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A new representation concerning the influence of rotations on inner motions of particles in atomic and molecular systems

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Abstract

A new theoretical representation on a connection of the rotation as a whole and inner motions of a free system of particles is suggested on the base the usage of the quantum mechanical conservation law for the system angular momentum. A derivation of a faithful relationship of the kinetic energy of a system of particles and their full angular momentum has been represented which has been made by the author firstly in the literature. A difference of the obtained relationship for a system of particles from the formula for one particle, which well-known in the theoretical mechanics, is in the appearance additional yields to the inner energy of the system of particles from partial angular momenta of particles that leads to an additional degeneration of rotational states due to counter pendulum movements of the particles not violating the conservation of the quantity of the system angular moment. As a result, a principal plurality of rotational states for a multiparticle system at a given angular moment was shown. This peculiarity of the conservation law of the full angular momentum provides some additional spectral and structural properties of atoms and molecules which had not earlier taken into consideration in the theory of their quantum states. A principal importance of the angular momentum conservation law in the theoretical analysis of molecular structures for astrophysical and physical and chemical applications has been pointed out.

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References

- [1] A. Messiah. Quantum mechanics. *North-Holland Pub. Co.* 1961.
- [2] B.K. Novosadov. Analytical mechanics of atom. *Moscow: Book on demand.* 2014. Ch.9. (Russian)

- [3] A.S. Makhnev. Theory of vibrations and calculation of molecular constants in different coordinate representations. *PhD Thesis in Phys. and Math. Sci. Doct. Ivanovo*. **2010**. (Russian)
- [4] D.A. Varshalovich, A.N. Moskalev, V.K. Khersonsky. Quantum theory of angular momentum. *Leningrad: Nauka*. **1975**. P.141. (Russian)
- [5] L.A. Gribov. Vibrations of molecules. *Moscow: Book House "LIBROKOM"*. **2009**. P.62. (Russian)
- [6] Boris K. Novosadov. A new representation concerning the influence of rotations on inner motions of particles in atomic and molecular systems. *Butlerov Communications*. **2021**. Vol.65. No.3. P.16-24. DOI: 10.37952/ROI-jbc-01/21-65-3-16 (Russian)