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Stochastic differential equations for non-linear hydrodynamics

Pep Español *

Departamento de Física Fundamental, UNED, Apartado 60141, 28080 Madrid, Spain

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Abstract

We formulate the stochastic differential equations for non-linear hydrodynamic fluctuations. The equations incorporate the random forces through a random stress tensor and random heat flux as in the Landau and Lifshitz theory. However, the equations are non-linear and the random forces are non-Gaussian. We provide explicit expressions for these random quantities in terms of the well-defined increments of the Wiener process.

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1. Introduction

Two physical phenomena affect in a crucial manner the dynamics of concentrated submicron colloidal suspensions. On the one hand, the hydrodynamic interaction between the colloidal particles is responsible for the complex behavior of these systems. The motion of a colloidal particle affects the state of motion of the other particles through the perturbation of the mediating solvent. Because of the long-range nature of these interactions, this is essentially a many-body problem for which obtaining analytical results is very difficult. The second physical phenomena that intervenes crucially in the dynamics of these systems is Brownian diffusion that keeps the particles in constant thermal agitation.

Hydrodynamic interactions and Brownian diffusion are the macroscopic and mesoscopic manifestations of the hydrodynamic behavior of the solvent in which the colloidal particles are immersed. Actually, the origin of the Brownian diffusion can be traced back to the fluctuations of the hydrodynamic fields surrounding the particles. This explanation of Brownian diffusion constitutes the hydrodynamic theory of

* E-mail: pep@fisfun.uned.es.

Brownian motion [1–4] which has been successfully used to predict the celebrated long-time tails in the velocity autocorrelation of a single Brownian particle. This prediction has been confirmed by experiments [5–8].

For the case of undiluted suspensions there is no analytic theory that describes simultaneously the rheological and diffusive aspects of the system. It seems that the only viable way is to recourse to numerical simulations. For this reason, there is at present great interest in mesoscopic levels of description for complex fluids that allow to address such problems with affordable computation work. In this respect, lattice Boltzmann automata [9–12] and dissipative particle dynamics [13–18] have been useful tools in studying hydrodynamic problems as those occurring in immiscible fluids and colloidal and polymeric suspensions.

In the lattice Boltzmann technique for colloidal suspensions, one solves a simplified version of the fluctuating Boltzmann equation on a lattice [11]. The advantage of the technique is that, due to the local description of the hydrodynamic behavior, the computational time grows linearly with the number of colloidal particles instead of cubically as in Stokesian dynamics [19]. The drawback lies in the difficulty of handling irregular moving boundary conditions on a lattice. On the other hand, the spirit of dissipative particle dynamics is to formulate point particles that move similarly as the “droplets” of the fluid would move, thus capturing the hydrodynamic behavior in an off-lattice technique. This approach is similar to the smoothed particle hydrodynamics technique [20,21] in which the macroscopic hydrodynamic equations are discretized on moving points. Smoothed particle dynamics, as opposed to dissipative particle dynamics, does not include any thermal randomness into account. Therefore, it is not clear how the fluctuations induced by the discreteness of the system are consistent with thermal fluctuations that have a microscopic origin. In order to clarify this point it is desirable to have a well-defined formulation for the Langevin equations for hydrodynamic fields.

There exists a well-known theory for hydrodynamic fluctuations which was formulated by Landau and Lifshitz in 1957 [22]. It consists basically on adding stochastic fluxes to the stress tensor and heat flux. The noise amplitude is determined by the temperature and the transport coefficients of the fluid. The main problem in trying to apply the Landau–Lifshitz theory for numerical simulations of time-dependent flows as those arising in fluctuating fluid solvents in colloidal suspensions can be summarized in the question, what value of the temperature (fluctuating and in general non-uniform) should one use in the noise amplitude? And, if the transport coefficients depend on the state of the fluid, what values of the hydrodynamic variables should one use, fluctuating or average values? These questions should be answered satisfactorily in any attempt to conduct numerical simulations of non-equilibrium time-dependent fluctuating fluids.

The Landau and Lifshitz theory deals with *linear* fluctuations around equilibrium states but the theory has been further generalized to linear fluctuations around non-equilibrium steady states [23]. However, hydrodynamics contains non-linearities coming from the dependence of the transport coefficients on the state variables and to the presence of quadratic terms in the Raighley dissipation function. There have been several attempts to study non-linear hydrodynamic fluctuations within the framework

of Fokker–Planck descriptions [24–28]. Fokker–Planck equations (FPEs) for hydrodynamic fluctuations are well-known since the early 1980s. What does not seem to be known are the stochastic differential equations (SDE) associated to the FPE. In the most general and complete work dealing with FPE for hydrodynamic variables, Zubarev and Morozov conclude that “the problem of the adequate Langevin equations describing *nonlinear* hydrodynamic fluctuations seems to be still open” [28]. In another important paper, van Saarloos et al. [27] formulate the Langevin equations for non-linear fluctuations by assuming that the random fluxes are Gaussian processes with white noise. This leads to an inconsistency in the form of particular unrealistic functional dependences of the transport coefficients on the temperature. In addition, the Einstein distribution function is not the equilibrium solution of the corresponding Fokker–Planck equation [28].

