

QUANTUM MECHANICS WITH NONNEGATIVE PROBABILITY FUNCTION – ONE OF THE METHODS OF ATOMIC STRUCTURES SIMULATION

The quantum theory has arisen from requirement to explain the character of electromagnetic radiation by atomic structures. Attempt to describe a stationary structure of atom by means of quantum mechanics further followed. In 1923 N. Bohr has offered the «Aufbau rule» – the rule of filling the electron shells in atoms which can be considered as an additional postulate to Bohr quantization rules in the old quantum mechanics.

In new quantum mechanics Heisenberg - Schrödinger the rule of quantization for hydrogen atom was introduced automatically. For the atoms following lithium, it did not fit experimental data; therefore the Runge rule was widely used. It is analogue to the Bohr «Aufbau rule» and does not follow from a formalism of wave mechanics with the Schrödinger equation.

Klechkovsky has received an indirect substantiation of the rule $(n+1, l)$ for filling the electron shells in atoms on the basis of Thomas-Fermi's statistical method approximately describing atomic structures. Such researches have been continued in works of Demkov and Ostrovsky, and also Barut and Kitagawara.

The majority of the theoretical works using approached and numerical methods (in more details see in Frisch, Veselov and Sobelman books), consider atomic structures in the form of two cooperating subsystems: selected electron and the remained part of atom (effective core potential).

In the given approach is present extended not spherically symmetric center and moving at its field extended electron. This situation, in our opinion, reflects the quantum-theoretical description of structurally-dot objects. Adequate model of this description is the quantum mechanics with non-negative quantum probability function, realizing «a principle of statistical conformity» by Blokhintsev-Terletsky, generalizing Bohr «principle of conformity».

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