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Correlation functions in Couette flow from group theory and molecular dynamics

by MYRON W. EVANS and DAVID M. HEYES
Department of Chemistry, Royal Holloway and Bedford New College, University of London, Egham, Surrey TW20 0EX, England

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We describe group theory statistical mechanics, GTSM, which enables us to predict *new* non-vanishing time correlation functions in fluids at steady state subjected to planar couette flow. These are by symmetry trivially zero at equilibrium. An ensemble average is treated using the rules of group theory in the laboratory XYZ frame and in the molecule-fixed xyz frame of the point group character tables. In this paper we determine the effect of couette flow on a range of ensemble averages by establishing the symmetry of the strain rate tensor in terms of the irreducible representations of the $R_h(3)$ rotation reflection group in the XYZ frame. This symmetry, $D_g^{(0)} + D_g^{(1)} + D_g^{(2)}$, is the same as the pressure tensor, **P** and consists of an antisymmetric vorticity term, $D_g^{(1)}$ and a symmetric strain rate component of symmetry $D_g^{(0)} + D_g^{(2)}$. This allows non-zero ensemble averages of the same symmetry in the XYZ frame. Depending on the number of off-diagonal elements in the strain rate tensor, up to six *new* off-diagonal elements of microscopic time-autocorrelation functions of type, $\langle \mathbf{A}(0)\mathbf{A}^T(t)\rangle$ appear by GTSM in the XYZ frame. We confirm this theory for monatomic fluids using molecular dynamics computer simulation. The SLLOD equations of motion for couette dv_X/dZ flow were implemented. We calculated non-vanishing peculiar quantity autocorrelation functions, ACF, of the generic form, $\langle \tilde{v}_\alpha(0)\tilde{v}_\beta(t)\rangle$, $\langle \tilde{v}_\alpha(0)\tilde{R}_\beta(t)\rangle$ (R is the position of a molecule) and $\langle P_{\alpha\beta}(0)P_{\gamma\delta}(t)\rangle$ for the Lennard-Jones fluid. The *new* correlation functions are highly structured and generally have a finite negative value at $t = 0$. They can exhibit time reversal dissymmetry, especially at low density.

1. Introduction

There have been a number of recent treatments of non-equilibrium fluids, characterizing their microscopic dynamical evolution [1–3]. They illustrate the difficulties in characterizing even the 'simplest' of non-equilibrium fluids. Time-correlation functions are natural and sensitive probes of non-equilibrium states. A shear field, for example, has a pronounced effect on the time correlation functions of a simple fluid, although their underlying significance is still not clear yet. The objective of this report is to describe the theory and provide verification of a route which predicts those time-correlation functions existing in (symmetry breaking) simple planar shear flow, which are trvially zero in the absence of shear flow for symmetry reasons. The effect of a shearing field is to change the time dependence of the diagonal elements of the pressure tensor and their time correlation functions. This promotes the existence of hitherto unmeasured off-diagonal elements which cannot be predicted from finite-element analysis. The latter are responsible for experimental observables such as the Weissenberg effect, which is the flow imparted to a sheared liquid in an axis perpendicular to that of the applied shear plane. There is no way of explaining the Weissenberg effect in terms of the molecular dynamics of shear without involving the effect of the time cross-correlation functions of the type described in the paper.

Whiffen has recently introduced the concept of 'group theoretical statistical mechanics', GTSM, based on the novel application of group theory to the thermodynamic ensemble average, $\langle \dots \rangle$ [4]. Symmetry can be used to predict those averages existing and vanishing in both the laboratory fixed frame XYZ and the molecule fixed frame xyz, applying group theory to the ensemble averages [5, 6]. Applications of this approach have recently been described [7–11]. Here, we make the *first* application of this theory to planar couette flow, and verify it by molecular dynamics computer simulation on model atomic fluids. At the present we are not directly interested in the nature of the non-equilibrium states nor in the precise form of the time correlation functions; only in predicting the 'allowed' time fluctuations of microscopic variables in fluids under shear flow, which become non-zero because of the shear flow.

This paper is organized as follows. In § 2 the GTSM theory is applied to simple planar shear or couette flow. In § 3 the NEMD molecular dynamics model is described and applied to determine shear flow time-correlation functions. Discussion of the results is given in § 4. Conclusions are given in § 5.

2. Group theory statistical mechanics

The irreducible representations of the rotation-reflection group, $R_h(3)$ in the XYZ frame are denoted by $D_g^{(0)}, \dots, D_g^{(n)}$ and $D_u^{(1)}, \dots, D_u^{(n)}$, respectively; where the subscript, g (or gerade) denotes even to parity reversal symmetry and u (or ungerade) denotes odd to parity reversal symmetry. The superscripts refer to the order of the spherical harmonics. In couette flow in an incompressible liquid (a frequently employed macroscopic simplification) Newton first derived the relationship between shear strain rate and stress, Π,

$$\Pi_{XZ} = \eta \frac{dv_X}{dZ}, \tag{1}$$

where η is the viscosity, a simple scalar of D_g^0 symmetry. The streaming velocity is $v_X(Z)$. This formula (1) applies in the limit $dv_X/dZ \to 0$. At finite shear rate η is a function of $\dot{\gamma} = dv_X/dZ$ and a more complicated stress tensor is required. In general,

$$\mathbf{\Pi} = 2\eta(\dot{\boldsymbol{\gamma}})\dot{\boldsymbol{\gamma}}. \tag{2}$$

In both situations GTSM applies at steady state in the presence of shear flow, where the isotropic $R_h(3)$ symmetry of the fluid is distorted, showing up in new non-zero terms in the stress tensor. The latter is found by considering the tensor product,

$$\dot{\boldsymbol{\gamma}} = \mathbf{v}(\mathbf{r}^{-1}), \tag{3}$$

making up nine elements of the velocity gradient. Here, $\mathbf{r}$, is the position vector whose single laboratory frame component is Z. This product has the D symmetry,

$$\Gamma(\mathbf{v})\Gamma(\mathbf{r}^{-1}) = D_u^{(1)}D_u^{(1)} = D_g^{(0)} + D_g^{(1)} + D_g^{(2)}, \tag{4}$$

where we have used the Clebsch–Gordon theorem [5],

$$D^{(n)}D^{(m)} = D^{(n+m)} + \dots + D^{|(n-m)|}. \tag{5}$$

In (1) and (2) the symmetry of the shear viscosity, η, is that of a scalar, $D_g^{(0)}$; with negative time reversal symmetry because it has units of pressure multiplied by time. The symmetry of the shear stress tensor is the product of that of the shear rate and that of the shear viscosity. The time reversal symmetry of the shear stress (or pressure) tensor is therefore positive. It follows that the shear stress tensor must also have the symmetry, $D_g^{(0)} + D_g^{(1)} + D_g^{(2)}$, along with the pressure tensor ($\mathbf{P} = -\mathbf{\Pi}$). *The representation, $D_g^{(0)} + D_g^{(1)} + D_g^{(2)}$, of the strain rate tensor reflects the fact that it* has an antisymmetric component of vorticity, of symmetry, $D_g^{(1)}$, and a symmetric traceless component of symmetry, $D_g^{(0)} + D_g^{(2)}$. (The mathematical treatment of these effects in a molecular fluid is formidably complicated. Evans showed that there are five conservation equations and eight constitutive equations [12].) A system under shear at steady state causes the $R_h(3)$ symmetry to be broken by the strain rate tensor of symmetry, $D_g^{(0)} + D_g^{(1)} + D_g^{(2)}$, whose effect is to make possible the existence of ensemble averages of this symmetry according to GTSM. On the molecular scale, the strain rate tensor applied in couette flow makes possible the existence of time correlation functions of the same symmetry both in the XYZ frame and in the molecule fixed xyz frame. (In atomic fluids the second case is inapplicable.) The tensor symmetry of all time correlation functions of the type: $\langle \mathbf{A}(0)\mathbf{A}^T(t)\rangle$, where $\mathbf{A}$ is a polar or axial vector is also, $D_g^{(0)} + D_g^{(1)} + D_g^{(2)}$. Thus all nine elements may exist in an atomic fluid under shear. Where there is only one component of the velocity gradient in the planar couette flow, e.g. dv_X/dZ, then only one independent off-diagonal element of the time *ACF*, $\langle \mathbf{A}(0)\mathbf{A}^T(t)\rangle$ appears in the laboratory XYZ frame. However, this may appear in all time cross correlation functions of this type (i.e. containing the X and Z superscripts) and will be the microscopic characteristic of the applied strain rate tensors. The strain rate tensor will also allow the existence in the XYZ frame of time cross correlation functions of type, $\langle \mathbf{A}(0)\mathbf{B}^T(t)\rangle$, with $D_g^{(0)} + D_g^{(1)} + D_g^{(2)}$, symmetry.

