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COMMENT

# Comment on 'Velocity autocorrelation function in fluctuating hydrodynamics'

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**Abstract.** Tsekov and Radoev recently studied the velocity autocorrelation function in a hydrodynamic model using the generalized Langevin equation formalism originally due to Mori and Zwanzig. The more recent recurrence relations formulation of the generalized Langevin equation provides a simplification. It also lends a perspective on the model of Tsekov and Radoev and points out the model's limitations. A refinement of the model is possible by consideration of the Hilbert space geometry as developed by the recurrence relations formulation.

Microscopic studies of hydrodynamics are of contemporary interest. In these studies the velocity autocorrelation function of a particle in a fluid is a focus of attention since it is measurable by scattering experiments [1]. Also, there exists a wealth of theoretical approaches to obtaining it from first principles. Recently Tsekov and Radoev [2] have added an interesting contribution to such a study of hydrodynamics. Specifically, they have considered the time evolution of the fluctuating local hydrodynamic velocity $V(t)$ via the original form of the generalized Langevin equation due to Mori [3] and Zwanzig [4]. (From a microscopic point of view, $V$ may be regarded as the velocity of one fluid particle under observation, e.g., a Brownian particle.) The generalized Langevin equation is an exact microscopic equation of motion defined in terms of a random force, which in a fluid context may be said to arise from molecular interaction.

In their model of hydrodynamics, Tsekov and Radoev assume that the force on a moving fluid particle, i.e., the drag force, is linear in $V - U$, where $U$ is an effective velocity field representing the surrounding medium. Here the first term, one which is linear in $V$, is the friction force for steady motion. The second term, linear in $U$, presumably represents the whole of the friction force for non-steady motion (i.e., Boussinesq term). They interpret it as a retarded effect due to a moving particle, hence a field. To solve the generalized Langevin equation, they introduce an approximation of the form $(U(t), U) = (V(t), V)$, i.e., $C_{UU}(t) = C_{VV}(t)$ in their notation. The resulting solution for the velocity autocorrelation function is of damped oscillation, a feature observed in numerical simulation results.

The purpose of this comment is to point out that during the past decade much progress has been made in the generalized Langevin equation formalism, especially in terms of the Hilbert space by the recurrence relations method [5]. This method has been applied to classical and quantum electron fluids, magnetic solids, harmonic-oscillator chains, etc [6]. In these studies, the Hilbert space geometry has played a critical role in elucidating the complex physical processes. The hydrodynamic model of Tsekov and Radoev can also benefit from this analysis. For example, the approximation introduced by Tsekov and Radoev denotes a certain shape of the Hilbert space. There are several many-body results in which exactly the same shape is also realized, indicating the existence of a common dynamical mechanism. Furthermore, the recurrence relations analysis shows that their approximation has other implications, not apparent in their work. Finally, this analysis also provides a systematic way of obtaining a refinement of their model.

The recurrence relations formulation is briefly summarized here in order to analyse the work of Tsekov and Radoev. Let $V(t)$ be the velocity of a particle in a fluid at time $t$. The proper equation of motion for this particle is the generalized Langevin equation

$$\frac{\mathrm{d}V(t)}{\mathrm{d}t} + \int_0^t \phi(t-t')V(t')\,\mathrm{d}t' = F(t) \tag{1}$$

where $\phi(t)$ is the memory function and $F(t)$ is the random force. For simplicity, we have adopted $\rho = 1$, where $\rho$ is the particle density. We have also suppressed the dependence on the wave vector $k$ therein. Equation (1) is the starting point of Tsekov and Radoev. The formal solution for the dynamical variable $V(t)$ is given by the recurrence relations method [5] as follows: $V(t)$ is a vector in a $d$-dimensional Hilbert space $\mathcal{S}$, spanned by basis vectors $f_0, f_1, \ldots f_{d-1}$, where $(f_n, f_{n'}) = 0$ if $n' \neq n$, $0 \leqslant n, n' \leqslant d-1$. Hence, $V(t)$ is an orthogonal expansion

$$V(t) = \sum_{n=0}^{d-1} a_n(t) f_n \tag{2}$$

where $\{a_n(t)\}$ is a family of real functions. The dimensionality $d$ is model-dependent. The distinguishing feature of this approach is that $f_n$ and $a_n(t)$ each must satisfy a unique recurrence relation.

The formal solution (2) is sufficient to describe all the physical quantities of interest implied in (1). For example, the random force $F(t)$ is an orthogonal expansion in a subspace $\mathcal{S}_1$, spanned by $f_1, f_2, \ldots f_{d-1}$

$$F(t) \equiv f_1[t] = \sum_{n=1}^{d-1} b_n(t) f_n \tag{3}$$

where $\{b_n(t)\}$ is another family of real functions but attached to the subspace $\mathcal{S}_1$. In this subspace, the $b_n(t)$ satisfy the same recurrence relation as the $a_n(t)$. The memory function is

$$\phi(t) \equiv \phi_1(t) = \left(f_1[t], f_1\right) / \left(f_0, f_0\right) = \Delta_1 b_1(t) \tag{4}$$

where $\Delta_1 = (f_1, f_1)/(f_0, f_0)$.

