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Exploring the Analogy Between Freezing of a 2D Yukawa Liquid and 2D Decaying Turbulence in Fluids

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Abstract. In Langevin-Dynamics simulations of large aggregates of up to 10^6 dust grains we study the continuous transition from a liquid-like to a solid state. In this freezing two-dimensional Yukawa liquid the hexagonal solid phase cascades to larger scales by domain merging, while defects pile up on the domain boundaries creating filamentary regions of enhanced grain mobility. The formation of larger crystal domains from merging is the analogy of vortex merging in two-dimensional fluid turbulence, and the filaments of enstrophy dissipation in the fluid is the analogy of the thin strands of enhanced mobility surrounding the domains. The geometry of these filaments exhibit similar intermittent properties in the two systems and are characterized by an evolving multifractal dimension spectrum.

Keywords: Yukawa liquid, turbulence, phase transition, self-organization, intermittency
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INTRODUCTION

In [1] Langevin-Dynamics (LD) simulations of large aggregates of up to 10^6 dust grains were performed to study the continuous transition from a liquid-like to a hexatic state. In this freezing two-dimensional (2D) Yukawa liquid the domains of hexagonal solid phase cascades to larger scales by domain merging, while defects pile up on the domain boundaries. These simulations shed new light on studies of much smaller clusters made in [2-5]. In [3] and [4] we explored the analogy between the Yukawa liquid and 2D fluid turbulence, but in systems strongly influenced by finite size and spatial inhomogeneity. The large simulations in [1] allow us to explore the analogy between the continuous phase transition and freely decaying 2D turbulence further, based on the following observations: In a 2D turbulent fluid energy injected on small scales undergo an inverse cascade to larger scales where viscous dissipation is very weak. This inverse cascade can be thought of as a process of merging of smaller vortices into larger ones. On the other hand the enstrophy (square of vorticity) undergoes a forward cascade to smaller scales, and can be thought of as stretching of the dissipation rate of enstrophy into thin filaments between the vortices. The formation of larger crystal domains from merging of smaller ones is the analogy of vortex merging in 2D fluids, and the filaments of enstrophy dissipation rate in the fluid is the analogy of the filamentary structure of the mobility field of dust grains, which is due to the thin strands of defects surrounding the domains. The geometry of these filamentary structures may have intermittent properties that are characterized by an evolving multifractal dimension spectrum.

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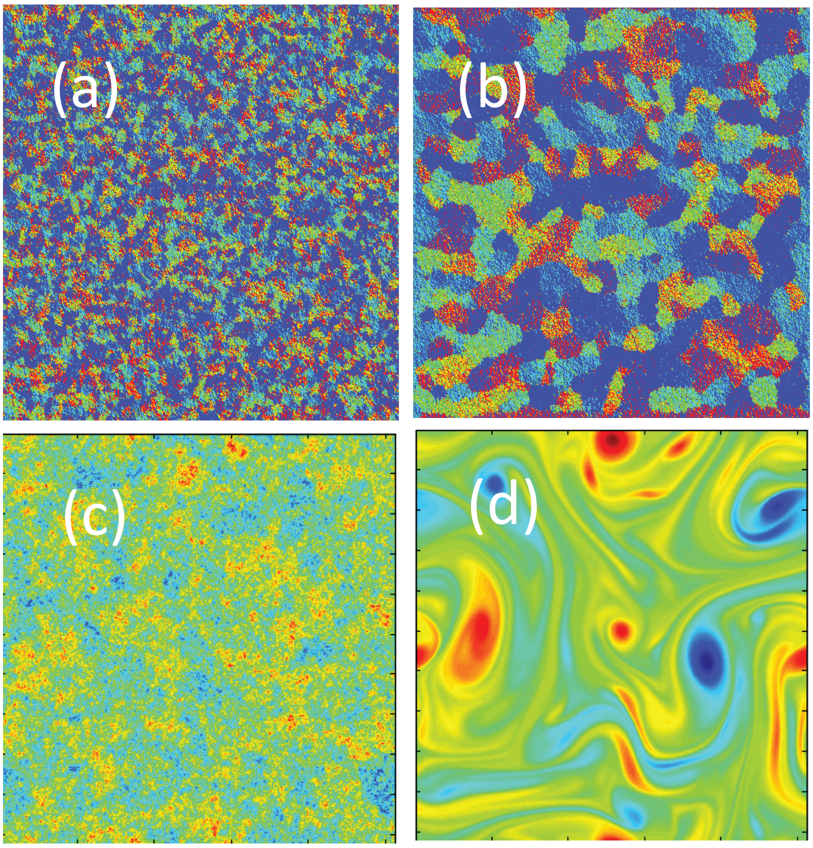

FIGURE 1. (a) Crystallite orientation in the initial stage of the LD-simulation. (b) The same in the late stages. (c) Vorticity field in initial stage of the fluid simulation. (d) The same in the later stage.