In the special case of shear applied to an atomic liquid, treated in this work, the $D_g^{(0)} + D_g^{(1)} + D_g^{(2)}$ symmetry of the applied field (1) causes the off-diagonal peculiar velocity time correlation function, $\langle \tilde{v}_X(0)\tilde{v}_Z(t)\rangle$ to appear in the laboratory frame, along with the off-diagonal element of the pressure tensor time correlation functions, $\langle P_{XY}(0)P_{YZ}(t)\rangle$, $\langle P_{XZ}(0)P_{XX}(t)\rangle$, $\langle P_{XZ}(0)P_{YY}(t)\rangle$ and $\langle P_{XZ}(0)P_{ZZ}(t)\rangle$. These results are obtained recognizing that, $\langle P_{XY}(0)P_{ZY}(t)\rangle$, contains the component $\langle v_Y(0)v_Y(t)v_X(0)v_Z(t)\rangle$. The two correlation functions contained within this time average are non-zero. Similar remarks can be made for $\langle P_{XZ}(0)P_{XX}(t)\rangle$ and $\langle P_{XZ}(0)P_{ZZ}(t)\rangle$. In each of these cases the component velocity time correlation functions exist by symmetry. Thus the existence of $\langle v_X(0)v_Z(t)\rangle$ implies the existence of certain elements of the pressure tensor autocorrelation function. The full symmetry of the time correlation function of the pressure tensor in the laboratory XYZ frame is

$$(D_g^{(0)} + D_g^{(1)} + D_g^{(2)})(D_g^{(0)} + D_g^{(1)} + D_g^{(2)}),$$

which is

$$(D_g^{(1)} + D_g^{(2)} + D_g^{(3)} + D_g^{(4)}) + 2(D_g^{(1)} + D_g^{(2)} + D_g^{(3)}) + 3(D_g^{(0)} + D_g^{(1)} + D_g^{(2)}),$$

which includes scalar, vector and tensor symmetry up to rank (4). For a shearing field of the type, dv_X/dZ, the above symmetry allows the existence of the foregoing off-diagonal elements of the pressure tensor time correlation functions, together with the usual diagonal elements. These time correlation functions are the dynamical manifestation of the Weissenberg effect, the occurrence of changes in $P_{\alpha\alpha}$ due to shear [13, 14]. The existence of this series of time correlation functions tests the validity of the GTSM theory out of conventional thermodynamic equilibrium. The details for the evaluation of these functions are given in the next section.

3. Simulation details

The MD simulations used particles interacting via the Lennard-Jones potential,

$$\phi(r) = 4\varepsilon((\sigma/r)^{12} - (\sigma/r)^6), \tag{6}$$

The basic technique has been described elsewhere [15]. The MD simulations were performed on a cubic unit cell of volume V containing $N = 108$ Lennard-Jones (LJ) particles of mass, m. The interactions were truncated at $2{\cdot}5\sigma$. A large time step version of the Verlet algorithm was used to increment the positions of the molecules [16]. We use LJ reduced units throughout, i.e. $k_B T/\varepsilon \to T$, and number density, $\rho = N\sigma^3/V$. Time is in $\sigma(m/\varepsilon)^{1/2}$, shear rate is in $(\varepsilon/m)^{1/2}/\sigma$, viscosity is in $(m\varepsilon)^{1/2}/\sigma^2$ and stress is in $\varepsilon\sigma^{-3}$. The temperature was fixed by the gaussian isokinetic scheme [17]. The time step was 0·0075. The production simulations extended for over 500 000 time steps for unsheared and sheared LJ states. Each state point was performed twice in individual segments of ca. 600 000 time steps. Two state points were examined. There was a near triple point state, at $\rho = 0{\cdot}8442$ and $T = 0{\cdot}722$. In the sheared case, $\dot{\gamma} = 1{\cdot}0$, producing $\eta = 2{\cdot}1$, about 30 per cent shear thinning [18]. A time origin for the correlation functions was taken at each time step. The shear velocity profile was introduced in the fluid using isokinetic SLLOD equations of motion [17, 18]. A low density state $\rho = 0{\cdot}1$ and $T = 2{\cdot}5$ was also examined. At this density the shear viscosity is dominated by the kinetic component, η_k. Here in the $\dot{\gamma} \to 0$ limit, $\eta = 0.27$ and $\eta_k = 0{\cdot}26$ [19]. The sheared state was at $\dot{\gamma} = 1{\cdot}0$. The shear viscosity ($\dot{\gamma} \doteq 1{\cdot}0$) at this state was 0·149 with $\eta_k = 0{\cdot}132$. The low density state is dominated by kinetic effects arising from $\dot{\gamma}$, whereas the high density state is governed mainly by the change in the local structure induced by the shear.

The peculiar or thermal velocity is denoted by $\tilde{v}_\alpha$

$$\dot{R}_X = v_X\tilde{v}_X + \dot{\gamma}R_Z, \tag{7}$$

$$\dot{R}_Y = v_Y = \tilde{v}_Y, \tag{8}$$

$$\dot{R}_Z = v_z = \tilde{v}_Z, \tag{9}$$

$$\frac{d\tilde{v}_X}{dt} = F_X/m - \dot{\gamma}\tilde{v}_Z - \beta\tilde{v}_X, \tag{10}$$

$$\frac{d\tilde{v}_Y}{dt} = F_Y/m - \beta\tilde{v}_Y, \tag{11}$$

and

$$\frac{d\tilde{v}_Z}{dt} = F_Z/m - \beta\tilde{v}_Z, \tag{12}$$

where the α component of the force on a particle is F_α, the velocity is v_α, the peculiar velocity is $\tilde{v}_\alpha$, and β is the coefficient in the gaussian isokinetic thermostatting control [18].

We can also define a quantity, $\tilde{R}_\alpha$, a 'peculiar' position, $\tilde{R}_\alpha(t) = R_\alpha(t) - R_\alpha(0)$, neglecting the streaming component,

$$\tilde{R}_\alpha(t) = \int_0^t \tilde{v}_\alpha(t')\, dt'. \tag{13}$$

Computations were carried out on a CRAY-1S at the University of London Computer Centre.

4. Results and discussion

We evaluated over at least two independent segments of 500 000 steps each, the correlation functions, $\langle \tilde{v}_Z(0)\tilde{v}_X(t)\rangle$ $\langle \tilde{v}_Y(0)\tilde{v}_Z(t)\rangle$, $\langle \tilde{v}_Y(0)\tilde{v}_X(t)\rangle$, $\langle \tilde{v}_Z(0)\tilde{R}_X(t)\rangle$, $\langle \tilde{v}_Y(0)\tilde{R}_X(t)\rangle$, $\langle \tilde{v}_Z(0)\tilde{R}_Y(t)\rangle$, $(V/k_B T)\langle P_{XY}(0)P_{XY}(t)\rangle$, $(V/k_B T)\langle P_{XZ}(0)P_{XZ}(t)\rangle$, $(V/k_B T)\langle P_{YZ}(0)P_{YZ}(t)\rangle$, $(V/k_B T)\langle P_{XZ}(0)P_{YZ}(t)\rangle$, $(V/k_B T)\langle P_{XZ}(0)P_{XY}(t)\rangle$, $(V/k_B T)\langle P_{XY}(0)P_{YZ}(t)\rangle$, $(V/k_B T)\langle P_{XZ}(0)P_{XX}(t)\rangle$, $(V/k_B T)\langle P_{XZ}(0)P_{YY}(t)\rangle$ and $(V/k_B T)\langle P_{XZ}(0)P_{ZZ}(t)\rangle$. In the absence of shear we note that reversal of the time arguments in the above correlation functions leaves them unchanged. This was also checked numerically. However, with shear there could be a departure from this stationarity principle. An estimate of the noise level in each time correlation function is the difference between the results of two segments. Therefore in the figures we show the results from both segments to estimate the statistical uncertainty. This permits the isolation of real effects from noise.

We predict by GTSM that the following correlation functions *could* exist in dv_X/dZ shear flow: $\langle \tilde{v}_Z(0)\tilde{v}_X(t)\rangle$, $\langle \tilde{v}_Z(0)\tilde{R}_X(t)\rangle$, $\langle v_X(0)v_Z(t)\rangle$, $\langle \tilde{v}_X(0)\tilde{R}_Z(t)\rangle$, $(V/k_B T)\langle P_{XY}(0)P_{YZ}(t)\rangle$, $(V/k_B T)\langle P_{XZ}(0)P_{XX}(t)\rangle$, $(V/k_B T)\langle P_{XZ}(0)P_{YY}(t)\rangle$ and $(V/k_B T)\langle P_{XZ}(0)P_{ZZ}(t)\rangle$. We also predict the same for these time correlation functions with time arguments reversed.

