Semiclassical calculation of electron spectra in atoms through two universal functions

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The features of the one-electron spectra in the spherically symmetric self-consistent attraction potentials have been under study in the paper [1] (also, reviews [2, 3]). Specifically, the potentials with the Coulomb singularity have been there considered. As is well known, the screening of the Coulomb potential leads to the lift of the degeneracy in the orbital momentum . It has been shown in [1], that the corresponding splitting  quadratically depends on the orbital momentum  (here  is a principal quantum number). In addition an analysis of the energy levels calculated in the nonrelativistic Hartree-Fock model for some heavy elements has confirmed the dependence even for not small orbital momentum . That was a basis of the proposed method to calculate the electron spectra in atoms.

The semiclassical approach is applied to calculate one-electron spectrum in a free atom. The atomic number scaling in the Thomas-Fermi model and Bohr-Zommerfeld quantization condition are used. Then on the assumption of the square dependence on the orbital momentum it is possible to calculate a spectrum of any element through the two universal functions, computed for the hydrogen (atomic number ). One of the functions is the classical electron action  for the *s*-state ().

At first the *s*- level energy  is calculated from the quantization condition

  (1)

Then one can use the square-law equation

  (2)

to calculate the other levels .

The algorithm to define the second universal function , the tables and plots of the both functions are given. It is demonstrated the comparison with the results of - computation from the Bohr-Zommerfeld condition and with the nonrelativistic Hartree-Fock model.

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References

1. Shpatakovskaya G.V. JETP Lett., 2001, 73, 268.
2. Shpatakovskaya G.V. Phys. Usp., 2012, 55, 429.
3. Shpatakovskaya Galina, Quasiclassical Method in Quantum Physics Problems (LAP LAMBERT Academic Publishing GmbH, 2012) , ISBN 978-3-8465-2681-1 (in Russian)