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LETTER TO THE EDITOR

Velocity autocorrelation function in fluctuating hydrodynamics: frequency dependence of the kinematic viscosity

Roumen Tsekov and Boryan Radoev
Department of Physical Chemistry, University of Sofia, Sofia 1126, Bulgaria

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Abstract. The memory effects in fluids are studied using Mori–Zwanzig formalism. An explicit form of the velocity autocorrelation function (VACF) of the hydrodynamic fluctuations and the corresponding frequency dependence of the kinematic viscosity are obtained. The reasoning is based on a modelling of the Langevin force resulting from an effective collision. The damped, oscillating VACF obtained is in agreement with the known numerical simulation results.

It is well known that the momentum balance of fluid motion can be presented as a generalised Langevin equation [1–3]

$$\rho(\mathrm{d}V_k/\mathrm{d}t) + \hat{G}(t)V_k = F_k(t) \qquad \langle V_k(t)F_k(t+\tau)\rangle = 0 \qquad \forall\tau > 0 \tag{1}$$

where ρ is the mass density of the fluid, $V_k(t)$ is the spatial Fourier image of the fluctuating hydrodynamic velocity, $\hat{G}V_k$ is the friction force and F_k is the Langevin force with mean value zero. Because of the common molecular-kinetic origin of two *ad hoc* introduced forces $\hat{G}V_k$ and F_k, these are not independent. Their relationship, identified by Kubo [1], the second fluctuation-dissipation theorem, is formulated most generally by Mori [2] and Zwanzig [4]

$$\hat{G}(t)V_k = \int_0^t C_{FF}(k, t-t_1)\cdot\left[\rho C_{VV}(k,0)\right]^{-1}\cdot V_k(t_1)\ \mathrm{d}t_1$$

where $C_{FF}(k,\tau)$ and $C_{VV}(k,\tau)$ are the spatial spectral densities of the time autocorrelation functions of the Langevin force and the hydrodynamic velocity fluctuations.

An equation for the evolution of the velocity autocorrelation function (VACF) $C_{VV}(k,\tau)$ can be obtained from (1) [3,5]:

$$\rho\frac{\mathrm{d}}{\mathrm{d}\tau}C_{VV}(k,\tau) + \int_0^\tau C_{FF}(k,\tau-\tau_1)\cdot\left[\rho C_{VV}(k,0)\right]^{-1}\cdot C_{VV}(k,\tau_1)\ \mathrm{d}\tau_1 = 0.$$

For the sake of convenience we will employ the Laplace transformation of the time-dependent functions, with the help of which and the well-known relation for the velocity spatial spectral density [6] $C_{VV}(k,0) = (k_B T/\rho)\mathsf{I}$, the above equation takes the form

$$\left[\rho k_B T \mathsf{I} s + \tilde{C}_{FF}(k,s)\right] \cdot \tilde{C}_{VV}(k,s) = (k_B T)^2 \mathsf{I}. \tag{2}$$

Here I denotes the unit tensor and $k_B T$ is the Boltzmann factor. The main aim of this letter is to obtain in explicit form the autocorrelation function of the Langevin force and the corresponding VACF of the fluid fluctuations. This goal is achieved by modelling of the random force F_k resulting from an effective collision [7].

The interaction between fluid particles can generally be presented by an operator $\hat{S}t(U-V)$, acting on the difference between the local hydrodynamic velocity $V(r,t)$ and an effective velocity field $U(r,t)$ accounting for the surrounding medium. In accordance with the classical theory of collisions [6, 7], the operator $\hat{S}t$ is linear and the momentum balance of the motion has the form $\rho(\mathrm{d}V/\mathrm{d}t) = \hat{S}tU - \hat{S}tV$. This result is equivalent to (1), and assuming the identity of operators $\hat{S}t$ and $\hat{G}$ for the Langevin force the following is obtained

$$F_k(t) - F_k(0) = \hat{G}(t)U_k = (k_B T)^{-1} \int_0^t C_{FF}(k, t-t_1) \cdot U_k(t_1)\, \mathrm{d}t_1.$$

Using this equation, its obvious consequences: $\langle U_k(t)\rangle = 0$ and $k_B T(\mathrm{d}F_k/\mathrm{d}t)(0) = C_{FF}(k,0) \cdot U_k(0)$, and the stationary nature of the considered processes, a link between the autocorrelation function of the Langevin force and the VACF of the effective field

$$\frac{\mathrm{d}}{\mathrm{d}\tau} C_{FF}(k,\tau) = -(k_B T)^{-2} C_{FF}(k,0) \cdot \int_0^\tau C_{UU}(k,\tau_1) \cdot C_{FF}(k,\tau-\tau_1)\, \mathrm{d}\tau_1$$

is obtained, which, by application of Laplace transformation, assumes the form

$$C_{FF}(k,0) - s\tilde{C}_{FF}(k,s) = (k_B T)^{-2} C_{FF}(k,0) \cdot \tilde{C}_{UU}(k,s) \cdot \tilde{C}_{FF}(k,s). \tag{3}$$

The use of this result requires knowledge of an adequate expression of $\tilde{C}_{UU}(k,s)$. The basic assumption in the present letter is the equivalence of the VACF of the local and effective fields $\tilde{C}_{UU}(k,s) \equiv \tilde{C}_{VV}(k,s)$. Such interpretation of the velocity $U(r,t)$ is in accordance with the Faxen theorem [8], according to which U is the fluctuating velocity field generated by the surrounding medium at the point r. From this consideration and the isotropy of the system described it follows that the velocity U is just another stochastic realization of the random process $V(r,t)$, i.e. they have the same statistical properties.

A consequence of the obtained results is the discovery of the autocorrelation function of the Langevin force and the VACF in explicit form. Substituting the correlation $\tilde{C}_{VV}(k,s)$ from (2) into (3) as $\tilde{C}_{UU}(k,s)$ leads to the following expression of the spectral density of the Langevin force autocorrelation function

$$\tilde{C}_{FF}(k,s) = (k_B T\rho/\tau_c)\mathsf{I}\left[\sqrt{1+(2s\tau_c)^2} - 2s\tau_c\right] \equiv k_B T \rho \nu(k,s) k^2 \mathsf{I} \tag{4}$$

where $\tau_c(k) = \sqrt{3k_BT\rho C_{FF}^{-1}(k,0)}$ is the correlation time and a generalized kinematic viscosity [6] $\nu(k,s)$ is introduced. Using this equation the frequency dependence of $\nu(k,s)$ and an alternative expression for τ_c

$$\nu(k,s) = \nu(k,0)\left[\sqrt{1+(2s\tau_c)^2} - 2s\tau_c\right] \qquad \tau_c^{-1} = \nu(k,0)k^2$$

can be derived. The reverse Laplace transformation of (4) affords the Langevin force autocorrelation function time dependence in analytical form, $C_{FF}(k,\tau) = (k_BT\rho/\tau_c^2)\mathrm{I}(\tau_c/\tau)J_1(2\tau/\tau_c)$. Here $J_1(\cdots)$ is the Bessel function of the first kind. Equations (2) and (4) also allow one to find the spectral density of the VACF, the reverse Laplace transformation of which is

$$C_{VV}(k,\tau) = (k_BT/\rho)\mathrm{I}(\tau_c/\tau)J_1(2\tau/\tau_c). \qquad (5)$$

It is seen from (5) that $C_{VV}(k,\tau)$ has the same τ dependence as $C_{FF}(k,\tau)$. The correctness of the obtained results is confirmed by the fact that a similar damped oscillating VACF of the fluid particles is computed in the known numerical simulation results [5].

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