We first consider the simulations performed on the high density state. In figure 1 $\langle \tilde{v}_Z(0)\tilde{v}_X(t)\rangle$ is given. The results from the two independent segments reveal unquestionably that this function exists. Unlike at $\dot{\gamma} = 0$ it starts from a finite negative value, achieves a maximum at $t \sim 0{\cdot}1$ and then decays to zero in an oscillatory manner. The function $\langle v_Z(0)v_X(t)\rangle$ is statistically indistinguishable from $\langle \tilde{v}_Z(0)\tilde{v}_X(t)\rangle$. The insert in figure 1 shows $\langle \tilde{v}_X(0)\tilde{v}_Z(t)\rangle$, which is very similar but has a slightly deeper minimum. In figure 2 $\langle \tilde{v}_Z(0)\tilde{R}_X(t)\rangle$ is given. The results from the simulations reveal its existence also. The function $(V/k_B T)\langle P_{XY}(0)P_{YZ}(t)\rangle$, is presented in figure 3. This function is zero in the $\dot{\gamma} \to 0$ limit. This cross-correlation function exists also for $\dot{\gamma} > 0$, commencing from a finite value at $t = 0$ and rising steadily to zero by $t \sim 1{\cdot}0$. The generic functions, $(V/k_B T)\langle P_{XZ}(0)P_{\gamma\gamma}(t)\rangle$ (where $\gamma = X$, Y or Z), are shown in figures 4–6. They all start at $t = 0$ from a finite negative value and rise smoothly to a negative value, which is somewhat smaller. The extent of rise is more pronounced in the order $X \sim Z > Y$. This is expected as the relative changes in the values of the normal pressure components, $(P_{\alpha\alpha})$ are also in this order. We found $P(\dot{\gamma} = 0) = 0{\cdot}025$, $P_{XX}(\dot{\gamma} = 1{\cdot}0) = 1{\cdot}17$, $P_{YY}(\dot{\gamma} = 1{\cdot}0) = 0{\cdot}79$, $P_{ZZ}(\dot{\gamma} = 1{\cdot}0) = 1{\cdot}25$ and $P(\dot{\gamma} = 1{\cdot}0) = 1{\cdot}07$. Note also that the average value of P_{XZ} is negative under shear ($P_{XZ} = -2{\cdot}08$). We found that the other correlation functions were statistically zero under shear as predicted by the group theory.

These non-equilibrium steady state cross-correlation functions can be related to the temperature dependence of ensemble averages through [20, 21],

$$\frac{\partial \langle B\rangle_{ss}}{\partial \beta} = -\langle \Delta B \Delta H_0\rangle_{ss} - F_e \int_0^\infty dt \langle \Delta B(0) \Delta J(t)\rangle_{ss}, \tag{14}$$

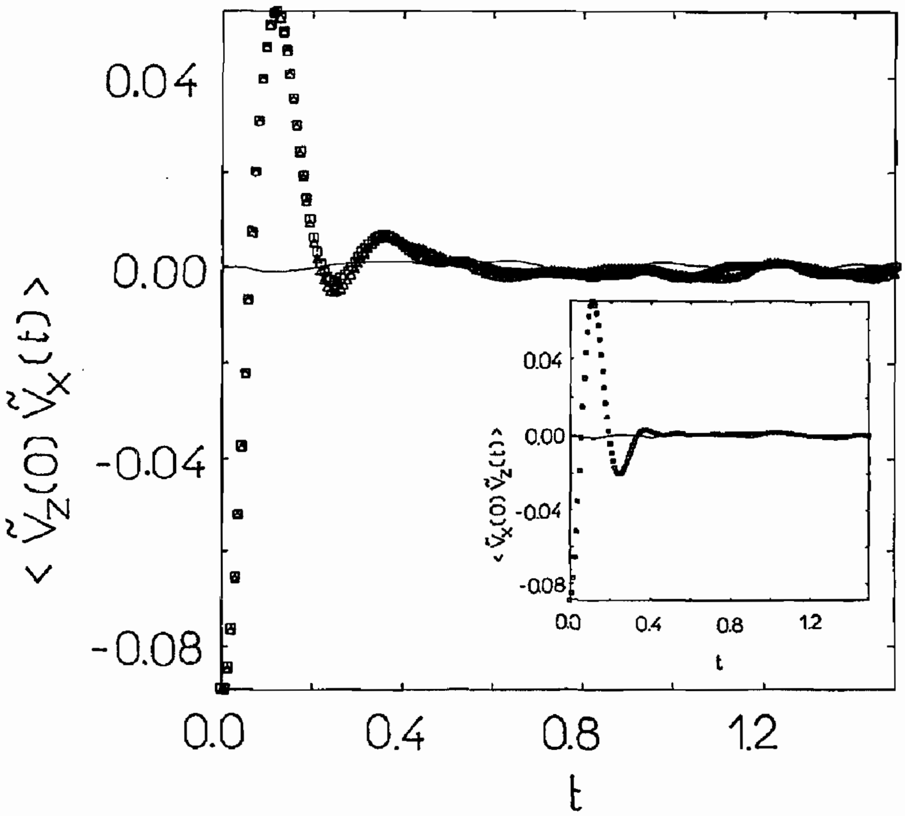

Figure 1. The time correlation function $\langle \tilde{v}_Z(0)\tilde{v}_X(t)\rangle$ for the unsheared system (solid line) and two independent contiguous segments of shear, Δ, and squares. $\rho = 0{\cdot}8442$ and $T = 0{\cdot}722$. The insert is, $\langle \tilde{v}_X(0)\tilde{v}_Z(t)\rangle$.

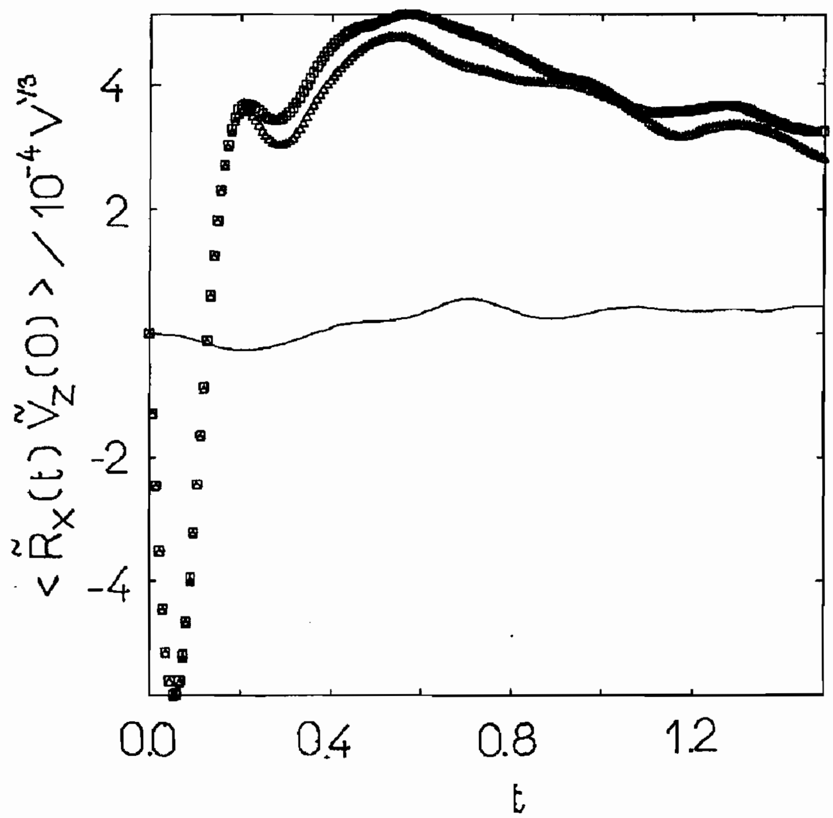

Figure 2. The time correlation function $\langle \tilde{v}_Z(0)\tilde{R}_X(t)\rangle$, for the unsheared system (solid line) and two independent contiguous segments of shear, Δ, and squares. $\rho = 0{\cdot}8442$ and $T = 0{\cdot}722$.