In this paper we formulate the appropriate SDE for nonlinear hydrodynamic interactions starting from first principles, i.e. from the FPE for hydrodynamic fields derived in Ref. [28]. The derivation of these Langevin equations is a necessary initial step in order to have well-defined starting points for numerical algorithms in which both the macroscopic and mesoscopic aspects of hydrodynamics are captured consistently. We provide explicit expressions for the random stress tensor and the random heat flux in terms of the increments of the Wiener process. The fluxes are shown to be non-Gaussian processes. These explicit forms for the random fluxes allow to implement a numerical simulation of the fluctuating hydrodynamic equations straightforwardly.

The formulation of the stochastic differential equations as appearing in this paper has an additional advantage when performing numerical simulations over the usual linear hydrodynamic fluctuations approach [29,30]. For the case of linear hydrodynamic fluctuations around non-equilibrium states, one has to first compute the non-equilibrium state of the system (usually assumed to be stationary) and then linearize the equations around this steady state. This involves a two-step procedure, whereas in the formulation of the present paper a single simulation produces simultaneously the mean motion and the fluctuations in one go. This is similar in spirit to the hydrostochastic formulation of Breuer and Petruccione, where a master equation is formulated for the hydrodynamic fields [31]. It is apparent that for the simulation of the hydrodynamic solvent between colloidal particles where the non-equilibrium (non-stationary) state is not even known, the approach of linear hydrodynamics is completely useless.

A word is in order about the procedure we follow for deriving the stochastic differential equations for the hydrodynamic equations. It is possible to obtain from first principles (for example with projection operator techniques) the Langevin equations governing the hydrodynamic variables. However, we have discussed at length in Ref. [32] that this procedure has the shortcoming that it does not provide information about moments of the random forces higher than the second one. Therefore, issues about the Gaussian nature of the noise cannot be resolved. For this reason, we follow in this paper a different route that is based on the mathematical equivalence between the Fokker–Planck equation and the corresponding stochastic differential equation [33]. Given a Fokker–Planck equation one can read from the coefficients of the equation

which is the corresponding Langevin equation for the stochastic process (with its appropriate stochastic interpretation, Ito or Stratonovich). There are no physical approximations involved in this procedure. A close analogy arises with the connection between the Liouville equation and the Hamilton equations in classical mechanics. They are mathematically equivalent representations of the same process (in this case a deterministic process). The actual interest of looking at Langevin equations instead of Fokker–Planck equations arises from a computational point of view. Langevin equations are much more easier to simulate than to solve a partial differential equation as the Fokker–Planck equation.

This paper is notationally a bit cumbersome. This is quite an inescapable situation given that we are dealing with five continuous hydrodynamic fields. In order to alleviate a bit this we have decided to give the structure of the Fokker–Planck equation and the corresponding stochastic differential equation for arbitrary fields before particularizing to the case of hydrodynamic fields. In any case, the final results have a very compact structure closely reminiscent to the Landau and Lifshitz theory.

The paper is distributed as follows. In Section 2 we discuss the definition of the coarse-grained hydrodynamic variables in some detail. In Section 3 we rewrite the standard FPE for the case that the set of relevant variables are extensive variables characterized by a discrete index associated to a lattice (i.e. a field defined on a lattice). We also write the FPE equation corresponding to the densities of the extensive variables. This FPE is then expressed in terms of functional derivatives. Section 4 is devoted to the equivalent SDE for fields on a lattice and its corresponding functional Langevin equation where precise meaning to the white noise term is given. In Section 5, the general FPE for fields on a lattice obtained in Section 3 is particularized to the case that the fields are the hydrodynamic fields. Section 6 is devoted to the derivation of the SDE for hydrodynamic fields. Finally, we discuss the results in the last section.

2. Hydrodynamic variables

Our aim is to obtain the FPE for the hydrodynamic continuous fields. From a mathematical point of view there are subtleties regarding the existence of the continuum limit for stochastic variables and for this reason we will restrict ourselves to the case that the fields are defined on a lattice. In this section we discuss the discrete variables that are representative of the hydrodynamic fields. A word is in order about the definition of the lattice of points \mathbf{r} . This lattice is usually taken as a regular cubic lattice [27]. In the formulation that follows there is no restriction, however, to the kind of lattice that can be used and irregular lattices are also possible. To each lattice point we associate a *volume element* of volume v_r that defines the region of space associated to each lattice point. In the case of the cubic lattice it is natural to associate a cubic cell of volume e^3 . For irregular lattices, the Voronoi tessellation allows to define non-overlapping volume elements that cover all the space [34]. Note that the cubic cell is a special case of Voronoi tessellation for the case of a regular cubic lattice.

