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Numerical Simulations of Complex Systems in Quantum and Classical Physics

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Abstract. In this talk we review our recent research on numerical simulations of various complex may-body systems. First, we will give an overview of the effective action approach [1–7] for numerical calculation of path integrals for non-relativistic many-body quantum system using a hierarchy of recursive relations derived from the underlying Schrödinger equation for general transition amplitudes. The use of the effective propagator expanded to high orders in the short time of propagation substantially speeds up the convergence of Path Integral Monte Carlo algorithm for calculation of general transition amplitudes, partition functions and expectation values. We will also present time-dependent formalism that allow numerical study of dynamics of quantum systems in time-dependent potentials.

In the second part of the talk, we will present molecular dynamics numerical simulations of granular materials [8–10]. In particular, we will present study of compaction of dense granular materials under the influence of vertical tapping. We analyze the compaction process for various values of friction coefficient and coefficient of normal restitution, and find that the time evolution of the density is described by the Mittag-Leffler function of order $0 < \alpha < 1$. We characterize the local organization of granular material in terms of contact connectivity and distribution of the Delaunay free volumes. Our analysis at microscopic scale provides evidence that compaction is mainly due to a decrease of the number of the largest pores. An interpretation of the memory effects observed for a discontinuous shift in tapping intensity is provided by the analysis of the time evolution of connectivity numbers and volume distribution of pores.

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