

# Quantum Mechanics 2021

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### Quantum-classical mechanics: Principles, applications, and prospects

In quantum mechanics, the theory of quantum transitions is grounded on the convergence of a series of time-dependent perturbation theory. In nuclear and atomic physics, this series converges because the dynamics of quantum transitions are absent by definition. In molecular and chemical physics, the dynamics of “quantum” transitions, being determined by the joint motion of a light electron (or electrons) and very heavy nuclei, are present by definition, and this series becomes singular. An exception is the dynamic problem for stationary states in the Born-Oppenheimer adiabatic approximation, when the electronic subsystem turns out to be “off” from the general dynamic process and therefore is not dynamically full-fledged: it only forms an electric potential in which the nuclei oscillate. Removing the aforementioned singularity can be accomplished in two ways. The first method was consisted of introducing an additional postulate in the form of the Franck-Condon principle into molecular quantum mechanics, in which the adiabatic approximation is used. The second method was proposed by the author and consisted of damping the singular dynamics of the joint motion of an electron and nuclei in the transient state of molecular “quantum” transitions by introducing chaos. This chaos arises only during molecular quantum transitions and is called dozy chaos. Dozy chaos leads to the continuity of the energy spectrum in the molecular transient state, which is a sign of classical mechanics. Meanwhile, the initial and final states of the molecule obey quantum mechanics in the adiabatic approximation. Molecular quantum mechanics, which takes into account the chaotic dynamics of the transient state of molecular “quantum” transitions, can be called quantum-classical mechanics (QCM). The efficacy of the damping for the aforementioned singularity is shown by different QCM applications, in particular, by applications of the so-called Egorov resonance to optical spectra in polymethine dyes and J-aggregates both for single-photon and two-photon processes, which, in particular, are rationalizing experimental studies in the field of bioimaging and photodynamic therapy. Prospects for further developments in QCM and their applications to problems of cancer and viral infections are discussed.

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## Biography

Vladimir Valentinovich Egorov has his expertise in theoretical molecular and chemical physics. Education: National Research Nuclear University MEPhI, Faculty of Theoretical and Experimental Physics (1966 – 1972), Moscow, USSR. He has completed his PhD from Theoretical Department of Institute of Chemical Physics, USSR Academy of Sciences (1981), and he has completed his Phys & Math Sci degree from Institute of Physical Chemistry, Russian Academy of Sciences (2004). He is leading researcher at FSRC “Crystallography and Photonics”, Russian Academy of Sciences, Moscow, Russia. He is working on the development of a fundamentally new physical theory – quantum-classical mechanics and its applications in physics, chemistry, biology and biomedicine.