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Anomalous pressure in fluctuating shear flow

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We investigate how the pressure in fluctuating shear flow depends on the shear rate S and on the system size L by studying fluctuating hydrodynamics under shear conditions. We derive anomalous forms of the pressure for two limiting values of the dimensionless parameter $\lambda = SL^2/\nu$, where ν is the kinematic viscosity. In the case $\lambda \ll 1$, the pressure is not an intensive quantity because of the influence of the long-range spatial correlations of momentum fluctuations. In the other limit $\lambda \gg 1$, the long-range correlations are suppressed at large distances, and the pressure is intensive. In this case, however, there is the interesting effect that the nonequilibrium correction to the pressure is proportional to $S^{3/2}$, which was previously obtained with the projection operator method [K. Kawasaki and J. D. Gunton, Phys. Rev. A **8**, 2048 (1973)].

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It has been confirmed for over a century of study that hydrodynamic equations describe macroscopic flow with high accuracy. However, a microscopic foundation of fluid mechanics has not yet been established except in the dilute limit gas. There seems to be no basis in microscopic physical laws on which to establish the validity of the local equilibrium assumption inherent in hydrodynamic equations. Indeed, it may be the case that any proper equation of state must be incorporated with nonequilibrium effects.

The anomalous form of equation of state under nonequilibrium conditions was first discussed by Kawasaki and Gunton [1]. They derived a nonanalytic dependence of the pressure tensor on the shear rate for an uniformly sheared simple fluid. Subsequently, the same problem was studied by several authors in detail [1–4], and the nonanalytic response due to mode-coupling effects has now become evident. Nevertheless, with regard to the normal stress, such predictions have not been fully confirmed by laboratory experiments or by numerical simulations [5].

In addition, quite recently, another type of anomalous nonequilibrium pressure has been reported by Aoki and Kusnezov [6]. They have studied numerically heat conduction problems of anharmonic oscillator models and have found that the nonequilibrium correction to the pressure is nearly proportional to the system size. This finding is remarkable because it implies the absence of the intensivity of the pressure in this nonequilibrium system. As far as we know, there is no theoretical explanation for this result so far.

In this paper, we propose a unified understanding of the two anomalies for a specific simple case, uniform shear flow in a fluid. We establish a general criterion that can distinguish between nonintensive and nonanalytic nature of the pressure. We also give a brief comment on numerical experiments that disagree with the mode-coupling theory.

The key idea of our study is to establish a possible relationship between the pressure anomalies and the long-range spatial correlation of momentum fluctuations. It has been recognized that a lack of detailed balance is responsible for various distinctive features. One of them is the generic existence of long-range spatial correlations of fluctuations of conserved quantities [7]. For example, a correlation of momentum fluctuations becomes spatially long ranged under shear conditions [8,9].

However, because the correlation function known at present is strongly divergent in a long wavelength limit, a certain appropriate length scale may be introduced as a cutoff. Therefore, we first need to know the momentum correlation function over the whole region of length scales. It may be suitable to study fluctuating hydrodynamics for this purpose.

Model. Let $v_i(\boldsymbol{r},t)$ be a fluctuating velocity field in an incompressible fluid with a constant temperature T that is far from the critical point. The time evolution of $v_i(\boldsymbol{r},t)$ is described by the continuity equation of the momentum,

$$\rho \partial_t v_i + \partial_j \Pi_{ij} = 0, \tag{1}$$

where the momentum flux tensor Π is given by

$$\Pi_{ij} = \rho v_i v_j + p\,\delta_{ij} - \nu\rho(\partial_i v_j + \partial_j v_i) + s_{ij}. \tag{2}$$

Here, ν is the kinematic viscosity, ρ is a constant density, and s represents a Gaussian random stress tensor satisfying the fluctuation-dissipation relation [10],

$$\langle s_{ik}(\boldsymbol{r},t) s_{lm}(\boldsymbol{r}',t')\rangle = 2\rho T\nu[(\delta_{il}\delta_{km} + \delta_{im}\delta_{kl}) - \tfrac{2}{3}\delta_{ik}\delta_{lm}]\delta^3(\boldsymbol{r}-\boldsymbol{r}')\delta(t-t'). \tag{3}$$

Throughout this paper, the Boltzmann constant is set to unity. The auxiliary field p in Eq. (2) can be replaced by use of the incompressible condition $\partial_l v_l = 0$, which implies the relation

$$p = p_{\mathrm{B}} - \partial_l \partial_m s_{lm} - \rho \Delta^{-1}(\partial_l v_m)(\partial_m v_l), \tag{4}$$

where p_{B} is a constant.