The time evolution of the random force $F(t) \equiv f_1[t]$ is itself also governed by equation (1). If $V(t)$ is replaced by $f_1[t]$ therein, it introduces a new random force, say $f_2[t]$. As in (3), then it too is an orthogonal expansion in a subspace $S_2$, spanned by $f_2, f_3, \ldots f_{d-1}$

$$f_2[t] = \sum_{n=2}^{d-1} c_n(t) f_n \tag{5}$$

where $\{c_n(t)\}$ similarly belongs to the subspace $S_2$ and satisfies the same recurrence relation. The corresponding memory function is

$$\phi_2(t) = (f_2[t], f_2)/(f_1, f_1) = \Delta_2 c_2(t) \tag{6}$$

where $\Delta_2 = (f_2, f_2)/(f_1, f_1)$. Evidently one can continue to define 'higher' random forces indefinitely or until the smallest subspace is reached if $d$ is finite. Now let $\hat{a}_n(z) = La_n(t)$, etc., where $L$ is the Laplace transform operator. Then,

$$\hat{a}_0(z) = 1/z + \Delta_1/z + \ldots + \Delta_{d-1}/z \tag{7a}$$

$$\hat{b}_1(z) = 1/z + \Delta_2/z + \ldots + \Delta_{d-1}/z \tag{7b}$$

$$\hat{c}_1(z) = 1/z + \Delta_3/z + \ldots + \Delta_{d-1}/z \tag{7c}$$

where $\Delta_n = (f_n, f_n)/(f_{n-1}, f_{n-1})$, and each right-hand side in the above equations denotes a continued fraction.

In the recurrence relations formulation one describes the time evolution process by means of an abstract space. This space is geometrically definable by the lengths of its basis vectors $\Delta_1, \Delta_2, \ldots \Delta_{d-1}$. If one chooses $V(t = 0) = f_0$, $V(t)$ traces a trajectory in this space. If the space has infinitely many dimensions, the trajectory is drawn as if towards an attractor embedded in the subspace $S_{n\to\infty}$. As a result, the velocity autocorrelation function $(V(t), V)$ may decay with or without an oscillation. If the space has a finite number of dimensions, there can be no decay. The autocorrelation function is purely oscillatory.

The problem which Tsekov and Radoev posed and solved can now be restated by the recurrence relations formulation. First, we shall identify Tsekov and Radoev's hydrodynamic quantities $C_{VV}$, $C_{FF}$ and $C_{UU}$. It is straightforward to recognize that $C_{VV}(t)/C_{VV}(0) = a_0(t)$ and $C_{FF}(t)/C_{FF}(0) = b_1(t)$. But to show that $C_{UU}(t)/C_{UU}(0) = c_2(t)$, it is necessary to know the second random force $f_2[t]$. From (3) it is possible to write

$$f_1[t] = b_1(t) f_1 + \int_0^t b_1(t - t') f_2[t']\, \mathrm{d}t'. \tag{8}$$

Comparing the above with their equations (2)–(3), we deduce that

$$f_2[t] = \{C_{FF}(0)/C_{VV}(0)\} U(t). \tag{9}$$

Equation (9) places the hydrodynamic model in the recurrence relations context.

The hydrodynamic model being a macroscopic model still does not contain sufficient information to be solved. Tsekov and Radoev introduce an approximation: $\hat{C}_{UU}(z) = \hat{C}_{VV}(z)$, which will be referred to as the Tsekov and Radoev model. In the recurrence relations language the Tsekov and Radoev model is given by

$$\Delta_1 \hat{a}_0(z) = \Delta_2 \hat{c}_2(z). \tag{10}$$

We shall now examine the conditions under which this model can be realized. By (7$a$) and (7$c$) the model is allowed if and only if (i) $d \to \infty$ and (ii) $\Delta_1 = \Delta_2 = \Delta_3 = \ldots \equiv u^2/4$. Then it follows at once that

$$\hat{a}_0(z) = \hat{b}_1(z) = \hat{c}_2(z) = \ldots = (2/u)\left[\sqrt{1+(z/u)^2} - z/u\right]. \tag{11}$$

Hence,

$$a_0(t) = b_1(t) = c_2(t) = \ldots = 2J_1(ut)/ut \tag{12}$$

where $J_1$ is the Bessel function. Equations (11) and (12) are what Tsekov and Radoev have obtained for their model.

