Opinion

on the dissertation of Prof. Dr. Rumen Tsvetanov Tsekov on "Classical and quantum Brownian motion", presented for the scientific degree "Doctor of Science" in the professional field 4.2 Chemical Sciences (Physical Chemistry)

by Prof. Boris Simeonov Galabov

The dissertation of Prof. Rumen Tsekov is a summary of his research, published in 35 scientific articles. A significant proportion of publications are in prestigious international scientific journals such as the Journal of Chemical Physics (5 articles), the Journal of Physics A (2 articles), the Journal of Physical Chemistry (2 articles), Phisica Scripta, the Journal of the Chemical Society Faraday Transactions, and a number of others.

In a series of articles / art. 2-6 / R. Tsekov theoretically treats the dynamics of a mechanical subsystem in a rigid body. The solid is modeled as a bath of interacting harmonic oscillators. An equation deriving the static interaction with the solid body by dissipative and fluctuation forces is derived, using both methods of classical mechanics and stochastic dynamics. The stochastic dynamics of a hydrocarbon molecule in a solid is considered as an example of application. A comparison of the theoretical predictions with the diffusion of n-paraffins in zeolite-T is made. A good correspondence of the theoretical estimates with the experimental data is obtained. A similar approach is used to explain the differences in diffusion coefficients between dimers and single rhenium atoms on a tungsten surface. A continuation of research on this topic theoretically describes the dynamics of a mechanical subsystem in an amorphous solid. The Langevin equations are also applied to describe the two-dimensional Brownian motion of single atoms and dimers on a solid surface. The dependences of the diffusion of alkanes on the surface of zeolites (J. Phys. Chem. 1998, 2003) are described by the formalism of stochastic equations. The periodic dependence of the value of the diffusion coefficient on the chain length of the alkanes is shown. A formula for calculating the diffusion coefficient for the motion of a single particle in a field of

periodic potential (Adv. Col. Interf. Sci. 2005). Research on this issue has been published in authoritative scientific journals (J. Chem. Phys., J. Phys. Chem.), which emphasizes their importance. The author demonstrates convincing capabilities for the application of the complex mathematical apparatus for theoretical research in the field of physicochemical description of Brownian motion and diffusion.

In a series of articles, the author discusses the theory of Brownian motion in systems in which quantum effects are significant. Fundamental in this direction is the author's first article on quantum Brownian motion (Chem. Phys. Lett., 1992), which derives equations based on the evolution of probability density. The approach allows to estimate the dispersion of the quantum Brownian particle in a harmonic external potential. In subsequent publications on this topic, the author derives equations describing the behavior of a quantum Brownian particle in a field of harmonic oscillators. However, it should be emphasized that the conclusions refer to an idealized system - a single particle in a thermal bath of harmonic oscillators. Further, R. Tsekov introduces a special temperature operator in the derivation of quantum equations, which consider the effect of quantum oscillators in a thermal bath on Brownian motion. It should be emphasized, however, that the validity of the derived equations cannot be verified experimentally, as they relate to an extremely simple, idealized system. This shortcoming was overcome, however, in subsequent research to arrive at the latest publication from 2021, where the formalism of Markov processes was further developed for an arbitrary system of N interacting quantum particles.

Tsekov's study of the movement of individual living cells in conditions modeling the environment of living organisms is interesting. Using a similar approach, already developed for the motion of a single Brownian particle in a thermal bath, the corresponding Klein-Kramers and Smoluchowski equations for the motion of a living cell are derived. Temperature, as a major factor in the movement of a Brownian particle, has been replaced by the so-called "temperament" of a living cell, considering its tendency to move. However, in addition to temperament in these conditions, temperature should also be a factor to consider.

Another important direction in R. Tsekov's research is the investigation on the relationship between quantum mechanics and Brownian motion. These studies are based on analogies between the probabilistic nature of the parabolic form of the Schrödinger equation and the diffusion equations. Without going into details of the conclusions that are the subject of theoretical physics, it should be noted that one of the most important results of the derived equations concerns one of the fundamental concepts in quantum mechanics, namely the dualistic nature of quantum particles. The derived equations can be interpreted as showing that quantum particles, such as an electron, are real particles, and the wave nature of motion results from the parallel presence of virtual particles that are waves in the coordinate subspace. In fact, the modern understanding of electrons is that they are real point particles of a certain mass, but whose motion has a wave character.

R. Tsekov conducted a number of studies illustrating the relationship between the equations of quantum mechanics and the theory of diffusion. For example, a stochastic Lorentz equation is derived, describing the Brownian-like behavior of point particles in quantum mechanics. It is shown that the Schrödinger equation resembles the diffusion equations in the presence of an imaginary diffusion coefficient. The idea of virtual quantum particles is used again, with the imaginary diffusion coefficient describing the Brownian motion of a real particle in a sea of virtual particles. The Brownian motion of a classical particle in a quantum neighborhood is also studied. The corresponding Smoluchowski equations are derived by introducing quantum operators for temperature and friction. In a recently published article, R. Tsekov offers an alternative interpretation of quantum mechanics, in which particles remain all the time, as in classical mechanics. The so-called force carriers that carry the fundamental interactions between particles are introduced. The force carriers are quantum particles, waves in the coordinate space.

It can be said that a number of the ideas in R. Tsekov's works dealing with the relations between the equations of Brownian motion and diffusion with the equations

of quantum mechanics have the character of hypotheses. However, they are protected supported in a convincing way by the derived numerous equations.

Rumen Tsekov's dissertation presents important for science results in the theory of Brownian motion and diffusion and the relationship between the classical equations for Brownian motion and diffusion and the equations of quantum mechanics. The author offers a series of bold ideas that are supported by the derived equations. The scientific results are presented in publications in a number of prestigious international scientific journals. I strongly suggest to the esteemed Scientific Jury to award the scientific degree "Doctor of Science" in the field of chemical sciences to Professor Rumen Tsvetanov Tsekov.

Signature:

(Prof. Boris Galabov)