

REVIEW

by Dr. **Alia Vitali Tadjer**

Professor of Theoretical Chemistry,

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of a dissertation for the award of the scientific degree 'Doctor of Science'

in the field of higher education 4. *Natural sciences, mathematics, informatics*

professional field 4.2. *Chemical sciences*

Author: Prof. Dr. **Rumen Tsvetanov Tsekov** - Department of Physical Chemistry, Faculty of Chemistry and Pharmacy at Sofia University “St. Kliment Ohridski ”

Topic: ***Classical and quantum Brownian motion***

1. Subject of review

By order № PD-38-245 of 18.05.2021 of the Rector of Sofia University “St. Kliment Ohridski” I have been appointed a member of the scientific jury for providing a procedure for the defense of a dissertation on “Classical and quantum Brownian motion” for obtaining the scientific degree 'Doctor of Science' in the field of higher education 4. Natural sciences, mathematics, informatics, professional field 4.2. Chemical sciences. The author of the dissertation is Prof. Dr. Rumen Tsvetanov Tsekov - Department of Physical Chemistry at the Faculty of Chemistry and Pharmacy at Sofia University “St. Kliment Ohridski”.

The set of materials presented by Prof. Dr. Rumen Tsvetanov Tsekov includes the following documents:

- declaration of originality and authenticity of the attached documents;
- CV in free format;

- a copy of the diploma for the master's degree;
- a copy of the diploma for the educational and scientific degree "Doctor";
- reference for compliance with the minimum national requirements for the scientific degree "Doctor of Sciences" in the scientific field 4. Natural sciences, mathematics and informatics professional field 4.2. Chemical sciences, containing a list of noticed citations;
- summary in Bulgarian and English;
- disk with the materials for the procedure (unreadable);
- a paper body containing:
 - summary in English
 - the scientific publications on the basis of which the dissertation was prepared.

The candidate has submitted 35 publications

- list of participations in conferences, projects, etc .;
- self-assessment of the contributions.

I would say that the documentation presented by Prof. Tsekov for the procedure is more than sparing. The parsimonious autobiography lists a number of facts for which detailed information is lacking, which makes it difficult for reviewers to work on scientometrics. There is no separate list of the author's publications - even those included in the dissertation are listed only in the list of noticed citations. It would be good to have a complete list of the mentioned 150 publications, distributed by participation in different procedures for academic degrees and titles. There is no way to understand from the attached documents whether the articles used in the dissertation have not been part of another procedure. The same applies to the other assets of the candidate - it is not clear whether among the 20 conference participations there are such related to the topic of the dissertation, as well as in what form the presentations were. It is not mentioned whether some of the projects in which he participated and / or supervised were related to the dissertation and what was the role of the candidate in these projects; whether the theses and dissertations he has been a supervisor or consultant of were/are related to the topic. The

attached reference for compliance with the minimum national requirements for the scientific degree "Doctor of Science" is just a table - I could not figure out how the reported number of points is determined. It would have been good if the candidate had attached a reference to the contributions of the individual publications included in the thesis.

2. Brief biographical data

Rumen Tsekov was born in 1963. He is a graduate of the Faculty of Chemistry at Sofia University "St. Kliment Ohridski", where in 1988 he graduated with a master's degree in chemistry. He was immediately appointed Assistant Professor in the Department of Physical Chemistry of the same institution. Five years later he defended his doctoral dissertation. After a series of specializations on 4 continents and several years of work in Germany, in 2009 he was elected Associate Professor, and 2 years later a Professor in the Department of Physical Chemistry at FCP-SU, where he was head of chair in the period 2012-2016. Tsekov combines teaching and research work – he has lecture courses, supervises / consults graduate and doctoral students, participates in / leads projects. He is the author of over 100 publications (115 according to SCOPUS) on which a total of 733 independent citations (SCOPUS) have been noticed. He is a member of several scientific societies and winner of several awards.

3. Topicality of the subject and expediency of the set goals and tasks

The dissertation is dedicated to a fundamental problem, which means that it is not one of the "hot" topics of the day, but one of the "eternal" ones, i.e., those that are always relevant and appropriate. Their study is a scientific challenge and their elaboration requires interdisciplinary approach.

4. Knowledge on the problem

The content of the dissertation clearly shows that the candidate is familiar in depth with the problem both with its history and with the assortment of theoretical approaches to its solution and the various connections between them. Previous and current research endeavors related to the topic are presented in satisfactory detail.

