Scientific report EPSD short visit grant 3656

Applicant: **Dr. A. S. de Wijn (Institute for Molecules and Materials, Radboud University Nijmegen, the Netherlands)**
Host: **Dr. S. Hallerberg (Institut für Physik, TU Chemnitz, Germany)**
Title: **Statistical inference of precursors for long jumps in molecular diffusion**

Purpose of visit

The goal of the collaboration which has led to this visit is to determine the physical mechanism which triggers long jumps in the diffusion of large molecules on surfaces by the use of statistical inference of their precursors in molecular dynamics simulations. Long jumps can strongly affect the surface diffusion and have been observed experimentally for organic molecules, nanoscale clusters, and adatoms [1, 2]. Recent studies [3, 4] highlight the existence of a relation between the diffusion of molecules and the dynamics of their internal degrees of freedom.

This visit was aimed at investigating the statistics of long jumps in molecular dynamics simulations performed by A. S. de Wijn and applying statistical inference methods designed by S. Hallerberg to the simulated trajectories, particularly to the dynamics of the internal degrees of freedom.

Work carried out during the visit and main results

We have used a numerical filter for long jumps designed during a previous visit (not funded by the ESF) to determine the distributions of jump lengths and recurrence times from trajectories generated by molecular dynamics simulations of benzene on graphite. Both distributions have long power-law tails with exponents consistent with the normal diffusion which was found directly from the numerical simulations.

Using the statistical inference and classifications algorithms [5, 6], we have identified precursors to long jumps within the multi-variate time series of the energies in various internal degrees of freedom. We have also begun to investigate precursors in several derived quantities, such as local time averages and fourier transforms. These have shown that during long jumps, the energy in the torsional degrees of freedom and one bond-bending vibration is reduced. Our results suggest that in a similar way to what was shown in [3], the chaos in the internal dynamics of the molecules contribute to the destruction of long jumps in the diffusion and by manipulating it with external forces, diffusion may be enhanced or reduced.

Future collaborations between the applicant and host (institution)

We will continue to collaborate on this and related topics. S. Hallerberg will apply to the EPSD program in the near future for a return visit. We would particularly like to use the newly gained information to design methods for increasing the survival of long jumps by applying external forces. Collaborations with others at the TU Chemnitz are also forseen, specifically on theoretical topics with Prof. G. Radons and analysis of experimental results on rotation and diffusion with Dr. D. Täuber.

Projected publications

More work is required from both sides to complete the analysis of the data and results, and to investigate possible ways to activate the precursors by external manipulation of the molecule. Additional numerical simulations are being performed for a variety of parameter values. When this data is fully analysed, the results will be published.

Bibliography

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