# Large-system hydrodynamic limit for color conductivity in two dimensions

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Nonequilibrium simulations of two-dimensional shear flow have shown that the viscosity is well defined in the large-system ''hydrodynamic'' limit. Those simulations, with up to a quarter million particles, were carried out at fixed energy and strain rate. Here we explore the mass current response to an external ''color field'' $E$ for $N$ particles, half with ''color charge'' $+1$, and half with $-1$. The fixed-field large-$N$ ''color conductivity'' $\kappa \equiv \langle \pm v/E \rangle$, with the energy per particle held constant, likewise indicates a well-defined large-system limit at moderate fields. [S1063-651X(98)06404-6]

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## I. INTRODUCTION

It was recently established, through extensive computer simulation over a wide range of system sizes [1,2], that the shear viscosity is a well-defined transport coefficient for a dense two-dimensional fluid. This is an interesting result because theoretical considerations [3,4] suggest that the usual transport coefficients are undefined in two-dimensional systems. That argument is based on the divergence of the Green-Kubo integral expressions. Because no boundary conditions are specified, despite their relative importance, in two dimensions, the actual situation is not completely clear. It may well be that the large-$N$ shear viscosity, though finite and well behaved for any fixed strain rate $\dot{\epsilon}$, diverges as $-\ln\dot{\epsilon}$ for sufficiently small strain rates. Although shear flows show no peculiarities, some evidence has accumulated that heat flows are anomalous in two dimensions. The artificial Evans-Gillan field [5], which is often used to generate a heat current, provides an unstable flow in two-dimensional fluids, even for vanishingly small fields, when the heat flow is stabilized by the usual homogeneous thermostat forces [1,6,7]. Though a phase-separating two-current instability has been seen in color conductivity simulations at high fields [8,9], the stability of the flow for larger systems, at moderate fields and for long times, has not been investigated.

Very recently it has been shown that hard-disk or hard-sphere trajectories in nonequilibrium thermostated simulations are identical to those generated in related adiabatic Hamiltonian simulations, though the time required to trace out the trajectories is quite different [10]. Thus the computer-generated trajectories for thermostatted systems, together with the multifractal phase-space structures which they generate, have fundamental significance for statistical mechanics. With this in mind we have extended our earlier small-system simulations of the ''color conductivity'' $\kappa$ for soft-disk systems [9]. This conductivity is the ratio of the (time-averaged) particle velocity to the strength of the accelerating field, where half the particles are accelerated to the right, and the remainder to the left, by the field. We investigate here whether or not this color conductivity,

$$\kappa \equiv \langle \pm (p_x/m) \rangle / E,$$

behaves in a peculiar way, perhaps symptomatic of a Green-Kubo divergence, as the number of particles is increased. A stationary nonequilibrium state is maintained, allowing us to determine the color conductivity, by using an isoenergetic thermostat variable $\zeta$, as is explained in Sec. II, which is devoted to our numerical results. Section III contains our conclusions.

## II. COLOR CONDUCTIVITY SIMULATIONS

The simulations were carried out in the usual way [5,11,12], using a special very smooth short-ranged repulsive pair potential,

$$\phi(r<\sigma) = 100\epsilon[1-(r/\sigma)^2]^4,$$

designed to minimize numerical errors. This soft-disk interaction has three vanishing derivatives at the cutoff distance, $r/\sigma = 1$. Otherwise, it is typical of soft repulsive interactions. With both the reduced number density $N\sigma^2/V$ and the reduced energy per particle $(\Phi + K)/N\epsilon$ set equal to unity, the collision diameter is about four-fifths of the interparticle spacing. Thus the model system represented here is a dense fluid, which we confine by using periodic boundaries.

