TEL AVIV UNIVERSITY אוניברסיטת תל-אביב

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הפקולטה למדעים מדויקים
ע"ש ריימונד ובברלי סאקלר
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הקתדרה לכימיה פיזיקלית ע"ש היינמן

April 12th, 2009

Re: Habilitation thesis of Dr Denis S Grebenkov

The habilitation thesis by Dr Denis S Grebenkov presents a clearly written summary of his achievements during recent years and demonstrates his deep knowledge and understanding of a broad spectrum of topics, theoretical tools and their applications. The thesis is written coherently, which makes the reading an interesting experience. I find impressive the emphasis put on both mathematical rigor and on trying to relate to real systems.

Studying Dr Grebenkov's activities I noted that his publications appear in high impact physics journals (in particular should be mentioned: Rev Mod Phys, Phys Rev Lett and PNAS). Moreover, the number of the invited lectures of Dr Grebenkov at the current stage of his career points toward an increase in visibility and reputation.

Let me state already here that this habilitation thesis acknowledges the high scientific level of Dr Grebenkov, his ability to carry out independent and original research and, I believe, to supervise young researchers.

Restricted diffusion plays a central role in a broad range of areas as diverse as physics, chemistry and biology. In particular, the latter provides many examples, some of which are mentioned in the thesis and others due to recent advances in measurement techniques on the level of single molecule (still to benefit from the results derived in the thesis). This is also what connects some of my own research to the thesis: diffusion in complex restricted systems such as cells or protein structures.

I would like to start with what is closer to some of my own recent research: first passage time statistics (Chapter 2 in the thesis). Dr Grebenkov chooses fractal surfaces to model geometrical restrictions on diffusion. This allows him to tune the "roughness" of boundaries from flat surfaces with dimension $D_0=2$ to higher fractal dimensions $D_0>2$. Two quantities are calculated: $\psi(t)$, the probability density function (pdf) of returning to an interface at time t having started at t=0 in a close vicinity of the interface, and $\theta(r)$, the pdf of the bridge distances. The dependence of the two quantities on D_0 is obtained and the results are verified numerically. I believe there is a misprint in Fig 2.11 (in the x-axis plot of α). Both pdfs appear in problems related to search and to reactivity at interfaces when a reactant displays exchange with the environment. In the case of facilitated search for a target by a diffusing enzyme along a DNA strand the power law behaviors of $\theta(r)$ and $\psi(t)$ are relevant. They control the mean first passage times to the target. The author recognizes this relevance and proposes an application of his results to such target search as a future program.

Dr Grebenkov skillfully extends his earlier geometry-adapted fast random walks algorithm to be able to handle issues related to catalytic surfaces. In particular he investigates progressive passivation of irregular surfaces accessed by diffusion. The passivation process actually "poisons" the surface by modifying its structural details and reduces its activity. Understanding the nature of the passivation is of great importance for maintaining efficient catalytic activity. Similar "poisoning" effects might appear also in biological tissues and organs (skin, lungs and placenta). Although the similarity between porous (chemical) materials and porous biological tissues, when it comes to modeling, has been noted, Dr Grebenkov manages to go beyond previous contributions and analyze the way structural details effect diffusion properties that might show up for instance in NMR diagnostics.

Dr Grebenkov's spectral description of restricted diffusion, by analyzing the Laplace operator eigenfunctions, is an important contribution to the understanding of NMR results in complex chemical and biological systems. NMR experiments on such systems display a rich spectrum of behaviors that have to be translated into structural and relaxation data. In his habilitation thesis, and summarized in a detailed Rev Mod Phys "NMR survey of reflected Brownian motion" , Dr Grebenkov describes the different diffusion regimes in various geometries and provides tools to analyze them. This may open the possibility for "reverse engineer"; namely, to design efficient geometries that fulfill some required characteristics.

The time dependent diffusion coefficient method to characterize confinements is interesting and relies on second moments being a good enough approximation. Dr Grebenkov shows again how previous results could be extended. I should comment here that analysis is done based on reflected Brownian motion. Both biological and chemical porous system might display also anomalous diffusion that can be a project for the future.

In Summary, this is an impressive habilitaion thesis that demonstrates mastering of theoretical tools and familiarity with the up to date open problems at the interface of physics, chemistry and biology.

Joseph Klafter