We take as relevant variables the total mass $M_{\mathbf{r}}$, the total momentum $\mathbf{P}_{\mathbf{r}}$ and total energy $E_{\mathbf{r}}$ of that set of particles that are within the volume element associated to the lattice point \mathbf{r} . In compact form, $M_{\mathbf{r}}, \mathbf{P}_{\mathbf{r}}, E_{\mathbf{r}} \rightarrow A_{\mathbf{r}}^m$ with $m = 0, \dots, 4$. Because these variables are conserved variables, one expects that their dynamics is much slower than any other set of dynamic variables in such a way that they form a closed description for the system. The size of the volume elements should be so large that the relevant variables can be considered as continuous. For example, if a single particle enters the cell, the variation of the mass of the cell can be considered as infinitesimal.

In mathematical terms, the relevant variables are given by

$$M_{\mathbf{r}} = \sum_i m \chi_{\mathbf{r}}(\mathbf{q}_i), \quad \mathbf{P}_{\mathbf{r}} = \sum_i \mathbf{p}_i \chi_{\mathbf{r}}(\mathbf{q}_i), \quad E_{\mathbf{r}} = \sum_i e_i \chi_{\mathbf{r}}(\mathbf{q}_i), \quad (1)$$

where we denote by $\mathbf{q}_i, \mathbf{p}_i$ the position and momentum of particle i and its energy is

$$e_i = \frac{\mathbf{p}_i^2}{2m} + \frac{1}{2} \sum_j' \phi(\mathbf{q}_i, \mathbf{q}_j). \quad (2)$$

The function $\chi_{\mathbf{r}}(\mathbf{q})$ is the characteristic function of the cell centered at \mathbf{r} , which takes values 1 if \mathbf{q} belongs to the cell and 0 otherwise. The volume of the cell at \mathbf{r} is given by

$$v_{\mathbf{r}} = \int d\mathbf{r}' \chi_{\mathbf{r}}(\mathbf{r}'). \quad (3)$$

If we displace the position \mathbf{q}_i of all the particles a vector \mathbf{r}' and simultaneously displace the location of the cell at \mathbf{r} the same vector \mathbf{r}' , the numerical value of $\chi_{\mathbf{r}}(\mathbf{q}_i)$ will not change. This translational invariance implies that $\chi_{\mathbf{r}}(\mathbf{q}_i) = \chi_{\mathbf{r}}(\mathbf{q}_i - \mathbf{r})$. It is apparent that if all cells are identical in shape as occurs in regular lattices, we can suppress the label \mathbf{r} of the characteristic function, i.e. $\chi_{\mathbf{r}}(\mathbf{q}_i - \mathbf{r}) = \chi(\mathbf{q}_i - \mathbf{r})$.

The density variables associated to our selected extensive variables are

$$\begin{aligned} \rho_{\mathbf{r}} &= \frac{M_{\mathbf{r}}}{v_{\mathbf{r}}} \equiv \sum_i m \bar{\delta}_{\mathbf{r}}(\mathbf{r} - \mathbf{q}_i), \\ \mathbf{g}_{\mathbf{r}} &= \frac{\mathbf{P}_{\mathbf{r}}}{v_{\mathbf{r}}} \equiv \sum_i \mathbf{p}_i \bar{\delta}_{\mathbf{r}}(\mathbf{r} - \mathbf{q}_i), \\ e_{\mathbf{r}} &= \frac{E_{\mathbf{r}}}{v_{\mathbf{r}}} \equiv \sum_i e_i \bar{\delta}_{\mathbf{r}}(\mathbf{r} - \mathbf{q}_i), \end{aligned} \quad (4)$$

where we have introduced

$$\bar{\delta}_{\mathbf{r}}(\mathbf{r}') = \chi_{\mathbf{r}}(\mathbf{r}')/v_{\mathbf{r}} \quad (5)$$

that satisfies by virtue of Eq. (3) the normalization condition

$$\int d\mathbf{r}' \bar{\delta}_{\mathbf{r}}(\mathbf{r}') = 1. \quad (6)$$

The velocity field is defined by

$$\mathbf{v}_r \equiv \frac{\mathbf{g}_r}{\rho_r}. \quad (7)$$

Note that $\sum_r v_r \rho_r = \sum_r M_r$, etc. We want to have $\sum_r M_r$ equal to the total mass of the systems and this is only possible if the cells are non-overlapping and cover all the space. If this condition is not met, then $\sum_r M_r$ is not a conserved variable and one does not expect it to be a slow variable.

