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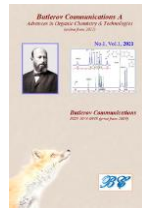

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Investigation of the Schroedinger equation for a molecule as an equation with a small parameter at some derivatives

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Abstract

Solutions of a Schroedinger equation for a molecule as a differential equation with a small multiplier at nuclear derivatives (which is a ratio of the electron mass to the atomic mass unit) possess a peculiar analytical properties. A presence of the small parameter at some derivatives says on a sharp difference in scales of electronic and nuclear density of a molecule that defines the structural peculiarities of molecular systems. In mathematical physics such equations are singularly perturbated, and their solving needs in application of asymptotical methods relative to the small parameter. In this work some questions are discussed connected with integrating of the Schroedinger equation for a molecule. A problem is put on an asymptotic decomposition of a molecular wave function by the small parameter and an analysis of the equation is fulfilled using a variational functional which tends to the functional of the degenerated problem when zeroth small parameter. It is pointed out that investigation of the degenerated Schroedinger equation (which answers to the Born-Oppenheimer approximation) allows one to give a deductive method of defining a chemical structure in a form of a variational geometrical problem with varying not only electronic wave function but parameters of nuclear coordinates, also. Extreme points of the auxiliary functional give a set of isomer structures of a molecule with a given atomic brutto formula. An existence of such a peculiarity of solutions of the degenerated (electronic) Schroedinger equation produces to a theoretical ground for observed experimentally chemical structures to which a clear hint in the input Schroedinger equation for a system of heterogeneous Coulombic charges is absent. When analyzing the electronic equation an explicit solution of a fundamental model problem on a motion of an electron in a field of fixed nuclei was considered and it was shown that a general form of the solution is represented by LCAO. To this end, a relativistic generalization of this important model quantum chemical problem was given and it was shown the descendance of the faithful solution with the nonrelativistic LCAO MO. The originality of the angular momentum

conservation law for molecular systems is discussed and it was shown that it introduces some new details into their optical spectra interpretation. Absence of atomic collisions within molecules and presence of the small parameter at nuclear derivatives allow one to formulate a local theory of nuclei motion within electronic shells of atoms with localization at nodes of a molecular structure frame.

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References

[1] L.A. Gribov. A variance of basic aspects in quantum theory of molecules. *Moscow: Nobel Press.* **2015**. 188p. (Russian)
[2] G.M. Zhislin. *Proceedings of the Moscow Math. Soc.* **1960**. No.9. P.82. (Russian)
[3] G.M. Zhislin. *Theor. and Math. Phys.* **1971**. No.7. P.332. (Russian)
[4] M.A. Antonets et al. *Theor. and Math. Phys.* **1973**. No.16. P.235. (Russian)
[5] M. Born et al. *Ann. d. Phys.* **1927**. No.84. P.457.
[6] B.K. Novosadov. Analytical mechanics of atom. *Moscow: Nobel Press.* **2014**. 332p. (Russian)
[7] L.A. Gribov. Vibrations of molecules. *Moscow: Bookhouse "LIBROKOM".* **2009**. 544p. (Russian)
[8] R.S. Mulliken. *Phys. Rev.* **1932**. Vol.41. P.49.
[9] G. Herzberg. Molecular Spectra and Molecular Structure I, Spectra of Diatomic Molecules. 2-nd ed. **1950**. *N.Y. Van Nostrand, Princeton*. 404p.
[10] H. Essén. *Int. J. Quantum Chem.* **1977**. Vol.12. P.721.
[11] B.K. Novosadov. Methods of mathematical physics of molecular systems. *Moscow: Bookhouse "LIBROKOM".* **2010**. 384p. (Russian)
[12] B.K. Novosadov. Quantum theoretical models and methods in chemical physics. *Moscow: Book on Demand Ltd.* **2017**. 282p. (Russian)
[13] Boris K. Novosadov. Investigation of the Schroedinger equation for a molecule as an equation with a small parameter at some derivatives. *Butlerov Communications.* **2021**. Vol.65. No3. P.1-15. DOI: 10.37952/ROI-jbc-01/21-65-3-1 (Russian)