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Analytical and Computational Studies of Correlations of Hydrodynamic Fluctuations in Shear Flow

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Abstract. We study correlations of hydrodynamic fluctuations in shear flow analytically and also by dissipative particle dynamics (DPD) simulations. The hydrodynamic equations are linearized around the macroscopic velocity field and then solved by a perturbation method in Fourier-transformed space. The autocorrelation functions (ACFs) from the analytical method are compared with results obtained from DPD simulations under the same shear-flow conditions. Up to a moderate shear rate, various ACFs from the two approaches agree with each other well. At large shear rates, discrepancies between the two methods are observed, hence revealing strong additional coupling between different fluctuating variables, which is not considered in the analytical approach. In addition, the results at low and moderate shear rates can serve as benchmarks for developing multiscale algorithms for coupling of heterogeneous solvers, such as a hybrid simulation of molecular dynamics and fluctuating hydrodynamics solver, where thermal fluctuations are indispensable.

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1 Introduction

The complex behavior of many particles plays a significant role in atomic fluids [1, 2], chemical and biological processes [3, 4], granular materials [5], and astrophysics [6]. On the one hand, given interparticle potentials, a kinetic-theory type of description from first

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principles can be formulated, which, however, may be too complex to apply. On the other hand, if physical quantities vary rather slowly in space and time, a local thermodynamic equilibrium may be valid. Therefore, the system can be represented by continuous hydrodynamic fields described by the Navier-Stokes-Fourier (NSF) equations, which take into account the conservation of mass, momentum and energy. Although such partial differential equations (PDEs) are concise and practically powerful, the thermodynamic derivatives and transport coefficients must be obtained from a more fundamental theory to complete the phenomenological description. Through the seminal efforts of Einstein, Onsager, Callen, Welton, Green, Kubo and many others [1,7], a general linear response theory has been established. Furthermore, the transport coefficients are connected to the corresponding correlation functions (CFs) of the microscopic fluctuating variables. These connections are all embraced in the fundamental Green-Kubo relations. At equilibrium or small deviations from equilibrium, a systematic connection between the CFs and the hydrodynamics equations has been established for the long wave-length and small-frequency hydrodynamic limit [1,8,9]. In this hydrodynamic limit, the effects of the solvent fluctuations on suspended Brownian particles have also been studied extensively [10]. A further extension for small wave-length of the fluid has been made, which connects the microscopic dynamics to the generalized hydrodynamic equations [9]. Another breakthrough is the development of the fundamental fluctuation relations at transient or stationary nonequilibrium state far from equilibrium, which was initiated by Evans et al. [11] and has later engaged many others [12–14]. Many of these works on statistical mechanics are closely related to the large deviation theory in probability theory [15].

At a stationary nonequilibrium state, it seems relatively simpler to start with the phenomenological hydrodynamic equations and work reversely to obtain various CFs of the fluctuating variables [16–25]. This strategy has been applied by Lutsko&Dufty [26] and has been receiving continuous attention [27–29]. In the present work, we consider an isothermal shear flow at steady state as a typical setting for the nonequilibrium behavior of many particles. Following the pioneering derivations of Lutsko&Dufty [26], the equations of fluctuating hydrodynamics are linearized around the steady state by assuming small fluctuations, before they are transformed into the Fourier space. Thereafter, an equivalent generalized eigenvalue problem is solved perturbatively to provide the temporal evolution of the hydrodynamic fluctuations. Finally, various autocorrelation functions (ACFs) can be constructed in the Fourier space and transformed into the real space if needed. Some analytical ACFs have been recently compared with inelastic hard-sphere simulations and multi-particle collision dynamics at low shear rates [27–29]. As the first objective of this work, we aim to verify the analytical ACFs at low/moderate shear rates and search for deviations from the theory at large shear rates via numerical simulations. We expect that our computations will reveal a transition from decoupling to the coupling of different fluctuating variables and may shed light on the possible extension of the theory at large shear rates. To this end, we employ a mesoscopic method called dissipative particle dynamics (DPD) to quantify such deviations.