For the case of a cubic lattice with cubic volume elements, the characteristic function can be represented as a product of square step functions in the x, y, z directions. One can argue that if the particles have some finite size, then it is meaningful to smooth out the step functions at the borders of the cell and to talk about fractions of a particle being in different cells. Actually, one could use coarsening functions other than $\bar{\delta}_r(\mathbf{r}')$ or these smoothed square step functions defining the “shape” of the cell. Zubarev and Morozov make use of a particular coarse-graining procedure in which the hydrodynamic fields are represented in a Fourier basis and then only the small $k < k_0$ components are retained [28]. In real space this is equivalent to use a coarse graining function of the form

$$\chi(r) = \frac{k_0^3}{2\pi^2} \left[\frac{\sin k_0 r}{(k_0 r)^3} - \frac{\cos k_0 r}{(k_0 r)^2} \right]. \quad (8)$$

This particular coarse-graining produces a coarse-grained density field that is not everywhere positive. This can be cured, for example, by using a Gaussian function

$$\Delta(r) = \frac{1}{\pi^{3/2}} \exp - (r/\varepsilon)^2, \quad (9)$$

where ε is a coarse-graining length. Nevertheless, in this paper we will restrict ourselves to the use of the coarse-graining function $\bar{\delta}_r(\mathbf{r}')$ derived from the characteristic function of each cell, Eq. (5).

We will need the time derivatives of the hydrodynamic variables. They have the form

$$\begin{aligned} iL\rho_r &= -\nabla_r \cdot \mathbf{g}_r, \\ iL\mathbf{g}_r &= -\nabla_r \cdot \sigma_r, \\ iLe_r &= -\nabla_r \cdot \tau_r, \end{aligned} \quad (10)$$

where the coarse-grained stress tensor and energy flux are given by the usual expressions (see, for example, Ref. [35]).

A remark on the meaning of ∇_r is in order. In obtaining Eq. (10) we have used

$$\frac{\partial}{\partial \mathbf{q}_i} \bar{\delta}_r(\mathbf{r} - \mathbf{q}_i) = -\frac{\partial}{\partial \mathbf{r}} \bar{\delta}_r(\mathbf{r} - \mathbf{q}_i), \quad (11)$$

where we assume that the index \mathbf{r} is continuous. In fact, Eq. (11) is a mathematical identity. However, we will evaluate the right-hand side of Eq. (11) only at the discrete values of the vector \mathbf{r} . There is no need to use discretized forms for the nabla operator with this understanding [27].

3. FPE for fields

Zwanzig derived from first principles the Fokker–Planck equation for the distribution function of a discrete set of variables with the aid of a projection operator technique [36]. The derivation provided explicit expressions for the drift and diffusion terms of the equation in terms of microscopic quantities. In this section, we will present the FPE for the case that the set of discrete variables are extensive variables A_r^m (or simply A) defined in each cell. We will also give the FPE for the distribution function of the densities $\tilde{A}_r^m = A_r^m/v_r$.

Let us consider an isolated system governed by Hamilton's equation of motion ($H(z)$ is the Hamiltonian and iL is Liouville's operator for the dynamics). The microscopic degrees of freedom are denoted by z . The FPE is a differential equation for the probability density $p(\alpha, t)$ that the system takes values α at time t for the phase functions $A(z)$, i.e.,

$$p(\alpha, t) \equiv \int \rho_t(z) \delta(A(z) - \alpha) dz, \quad (12)$$

where $\delta(A(z) - \alpha)$ is a product of Dirac's delta functions, one for each relevant variable, and $\rho_t(z)$ is the solution of Liouville's equation.

The FPE is [28,32,36,35]

$$\partial_t p(\alpha, t) = - \sum_{mr} \frac{\partial}{\partial \alpha_r^m} K_r^m(\alpha) p(\alpha, t) + \frac{1}{2} \sum_{mr} \sum_{m'r'} \frac{\partial}{\partial \alpha_r^m} \frac{\partial}{\partial \alpha_{r'}^{m'}} D_{rr'}^{mm'}(\alpha) p(\alpha, t) \quad (13)$$

with the following definitions:

$$K_r^m(\alpha) \equiv v_r^m(\alpha) + \sum_{m'r'} \zeta_{rr'}^{mm'}(\alpha) F_{r'}^{m'}(\alpha) + \sum_{m'r'} \frac{\partial}{\partial \alpha_r^m} \zeta_{rr'}^{mm'}(\alpha) \quad (14)$$

with

$$\begin{aligned} v_r^m(\alpha) &\equiv \langle iLA_r^m \rangle^\alpha, \\ \zeta_{rr'}^{mm'}(\alpha) &\equiv \int_0^\infty du \left\langle (\delta iLA_r^m \delta iLA_{r'}^{m'}(u)) \right\rangle^\alpha, \\ F_r^m(\alpha) &\equiv \frac{\partial}{\partial \alpha_r^m} \ln \Omega(\alpha), \\ \Omega(\alpha) &\equiv \int \delta(A(z) - \alpha) dz, \\ D_{rr'}^{mm'}(\alpha) &\equiv \zeta_{rr'}^{mm'}(\alpha) + \zeta_{r'r}^{m'm}(\alpha), \end{aligned} \quad (15)$$

where we have defined the projected part $\delta iLA_r^m \equiv iLA_r^m - \langle iLA_r^m \rangle^\alpha$.