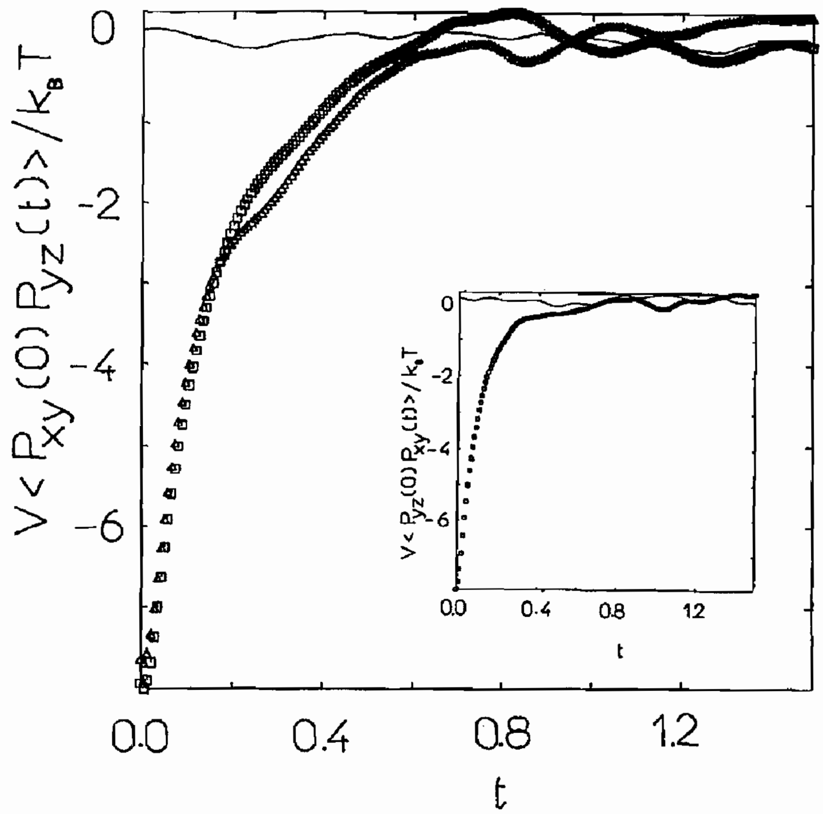

Figure 3. The time correlation function $(V/k_B T)\langle P_{XY}(0)P_{YZ}(t)\rangle$, for the unsheared system (solid line) and two independent contiguous segments of shear, Δ, and squares. $\rho = 0{\cdot}8442$ and $T = 0{\cdot}722$. The insert is the same function with reversal of the time-arguments: $(V/k_B T)\langle P_{YZ}(0)P_{XY}(t)\rangle$.

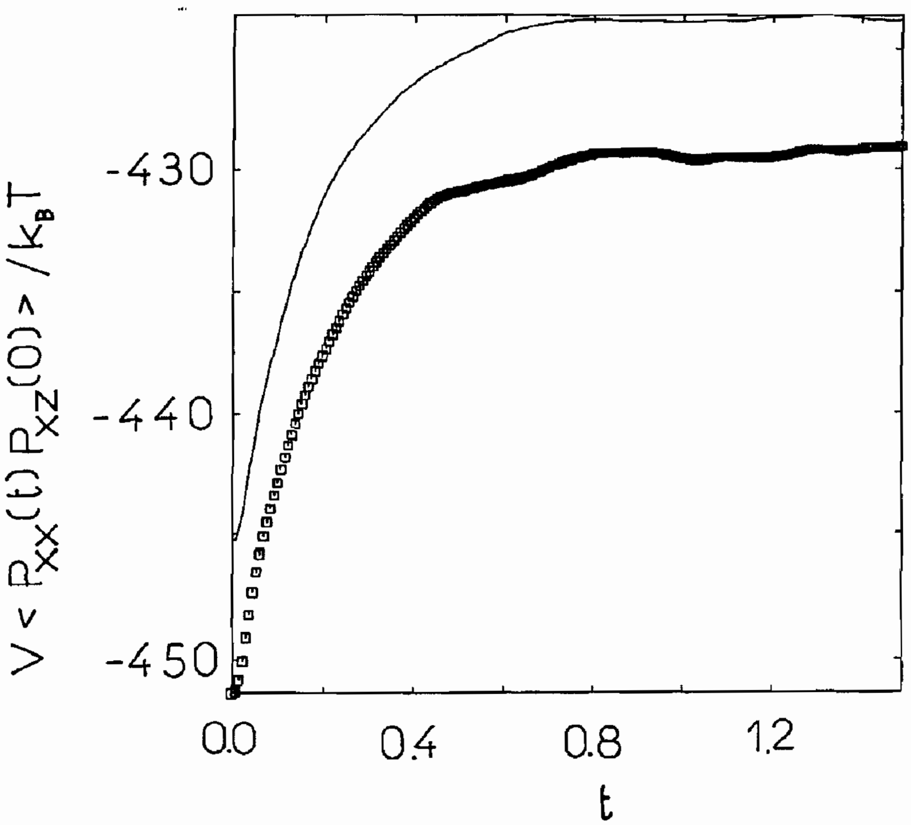

Figure 4. The time correlation function $(V/k_B T)\langle P_{XZ}(0)P_{XX}(t)\rangle$, for two independent contiguous segments of shear. $\rho = 0{\cdot}8442$ and $T = 0{\cdot}722$.

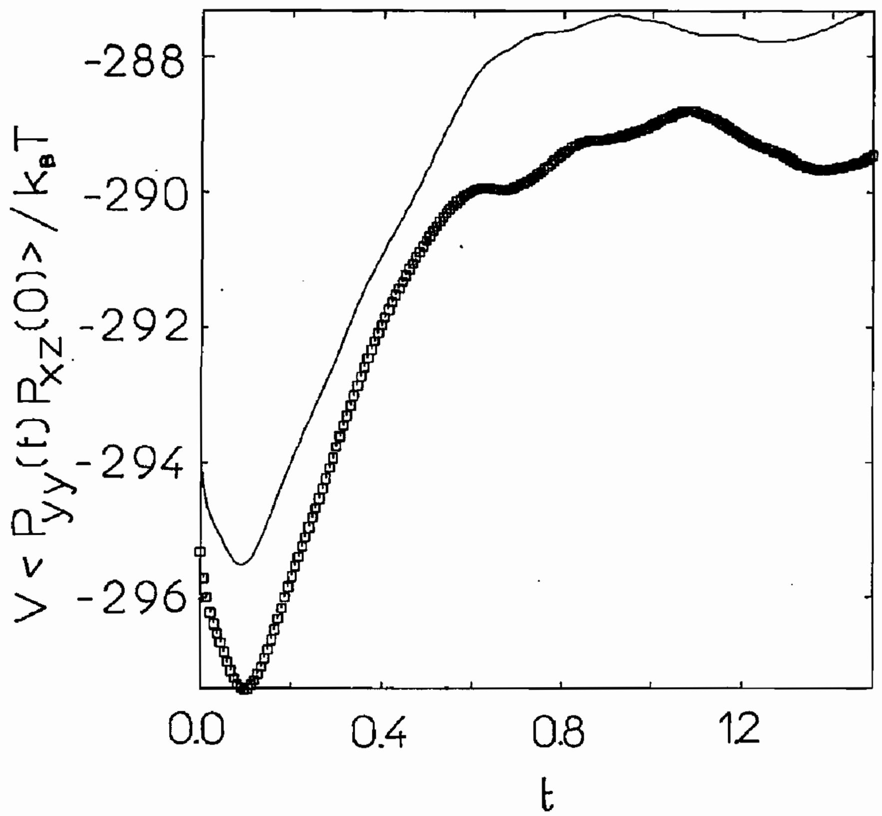

Figure 5. The time correlation function $(V/k_B T)\langle P_{XZ}(0)P_{YY}(t)\rangle$ for two independent contiguous segments of shear. $\rho = 0{\cdot}8442$ and $T = 0{\cdot}722$.

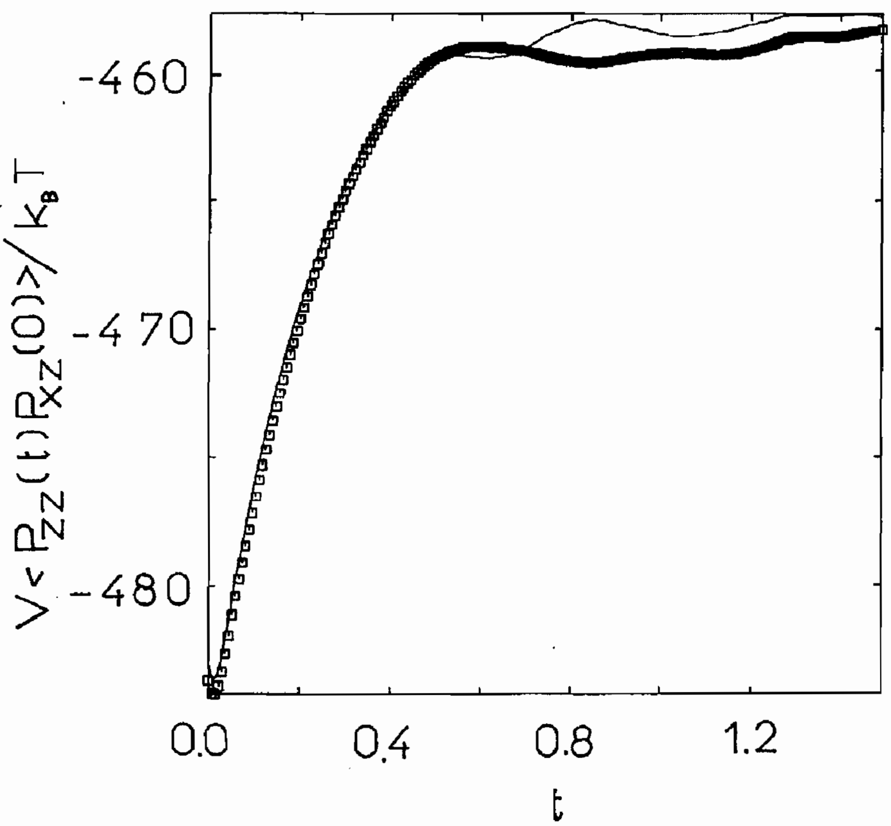

Figure 6. The time correlation function $(V/k_B T)\langle P_{XZ}(0)P_{ZZ}(t)\rangle$ for two independent contiguous segments of shear, $\rho = 0{\cdot}8442$ and $T = 0{\cdot}722$

where $\beta = 1/k_B T$, B is a phase variable, H_0 is the internal energy, $\Delta B = B - \langle B \rangle$, $\Delta H_0 = H_0 - \langle H_0 \rangle$, F_e is the external field ($=\dot{\gamma}$, here), J is the dissipative flux ($= P_{XZ} V$, here). In our study, B is P_{YZ}, P_{XX}, P_{YY}, and P_{ZZ}, for example.