5. Research methodology

The chosen methodology is presented extremely briefly and concisely, both as a physical and as a mathematical representation. I find that it is original and completely suitable for searching of a possible solution to the task. On the other hand, there is still room to enrich it in case the candidate decides to continue working on this topic.

6. Characteristics and evaluation of the dissertation

The dissertation has a strange format, atypical for the Bulgarian practice. The total volume of the printed body is 247 pages, 35 of which are a hybrid between an abstract and a description of the contributions and the remaining 210 are copies of the 35 publications on which this prologue is based. I would refrain from commenting whether such a format is acceptable or not. I know that this is an established model for obtaining a PhD degree in many European universities, but as far as the degree of 'Doctor of Science' is present in the academic life of modern countries, it is acquired on the basis of work with the character of a monograph (and often published as such in the form of a book), summarizing research on a particular topic. In the present case, it is something like a collection of articles with an extended preface, the size of a not very voluminous review article. I admit that I have not seen such either at home or abroad. The abstract in Bulgarian and English is presented as a separate body. Surprisingly, there are more spelling/grammar mistakes in the Bulgarian text than in the English.

According to the attached table of contents, the text is divided into 5 sections. After a concise introduction to the problem, showing that the subject excited almost all physicists of the late 19th and first half of the 20th century (including all the Nobel laureates of the time), sections devoted to the Brownian motion of classical and quantum particles followed. To the classical aspects of the Brownian motion are entirely devoted 12 relatively early in the candidate's career publications (2,3,4,5,6,8,9,11,12,22,23,24) and part of two later ones (21 and 30). The latter two, as well as the remaining 21, are related to quantum aspects of the Brownian motion.

7. Contributions and significance of the findings/derivations for science and practice

The candidate has set goals that gradually swell and evolve. In contrast to the laconic presentation, the contributions are presented in detail by the author within 10 points.

In the classical aspect, the derivation of a generalized Langevin equation for the interaction of an arbitrary system with a structured environment with harmonic behavior is a contribution, while the ordinary Langevin equation itself is employed to describe resonant Brownian motion in real systems, which is compared with experimental results and model simulations. Among the quantum achievements there are such of an “ideological” nature, some of which I find formal rather than essential and come down to the type of interpretation of quantum mechanics. I appreciate the derivation of a stochastic analogue of the Langevin equation, as well as the proposed projection operator describing the collapse of the wave function of a quantum particle in a classical environment. For me, as for other colleagues, the most original concept is the introduction of a temperature operator and its application to describe the mobility / vitality of living cells.

For the most part, the contributions are related to mathematical formalism for describing incidental events and searching for a connection between statistical thermodynamics and quantum mechanics in Bohm's interpretation. Like the three "B's" in music (Bach, Beethoven and Brahms) the interpretation of quantum mechanics, also features three "B's" - Bohr, Born and Bohm (if we don't count de Broglie). In both cases, these are not the only significant representatives, but they are the brightest identifiers in the respective field. And if the three musicians are a kind of definition for three epochs in music spanning almost three centuries, then the three physicists mark the debatable interpretation of quantum mechanics within about 50 years. Although not always of the same opinion, Bohr and Born belong to the *Copenhagen school*, which to this day is dominating in the guild. Bohm's interpretation enjoys variable success, which has its ups and downs, but is generally more applicable to the description of physical properties and is unsuitable for chemistry. Prof. Tsekov is not a "citizen of Copenhagen", as are the prevailing number of quantum chemists in the world and in our country, including me. For this reason, I am somewhat skeptical of some of Bohm's conventions in the interpretation, which the candidate

has fully confided. These include the rejection of the dualistic nature of the electron, as well as the argument proposed in the thesis; here is friction as a term to describe / replace certain types of interactions. From a mathematical point of view, all conclusions seem completely correct. Using his excellent training in statistical mechanics and thermodynamics, Tsekov relied on Wigner-Wayl representation and Liouville's equation. From a chemical point of view, in particular at the molecular level, the idea of Brownian motion of a charged particle in the potential of charged (with a higher charge in the general case) nuclei seems to me, if not ludicrous, then insignificant. This is probably the result of paradigms instilled in the course of our education, but we generally associate Brownian motion with the stochastic behavior of neutral particles, while charged ones always have much stronger and more clearly oriented interactions that mask it, if present at all.