The equations of motion were solved with fourth-order Runge-Kutta integration, using a time step $0.01\sigma(m/\epsilon)^{1/2}$. There were no significant changes when a time step half that size was used. A time-reversible friction coefficient $\zeta$ was chosen to constrain the internal energy to its original value:

 

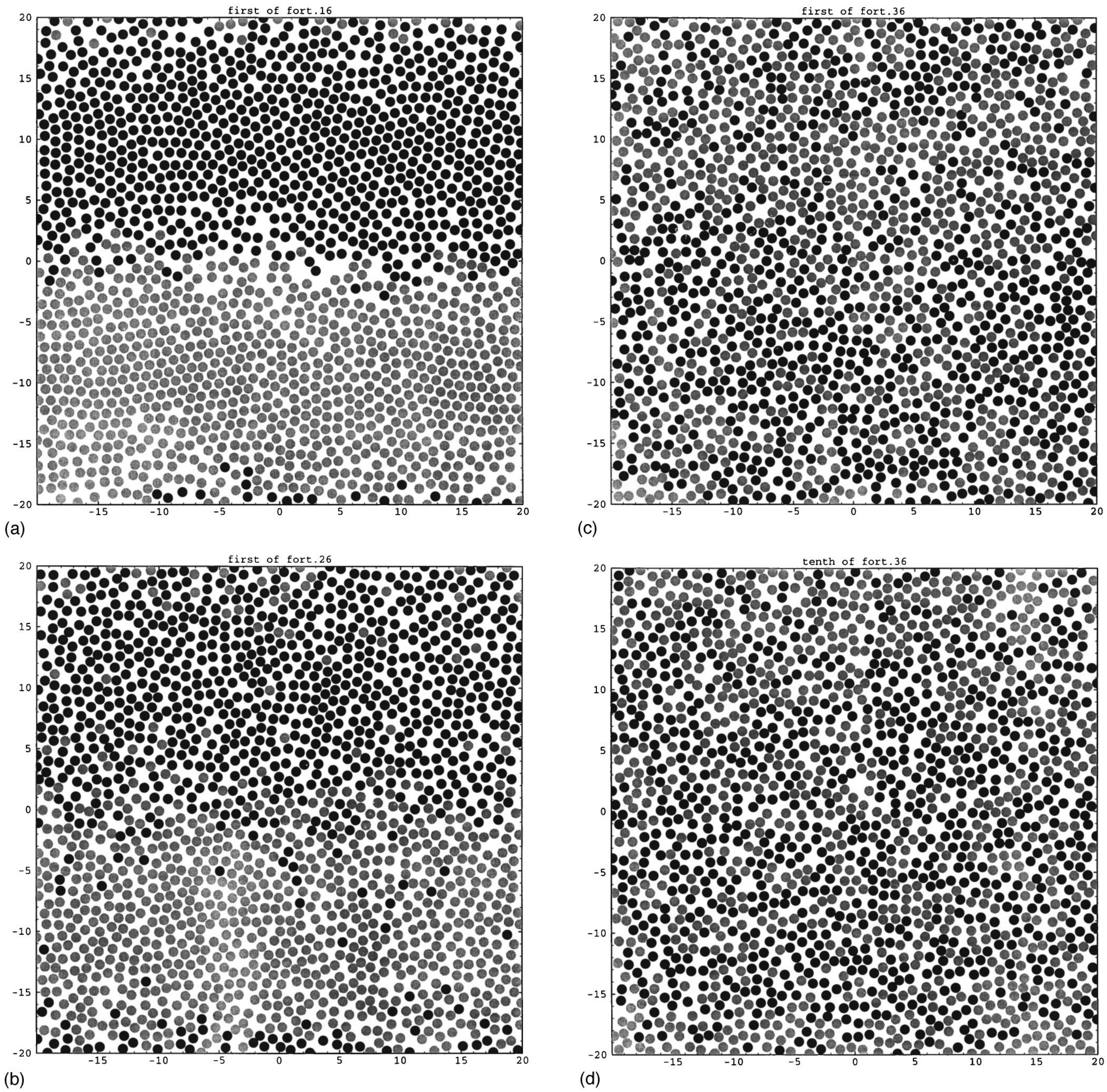


FIG. 1. Time development of 1600 soft disks at a field strength of $0.25\epsilon/\sigma$. The particles initially were arranged in two strips parallel to the field direction. The figure shows the right-going and left-going particles at reduced times of 50, 550, 1050, and 1550. Mixing is essentially complete at a time of $1500\sigma(m/\epsilon)^{1/2}$.

