Review

of the dissertation of Prof. Dr. Rumen Tsekov
"Classical and quantum Brownian motion"
to obtain the degree of ***Doctor of Science***
Field of higher education 4. Natural sciences, mathematics and informatics
Professional field 4.2. Chemical sciences

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The set of hard copy materials presented by Prof. Dr. Rumen Tsekov includes the following documents: dissertation, declaration of authorship and reference for compliance with the minimum national requirements for the degree of *Doctor of Science* (only the number of points is presented). On electronic media are presented: CV, diploma of higher education, diploma of educational and scientific degree *Doctor*, dissertation (in English), summary of the dissertation (in Bulgarian and English); 35 scientific publications, which are included in the dissertation and reference for compliance with the minimum national requirements for the scientific degree of Doctor of Sciences. No evidence for participation in scientific conferences has been attached, although there are listed in the abstract. There is also no protocol from the extended departmental council of the Department of Physical Chemistry at the Faculty of Chemistry and Pharmacy of Sofia University, related to the preliminary discussion of the dissertation and the opening of the defense procedure.

Biographical data

Rumen Tsekov began studying chemistry at the Faculty of Chemistry of Sofia University in 1983 and graduated in 1988 with full honors as a master's degree in Chemical Physics and Theoretical Chemistry. Immediately after graduating, he began his scientific career in the same faculty, following the scientific hierarchy - assistant (1988), senior assistant (1991), chief assistant (1996) and defending a dissertation in physical chemistry on "Fluctuation phenomena on fluid surfaces" in 1993 under the supervision of Prof. Boryan Radoev. From 1993 to 2002 he specialized at the University of Buffalo (USA), he was a visiting professor at the Universities of Cincinnati (USA) and Tsukuba (Japan) and was a Humboldt Fellow at the Technical University of Freiberg (Germany). He left Sofia University in 2002 and worked in Germany as a Mercator professor and guest researcher, at the University of Karlsruhe (2002-2006) and at the Technical University of Aachen (2007-2009), respectively, and for a short time (3 months) in University of Brisbane (Australia). He returned to

Alma Mater in 2009 as an associate professor in the Department, where he began his scientific career. Two years later he was elected professor of physical chemistry.

Evaluation of dissertation publications

The dissertation is written on 35 pages. The introduction is presented on five of them, the main part of the dissertation is listed on 28 pages, and the other two contain contributions. A list of the author's articles included in the dissertation is given on 3 more pages, and the articles themselves follow the main text. If the attached articles are taken into account, then the total number of pages becomes 347.

The dissertation is based on 35 scientific publications, of which 19 are by Rumen Tsekov (№№ 7,8, 10, 13-17, 19, 21, 23-25, 28, 30-35), and of the remaining 16, Prof. Tsekov is the first author in 11 (№№ 1-6, 9, 12, 22, 27, 29, 32) and the second author in 5 (№№ 4, 11, 18, 20, 26). Eleven of these 16 articles are with only two authors. In six of all 16 publications with two or more authors, Prof. Tsekov is a corresponding author. All publications are in international scientific journals with impact factor. They are arranged by quartiles as follows:

Q1: publications. Five of them in the *Journal of Chemical Physics* (IF 3.220), two each in the *Journal of Physical Chemistry B* (IF 3.266) and *Journal of Physics A* (IF 1.186), and one each in *Chemical Physics Letters* (IF 2.330), *Surface Science* (IF 1.839) и *Advances in Colloid and Interface Science* (IF 4.481).

Q2: 8 publications. Two of them in *Доклади на БАН* (IF 0.343) and one each in the *Journal of Chemical Society Faraday Transactions* (IF 1.757), *Physica Scripta* (IF 1.164), *Foundations of Physics* (IF 1.147), *Europhysics Letters* (IF 1.978), *Physics Letters A* (IF 2.236) и *Annalen der Physik (Berlin)* (IF 1.401).

Q3: 14 publications. Six of them in the *Fluctuation and Noise Letters* (IF 1.208), four in *International Journal of Theoretical Physics* (IF 0.659), three in *Chinese Physics Letters* (IF 0.943) and one in *Reports in Advances of Physical Sciences*.

Q4: One publication in *International Journal of Molecular Science* (IF 0.333).

According to the SCOPUS information database, a total of 183 citations in the specialized literature have been noted in the articles included in the dissertation.

The presented information about the publications on the dissertation and their respective quartiles, as well as the number of the citations on these articles, shows that the minimum national requirements for the degree *Doctor of Science* have been exceeded 5 and 4 times, respectively.

Dissertation contributions

The dissertation consists of three parts. In the first part, the focus is on Brownian motion of classical particles. Within classical mechanics, a generalized Langevin equation is derived for an arbitrary mechanical subsystem interacting with the harmonic bath of a solid environment.