PHENOMENOLOGY OF THE LD SIMULATIONS

The LD simulations are Molecular-Dynamics simulations of dust grains interacting via electrostatically screened potentials (Yukawa-potentials) and subject to dynamic friction and stochastic forcing simulating the effect of collisions with the neutral gas. The equations describing this system is a set of Langevin equations for the dust grains coupled through the mutual electrostatic interaction. The modeling of the interaction with the neutral gas is called a Langevin thermostat, and tends to equilibrate the dust dynamics to the fixed temperature T_g of the gas. The simulations we analyze in this paper are made on a square domain with hard-wall boundary conditions. The gas temperature T_g is chosen slightly below the critical temperature T_c for the liquid-solid phase transition, and the initial temperature of the dust grains is chosen slightly above T_c. The phenomenological description of the relaxing evolution of this system is the initial formation of small domains of crystallized matter (crystallites) with well-defined crystallite orientation, surrounded by strands of 5- and 7- order crystal defects. Along these strands dust grains undergo cooperative hopping in the lattice, and are much more mobile than those residing in the hexagonal lattice in the interior of domains. The system then self-organizes further through merging of domains to form increasingly larger domains, and hence a reduction of the total number of defects. A particle "mobility field" can be constructed by computing the displacement of dust grains during a time interval much longer than the wobbling period for caged grains, as shown in Fig. 2a. It is apparent that this mobility field accumulates large values at the boundaries between the domains where we have numerous crystal defects. The formation and merging of domains are shown in Fig.1a,b. After the initial phase of domain formation the number of defects decrease with time t according to the power-law $N \sim t^{-2/5}$. The details of the simulations and the analysis of this relaxation process perceived as a second order phase transition is thoroughly described in [1]. In this paper we focus on the aspects that emphasizes the similarities with decaying 2D fluid turbulence.

PHENOMENOLOGY OF THE TURBULENCE SIMULATIONS

These are numerical solutions to the 2D Navier-Stokes equations on a square 1024×1024 grid. A spectral method is employed, and hence periodic boundary conditions. The initial state is chosen to provide a broad spectrum of scales in the vorticity field $\omega = \nabla^2\psi$, as shown in Fig. 1c. Here ψ is the stream function for the 2D potential flow. The simulation contains no input of energy and enstrophy, i.e. we are simulating decaying turbulence. The inverse energy cascade proceeds by vortex merging into vortices of increasing size as shown in Fig. 1c. But since there is no boundary dissipation, the total energy decays very slowly due to the weak viscous dissipation at large spatial scales. The enstrophy $z = |\omega^2|$ undergoes a forward cascade towards smaller scales where it is effectively dissipated by viscosity. The enstrophy dissipation rate is given by $d_t z = \mu = \nu |\nabla\omega|^2$, where ν is the viscosity. The enstrophy dissipation rate field $\mu(x,y)$ at a late stage of the simulation is shown in Fig. 3a. It shows that the shears in vorticity make the enstrophy dissipation rate accumulate at the edges between vortices, not quite unlike the large grain displacements are accumulating at the edges of the crystallite domains in the Yukawa liquid.

SELF-ORGANIZATION AS DISSIPATION OF DISORDER

In the self-organizing Yukawa liquid disorder decreases through domain merging. Domains a are characterized by their lattice orientation, as shown in Fig. 1 a,b, and must be bordered by defects. Domains can only merge when their lattice orientation become the same, hence evolution towards larger domain through merging can only occur as long as there is some rotational motion of domains. This presupposes some slipping along the boundaries involving cooperative hopping of grains associated with defect dynamics. The empirical law $N \sim t^{-2/5}$ is solution to the evolution equation $d_t N \sim N^{7/2}$ and that the defect decay rate decreases as $\gamma = N^{-1} d_t N = N^{5/2} \sim t^{-1}$. This slowing of defect loss due to domain merging is due to the decreased rotational mobility of the domains as they grow in size. The grain mobility field shown in Fig. 2a at a late stage of the simulation indicates that energy loss by friction against neutrals takes place primarily at the domain boundaries, and (in slightly vague terms) we can perceive the lattice disorder as being dissipated in these regions of high mobility.

