Chaos and regular dynamics of complex atomic systems in magnetic fields

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The numerical solution of the Schroedinger equation for atomic hydrogen in a static magnetic field has been found with the use of the operator perturbation theory (OPT) form method and the known in the scattering theory "distorted-wave" approximation. It has been shown that the wave functions and spectrum structure are intermediate between the regular structure and the chaotic one [1]. The estimates of the resonance widths have been performed.

The hydrogen atom in a static magnetic field has been considered as a prototype of the quantally chaotic system. The interest to this problem has been stimulated in last years by an experimental observation of complicated spectra with narrow resonances coexisting with broad one (c.f.[1-10]). Theoretical estimates of its spectrum have been performed in the frame of different approaches, in particular, Random Matrix theory, the WKB approximation (c.f.[1-8]). It has been shown that the predictions of the theory in the immediate vicinity of the ionization threshold are to be improved. The present paper is devoted to a study of the structure of the quantum states of the H atom in a static magnetic field near the ionization. A correct numerical solution of the Schroedinger equation has been found with the use of the early developed method - the operator perturbation theory form and the well-known in the scattering theory "distorted -wave" approximation [1].

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

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

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

$$H = \frac{1}{2}(P_z^2 + P_\rho^2) - \frac{1}{z} + \frac{1}{8}\omega^2\rho^2 \; . \qquad (2)$$

The corresponding spectrum is:

$$E(n_\rho, n_z) = (n_\rho + \frac{1}{2})\omega - \frac{1}{2}n_z^2) \; . \qquad (3)$$

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

We have fulfilled the estimates of the resonances widths G for different energy intervals. To calculate G we have used the OPT method (see detailes in ref.[1]). Here we only note that the resonance width is defined by the imaginary part of the state energy in the lowest PT order:

$$\mathrm{ImE} = \frac{\mathrm{G}}{2} = \pi < \Psi_{\mathrm{Eb}}|\mathrm{H}|\Psi_{\mathrm{Es}} >^2 \tag{4}$$

with the total Hamiltonian. For interval $(n - 1/2)\omega < E < (n + 1/2)\omega$ we have found that the resonances widths are $\sim$ 0.003-0.005, which is reasonably in agreement with the experimental data [4,5] and theoretical predictions [7,8]. For $-1/2\omega < E < 1/2\omega$ interval a regular dynamics behaviour takes place, under $E \sim \omega$ a chaotic one. The Landau levels are strongly mixed [10].

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