We see that the model of Tsekov and Radoev means that the Hilbert space of $V(t)$ has an infinite number of dimensions and is hyperspherically shaped. It is evidently the simplest of all infinite-dimensional shapes. The same shaped Hilbert space is realized in several microscopic models [7]. In these models, the shapes of the Hilbert space are calculated *ab initio*, not given as in the model of Tsekov and Radoev. Classically, the NN coupled harmonic-oscillator chain with one impurity can yield such a Hilbert space. Quantum mechanically, the two-dimensional ideal electron gas at $T = 0$ can also yield the same. In these physical models an infinite-dimensional hyperspherical Hilbert space is obtained under only very special values of their parameters. It is not a general property of these models. It indicates therefore that the model of Tsekov and Radoev is very restrictive. It may still be physically realizable under certain hydrodynamic constraints.

The hydrodynamic model of Tsekov and Radoev belongs to a class of Hermitian many-body models whose dynamics is uniquely determined by an infinite-dimensional hyperspherical Hilbert space. For this class of models, the memory functions are all the same, i.e., $\phi_1(t) = \phi_2(t) = \ldots$. It means that the relationship between, say, the stochastic velocity $V$ and its random force $F \equiv f_1$ is identical to the relationship between $f_1$ and its random force $f_2$ and so on. Although the model of Tsekov and Radoev does not directly assume this feature, it is nevertheless implied therein.

Equation (9) shows that the effective velocity field $U$ represents the second random force if the interaction between fluid particles is linear in $V - U$. In this linear model of a fluid, the velocity field $U$ is what drives the random force $F$, which in turn drives $V$. According to the recurrence relations formulation, the velocity field $U$ is itself driven by other 'higher' random forces. A macroscopic model is thus incompletely defined if these forces are not given *a priori*. By assuming a particular shape of the Hilbert space, Tsekov and Radoev have in effect defined them, if in a very limited way.

When certain simplifying approximations (e.g., RPA) are made in microscopic many-body models, one finds regular shapes of the Hilbert space. These shapes correspond to solvable zeroth-order solutions [6]. Corrections to them are obtained if these shapes are approximately deformed successively [8]. Thus, if it is necessary to refine the model of Tsekov Radoev to be more realistic, the recurrence relations formulation provides a formal procedure by means of the Hilbert space geometry.

Also, an infinite-dimensional hyperspherical Hilbert space implies a damped oscillation in the autocorrelation function of $V(t)$. But this is not unique. There are other possible infinite-dimensional shapes which can also give rise to similar behaviour. What is more general is whether slow decay exists in the velocity autocorrelation function. It exists in a Hermitian system if and only if the Hilbert space has infinite dimensions. The existence and mechanisms of slow decay are of current interest [9].

Finally, one might ask what information is being lost, or made inaccessible, by assuming at the outset a regular shape of the Hilbert space as in the model of Tsekov and Radoev. The solution of the hydrodynamical equation or its equivalent Langevin equation depends on the random force. The random force itself depends on the interaction between fluid particles, which implies a singular shape of the Hilbert space in one-to-one correspondence. To be fully developed, it is thus necessary to specify the nature of the random force or the interaction. The hydrodynamic problem of Tsekov and Radoev, as is given, is not fully developed in this sense. Nevertheless, to uncover physical implications of the Tsekov and Radoev model, we shall employ the idea of dynamic equivalence in considering two examples, one fully developed and the other not.

Density fluctuations in a 2D electron gas at low temperatures [10] represent a fully developed problem since the interaction is known. Viewed at long wavelengths, the shape of the Hilbert space for the density fluctuations seems regular. This is the regime where the RPA becomes exact. What is not seen are irregular parts ('wrinkles') arising from the short-range correlation. The fine structure is apparent if viewed at shorter wavelengths, where the RPA breaks down. The Tsekov and Radoev model is an RPA, containing but gross features.

Next, consider a very long 1D classical harmonic-oscillator chain. Let the momentum of one end particle, say $p_1$, be the dynamical variable of interest. If the chain is monatomic and the interaction is limited to NN only, the shape of the Hilbert space for $p_1(t)$ is hyperspherical, exactly as the Tsekov and Radoev model. The hypersphere will be distorted if next NN are added. If the NN interaction is dominant, the distortion is slight and the dynamics of this harmonic oscillator chain are well described by a hyperspherical Hilbert space. Such a Hilbert space is insufficient to describe the dynamics fully if the more-distant-neighbour interaction is not weak, or if some impurities are present. What is missed is contained in the distorted part of the Hilbert space, which is inaccessible to the Tsekov and Radoev model.

As a model of hydrodynamics, the Tsekov and Radoev model is thus a long-wavelength picture of molecular collisions. Fine details are absent, as if smoothed over, as a result of 'regularizing' the shape of the Hilbert space. The fine dynamic structure, which, as noted, would reflect the short-range correlation, is typically incoherent and dominating over a short time. Some of the more coherent and long-lived modes of the correlation are, however, contained in the Tsekov and Radoev model, as evidenced by the slow decay in the velocity autocorrelation function. Not fully developed, the Tsekov and Radoev model cannot be further delineated.

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