We have introduced the average of an arbitrary phase function G over the submanifold $A(z) = \alpha$ by

$$\langle G \rangle^\alpha \equiv \frac{1}{\Omega(\alpha)} \int \delta(A(z) - \alpha) G(z) dz. \quad (16)$$

The derivation of the FPE from the underlying microscopic dynamics of the system relies on the fact that the relevant variables A are much slower than the rest of variables of the system. This allows for a Markovian memoryless description of the dynamics of these relevant variables. A systematic expansion of a microscopically exact master equation in terms of a slowness parameter (which is, essentially, the ratio between time scales between relevant and irrelevant variables) has been carried out by Mori et al. [37]. To second order in the slowness parameter the non-linear FPE (Eq. (13)) is obtained.

In the microscopic formulation of the FPE the drift K_r^m and the diffusion tensor $D_{rr'}^{mm'}$ are defined in terms of microscopic quantities. The problem is that these quantities are difficult to compute. Basically, three difficulties have to be resolved: the calculation of the averages $\langle \dots \rangle^\alpha$, the calculation of the thermodynamic forces F_r^m (or equivalently of the phase-space volume $\Omega(\alpha)$) and finally the calculation of the correlation functions in the kinetic tensor $\zeta_{rr'}^{mm'}$. The first two are closely related and can be resolved for the case of hydrodynamic variables by resorting to the local equilibrium approximation. The explicit calculation of the kinetic coefficients is much more difficult and they are simply left as phenomenological coefficients.

The rest of the section is devoted to the FPE equation for the distribution function of the densities $\tilde{A}_r^m = A_r^m/v_r$. The corresponding FPE is obtained by a simple change of variables:

$$\begin{aligned} \partial_t p(v_r \tilde{\alpha}, t) = & - \sum_{mr} \frac{\partial}{\partial \tilde{\alpha}_r^m} \frac{1}{v_r} K_r^m(v_r \tilde{\alpha}) p(v_r \tilde{\alpha}, t) \\ & + \frac{1}{2} \sum_{mr} \sum_{m'r'} \frac{\partial}{\partial \tilde{\alpha}_r^m} \frac{\partial}{\partial \tilde{\alpha}_{r'}^{m'}} \frac{1}{v_r^2} D_{rr'}^{mm'}(v_r \tilde{\alpha}) p(v_r \tilde{\alpha}, t), \end{aligned} \quad (17)$$

where $\tilde{\alpha}_r^m = \alpha_r^m/v_r$. We therefore introduce in a natural way the following quantities:

$$\begin{aligned} P[\tilde{\alpha}, t] & \equiv \prod_r^M v_r p(v \tilde{\alpha}, t), & K_r^m[\tilde{\alpha}] & \equiv \frac{1}{v_r} K_r^m(v \tilde{\alpha}), \\ D_{rr'}^{mm'}[\tilde{\alpha}] & = \frac{1}{v_r^2} D_{rr'}^{mm'}(v \tilde{\alpha}), & F_r^m[\tilde{\alpha}] & \equiv F_r^m(v \tilde{\alpha}), \\ v_r^m[\tilde{\alpha}] & \equiv \frac{1}{v_r} v_r^m(v \tilde{\alpha}), & \zeta_{rr'}^{mm'}[\tilde{\alpha}] & \equiv \frac{1}{v_r^2} \zeta_{rr'}^{mm'}(v \tilde{\alpha}), & \Omega[\tilde{\alpha}] & \equiv \Omega(v \tilde{\alpha}). \end{aligned} \quad (18)$$

We use square brackets to denote that the left-hand sides have different functional forms from the right-hand side (for example, $F_r^m[\tilde{\alpha}]$ is a different function of its argument from $F_r^m(v \tilde{\alpha})$ even though they are named with the same symbol F_r^m). M is the total number of variables. In this way, the probability density $P[\tilde{\alpha}, t]$ is normalized to unity, i.e., $\int \mathcal{D}\tilde{\alpha} P[\tilde{\alpha}, t] = 1$, where $\mathcal{D}\tilde{\alpha}$ is a short hand for $d\tilde{\alpha}^M$.

Note that these definitions (Eq. (18)) allow to express the reversible part of the drift and the kinetic tensor in terms of averages over density fields:

$$\begin{aligned} v_r^m[\tilde{\alpha}] &= \langle i\tilde{L}_r^m \rangle^{v\tilde{\alpha}}, \\ \zeta_{rr'}^{mm'}[\tilde{\alpha}] &= \int_0^\infty du \langle (\delta i\tilde{L}_r^m)(\delta i\tilde{L}_{r'}^{m'}(u)) \rangle^{v\tilde{\alpha}}, \end{aligned} \quad (19)$$

where we have defined the projected part $\delta i\tilde{L}_r^m \equiv i\tilde{L}_r^m - \langle i\tilde{L}_r^m \rangle^{v\tilde{\alpha}}$. With the definitions (Eq. (18)) the FPE for the density fields is