Contributions could be defined as the achievement of new and extension of existing knowledge by applying modern methods, building and proving hypotheses, confirming or disputing existing ones. The subject has a future and can be expanded both in terms of objects and in terms of formalism.

8. Evaluation of the publications on the dissertation

34 out of 35 attached publications have undergone independent peer-review process and are in journals with an impact factor, although this factor in many cases is well below 1,000; yet, this does not prevent the journals from being in decent quartiles. In particular, there is one article in a journal with $IF > 4$, five with $IF > 3$, three with $IF > 2$, 14 with $IF > 1$ and 11 with $IF < 1$; but by quartiles the distribution is: 12 in Q1, 8 in Q2, 13 in Q3 and only 1 in Q4. Since the reviewers of these publications are certainly better specialists in the field than I am, I do not intend to discuss their assessment. Rather, I would like to draw attention to the acceptance that these articles have met with the scientific community. According to the author, 182 citations were noticed in the literature. Distributed over 35 publications, this makes an average citation rate of about 5 citations per article. But this is not actually the case. In fact, there are five articles with more than 10 citations, mostly those on the classic Brownian motion, and the rest enjoy little or no interest (6 with 0, 6 with 1, 3 papers with respectively 2, 3 and 4 citations). Moreover, the citing authors

are almost the same people, united in quite large groups of co-authors, unlike the publications of the candidate. The fact that the candidate's articles are in not very popular journals probably also played a role, but it is good that the author did not rely on these publications for its h-factor.

I cannot comment on the candidate's performance at conferences and in contracts, as there is no information about them.

9. Personal participation of the author

The personal participation of the candidate is not only indisputable, it is obviously leading. Out of 35 attached articles, Tsekov is the first author in 32, in 19 of which he is the single author. I also believe that the results obtained in the few co-authored papers are mainly his input. Even if some of his notable co-authors in the publications have made a significant contribution to the analysis of the results, the dissertation itself is obviously entirely his merit.

10. Summary

The summary accurately reflects the content of the dissertation. In fact, the summary IS the dissertation.

11. Critical remarks and recommendations

The dissertation is not easy to read. There are references to at least 100 equations, theories, rules, hypotheses, interpretations, methods that the reader is supposed to be well familiar with. If not, that's his/her problem. There is no bibliography and the only option is to look for the source in the respective article. The lack of a common bibliography makes it impossible to assess the number and type of sources cited. I may have missed some citations, but I have not seen references to authors such as Sbitnev and his open system formalism, where coordinates and momentum are treated equally, or to Goldstein's work on Bohm's relativistic method and the use of density matrices in Bohm's mechanics. It would have been great to have something like an abstract, where it is clear – “so far we knew this and that (not the equation of somebody), but it does not allow us to evaluate / understand this and that, so I have developed / shown this and that and I have applied it to explain this and that, which is useful for this and that”. I think that the difference between a beginner and an established scientist is in this - the beginner tries to

show how complex a task he has undertaken and how many difficulties he has faced, and therefore the PhD theses are usually pretentiously written to demonstrate how serious a scientist the author is; the established scientist has outgrown this and knows that his work is significant, but he is able to present it simply and understandably, so the Dr.Sci. theses are usually a useful read and aid even beginners in the field. I would not describe the present thesis as such.

Tsekov's research is definitely non-standard and the results are a contribution to the field, but the text of the dissertation sounds more like a self-indulging hobby, like derivation for derivation sake.

12. Personal impressions

My personal impressions are long-standing - I have known the candidate for about 35 years. I have no joint activities with the candidate. As a scientist he is an erudite, as a colleague he is honest. Tsekov makes an impression of a motivated, purposeful and systematic researcher.

CONCLUSION

The dissertation contains scientific results that represent an original contribution to science and in this sense it meets the requirements of the Law for the Development of Academic Staff in the Republic of Bulgaria, the Regulations for implementation of this law and the relevant Regulations of Sofia University "St. Kliment Ohridski". The dissertation shows that the candidate possesses in-depth theoretical knowledge and professional skills in the scientific field, demonstrating qualities and skills for conducting research with the receipt of original and significant scientific contributions.

Due to the above, I give my positive assessment of the research and the results and contributions, and I propose to the esteemed scientific jury to award to Prof. Dr. Rumen Tsvetanov Tsekov the degree 'Doctor of Science' in the field of higher education: 4. Natural Sciences, mathematics, informatics, professional field 4.2. Chemical sciences.

25.08. 2021

Reviewer:

Prof. Dr. Alia Tadjer