Having first considered those correlation functions which become non-zero in the presence of shear, we now discuss briefly the change in form in the correlation functions due to shear that are still non-zero in the absence of shear. With increasing $\dot{\gamma}$ the $\dot{\gamma} = 0$ allowed correlation functions are known to become highly structured in two dimensions [22] and three dimensions [18], reflecting a restriction in accessible phase space.

At the onset of shear thinning we observe a change in $\langle P_{XY}(0)P_{XY}(t)\rangle$, and $\langle P_{YZ}(0)P_{YZ}(t)\rangle$. Figures 7 and 8 demonstrate an increase in the $t = 0$ values for these functions and a more rapid decay than the corresponding $\dot{\gamma} = 0$ functions. The change in $\langle P_{XZ}(0)P_{XZ}(t)\rangle$ (shown in figure 9), is much more dramatic as the limiting $t \to \infty$ value is $\langle P_{XZ}\rangle^2$ which is non-zero in dv_X/dZ planar shear flow.

We now consider these correlation functions of the low density state. In the absence of shear all diagonal elements of the pressure manifest a value of 0·236. We found $P(\dot{\gamma} = 1) = 0{\cdot}234$, $P_{XX}(\dot{\gamma} = 1{\cdot}0) = 0{\cdot}363$, $P_{YY}(\dot{\gamma} = 1{\cdot}0) = 0{\cdot}171$ and $P_{ZZ}(\dot{\gamma} = 1{\cdot}0) = 0{\cdot}167$. As for the high density state, the function $\langle v_Z(0)v_X(t)\rangle$ is statistically indistinguishable from $\langle \tilde{v}_Z(0)\tilde{v}_X(t)\rangle$. However, there is a noticeable difference between $\langle \tilde{v}_X(0)\tilde{v}_Z(t)\rangle$ and $\langle \tilde{v}_Z(0)\tilde{v}_X(t)\rangle$ as figure 10, and insert reveal. (There is some evidence of this at the high density also; see figure 1 and insert.) The failure of time reversibility is a feature of non-equilibrium states. The time correlation functions therefore provide a rich *reproducible* characterization of the dynamics of non-

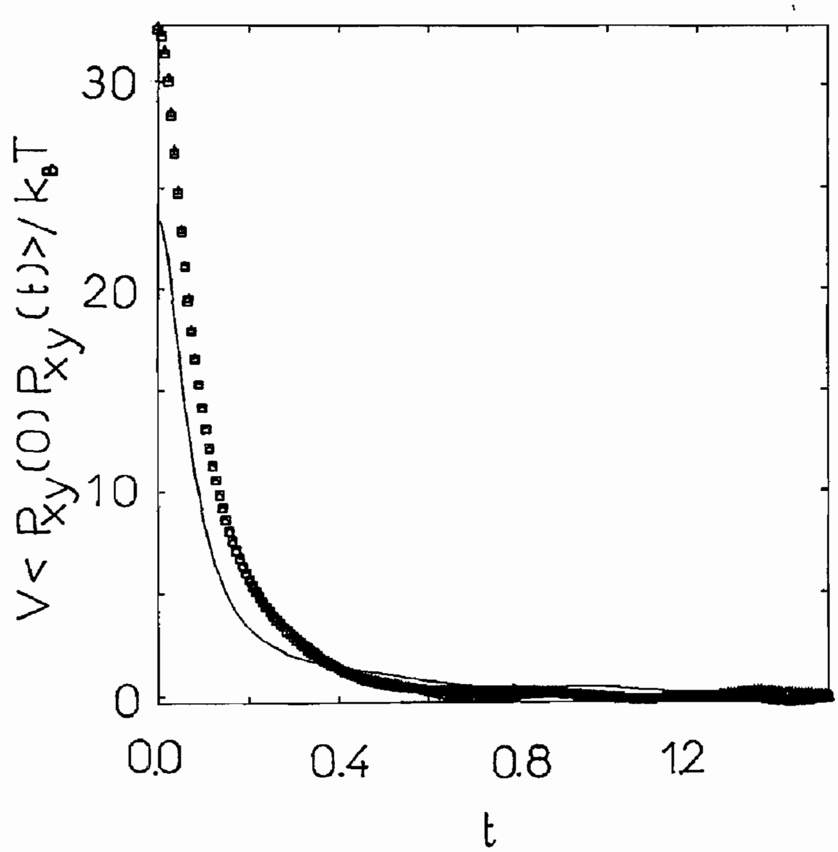

Figure 7. The time correlation function $(V/k_B T)\langle P_{XY}(0)P_{XY}(t)\rangle$ for the unsheared system (solid line) and two independent contiguous segments of shear, Δ and squares.

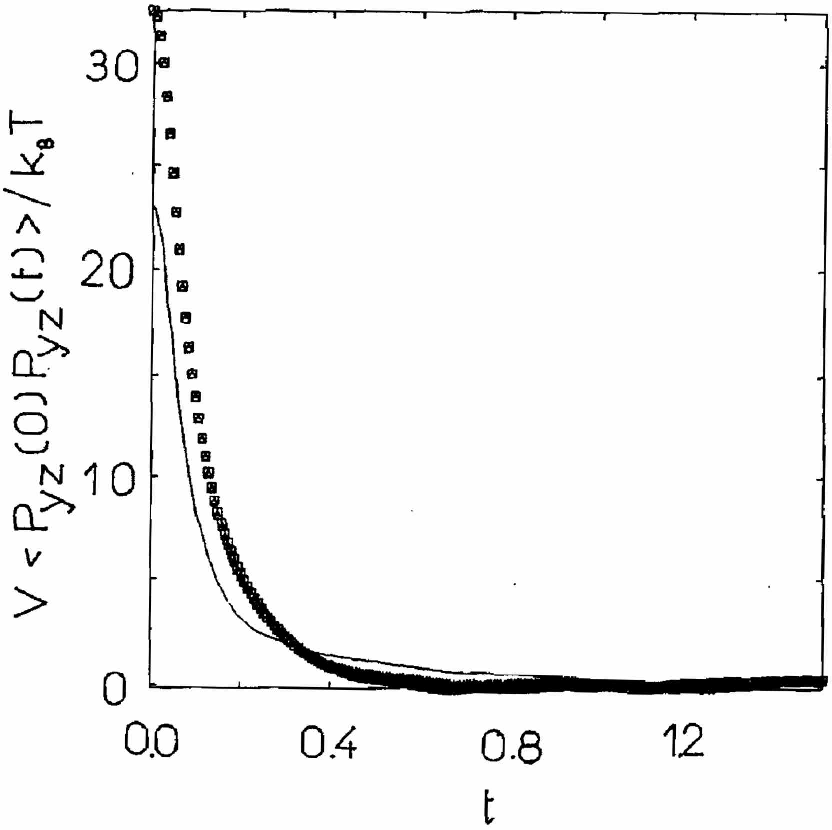

Figure 8. The time correlation function $(V/k_B T)\langle P_{YZ}(0)P_{YZ}(t)\rangle$ for the unsheared system (solid line) and two independent contiguous segments of shear, Δ, and squares. $\rho = 0{\cdot}8442$ and $T = 0{\cdot}722$.