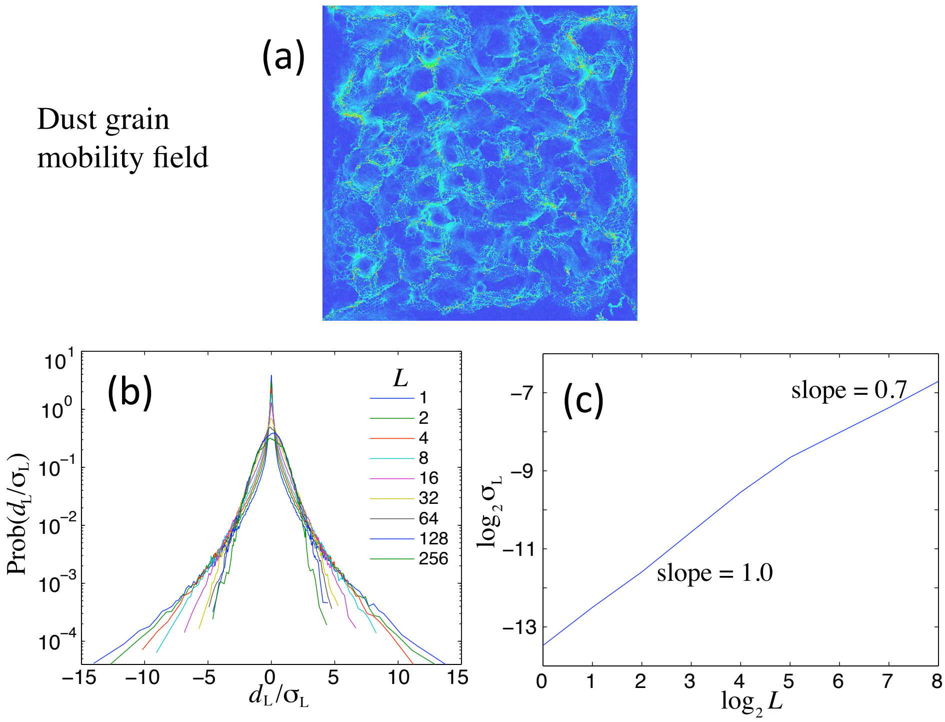

FIGURE 2. (a) Field of mobility d of dust grains in a given time interval. (b) PDFs of normalized fluctuation of displacement d_L/σ_L integrated over a box of dimension L x L for L varying from 1 to 256, in units of the mean interparticle distance. Here d_L is the deviation of the integrated displacement field over the box from its ensemble mean. σ_L is the standard deviation of d_L. (c) $\log_2\sigma_L$ plotted against $\log_2 L$. The slope of the curve for $L<2^5$ is 1.0, and for $L>2^5$ it is 0.7.

The spatial structure of the mobility field has a complex intermittent (multifractal) structure as illustrated in Fig. 2a and Fig. 10 of reference [1]. Intermittency means that the probability density functions (PDFs) of fluctuations on increasing spatial scales change shape from leptokurtic (heavy-tailed) on short scales towards Gaussian on large scales. When this is the case the field has a "bursty" appearance. Since the field is non-negative we can perceive it as a density field and compute the "mass" in boxes of varying size L^2. In Fig. 2b we have computed PDFs of such masses on varying scales L in a semi-logarithmic plot by dividing the area into boxes of linear size L and integrating the mobility field in each box. The PDFs in the figure have been rescaled so that they all have the same standard deviation and they have all been shifted to have zero mean. This has been done in order to highlight the change in shape from small to large L. In Fig. 2c the change in standard deviation of these PDFs as a function of L (the first-order structure function) has been plotted in a log-log plot. A linear shape of this curve indicates that the field can be characterized by a multifractal spectrum. We observe that there is a break of the curve at the scale L=2^5. This is the typical scale of the border region between domains where numerous defects exist. It is on this scale and shorter that we can give a quantitative multifractal characterization of the intermittent mobility field. The slope $D_B = \log_2 \sigma_L / \log_2 L$ is the main fractal dimension (box dimension) of the multifractal field, and for the curve in Fig. 2c we have $D_B \approx 1.0$, reflecting the filamentary structure of the field.