The Langevin equation is applied to describe several different cases of resonant Brownian motion of atoms and of rigid, rotating, and vibrating dimers on solid surfaces, as well as of n-alkanes in zeolites. In these cases, a non-monotone dependence of the classical diffusion coefficient on the structure of the diffusing particle is observed, and the calculations correlate well with the experiment. The calculated diffusion coefficients of atoms and dimers of rhenium on the surface of tungsten crystals coincide with the experimentally determined values. These studies, conducted together with Prof. Eli Ruckenstein, are included in 6 papers (№№ 2-6), cited a total of 59 times, among which is the most cited publication (№ 2) in the dissertation. The obtained numerical results from the diffusion coefficients are in excellent agreement with the experimental results for the diffusion of n-alkanes in zeolites. The research published in two articles (№№ 9 and 11), together with colleagues from the University of Cincinnati, is also among the most cited - a total of 39 citations.

In biology, the transport of molecules across highly structured biological membranes is also an example of resonant diffusion. In the dissertation, through the generalized Langevin equation, the driving force of cell migration is theoretically studied, proposing a model for their Brownian motion, and by analogy with the temperature that determines the Brownian motion of non-living objects, an important biophysical parameter called temperament of living cells, describing the desire to move living biological objects. Klein-Kramers and Smoluchowski equations are obtained, where thermal energy is replaced by temperament. Thus, the Maxwell-Boltzmann equilibrium distribution also describes the probability density for the velocity and position of living cells.

The second part of the dissertation presents the idea that electrons are particles that can also perform Brownian motion. A new interpretation of quantum mechanics has been proposed, in which, like classical mechanics, particles are point-like at all times. It has been shown that quantum mechanics is caused only by virtual quasi-particles that carry fundamental interactions. These virtual particles are waves in the coordinate subspace and quasi-particles in the impulse subspace. They are also the reason for the wave nature of quantum mechanics, not the point particles it describes. Schrödinger's fundamental equation is explained as a result of collisions between point and virtual particles.

A stochastic Lorentz equation describing the Brownian motion of point particles in quantum mechanics is derived as an analogue of the Langevin

equation. It is shown how, by means of a calibration transformation, the Schrödinger equation is obtained from the Lorentz-Langevin equation.

The third part of the dissertation proposes a stochastic Bom-Langevin equation, obtained by combining the ideas of Bohm and Langevin. It describes Brown's dynamics within Bohm's mechanics. The corresponding Smoluchowski-Bohm equation is then derived, which describes the evolution of the probability density in the configuration subspace of a quantum subsystem interacting with the classical environment. This equation reflects the stochastic Bom-Langevin dynamics described by a density functional. For numerical calculations in chemistry, a nonlinear dissipative Kon-Sham equation has been proposed, which improves the kinetic functionality of Thomas-Fermi-Weizsäcker. In this part of the dissertation a nonlinear master equation is derived, which correctly reflects the entropy of open quantum systems and, unlike linear alternatives, its equilibrium solution is the exact canonical Gibbs density matrix.

It is noteworthy that the articles describing the research in the second and third parts of the dissertation (№ 1,7,10, 13-19, 21, 25-29, 31-35) have only one author, Rumen Tsekov, they are about 80% of the total number of papers. The leading role of Tsekov in other publications is also undoubted. The number of citations found in the articles on which these two parts of the dissertation are based is less than half of the total number of citations. This is understandable, given the very specific field in which Prof. Tsekov's dissertation is. We should not ignore the fact that many of the articles have been published in the last five years.

Summary of the dissertation

The summary of the dissertation is a translation from English into Bulgarian of its content and contributions. Only there is a very short list of participations in research projects and conferences. The titles of the presented reports or posters are not even given. There are several typographical errors that need to be corrected in the final version of the abstract.

Remarks

Although written in a way that is not standard for our latitudes, the dissertation as a whole makes a good impression on the reader. I have a remark related to its technical layout. Only the author's articles are listed as bibliography. This way of presentation is very good when preparing a summary of the dissertation, but in the dissertation, in my opinion, it would be good to cite also other scientific papers.

Conclusion

In conclusion, I believe that the Dissertation summarizes significant scientific results with a leading contribution of the author. In the majority of articles he is the only author. Prof. Rumen Tsekov is an erudite scientist with many interesting ideas in the field of chemical physics and theoretical physics. These own ideas and views will surely lead to new interesting results.

I am convinced of the high level of his research work. Prof. Tsekov has left a visible trace with the scientific production presented in the Dissertation. This gives me every reason to recommend to the esteemed Jury to award Prof. Dr. Rumen Tsekov the scientific degree *Doctor of Science*.

August 27, 2021

Prof. Venelin Enchev