$$\partial_t P[\tilde{\alpha}, t] = - \sum_{mr} \frac{\partial}{\partial \tilde{\alpha}_r^m} K_r^m[\tilde{\alpha}] P[\tilde{\alpha}, t] + \frac{1}{2} \sum_{mr} \sum_{m'r'} \frac{\partial}{\partial \tilde{\alpha}_r^m} \frac{\partial}{\partial \tilde{\alpha}_{r'}^{m'}} D_{rr'}^{mm'}[\tilde{\alpha}] P[\tilde{\alpha}, t] \quad (20)$$

with

$$\begin{aligned} K_r^m[\tilde{\alpha}] &= v_r^m[\tilde{\alpha}] + \sum_{r'} v_r \zeta_{rr'}^{mm'}[\tilde{\alpha}] F_{r'}^{m'}[\tilde{\alpha}] + \sum_{r'} \frac{\partial}{\partial \tilde{\alpha}_{r'}^{m'}} \zeta_{rr'}^{mm'}[\tilde{\alpha}], \\ F_{r'}^{m'}[\tilde{\alpha}] &= \frac{1}{v_r} \frac{\partial}{\partial \tilde{\alpha}_{r'}^{m'}} \ln \Omega[\tilde{\alpha}], \\ D_{rr'}^{mm'}[\tilde{\alpha}] &= \zeta_{rr'}^{mm'}[\tilde{\alpha}] + \zeta_{r'r}^{m'm}[\tilde{\alpha}]. \end{aligned} \quad (21)$$

The FPE for the densities (Eq. (20)) admits a suggestive continuum notation. By making the substitutions of partial derivatives by functional derivatives according to

$$\frac{1}{v_r} \frac{\partial}{\partial \tilde{\alpha}_r^m} \rightarrow \frac{\delta}{\delta \tilde{\alpha}_r^m} \quad (22)$$

and sums by integrals

$$\sum_r v_r \rightarrow \int d\mathbf{r}, \quad (23)$$

we can write Eq. (20) in functional form,

$$\partial_t P[\tilde{\alpha}, t] = - \int d\mathbf{r} \frac{\delta}{\delta \tilde{\alpha}_r^m} K_r^m[\tilde{\alpha}] P[\tilde{\alpha}, t] + \frac{1}{2} \int d\mathbf{r} \int d\mathbf{r}' \frac{\delta}{\delta \tilde{\alpha}_r^m} \frac{\delta}{\delta \tilde{\alpha}_{r'}^{m'}} D_{rr'}^{mm'}[\tilde{\alpha}] P[\tilde{\alpha}, t] \quad (24)$$

with

$$\begin{aligned} K_r^m[\tilde{\alpha}] &= v_r^m[\tilde{\alpha}] + \int d\mathbf{r}' \zeta_{rr'}^{mm'}[\tilde{\alpha}] F_{r'}^{m'}[\tilde{\alpha}] + \int d\mathbf{r}' \frac{\delta}{\delta \tilde{\alpha}_{r'}^{m'}} \zeta_{rr'}^{mm'}[\tilde{\alpha}], \\ F_{r'}^{m'}[\tilde{\alpha}] &= \frac{\delta}{\delta \tilde{\alpha}_{r'}^{m'}} \ln \Omega[\tilde{\alpha}], \\ D_{rr'}^{mm'}[\tilde{\alpha}] &= \zeta_{rr'}^{mm'}[\tilde{\alpha}] + \zeta_{r'r}^{m'm}[\tilde{\alpha}]. \end{aligned} \quad (25)$$

The functional FPE (Eq. (24)) is understood in this work simply as a notational device and the mathematically well-defined FPE is the discrete FPE (Eq. (20)).

4. Stochastic differential equation for fields

As it is well known [33], associated to the FPE there is a stochastic differential equation (SDE) describing the stochastic process $\alpha(t)$. The SDE corresponding to the FPE (Eq. (20)) is given by

$$d\tilde{\alpha}_{\mathbf{r}}^m(t) = K_{\mathbf{r}}^m[\tilde{\alpha}(t)] dt + \sum_{m'\mathbf{r}'} B_{\mathbf{r}\mathbf{r}'}^{mm'}[\tilde{\alpha}(t)] dW_{\mathbf{r}'}^{m'}(t), \quad (26)$$

where we have introduced the independent increments of the Wiener process associated to each cell \mathbf{r} . These increments satisfy the mnemotechnical rule for Itô calculus:

$$dW_{\mathbf{r}}^m(t) dW_{\mathbf{r}'}^{m'}(t') = \delta_{mm'} \delta_{\mathbf{r}\mathbf{r}'} dt \quad \text{if } t = t' \quad (27)$$

and zero if $t \neq t'$. The Kronecker delta $\delta_{\mathbf{r}\mathbf{r}'}$ is one if $\mathbf{r} = \mathbf{r}'$ and zero otherwise. The matrix $B_{\mathbf{r}\mathbf{r}'}^{mm'}[\tilde{\alpha}]$ is the square root in matrix sense of $D_{\mathbf{r}\mathbf{r}'}^{mm'}[\tilde{\alpha}]$, this is

$$\sum_{m'\mathbf{r}'} B_{\mathbf{r}\mathbf{r}'}^{mm'}[\tilde{\alpha}] B_{\mathbf{r}'\mathbf{r}'}^{m''m'}[\tilde{\alpha}] = D_{\mathbf{r}\mathbf{r}'}^{mm''}[\tilde{\alpha}]. \quad (28)$$

The SDE (Eq. (26)) is interpreted in Itô sense. This interpretation is most convenient for numerical simulations because the increment of the Wiener process is uncorrelated with the variables at the same time. For a discussion of the advantages of deriving stochastic differential equations from first principles through the FPE route instead of directly from the microscopic dynamics, see Ref. [32].