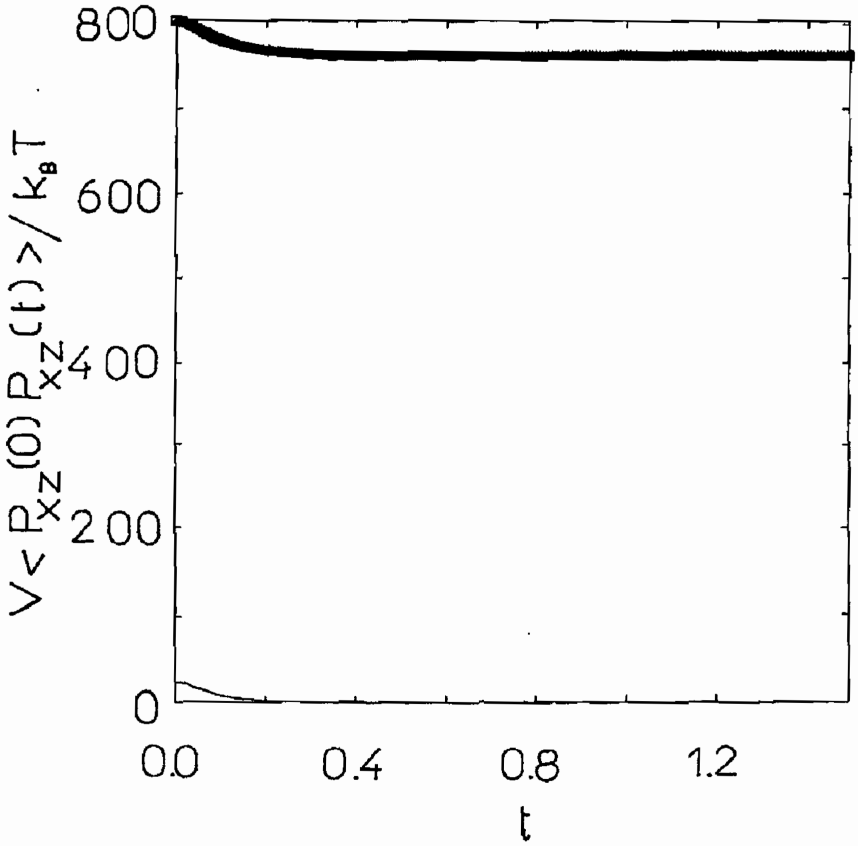

Figure 9. The time correlation function $(V/k_B T)\langle P_{XZ}(0)P_{XZ}(t)\rangle$ for two independent contiguous segments of shear, $\rho = 0{\cdot}8442$ and $T = 0{\cdot}722$.

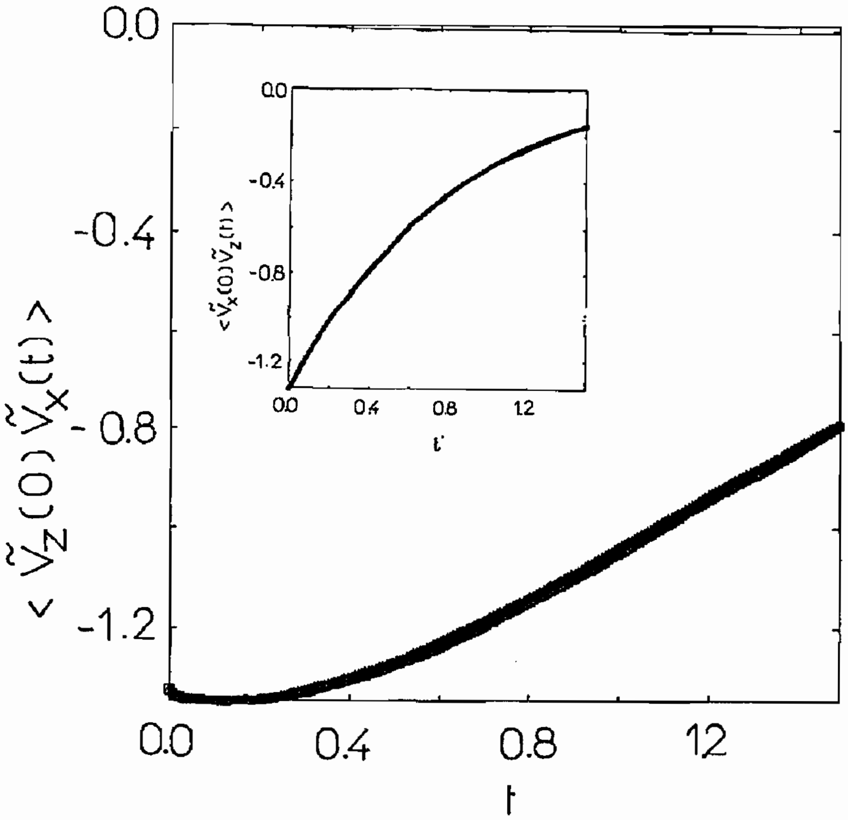

Figure 10. The time correlation function $\langle \tilde{v}_Z(0)\tilde{v}_X(t)\rangle$ for the unsheared system (solid line) and two independent contiguous segments of shear, Δ, and squares. $\rho = 0{\cdot}1$ and $T = 2{\cdot}5$. The insert is $\langle \tilde{v}_X(0)\tilde{v}_Z(t)\rangle$.

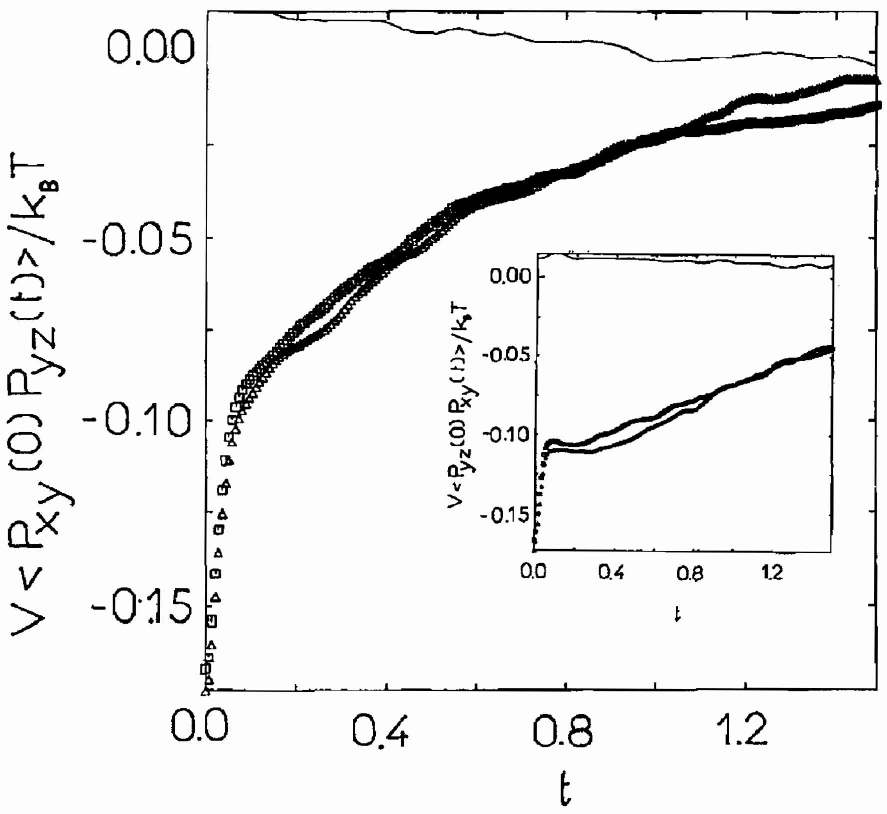

Figure 11. The time correlation function $(V/k_B\,T)\langle P_{XY}(0)P_{YZ}(t)\rangle$, for the unsheared system (solid line) and two independent contiguous segments of shear, Δ, and squares. $\rho = 0{\cdot}1$ and $T = 2{\cdot}5$. The insert is the same function with reversal of the time-arguments i.e. $(V/k_B\,T)\langle P_{YZ}(0)P_{XY}(t)\rangle$.

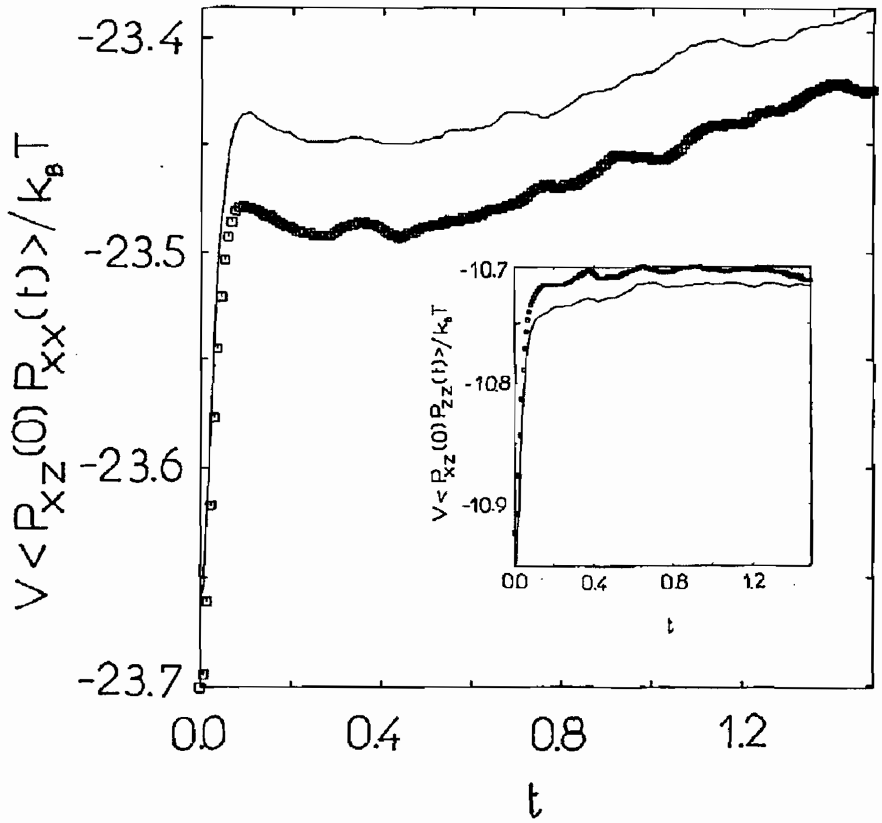

Figure 12. The time correlation function $(V/k_B\,T)\langle P_{XZ}(0)P_{XX}(t)\rangle$ for two independent contiguous segments of shear, $\rho = 0{\cdot}1$ and $T = 2{\cdot}5$. The insert is $(V/k_B\,T)\langle P_{XZ}(0)P_{ZZ}(t)\rangle$.