$$\{\dot{x}=(p_x/m);\dot{p}_x=F_x\pm E-\zeta p_x;\dot{y}=(p_y/m);\dot{p}_y=F_y-\zeta p_y\};$$

$$\zeta\equiv\sum \pm Ep_x/\sum p^2.$$

For convenience, in our numerical work, we set the particle mass $m$, as well as the potential parameters $\sigma$ and $\epsilon$ equal to unity. We chose the strength of the external field $E$, which drives the mass current, so as to approximate the dissipation rates, $0.01<\dot{S}/Nk<0.08$, of our earlier shear flow simulations [1,2]. As is usual, the pairs of interacting particles were stored in a ''linked list,'' constructed at every time step, so that the required computer time was proportional to the number of particles rather than to $N^2$. The largest of the Lyapunov exponents, $\lambda_1$, was also measured, because the shear flow work indicated that both the viscosity coefficient and the largest Lyapunov exponent have deviations of order $N^{-1/2}$ from the corresponding large-system limiting values.

The color conductivity simulations presented no special difficulties. In heat-flow simulations, with a relatively soft potential and the usual thermostats, a bothersome instability can occur, with one particle taking up most of the system energy and traveling through its fellows at high speed. We are currently investigating the sensitivity of this instability to thermostat type, with Markus Hartmann. Although the color

TABLE I. Color conductivity (mean velocity, divided by field strength $E$) for $N$ two-dimensional particles interacting with the soft potential $\phi(r<\sigma)=100\epsilon[1-(r/\sigma)^2]^4$. The largest Lyapunov exponent $\lambda_1$ and potential energy per particle $\Phi/N$ are tabulated for a total run time of $t$. The potential energy is given as a sum of like and unlike interactions. The total energy per particle and area per particle are both taken to be 1.00 in reduced units. Comparable data for $N=100$ are in excellent agreement with the considerably shorter simulations described in Ref. [11]. A simulation with $N=102\,400$ at the higher-field strength was unstable.

| $N$ | $E\sigma/\epsilon$ | $t(\epsilon/m)^{1/2}/\sigma$ | $\lambda_1(m/\epsilon)^{1/2}\sigma$ | $\kappa(m\epsilon)^{1/2}/\sigma$ | $\Phi/N\epsilon$ |
|---|---|---|---|---|---|
| 4 | 0.25 | 100 000 | 3.31 | 0.068 | 0.085+0.170 |
| 16 | 0.25 | 50 000 | 3.06 | 0.103 | 0.144+0.163 |
| 36 | 0.25 | 50 000 | 3.07 | 0.127 | 0.149+0.158 |
| 64 | 0.25 | 20 000 | 3.07 | 0.143 | 0.150+0.154 |
| 100 | 0.25 | 20 000 | 3.08 | 0.154 | 0.151+0.153 |
| 256 | 0.25 | 10 000 | 3.09 | 0.179 | 0.151+0.150 |
| 400 | 0.25 | 10 000 | 3.10 | 0.188 | 0.150+0.150 |
| 1600 | 0.25 | 10 000 | 3.09 | 0.219 | 0.148+0.146 |
| 6400 | 0.25 | 10 000 | 3.09 | 0.228 | 0.144+0.143 |
| 25 600 | 0.25 | 14 000 | 3.09 | 0.235 | 0.142+0.141 |
| 102 400 | 0.25 | 10 000 | 3.09 | 0.237 | 0.140+0.139 |
| 4 | 0.50 | 100 000 | 3.30 | 0.069 | 0.085+0.170 |
| 16 | 0.50 | 50 000 | 3.06 | 0.101 | 0.144+0.164 |
| 36 | 0.50 | 50 000 | 3.06 | 0.128 | 0.150+0.156 |
| 64 | 0.50 | 20 000 | 3.06 | 0.144 | 0.150+0.153 |
| 100 | 0.50 | 20 000 | 3.06 | 0.156 | 0.151+0.151 |
| 256 | 0.50 | 10 000 | 3.06 | 0.186 | 0.150+0.146 |
| 400 | 0.50 | 30 000 | 3.06 | 0.194 | 0.148+0.145 |
| 1600 | 0.50 | 20 000 | 3.03 | 0.216 | 0.142+0.136 |
| 6400 | 0.50 | 10 000 | 3.02 | 0.239 | 0.136+0.128 |
| 25 600 | 0.50 | 10 000 | 3.00 | 0.259 | 0.131+0.123 |

