Final Report on DOE grant
"Some Basic Research Problems Related to Energy"
E.G.D. Cohen

This is my report on the activities on my grant #DE-FG02-88ER13847 from July 1, 2005-June 30, 2006.

Following the work of my previous Progress Report, in which we proved a Theorem for the very short initial behavior of a Green's function, we developed the necessary theory to obtain explicit expressions for the coefficients of a series expansion of the Green's function for mass transport problems around a Gaussian. We have made a set of complicated numerical evaluations of the first few coefficients in this expansion, in the hope that on the very short time scales of interest, i.e. the pico and subpico time scales, already these first few terms would indicate for which times there are relevant corrections to the easily evaluated leading Gaussian term. At present our results point indeed to a time scale for this of about 0.1 ps. The would mean, if checking of our calculations confirms this, that one has an estimate for an upperbound for the applicability of the Gaussian alone of about 0.1 ps. Below this time scale the difficult series expansion contributions can then be neglected.

This would facilitate considerably to give engineers a sense to what short times an easy estimate of mass transport calculations can be made in a relatively simple fashion (i.e. via a Gaussian function alone).

4 Publications

1. "Theorem on the Distribution of Short-Time Particle Displacements with Physical Applications", R. Van Zon and E.G.D. Cohen, Journal of Statistical Physics, Vol. 123, No. 1 (2006).
2. "Theorem on the Distribution of Short Time Single Particle Displacements", R. Van Zon and E.G.D. Cohen (NEXT-Sigma Phi), Physica A (2006).
3. "Very Short Time Fluctuations of Displacements and Work", R. Van Zon and E.G.D. Cohen, Proceedings of the International Conference "Work, Dissapation and Fluctuations in Non-equilibrium Physics", March 22-25, 2006, ULB, Brussels, Belgium, to be published in Comptes Rendus de l'Académie des Sciences de Paris (2007).
4. "Numerical Investigations into Single Particle Correlations on the Pico and Subpico Time Scale of Lennard-Jones Fluids", Ashwin, S.S., R. Van Zon and E.G.D. Cohen, (to be submitted).

This work was carried out together with two post-docs, who were trained: Dr. Ramses Van Zon for 3 years, and Dr. Ashwin Selvarajan Sampangarij for 1 year.

With my best regards, E.G.D Cohen