equilibrium states. The function $(V/k_B\,T)\langle P_{XZ}(0)P_{YZ}(t)\rangle$ also manifests time irreversibility as revealed in figure 11. The cross-correlation functions $(V/k_B\,T)\langle P_{XZ}(0)P_{\gamma\gamma}(t)\rangle$ also reveal a statistically significant time development. Two examples for the sheared states are given in figure 12, where $\gamma = Z$ in the main figure and $\gamma = X$ in the insert. The $\gamma = Y$ is also structured, showing a maximum at $t \sim 0{\cdot}2$ before decaying to $(V/k_B\,T)\langle P_{XZ}(0)P_{YY}(t)\rangle \sim -11{\cdot}0$ at $t \sim 1{\cdot}5$. The $(V/k_B\,T)\langle P_{\alpha\beta}(0)P_{\alpha\beta}(t)\rangle$ correlation functions decay more rapidly under finite shear, with $(V/k_B\,T)\langle P_{\alpha\beta}(0)P_{\alpha\beta}(0)\rangle = 0{\cdot}43$.

4. Conclusions

In this paper we have established the link between a macroscopic applied field symmetry and the precise symmetry of the induced time correlation functions. We have looked at planar couette shear flow, showing that there are new time correlation functions in both the cartesian and peculiar frames of reference. It is not obvious that shear will produce these new correlation functions without this treatment. They do not arise from classical treatments of rheology. We believe that a description of couette flow is incomplete without these new correlation functions, which potentially provide new experimental probes for the microscopic consequences of non-newtonian flow. The Weissenberg effect (observed when a non-newtonian fluid climbs up a rod rotating in it) is the result of the existence of cross time correlation functions of the type first reported here. Therefore the Weissenberg effect could be used as an experimental probe for these correlation functions.

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Chapter 7

THE PHOTON'S MAGNETOSTATIC FLUX QUANTUM $\hat{B}_{\Pi}$:

ON THE ABSENCE OF FARADAY INDUCTION

by

M. W. Evans[1],

Department of Physics,

University of North Carolina,

Charlotte, NC 28223.

ABSTRACT

The relativistic theory of fields is used to show that the recently proposed *magnetostatic flux quantum* $\hat{B}_{\Pi}$ *of the photon does not result in Faraday induction* because the photon propagates at the speed of light. In consequence there cannot be components of the classical $\mathbf{B}_{\Pi}$ orthogonal to the propagation direction, and straightforward application of symmetry and the Lorentz transformations shows that components of the associated electric field strength $\mathbf{E}_{\Pi}$ perpendicular to the propagation direction Z vanish in all frames of reference. Thus $\mathbf{E}_{\Pi}$ can never be generated from $\mathbf{B}_{\Pi}$ in free space through Faraday's non-relativistic law of induction, in agreement with recent experimental observation.

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[1]Visiting Scientist and Leverhulm Senior Fellow, Cornell Theory Center, Ithaca, NY 14853; Senior Visiting Research Associate, Materials Research Lab., Penn State University, University Park, PA 16802.

1. INTRODUCTION

It has been deduced recently {1-7} that the photon generates the magnetostatic flux density operator

$$\hat{B}_{\text{II}} = B_0 \frac{\hat{J}}{\hbar} \tag{1}$$

where $\hat{J}$ is the photon's quantised angular momentum, a boson operator which has eigenvalues only in the propagation direction {8} of the photon. B_0 is the scalar magnetic flux density amplitude associated with a single photon, and $\hbar$ is the unit of angular momentum in quantum mechanics, the reduced Planck constant. The classical equivalent of $\hat{B}_{\text{II}}$ is an axial vector $\mathbf{B}_{\text{II}}$ which is defined through the conjugate product $\mathbf{E} \times \mathbf{E}^*$ of the electromagnetic plane wave solutions $\mathbf{E}$ and $\mathbf{E}^*$ of Maxwell's equations. Here $\mathbf{E}$ is the oscillating electric field strength vector in volts per metre and $\mathbf{E}^*$ is its complex conjugate {9-14}. The cross product $\mathbf{E} \times \mathbf{E}^*$ is not in itself a solution of Maxwell's equations, and is independent of the phase of the plane wave. It can be expressed in terms of the vector, or antisymmetric, part of the intensity of free space electromagnetic radiation

$$I_{ij} = \epsilon_0 c E_i E_j^* \tag{2}$$

where ϵ_0 is the free space permittivity and c the speed of light. It has been shown {1-7} that $\mathbf{E} \times \mathbf{E}^*$ has magnetic symmetry, i.e. is negative to motion reversal $\hat{T}$ and positive to parity inversion $\hat{P}$. It is a relative of the $\hat{T}$ *and* $\hat{P}$ negative Poynting vector

$$\boldsymbol{N} = \frac{1}{\mu_0}\boldsymbol{E}\times\boldsymbol{B}^* \qquad (3)$$

where μ_0 is the free space permeability. The Poynting vector can be expressed in terms of the scalar part, I_0, of the intensity tensor by

$$\boldsymbol{N} = 2I_0\boldsymbol{n} \qquad (4)$$

where **n** is a unit vector in the propagation direction of the electromagnetic radiation in free space. Since **E** x **E*** is a purely imaginary axial vector {1-7} with magnetic symmetry, it is straightforward to deduce {1-7} that there exists in the classical theory of fields a novel, purely real, axial flux density vector $\mathbf{B}_{\Pi}$ with the recquired units of tesla defined by

$$\boldsymbol{B}_{\Pi} = \frac{\boldsymbol{E}\times\boldsymbol{E}^*}{2E_0ci} = B_0\boldsymbol{k} = \frac{E_0}{c}\boldsymbol{k} = \left(\frac{I_0}{\epsilon_0c^3}\right)\boldsymbol{k} \sim 10^{-7}I_0 \qquad (5)$$

Here E_0 is the scalar electric field strength amplitude of the electromagnetic plane wave, and **k** is a unit axial vector.

The novel vector $\mathbf{B}_{\Pi}$ is the classical equivalent of the boson operator $\hat{B}_{\Pi}$, whose existence has been inferred theoretically using the relation {5} between the classical $\mathbf{B}_{\Pi}$ and the classical third Stokes parameter S_3 in the context of contemporary quantum field theory, in which S_3 becomes the third Stokes operator $\hat{S}_3$ defined recently by Tanaś and Kielich {15} in terms of creation and annihilation photon operators. Clearly, $\hat{B}_{\Pi}$ is a property of light, and interacts with matter to produce observable effects, such as magnetisation by circularly polarised light - the "inverse Faraday" effect {16-20}; and the recently demonstrated phenomenon of laser enhanced NMR {21}, in which circularly polarised light acts magnetically to shift NMR resonances in unexpected ways far from optical resonance. Also recently demonstrated {22} is the optical Faraday effect, in which circularly polarised light rotates the plane of polarization of a probe {23-26}. The existence of magneto-optic effects such as these was first proposed by Piekara, Kielich, and co-workers {23-30} and it is now possible to show {1-7} that they are all dependent on the existence of the novel operator $\hat{B}_{\Pi}$. The latter is therefore fundamental in physical optics, and it has been shown recently {31-33} that ubiquitous phenomena such circular dichroism, ellipticity, and antisymmetric Rayleigh/Raman scattering can also be expressed directly in terms of $\hat{B}_{\Pi}$ or in the classical approximation, $\mathbf{B}_{\Pi}$. Thus $\hat{B}_{\Pi}$ is fundamental in linear as well as nonlinear optics.