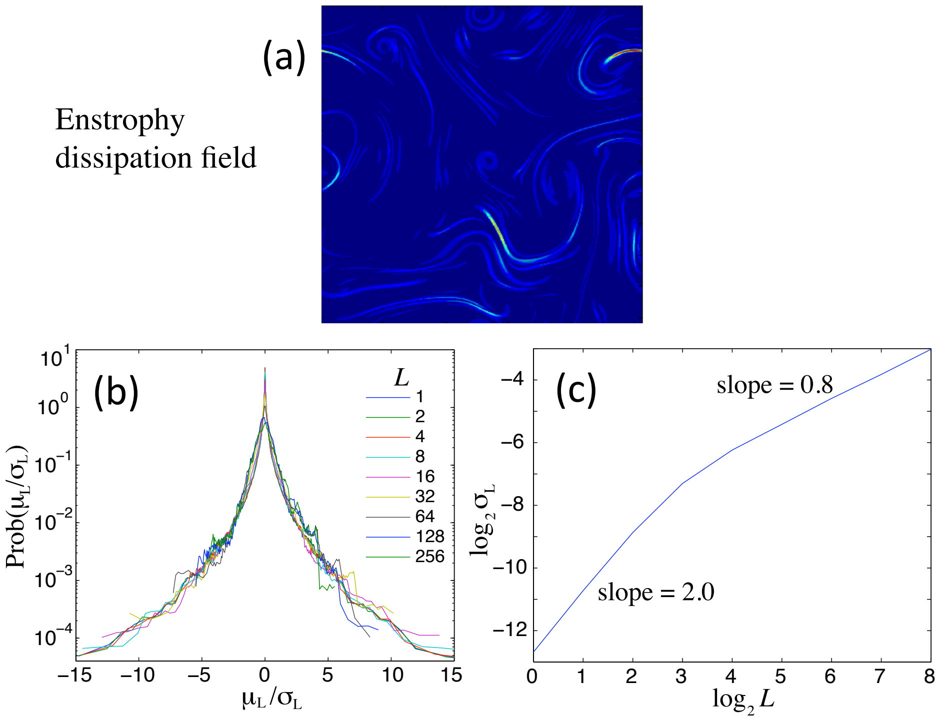

FIGURE 3. (a) Field of enstrophy dissipation rate in late stage of freely decaying 2D fluid turbulence. (b) PDFs of normalized fluctuation of enstrophy dissipation rate μ_L/σ_L in a box of dimension L x L for L varying from 1 to 256 grid points. Here μ_L is the deviation of the integrated enstrophy dissipation rate over the box from its ensemble mean. σ_L is the standard deviation of μ_L. (c) $\log_2\sigma_L$ plotted against $\log_2 L$. The slope of the curve for $L<2^3$ is 2.0, and for $L>2^4$ it is 0.8.

In 2D decaying turbulence with periodic boundary conditions the total energy is very weakly dissipated and accumulates at large spatial scales, whereas the enstrophy is subject to strong dissipation due to strongly sheared motions in elongated filaments at small scales. The developed turbulent flow will be weakly sheared and energetic in a large fraction of the flow area, but these weakly sheared regions are separated by filamentary structures of high shear where enstrophy is dissipated. The initial high disorder in the form of high enstrophy at all scales is reduced through forward cascade and dissipation in the system of thin filaments. Thus enstrophy dissipation is the mechanism by which disorder decreases in the 2D viscous fluid. Figure 3a shows the energy dissipation rate field at a late stage of the fluid simulation, and Fig. 3b the rescaled PDFs of the field on varying scales. The change in shape of the PDFs are apparent on scales up to $L=2^7$, which is the typical perpendicular size of the filamentary structures in the field. Figure 3c shows that in the fluid case the first-order structure function has a break at the scale $L=2^3$. For smaller scales than this the slope is $D_B \approx 2.0$, which just reflects that the numerically computed field is smooth on the scales of a few mesh constants due to hyperviscosity included to assure numerical stability. The interesting slope is in the range $\left(L^4, L^7\right)$ where we have $D_B \approx 0.8$, consistent with the filamentary structure of the enstrophy dissipation field.

DISCUSSION

By analyzing results from large-scale simulations of a freezing 2D Yukawa liquid and freely decaying turbulence in a 2D viscous fluid we have found striking similarities in how these systems self-organize as they relax towards equilibrium. We have demonstrated the intermittent nature of the fields that represent the dissipation of disorder, i.e. the self-organization, of the systems but limited space does not allow us here to show the multifractal dimension spectra and how these evolve with time. Such analyses show that the degree of multifractality increases as the systems evolve and that intermittency is a characteristic of the developed state where memory of the initial state has been lost.

The detailed physics of the freezing Yukawa liquid and a turbulent viscous fluid is of course very different. On the other hand, this can be seen as the major reason why the commonalities we have found in the statistical characterization of their dynamics can be of fundamental significance. It suggests that it might be possible to formulate common dynamic-stochastic descriptions of these systems on a mesoscopic level, which are not directly derived from first principles. Such descriptions would be less detailed than the Yukawa-Langevin or Navier-Stokes equations (for which analytical progress has been very slow), but still more than a phenomenological conceptual and statistical characterization as given in the present paper.

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