A DYNAMIC MODEL OF THE HYDROGEN MOLECULE. I. THE MODEL OF THE HYDROGEN MOLECULAR ION

Ostrovskiy N.V.
Vyatka State University, city of Kirov, Russia

Ostrovskiy N.V.
Vyatka State University

According to modern representations, electron in an atom or a molecule can be described by the so-called wave equation, which decision gives distribution of probability density of an electron finding (or density of a charge distribution) in the certain area of space named an electronic orbital (Schrödinger model). The strict decision of the wave equation is possible only for one-electronic systems. For more complex systems are used various semi-empiric methods, which allow to calculate electron energy, lengths and corners between bounds in molecules with comprehensible accuracy.

The basic lack of the given model is "static character" of electron, that specifies conditional character of it.

In 1913 Niels Bohr had been developed model of atom according to which electron in atom addresses around of a nucleus on a circular orbit so force of an electrostatic attraction is equal to centrifugal force. The model of the Bohr gives fine concurrence to experimental data for hydrogen atom, but for multielectronic systems, as well as in case of Schrödinger model, the mistake in calculations appears is unacceptable big.

At a sight of the author, the reason of it is inapplicability for multielectronic systems of Qulon equation. Replacement of Qulon equation on **the generalized equation of electrostatic interaction**, deduced by analogy to the generalized equation of gravitational interaction (see, for example, [2]), allows to eliminate these divergences. In system of *n* charges the chosen charge (we shall designate it as 1) interaction with a charge for which the size $\left|q_i / r_{1i}^3\right|$ is maximal will be defining (we shall designate it as 2). Then:

$$\vec{F}_{12} = q_1 r_{1i} \sum_{i=2}^{n} q_i \vec{r}_{1i} / r_{1i}^4 \cdot$$

In the given work on the basis of the advanced model of atom, with use of the generalized equation of electrostatic interaction, the dynamic model of a hydrogen molecular ion, including electron's movement around nucleus 1 and movement of nucleus 2 around hydrogen atom is constructed. Besides, in models is used the value of internal energy of electron, which the deformation of its orbit under the action of nucleus 2 is determined. The ionization potential of H_2^+, calculated in framework of this model, differs from experimental on 1,4% relatively.

References:

1. *Nikolay V. Ostrovskiy*. Physical model of the orbital movement of the Jupiter satellite Karme. Electronic conference "Computer Applications in fundamental and applied Physics and Mathematics". 29.03.06. URL: http://www.ivtn.ru/2006/physmath/enter/t_pdf/tp06_07.pdf.