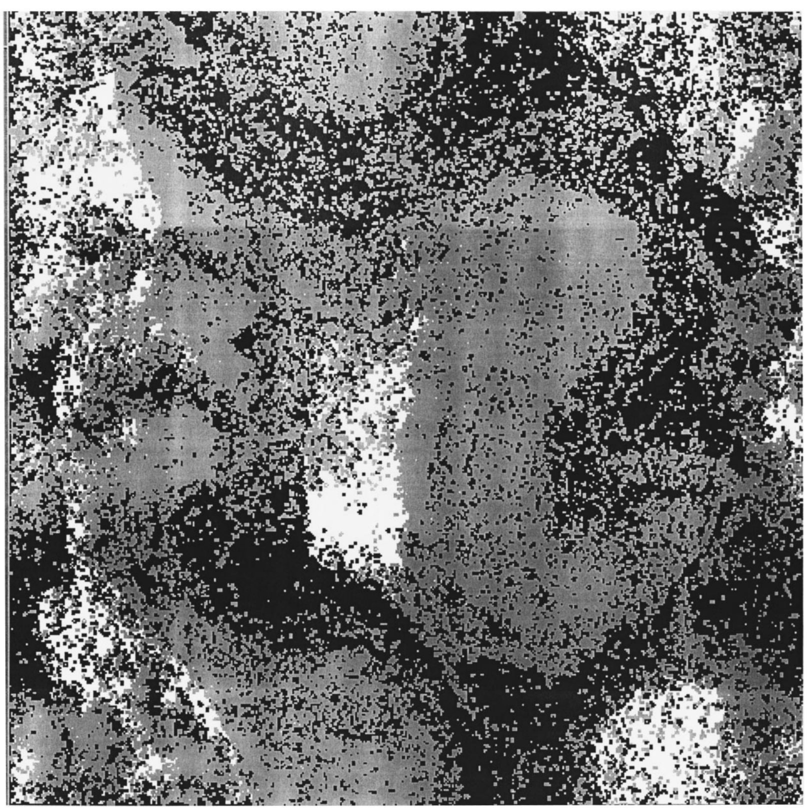

FIG. 2. Snapshot of 102 400 soft disks at a field strength of $0.50\epsilon/\sigma$, showing phase separation. The two species are shown as two shades of gray. The white patches are free of particles, indicating a local pressure near zero.

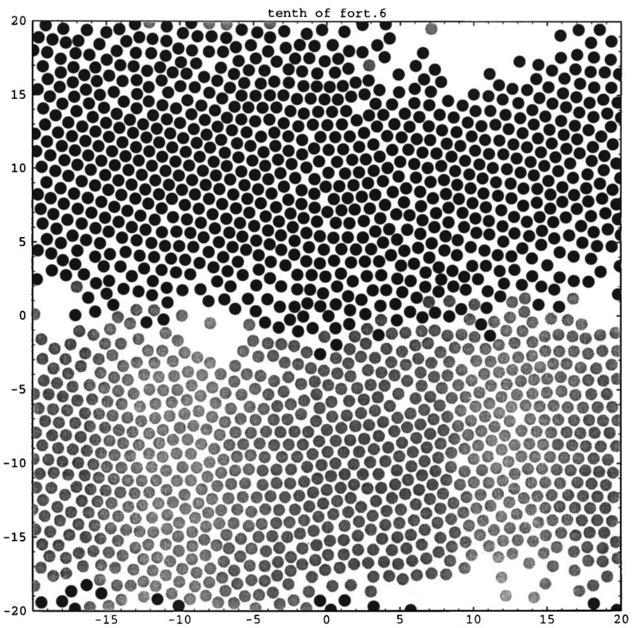


FIG. 3. Snapshot of 1600 soft disks at a field strength of $0.50\epsilon/\sigma$. The particles initially were arranged in two strips parallel to the field direction. Such an arrangement is quite stable, with the fluid freezing into two rapidly moving parallel slabs, as shown here.

conductivity problem is simpler than the heat-flow problem, and more stable—because the external forces are not velocity dependent—high-field color conductivity simulations have similarly shown a ''two-stream'' instability, with segregation of right-moving and left-moving particles into separate massive clumps. See the description in Ref. [8]. It is possible that such a phase separation could be understood by an extension of free-energy ideas taken from equilibrium thermodynamics. If the separated phases could cool sufficiently for the resulting free energy drop to offset the loss in mixing entropy, then separation should occur. For the dense fluid state which we study here, losing nearly the entire kinetic energy, $0.7N\epsilon$, would be required to offset the contribution of the mixed-phase mixing entropy to the free energy, $-NkT \ln 2$.