A physically suggestive way of writing the SDE (Eq. (26)) is by using white noise in space and time defined as

$$\eta^m(\mathbf{r}, t) \equiv \frac{dW_{\mathbf{r}}^m(t)}{\sqrt{v_{\mathbf{r}}} dt}. \quad (29)$$

We thus write Eq. (26) as an ordinary differential equation, i.e., in the form of a Langevin equation

$$\partial_t \tilde{\alpha}_{\mathbf{r}}^m(t) = K_{\mathbf{r}}^m[\tilde{\alpha}(t)] + \int d\mathbf{r}' \tilde{B}_{\mathbf{r}\mathbf{r}'}^{mm'}[\tilde{\alpha}(t)] \eta^{m'}(\mathbf{r}', t), \quad (30)$$

where we have introduced the “continuous” matrix $\tilde{B}_{\mathbf{r}\mathbf{r}'}^{mm'}[\alpha(t)] = B_{\mathbf{r}\mathbf{r}'}^{mm'}[\alpha(t)]/\sqrt{v_{\mathbf{r}}}$ that satisfies

$$\int d\mathbf{r}' \tilde{B}_{\mathbf{r}\mathbf{r}'}^{mm'}[\tilde{\alpha}] \tilde{B}_{\mathbf{r}'\mathbf{r}'}^{m''m'}[\tilde{\alpha}] = D_{\mathbf{r}\mathbf{r}'}^{mm''}[\tilde{\alpha}]. \quad (31)$$

The white noise term has the following correlation:

$$\begin{aligned} \left\langle \eta^m(\mathbf{r}, t) \eta^{m'}(\mathbf{r}', t') \right\rangle &= \left\langle \frac{dW_{\mathbf{r}}^m(t)}{\sqrt{v_{\mathbf{r}}} dt} \frac{dW_{\mathbf{r}'}^{m'}(t')}{\sqrt{v_{\mathbf{r}'}} dt'} \right\rangle \\ &= \delta_{mm'} \frac{\delta_{\mathbf{r}\mathbf{r}'}}{v_{\mathbf{r}}} \frac{1}{dt} \quad \text{if } t = t' \end{aligned} \quad (32)$$

and zero if $t \neq t'$. We can rewrite this correlation as follows:

$$\langle \eta^m(\mathbf{r}, t) \eta^{m'}(\mathbf{r}', t') \rangle = \delta_{mm'} \delta(\mathbf{r} - \mathbf{r}') \delta(t - t'). \quad (33)$$

The reason for such a procedure is that the expression given by Eq. (33) will give the same results as Eq. (32) when computing averages and correlations. Indeed, let us consider the noise term in Eq. (26) which is given by

$$f_{\mathbf{r}}^m(t) dt \equiv \sum_{\mathbf{r}'} B_{\mathbf{r}\mathbf{r}'}^{mm'} [\alpha(t)] dW^{m'}(\mathbf{r}, t). \quad (34)$$

The notation suggests that $f_{\mathbf{r}}^m(t)$ is related to the derivative of the Wiener process that does not exist in a strict sense. Nevertheless, with the understanding that $f_{\mathbf{r}}^m(t) dt$ will appear always inside integral expressions (which will be interpreted as stochastic integrals) such a procedure leads to correct results. For example, the correlation of the noise terms (Eq. (34)) will be

$$\begin{aligned} & \left\langle \int dt \int dt'' f_{\mathbf{r}}^m(t) f_{\mathbf{r}''}^{m''}(t'') \right\rangle \\ &= \left\langle \int \int \sum_{\mathbf{r}'} B_{\mathbf{r}\mathbf{r}'}^{mm'} [\tilde{\alpha}(t)] dW^{m'}(\mathbf{r}, t) \times \sum_{\mathbf{r}'''} B_{\mathbf{r}'''\mathbf{r}''}^{m''m'''} [\tilde{\alpha}(t')] dW^{m'''}(\mathbf{r}''', t') \right\rangle \\ &= \left\langle \int dt \sum_{\mathbf{r}'} B_{\mathbf{r}\mathbf{r}'}^{mm'} [\tilde{\alpha}(t)] B_{\mathbf{r}'\mathbf{r}'}^{m''m'} [\tilde{\alpha}(t)] \right\rangle \\ &= \int dt \int \mathcal{D}\tilde{\alpha} P[\tilde{\alpha}, t] D_{\mathbf{r}\mathbf{r}'}^{mm''} [\tilde{\alpha}] = \int dt \langle D_{\mathbf{r}\mathbf{r}'}^{mm''} \rangle_t \end{aligned} \quad (35)$$

where Itô rule (Eq. (27)) has been used. Note that one can write

$$\langle f_{\mathbf{r}}^m(t) f_{\mathbf{r}''}^{m''}(t'') \rangle = \delta(t - t'') \langle D_{\mathbf{r}\mathbf{r}''}^{mm''} \rangle_t \quad (36)$$

because if one integrates over t, t'' one recovers Eq. (35) and the integration limits are arbitrary.