We consider the system in a three-dimensional space, for which $-\infty < x,\ z < \infty$, and $-L/2 \leq y \leq L/2$. The boundary conditions are imposed satisfying

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$$\boldsymbol{v}(x,L/2,z)=\boldsymbol{v}(x,-L/2,z)+SL\boldsymbol{e}_x, \tag{5}$$

which are chosen so as to make the analysis as simple as possible. We study linear fluctuations around the average shear flow

$$\langle \boldsymbol{v}(x,y,z)\rangle=(Sy,0,0). \tag{6}$$

Without loss of generality, we set $S\geqslant 0$.

From Eq. (1), we have $\partial_j\langle\Pi_{yj}\rangle=0$ for the statistical steady state. Because this represents a force balance equation, the pressure in the y direction is given by $\langle\Pi_{yy}\rangle$. Then, using Eqs. (2) and (4), we write the pressure p_y as

$$p_y=p_{\rm B}+\rho\langle v_y^2\rangle-\rho\Delta^{-1}\langle(\partial_l v_m)(\partial_m v_l)\rangle. \tag{7}$$

Now, the problem is to determine how p_y depends on the shear rate S and on the system size L.

The most general form of fluctuating hydrodynamics consists of a set of stochastic evolution equations for the energy, density, and momenta [10]. In our model, the thermal diffusion constant and the sound damping constant are assumed to be much larger than the kinematic viscosity. This assumption is made for simplicity here, otherwise the calculation of the stress tensor becomes more complicated [3,4].

Now, we make a comment on the local equilibrium assumption that is involved in hydrodynamic descriptions. Let ℓ be a microscopic length, such as a mean-free path, and define a dimensionless parameter ϵ as

$$\epsilon=\frac{\ell^2 S}{\nu}. \tag{8}$$

In order to investigate the physical meaning of this parameter, we first consider the case $\epsilon\to 0$. In this case, the local equilibrium assumption is valid because of the separation of scales. This implies that the shear flow does not influence the thermodynamic properties of the system. However, if ϵ becomes of the order of unity, the molecular motion is violently disturbed by the shear. Although it may be interesting to study such systems, we cannot use fluctuating hydrodynamics for that aim. From this brief consideration of these two limiting cases, we regard the parameter ϵ as representing the extent of departure from the condition of local equilibrium states. Because we seek the nonequilibrium correction to the pressure under shear within the framework of fluctuating hydrodynamics, we consider the case of a small but finite ϵ.

As the final condition on our model, we assume $L\gg\ell$, so that the continuum description is valid. Note that our model does not include the parameter ℓ explicitly. It is included only as a cutoff length when we encounter an ultraviolet divergence.

Dimensional analysis. There are two independent dimensionless parameters in the system:

$$\lambda=\frac{L^2 S}{\nu},\quad D=\frac{T}{\rho\nu^2 L}. \tag{9}$$

Quite generally, we can write

$$p_y-p_y^{\rm eq}=\frac{T}{L^3}f\left(\frac{L^2S}{\nu},\frac{T}{\rho\nu^2 L}\right), \tag{10}$$

where $p_y^{\rm eq}$ is the equilibrium pressure. We have assumed that $p_y-p_y^{\rm eq}$ does not have ultraviolet divergences. The validity of this assumption is not obvious, and it should be confirmed by a concrete calculation.

Because we carry out a linear analysis of the fluctuations, we replace $f(\lambda,D)$ by $f_0(\lambda)\equiv f(\lambda,D=0)$. Then the problem is now reduced to deriving the form of the function $f_0(\lambda)$. However, because it is still difficult to find a general solution even in this simplified problem, we study two specific cases, $\lambda\ll 1$ and $\lambda\gg 1$.