In our initial calculations, at the lower of the two fields we investigated, $E=0.25\epsilon/\sigma$, and with the two particle ''colors'' initially interspersed on a square lattice, checkerboard fashion, we found no evidence of clumping. To check this finding, we carried out additional calculations in which the two colors were initially segregated into two strips parallel to the $x$ axis. These strips rapidly homogenized and disappeared, reinforcing our impression that the flow remains stable for large system sizes with $E=0.25\epsilon/\sigma$. Figure 1 shows a typical series of snapshots, starting from an initial configuration with the two particle types arranged in two broad two parallel strips, $N\times(N/2)$. It is interesting that simultaneous snapshots, showing the direction of each particle's velocity rather than its color, indicate relatively small-scale transient clumping at long times; but investigation reveals that the particles in the ''clumps'' are a relatively homogeneous mixture of the two colors, with those of the slightly predominant species entraining the other. This clumping simply indicates the inability of the two fluids to interpenetrate, and is quite distinct from the phase separation which occurs at higher fields. The separation of potential energy into like-color and unlike-color pairs (see Table I) is a useful indicator of phase separation, somewhat simpler than the corresponding pair distribution functions discussed in Ref. [8]. In the lower-field case the ratio is not far from the ideal-mixing value of $[\Phi_{\rm like}/\Phi_{\rm unlike}]=[1-(2/N)]$. The largest Lyapunov exponent for these simulations likewise shows very little size dependence, in contrast to its behavior in the higher-field simulations discussed next.

At a field of $0.50\epsilon/\sigma$ the situation is different. Larger systems show marked phase separation; see Fig. 2. The Lyapunov exponent for these larger systems is also significantly smaller, indicating a reduction in mixing activity in the phase space. The ratio of like to unlike energies also begins to deviate significantly from the ideal-mixing value, for systems of a few hundred particles or more. Finally, systems started out with the two colors arranged in strips parallel to the field direction freeze, with most of the energy taken up by the streaming velocity of the two resulting solid chunks of material; see Fig. 3.

It is clear from these data that a nonequilibrium phase transition separates the two field strengths. This finding corroborates that of Ref. [8], in which simulations were carried out at fixed current rather than fixed field. The lower-field conductivity data shown in Table I, when plotted as a function of $N^{-1/2}$, show no significant deviation from a straight line, with an intercept value of $0.24_0\sigma(m\epsilon)^{-1/2}$. The analogous linear dependence of the transport coefficient on the width of the system was likewise observed in our shear viscosity studies.

An unexpected and significant finding emerged from an analysis of our Lyapunov instability studies. We found that those particles which make the largest contribution to the maximum exponent, $\lambda_1$, tend to be localized in space. Figure 4, for $N=25600$, is typical. The top of the figure shows a homogeneous color distribution and a clumped velocity distribution. The bottom of the figure shows, more darkly, those particles which make an above-average contribution to $\lambda_1$, first in coordinate space, and then in momentum space. The clumps which result are nearly the same for the two representations. We could find no particular properties of these particles, such as temperature, energy, or stress, which were correlated with the instability. It is quite interesting to see macroscopic modes so highly correlated with microscopic dynamic instabilities. A detailed study of this correlation between microscopic dynamical instability and macroscopic modes should be taken up for a simple unstable hydrodynamic flow such as Kolmogorov or Rayleigh-Bénard flow.

### III. CONCLUSIONS

Both color conductivity and shear viscosity have well-defined large-system limits, for a fixed value of the driving from equilibrium, for dense two-dimensional fluids with short-ranged soft repulsive forces. The results are reproducible and independent of the initial conditions. At higher fields we confirmed the well-known two-phase instability studied by Hansen and Evans [7] and Evans, Lynden-Bell, and Morriss [8]. A phenomenological representation of these results is currently lacking, due to the failure of any theory to treat phase separation under nonequilibrium conditions. This, together with the correlation linking microscopic Lyapunov

