculate the energies of the high-field ground states of neutral hydrogen and helium atoms. The comparison of the obtained data with the recent calculations results [10–12] is presented.

The Hamiltonian in the cylindrical coordinates is (the atomic units are used):

$$H = 1/2(P_z^2 + P_\rho^2) - (\rho^2 + z^2)^{-1/2} + 1/8\omega^2\rho^2 \quad (1)$$

Here ω denotes the magnetic field (along the z axis). The paramagnetic term in (1) is dropped as we consider Lz =0. The diamagnetic potential $1/8\omega^2\rho^2$ confines the motion in the direction which is transverse to the magnetic field. We are interested in the states, strongly stretched along the magnetic field. The adiabatic-like separation in the Schrödinger equation is possible for the Hamiltonian

$$H = 1/2(P_z^2 + P_\rho^2) - 1/z + 1/8\omega^2\rho^2 \quad (2)$$

The corresponding spectrum is:

$$E(n_\rho, n_z) = (n_\rho + 1/2)\omega - 1/2n_z^2)$$

The Rydberg series is coupled by the non-adiabatic term: $V = 1/z - (\rho^2 + z^2)^{-1/2}$.

We prescribe to each electron a definite value of the magnetic quantum number. The corresponding differential equation system and the method of its solution are in detail presented in [1]. Note that the standard approach is based on the expansion of the problem Hamiltonian wave functions in the form of linear superposition with the further use of the atomic bases. We have estimated the resonances widths *G* for different energy intervals. To calculate the values of *G*, we have used the operator perturbation theory method (see details in [1, 13–14]). Here we only note that the resonance width is determined by the imaginary part of the state energy in the lowest PT order:

$$\operatorname{Im} E = G/2 = \pi < \Psi_{Eb} \mid H \mid \Psi_{Es} >^2$$

with the total Hamiltonian. For the energy interval of $[(n\text{-}1/2)w<E<(n+1/2)w]$ we have found that the resonances widths are ~0.003-0.005. Here we have a good agreement with the experimental data [4,5] and theoretical predictions [7,8]. For the energy interval of ($-1/2\ w < E < 1/2\ w$), a regular dynamical behavior takes place. However, when $E \sim w$, chaotic behavior is observed. The Landau levels are strongly mixed [14].

Table 1. Energies (in atomic units) of the ground state for neutral hydrogen and helium atoms at strong field

Z Ref.	Y=0.5	Y=1	Y=2	Y=5
1 [9-1]	-0.88996	-0.66223	-	-
[9-2]	-0.88910	-0.66049	-	-
[10]	-0.69721	-0.83117	-1.02221	-1.38040
This work	-0.78656	-0.85980	-1.16605	1.42620
2 [9-1]	-	-2.4000	-	-
[9-2]	-	-	-	-
[10]	-2.61555	-2.95969	-3.50205	-4.61725
This work	-2.70032	-3.02680	-3.52040	-4.62378

Table 2. Energies (in atomic units) of the ground state for neutral hydrogen and helium atoms at strong field

Z Ref.	Y=10	Y=20	Y=50	Y=100
1 [9-1]	-	-	-	-
[9-2]	-	-	-	-
[10]	-1.74780	-2.21540	-3.01786	-3.78980
This work	-1.75821	-2.22890	-3.04369	-3.80322
2 [9-1]	-	-	-	-
[9-2]	-	-	-	-
[10]	-5.82951	-7.42770	-10.26449	-13.07665
This work	-5.86001	-7.45012	-10.28789	-13.34278

Table 3. Energies (in atomic units) of the ground state for neutral hydrogen and helium atoms at strong field

Z Ref.	Y=200	Y=500	Y=1000	Y=10000
1 [9-1]	-	-	-	-
[9-2]	-	-	-	-
[10]	-4.72715	-6.25709	-7.66242	-14.14097
This work	-4.73942	-6.26854	-7.67380	-15.01276
2 [9-1]	-	-	-	-
[9-2]	-	-	-	-
[10]	-16.57908	-22.46665	-28.03209	-55.15140
This work	-16.60176	-22.47102	-28.34210	-56.62340

In Tables 1, 2, 3 we present the results of our calculation of the ground state energies for neutral hydrogen and helium atoms at strong field. For comparison we also show the data, obtained in [9] on the basis of the calculation within the expansion of the Hamiltonian wave functions as a linear superposition with the use of hydrogen-like (in the tables it is designated as [9-2]) and Slater functions (in the tables – [9-1]) bases. In Table 1 we present the results of calculations for the energies of the H and He atoms from Ref. [10] on the basis of the two-dimensional mesh Hartree-Fock method. The static magnetic field is changed in the interval: $y=B/B_0$=0.01–10000, where the units are $B_0 = m^2e^3c/h^3Z^3$. One can note a great difference between the presented data. This fact confirms the complexity of the problem considered. The data presented in the tables provide information about the behavior of the neutral hydrogen and helium atoms in the complete strong-field mode. Useful information about the behavior of an atomic system can be obtained on the basis of the analysis of the ionization energies of the atom versus the magnetic field strength.

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Н-ПОДІБНІ ТА Не-ПОДІБНІ СИСТЕМИ У СИЛЬНОМУ МАГНІТНОМУ ПОЛІ: ЧИСЕЛЬНИЙ РОЗРАХУНОК

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Досліджено структуру квантових станів для Н-подібних та Не-подібних атомних систем у статичному магнітному полі (y=0.01–10000 в одиницях $B_0 = m^2e^3c/h^3Z^3$). Розраховано енергії основних станів нейтральних атомів водню та гелію у сильному статичному магнітному полі. У розрахунках використано ефективне представлення для гамільтоніану хвильової функції. Шукане представлення одержано на основі чисельного розв'язку рівняння Шредінгера для атома в магнітному полі з використанням операторної теорії збурень.