In this communication, we prove in Section 2 that the classical $\mathbf{B}_{\Pi}$ does not obey the well known Faraday law of induction, essentially because the photon always propagates at the speed of light in any frame of reference. It follows that if a circularly polarised laser beam is modulated and passed through free space in an induction coil, no voltage will be observed on the grounds of Faraday induction due to $\mathbf{B}_{\Pi}$, however intense the laser, and whatever the magnitude of the term $-\delta \mathbf{B}_{\Pi}/\delta t$ produced by chopping the laser beam. A voltage will only be observed if the laser is also made to pass through material in the coil, producing the well known magnetization pulse of the inverse Faraday effect {17}.

Section 3 is a short discussion on the correct interpretation of the classical $\mathbf{B}_{\Pi}$ and the quantum $\hat{B}_{\Pi}$ operator of the photon.

2. THE ABSENCE OF FARADAY INDUCTION DUE TO $\hat{B}_{\Pi}$ IN FREE SPACE

Consider electromagnetic plane waves from a static source in frame (X, Y, Z) propagating in Z in free space. Let there be a frame (X$'$, Y$'$, Z$'$) which moves at a velocity v_Z with respect to (X, Y, Z). Lorentz transformation {34} produces the well known relations of classical relativistic field theory:

$$H_{\Pi Z}=H_{\Pi Z};\quad H_{\Pi Y}=\frac{H_{\Pi Y'}-\frac{v_Z}{c}E_{\Pi X'}}{\left(1-\frac{v_Z^2}{c^2}\right)^{\frac{1}{2}}};\quad H_{\Pi X}=\frac{H_{\Pi X'}+\frac{v_Z}{c}E_{\Pi Y'}}{\left(1-\frac{v_Z^2}{c^2}\right)^{\frac{1}{2}}};$$

$$E_{\Pi Z}=E_{\Pi Z'};\quad E_{\Pi Y}=\frac{E_{\Pi Y'}+\frac{v_Z}{c}B_{\Pi X'}}{\left(1-\frac{v_Z^2}{c^2}\right)^{\frac{1}{2}}};\quad E_{\Pi X}=\frac{E_{\Pi X'}-\frac{v_Z}{c}B_{\Pi Y'}}{\left(1-\frac{v_Z^2}{c^2}\right)^{\frac{1}{2}}};\qquad (6)$$

We also note that classical angular momentum transforms as

$$J_Z=J_{Z'};\quad J_Y=\frac{J_{Y'}}{\left(1-\frac{v_Z^2}{c^2}\right)^{\frac{1}{2}}};\quad J_X=\frac{J_{X'}}{\left(1-\frac{v_Z^2}{c^2}\right)^{\frac{1}{2}}}\qquad (7)$$

It is clear that for an object travelling at the speed of light, so that $v_Z = c$, the components $B_{\Pi Y}$, $B_{\Pi X}$, $E_{\Pi Y}$ and $E_{\Pi X}$ all become infinite in frame (X, Y, Z) unless

$$H_{\Pi Y'} = E_{\Pi X'} - H_{\Pi X'} = E_{\Pi Y'} = 0 \tag{8}$$

It is well known that the photon is massless, and travels at the speed of light in all frames of reference. In consequence, it cannot be described by non-relativistic mechanics. Its rigorous description requires relativistic quantum field theory, which shows {34-38} that its angular momentum has no eigenvalues orthogonal to its propagation direction Z. From eqn. (1), the same conclusion is reached about the novel magnetostatic flux quantum $\hat{B}_{\Pi}$. In the classical relativistic approximation, it also becomes clear that the magnetic field $\mathbf{B}_{\Pi}$ can have no components in frame (X, Y, Z) perpendicular to the propagation direction Z. It follows from the Lorentz transformation equations (6a) and (6b) that

$$B_{\Pi Z} = B_{\Pi Z'}; \quad B_{\Pi Y} = B_{\Pi X} = 0; \tag{9}$$

and

$$B_{\Pi Y'} = E_{\Pi X'} = B_{\Pi X'} = E_{\Pi Y'} = 0; \tag{10}$$

from which

$$E_{\Pi Z} = E_{\Pi Z'}; \quad E_{\Pi X} = E_{\Pi Y} = 0. \tag{11}$$

However, considerations {1-7} of $\hat{P}$ *and* $\hat{T}$ symmetry in the vector cross products $\mathbf{E} \times \mathbf{E}^*$, $\mathbf{B} \times \mathbf{B}^*$ and $\mathbf{E} \times \mathbf{B}^*$ of the usual oscillating plane wave electric and magnetic field vectors **E** and **B**, solutions of Maxwell's equations, show that products such as these cannot generate an electrostatic field in the propagation direction of an electromagnetic plane wave. This conclusion follows from the fact that **E** x **E*** and **B** x **B*** both have positive $\hat{P}$ and negative $\hat{T}$ symmetries; and **E** x **B*** has negative $\hat{P}$ *and* $\hat{T}$ symmetries, whereas the electric field $\mathbf{E}_{\Pi}$ would have to be positive to $\hat{T}$ and negative to $\hat{P}$. Thus, from this source

$$E_{\Pi Z} = E_{\Pi Z'} = 0 \tag{12}$$

and we are left only with the relativistically invariant classical magnetic flux density component

$$B_{\Pi Z} = B_{\Pi Z'} \neq 0 \tag{13}$$

which is the classical approximation to the operator $\hat{B}_{\Pi}$.

Note also that in classical relativistic theory, $\mathbf{B}_{\Pi}$ can only be proportional to angular momentum $\mathbf{J}_{\Pi}$ in frame (X, Y, Z), as implied by eqn. (1) if $E_{\Pi X'}$ *and* $E_{\Pi Y'}$ are identically zero, thus reinforcing our earlier conclusion. This follows from the structure of eqns (6a) and (7).

If, now, we attempt to assert that the nineteenth century, classical, non-relativistic and phenomenological Faraday Law of induction applies to $\mathbf{B}_{\Pi}$:

$$\nabla \times \boldsymbol{E}_{\Pi} = -\frac{\delta \boldsymbol{B}_{\Pi}}{\delta t} \tag{14}$$

having assumed that the uniform, intrinsically time independent, $\mathbf{B}_{\Pi}$ can be made time dependent by some device such as chopping a circularly polarised laser in free space inside an induction coil, we must obtain the results $E_{\Pi X} \neq 0$; $E_{\Pi Y} \neq 0$ from the integration of eqn (14); results which contradict the requirement (11) derived in turn from the fundamental, quantum relativistic, recquirement that the photon have no component of angular momentum perpendicular to its direction of propagation.

We conclude therefore that there cannot be a phenomenological Faraday Law of induction (14) for $\mathbf{B}_{\Pi}$ of the photon, because this would violate the quantum and classical relativistic theory of fields. There cannot be a non-zero $\mathbf{E}_{\Pi}$ associated with the photon in the axes X and Y orthogonal to Z, only a $\mathbf{B}_{\Pi}$ in its direction of propagation.

3. DISCUSSION : THE INTERPRETATION OF $\hat{B}_{\Pi}$ OR $\mathbf{B}_{\Pi}$

Clearly, the $\mathbf{B}_{\Pi}$ field is neither a plane wave nor an ordinary magnetostatic flux density $\mathbf{B}_S$ such as that produced by a magnet. It is not a plane wave because it is not a solution of the (non-relativistic) Maxwell equations, but, rather, constructed from the cross product $\mathbf{E} \times \mathbf{E}^*$ in an analogous way to the Poynting vector's definition in terms of the cross product $\mathbf{E} \times \mathbf{B}^*$. Significantly, the Poynting vector is a flux of energy density, and the vector $\mathbf{B}_{\Pi}$ is a flux of magnetic density. As discussed for example by Landau and Lifshitz (ref {34}, p.47) the Poynting vector is directly proportional to the **linear** momentum per unit volume of the electromagnetic field, whereas the $\mathbf{B}_{\Pi}$ vector is proportional to the **angular** momentum per unit volume of the electromagnetic field from eqn. (1). The relation between the energy and linear momentum of the electromagnetic plane wave is the same as for that of a particle (the photon) moving at the speed of light {34}. It follows that **N** is relativistic in nature, as is $\mathbf{B}_{\Pi}$, the former is related to the scalar part of the wave intensity, and the latter to its vector part.

The vector $\mathbf{B}_{\Pi}$ is not an ordinary uniform magnetostatic flux density because the photon travels at the speed of light and $\mathbf{B}_{\Pi}$ travels with it. Therefore, $\mathbf{B}_{\Pi}$ is a concept that can be described only by classical relativistic field theory and relativistic mechanics, and $\hat{B}_{\Pi}$ can be described only by relativistic quantum field theory. The deduction that $\mathbf{B}_{\Pi}$ does not obey Faraday's law of induction has recently been verified experimentally {39} by modulating a circularly polarised laser travelling in free space through an induction coil. No induced voltage was observed for any laser intensity.

Finally, we note that plane waves must be solutions of Maxwell's phenomenological equations in the classical, non-relativistic, approximation. Clearly, neither **N** nor $\mathbf{B}_{\Pi}$ can be solutions of the non-relativistic Maxwell equations because both vectors are phase independent cross products and both are relativistic in nature.

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