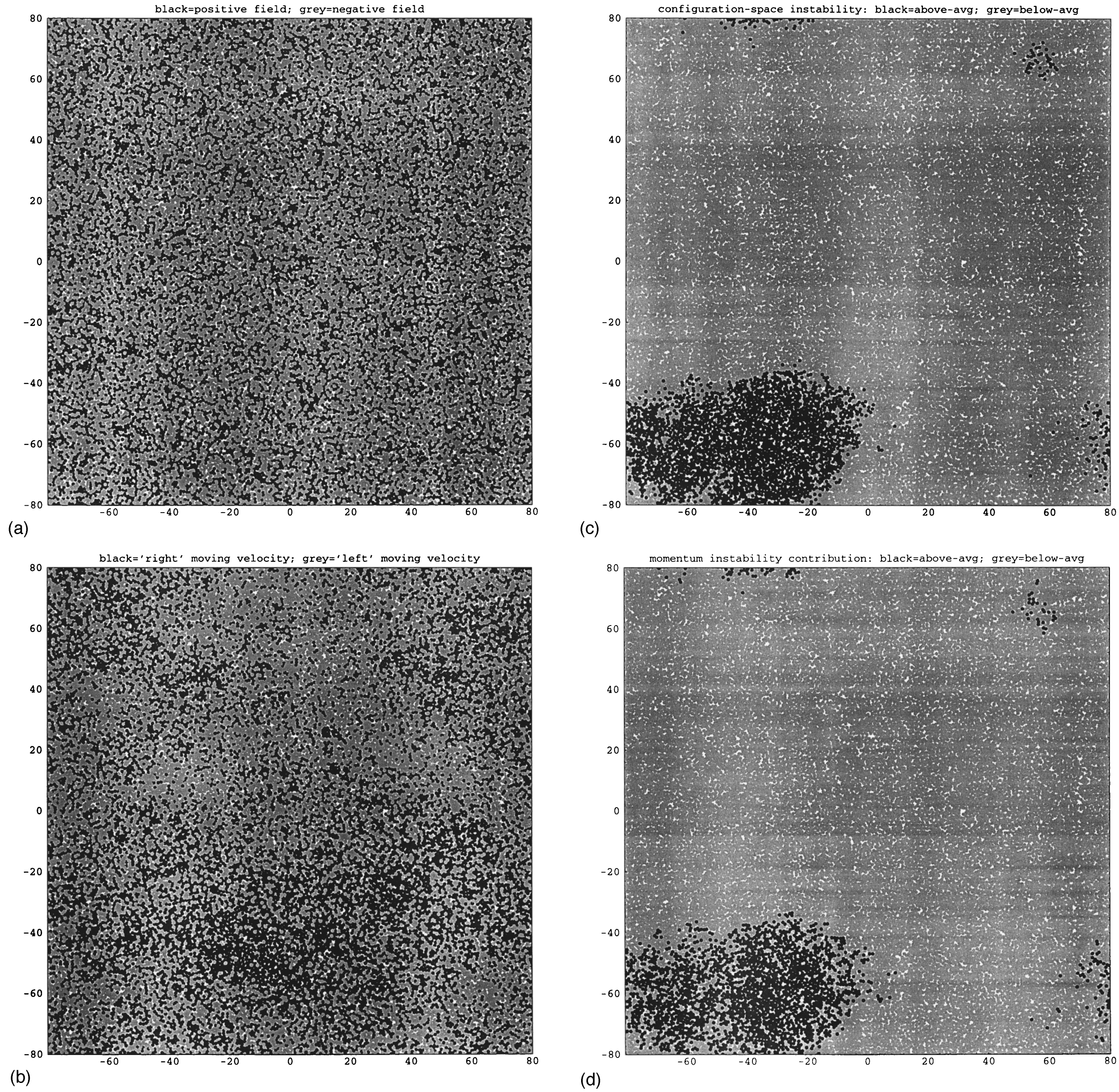


FIG. 4. Four views of a typical configuration of 25 600 particles at a field strength of $0.25\epsilon/\sigma$. In the left column the colors indicate (a) particle color (black indicates a positive field force and gray a negative field force) and (b) direction of motion (black denotes the ''right''-moving velocity and grey the ''left''-moving velocity). In the right column the colors indicate those particles making above-average contributions (black) to $\lambda_1$ in (c) configuration space and (d) momentum space.

instability to macroscopic hydrodynamic modes, suggests promising research areas.

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