When $\lambda\ll 1$, all quantities may be expanded in powers of λ. Due to the reflection symmetry, we have $f_0(\lambda)\simeq c_0\lambda^2$. Here c_0 is a constant whose value is calculated to be $1/1152\pi$ below. We thus obtain

$$p_y-p_y^{\rm eq}=c_0 TL\left(\frac{S}{\nu}\right)^2. \tag{11}$$

Note that this L dependence, which implies the breakdown of the intensive nature, is compatible with the result by Aoki and Kusnezov [6]. At the end of this paper, we discuss that this anomalous behavior can be attributed to the long-range correlation of momentum fluctuations.

Next, we shall consider the opposite case, $\lambda\gg 1$. Note that this condition does not necessarily imply the strong shear. For example, this asymptotic case is realized by taking the limit $L\to\infty$, while keeping the shear rate S small, in which case the shear stress obviously remains small. Note also that planar Couette flow is linearly stable for all values of λ. If we encounter no infrared divergence in the calculation of $p_y-p_y^{\rm eq}$, we obtain $f_0(\lambda)=c_1\lambda^{3/2}$, because $p_y-p_y^{\rm eq}$ should be independent of L. In this case we have

$$p_y-p_y^{\rm eq}=c_1 T\left(\frac{S}{\nu}\right)^{3/2}. \tag{12}$$

This S dependence is the same as that obtained by Kawasaki and Gunton. As we demonstrate below indeed, no infrared divergence is accompanied in the calculation of $p_y-p_y^{\rm eq}$, and that calculation yields Eq. (12) with $c_1=1.06\times 10^{-2}$.

Technical details. We first consider the case $\lambda\to\infty$ and begin by performing the Fourier expansion

$$v_y(\boldsymbol{r})=\int\frac{d\boldsymbol{k}}{(2\pi)^3}e^{i\boldsymbol{k}\cdot\boldsymbol{r}}\hat{v}_y(\boldsymbol{k}). \tag{13}$$

In a statistically steady state, an equal-time correlation function can be defined as

$$\langle\hat{v}_y(\boldsymbol{k})\hat{v}_y(\boldsymbol{k}')\rangle=C_{yy}(\boldsymbol{k})\delta^3(\boldsymbol{k}+\boldsymbol{k}'). \tag{14}$$

Equation (7) is then rewritten in the form

$$p_y=p_{\rm B}+\rho\int\frac{d\boldsymbol{k}}{(2\pi)^3}C_{yy}(\boldsymbol{k}), \tag{15}$$

where we have used the result $\langle(\partial_l v_m)(\partial_m v_l)\rangle=0$, which is readily obtained by $\partial_l v_l=0$ and Eq. (3). From Eqs. (1) and (2), we derive the equation of the correlation function $C_{yy}(\boldsymbol{k})$:

$$-Sk_x\frac{\partial C_{yy}(\boldsymbol{k})}{\partial k_y}=-2\left(\nu k^2-2S\frac{k_xk_y}{k^2}\right)C_{yy}(\boldsymbol{k})+\frac{2\nu T}{\rho}(k_x^2+k_z^2). \tag{16}$$

We can solve this equation by introducing the new wave vector $\boldsymbol{k}'=\boldsymbol{k}+Stk_x\boldsymbol{e}_y$, where t is a fictitious time parameter. Using the standard manipulation [9,11], we obtain

$$C_{yy}(\boldsymbol{k})=\frac{2\nu T}{\rho}(k_x^2+k_z^2)\int_0^\infty dt\, e^{-2\nu k^2(t+t^2S\hat{k}_x\hat{k}_y+t^3S^2\hat{k}_x^2/3)}\times(1+2tS\hat{k}_x\hat{k}_y+t^2S^2\hat{k}_x^2)^2. \tag{17}$$

