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COMMENTS ON REPLY BY EU ON CO-ROTATING FRAMES

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Abstract

The role of microscopic cross correlation functions in the rotating frame formalism is discussed in the context of remarks by Eu.

Introduction

Some comments are offered on the reply by Eu (1) to an earlier paper by Evans and Heyes (2) on the role of novel cross correlation functions as indicators of the non-Newtonian response of an ensemble of atoms to shear stress.

Comments

(1) The original paper (2) carefully distinguished the concept of fluid particle and atom. The former is a mathematical artifice and the latter a physical entity. The difference between these two concepts is hardly a subtle one, and was explained in the original article (2).

(2) The time cross correlation in question, that between the laboratory X and Z components of the linear velocity of a diffusing atom, has the new property (3–6) of being asymmetric

$$\langle v_X(t)v_Z(0)\rangle \neq \langle v_Z(t)v_X(0)\rangle \quad (1)$$

i.e. is a linear combination of the antisymmetric

$$D_g^{(1)}(t): \quad \langle v_X(t)v_Z(0)\rangle = -\langle v_Z(t)v_X(0)\rangle \quad (2)$$

nd symmetric

$$D_g^{(2)}(t): \quad \langle v_X(t)v_Z(0)\rangle = \langle v_Z(t)v_X(0)\rangle \quad (3)$$

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The time dependence (1) vanishes in the absence of shear stress, and is sensitive to the non-Newtonian relation between shear stress and shear strain rate (2-10) in a computer simulation of an atomic ensemble. It is NOT a vortex, and contrary to the understanding of Prof. Eu, was not described as such in ref. (2). The antisymmetric part (2) has the D SYMMETRY of a vortex, albeit with opposite (+) motion reversal symmetry (T). This D symmetry on the point group $R_h(3)$ of the atomic ensemble is $D_g^{(1)}$, which is the same as that of a vortex, and the same as that of angular velocity or momentum. The parity inversion symmetry (P) of all these quantities is positive, indicated by the subscript g, meaning "gerade", or "even".

(3) The original reference (2) pointed out that hydrodynamics generally does not use atoms, or molecular structure, and Eu's corotating frame theory appears not to be able to account for the existence of the correlation function $\langle v_x(t)v_z(0)\rangle$. Prof. Eu has not attempted to argue with this, but has built a straw man to conveniently scare ravens and readers alike, i.e. his spurious comments on vortices. If his equations can be modified to describe $\langle v_x(t)v_z(0)\rangle$, then some progress will have been made, but probably at the expense of many phenomenological parameters.

(4) The cross correlation function $\langle v_x(t)v_z(0)\rangle$ is one out of many recently discovered by simulation (2-10), which has also produced asymmetric cross correlation functions of stress tensor components, together with rise and fall transients and a new light scattering spectroscopy, showing clearly that Evans and Heyes are perfectly aware of how quantities are customarily defined, and that the stress tensor is not a vortex. Eu in his reply refers to none of this work, which has been available (2-9) for several months.

(5) Hydrodynamics is a major subject area, but its constitutive equations for molecular liquids are insoluble without major computational input. Prof. Eu has shown, perhaps without intending to do so, that it is still apparently incapable of describing fundamental atomic dynamical properties. In corollary

however, molecular dynamics is increasingly capable (11,12) of describing many of the phenomena of hydrodynamics, using only Newton's equations of motion.

(7) The original paper (2) was intended to "help to resolve" the remaining gaps in knowledge between the two subject areas, and to clear up what, for the non ultra specialist, appears to be an entirely confusing controversy involving Prof. Eu and other distinguished colleagues in classical hydrodynamics. It was a modest paper claiming only to suggest that $\langle v_x(t)v_z(0)\rangle$ might be an interesting subject of investigation for hydrodynamics, whatever frame of reference, whatever approach. Thus far, hydrodynamics has failed to meet the new challenges posed in a series of recent papers (2-10) by Evans and Heyes. To chemists, this is unsurprising, because hydrodynamics has always had difficulty in dealing with liquids at the fundamental (atomic or molecular) level. In contrast, molecular dynamics works directly from this level, using the Newton and Euler equations. Ref. (2) did not claim that molecular dyanmics was the answer to everything, and in this respect hydrodynamics and the Boltzmann equation have obvious everyday utility.

8) The way forward is quite clear, and I would be more than happy to see equations developed by Prof. Eu or others to describe the fundamentally new cross correlation functions (2-10), using as few unknown parameters as the original molecular dynamics methods (2-10). The latter rely only on the Lennard Jones potential, for a sample of atoms of the order of a 1000, over segments of about half a million time steps. I suspect that such a task is still beyond the reach of contemporary classical hydrodynamics, but I would be delighted to be persuaded otherwise by data from analytical equations used to describe those already available from computer simulation (2-8). Such work might also show more clearly the role, if any, of "objectivity", and distinguish between the confusing counter-claims which the original paper (2) attempted to address.

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