Combining Eqs. (15) and (17), we find an integral expression of the pressure [12]. When $S=0$, this merely gives the equilibrium pressure p_y^{eq}, which can be written as

$$p_y^{\mathrm{eq}}=p_{\mathrm{B}}+bT\ell^{-3}. \tag{18}$$

Here ℓ is introduced as a short scale cutoff to avoid the ultraviolet divergence, and b is a numerical constant. Because p_{B} remains undetermined, this ultraviolet divergence is renormalized into it appropriately so that p_y^{eq} coincides with the observable equilibrium pressure. In a nonequilibrium case $(S>0)$, we find that the correction to the equilibrium pressure is actually expressed in form (13), and c_1 is given by

$$c_1=\sqrt{\frac{\pi}{32}}\frac{1}{(2\pi)^3}\int_0^\infty dt\frac{1}{t^{3/2}}g(t), \tag{19}$$

with

$$g(t)=\int d\Omega\, A(\Omega)\frac{B(\Omega)+tC(\Omega)}{\left[1+tB(\Omega)+\frac{t^2}{3}C(\Omega)\right]^{3/2}}. \tag{20}$$

Here $\Omega=(\theta,\phi)$, $d\Omega=d\phi\, d\theta\sin\theta$ and A, B, C are polynomials of $\sin\theta$, $\cos\phi$, and $\sin\phi$, which are determined from Eq. (17). From numerical integrations, we obtain $c_1=1.06\times10^{-2}$.

In the case $\lambda\ll1$, we can utilize the calculation performed above by simply replacing $\int dk_y(2\pi)^{-1}e^{ik_yy}\cdots$ with $\Sigma_nL^{-1}e^{i2\pi ny/L}\cdots$ in Eq. (13). In this way, an expression similar to Eq. (17) with the replacement $k_y\rightarrow2\pi/L$ is found. Then the expansion of this correlation function in powers of λ leads to the desired form of the nonequilibrium pressure in Eq. (11), whose numerical factor is obtained as $c_0=1/1152\pi\approx2.8\times10^{-4}$.

Long-range correlations. Here we demonstrate that the anomalous forms of the pressure (11) and (12) are closely related to the long-range correlations of momentum fluctuations. For simplicity, we restrict our attention to the fluctuations with $\boldsymbol{k}=(k,0,0)$. Two asymptotic forms of the correlation function are given as

$$C_{yy}(k,0,0)\sim\frac{T}{\rho}\left(1+\frac{1}{2}\frac{S^2}{\nu^2k^4}\right), \tag{21}$$

for $k^2\gg S/\nu$, and

$$C_{yy}(k,0,0)\sim\frac{T}{\rho}\left(\frac{2}{3}\right)^{1/3}\Gamma\left(\frac{2}{3}\right)\frac{S^{2/3}}{\nu^{2/3}k^{4/3}}, \tag{22}$$

for $k^2\ll S/\nu$. Comparing these expressions with Eqs. (11) and (12), the dependence of the pressure on the long-range fluctuations in each case becomes clear. The $1/k^4$ dependence in Eq. (21) reflects highly anomalous behavior of the fluctuations with small wave numbers [13]. Note that there is a range of wave numbers that satisfy $k^2\gg S/\nu$ but are still much smaller than the characteristic wave number of equilibrium density fluctuations. On the other hand, Eq. (22) shows that this long-range correlation is suppressed at scales larger than $l\equiv\sqrt{\nu/S}$, crossing over to a weaker correlation (see also Fig. 1). This is equivalent to the stronger power-law decay of the correlation function than $1/r$ in a real space [14]. A new length scale l characterizes this crossover, which is intrinsic in the nonequilibrium system considering now.

These results provide the following physical picture. The momentum fluctuations exhibit the long-range correlation described by Eqs. (21) and (22). When $L\ll l$, this correlation yields the nonintensive contribution to the pressure given in Eq. (11). On the other hand, when L is chosen to be sufficiently large, the long-range correlation is suppressed at scales larger than l, and this leads to the nonanalytic shear rate dependence given by Eq. (12) instead.

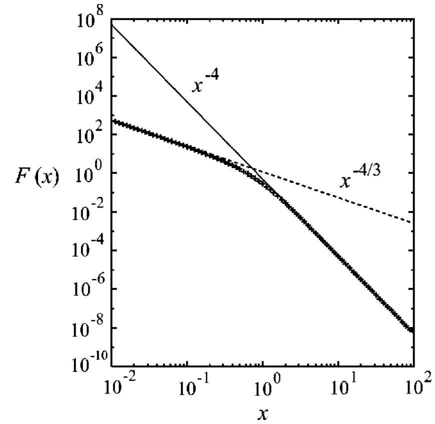

FIG. 1. Plots of numerically evaluated scaling function $F(x)$, where the correlation function $C_{yy}(k)$ is written in the form $C_{yy}(k)=\rho^{-1}T[1+F(kl)]$. Note that $\rho^{-1}TF(kl)$ corresponds to the nonequilibrium correction to the momentum correlation function. The solid line and the dotted line represent the asymptotic functions calculated from the exact integral form of $F(x)$ for large $x\gg1$ and for small $x\ll1$, respectively. These asymptotic functions are equivalent to results (21) and (22).

Discussion. In a nonequilibrium system, an external field having a spatial gradient (i.e., shear flow) induces the coupling of fluctuations with different wave vectors. In a perturbative expansion to the lowest order in shear rate, a correlation function has the same form as Eq. (21). This may cause an infrared divergence in the calculation of $p_y - p_y^{\rm eq}$. Roughly speaking, Eq. (11) is obtained when the cutoff scale is chosen as L, while Eq. (12) is obtained when it is chosen as l. We have demonstrated the validity of this intuitive argument by computing the correlation function rigorously.

The predicted finite-size dependence of pressure (11) under the condition $\lambda \ll 1$ is fairly striking. Since $l = \sqrt{\nu/S}$ may be less than 1 mm for water at standard temperature and pressure and for experimentally accessible shear rate, it is possible to design an experimental device corresponding to the condition $\lambda \ll 1$. On the other hand, from Eqs. (8), (12), and (18), $(p_y - p_y^{\rm eq})/p_y^{\rm eq}$ is found to be proportional to $\epsilon^{3/2}$ in the case $\lambda \gg 1$, and ϵ^2 in the case $\lambda \ll 1$, respectively. This indicates that the nonequilibrium correction vanishes in local equilibrium states (i.e., $\epsilon \to 0$), as expected. For example, ϵ is less than 10^{-8} when the shear rate is $10^3\ \mathrm{s}^{-1}$ for water considered above. Thus, unfortunately, the nonequilibrium correction may be too small to observe for simple fluids under ordinary experimental conditions in either case.

This fact, however, does not eliminate the fundamental significance of the present study. In constructing a theoretical framework of nonequilibrium statistical mechanics, this "ϵ-effect" must be taken into consideration, because a statistical distribution can be reduced to a local canonical ensemble only in the limiting case $\epsilon \to 0$. Furthermore, making use of the experimental technique developed in the micro- and nanofluid studies may enable us to detect the nonequilibrium effect for real fluids in the near future. We also expect that our findings stimulates further numerical studies such as molecular dynamic simulations.

Recently, Marcelli *et al.* reported the analytic dependence of pressure in shear flow observed in simulations of nonequilibrium molecular dynamics [5]. Because the shear conditions were chosen to satisfy $\epsilon \gg 1$ and $\lambda \gg 1$ in their simulations, their result is not directly comparable to ours. However, we believe that the qualitative feature of our result does not change even in the case $\epsilon \gg 1$. We suspect that their model system does not exhibit long-range momentum correlation because of the absence of the local conservation of momentum. That might be the reason why their result is inconsistent with the existing mode-coupling theories [1–4] and ours. We expect that measuring momentum correlation functions will help resolve the discrepancy, probably favorably with the mode-coupling theory.

Finally, we give a general remark on the possibility of describing an equation of state for a nonequilibrium steady state, using a thermodynamic function. An experimental test of this possibility has recently been proposed in Ref. [15], in which the intensivity of the pressure is postulated. Therefore, the recovery of the intensivity in our calculation has a significant meaning with regard to the construction of thermodynamics extended to steady states.

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