On the other hand, in the continuous version (Eq. (30)) the noise term is given by

$$f_{\mathbf{r}}^m(t) \equiv \int d\mathbf{r}' \tilde{B}_{\mathbf{r}\mathbf{r}'}^{mm'} [\tilde{\alpha}(t)] \eta^{m'}(\mathbf{r}', t). \quad (37)$$

Now, if we use the continuum version (Eq. (37)) and proceed with the ordinary calculus rules (and the fact that the noise is uncorrelated with the variables at the same time) we will have

$$\begin{aligned} & \left\langle \int dt \int dt' f_{\mathbf{r}}^m(t) f_{\mathbf{r}'}^{m'}(t') \right\rangle \\ &= \left\langle \int dt \int dt' \int d\mathbf{r} \tilde{B}_{\mathbf{r}\mathbf{r}'}^{mm'} [\tilde{\alpha}(t)] \eta^{m'}(\mathbf{r}, t) \right. \\ & \quad \times \left. \int d\mathbf{r}'' \tilde{B}_{\mathbf{r}''\mathbf{r}'}^{m''m'''} [\tilde{\alpha}(t')] \eta^{m'''}(\mathbf{r}'', t') \right\rangle \end{aligned}$$

$$\begin{aligned}
&= \int dt \int dt' \int d\mathbf{r}' \int d\mathbf{r}''' \left\langle \tilde{B}_{\mathbf{r}'''}^{mm'}[\tilde{\alpha}(t)] \tilde{B}_{\mathbf{r}',\mathbf{r}'''}^{m''m'''}[\tilde{\alpha}(t')] \right\rangle \left\langle \eta^{m'}(\mathbf{r}',t) \eta^{m'''}(\mathbf{r}''',t') \right\rangle \\
&= \int dt \int d\mathbf{r}' \left\langle \tilde{B}_{\mathbf{r}'}^{mm'}[\tilde{\alpha}(t)] \tilde{B}_{\mathbf{r}',\mathbf{r}'}^{m''m'''}[\tilde{\alpha}(t)] \right\rangle \\
&= \int dt \left\langle D_{\mathbf{r}'}^{mm'}[\tilde{\alpha}(t)] \right\rangle
\end{aligned} \tag{38}$$

which provides the same result as Eq. (35).

5. Fokker–Planck equation for a simple fluid

Now we wish to specify the FPE (Eq. (20)) for the case that the continuum variables $\tilde{A}_{\mathbf{r}}^m$ are the hydrodynamic variables. This has been done explicitly in Ref. [28] for the case that the coarse-grained hydrodynamic fields are defined in terms of the small $k < k_0$ Fourier components. In order to derive the SDE (Eq. (30)) we found it more convenient to work with the coarse-grained hydrodynamic fields defined in terms of the densities (i.e. extensive variables divided by the volume of the cell). For this case the derivation of the explicit forms for the drift and diffusion terms follows very similar lines as those of Ref. [28] and, therefore, only the final results are quoted here. The physical assumptions underlying the derivation of the Fokker–Planck equation for hydrodynamic variables are essentially that the fields are slowly varying in space and time. Therefore, a second-order expansion in gradients is allowed along with a Markovian assumption. Consistently, the concept of local equilibrium is advocated. These assumptions are thoroughly discussed by Zubarev and Morozov [28].

The thermodynamic forces $F_{\mathbf{r}}^m[\tilde{\alpha}]$ are given by

$$\begin{aligned}
F_{\mathbf{r}}^0[\tilde{\alpha}] &= -\frac{1}{T_{\mathbf{r}}} \left(\mu_{\mathbf{r}} - \frac{\mathbf{v}_{\mathbf{r}}^2}{2} \right), \\
F_{\mathbf{r}}^v[\tilde{\alpha}] &= -\frac{\mathbf{v}_{\mathbf{r}}^v}{T_{\mathbf{r}}}, \\
F_{\mathbf{r}}^A[\tilde{\alpha}] &= \frac{1}{T_{\mathbf{r}}} \equiv \beta_{\mathbf{r}},
\end{aligned} \tag{39}$$

where $T_{\mathbf{r}}$ is the temperature and $\mu_{\mathbf{r}}$ is the chemical potential which are given in terms of the equilibrium equations of state, which is

$$\begin{aligned}
T_{\mathbf{r}} &= T^{eq}(\rho_{\mathbf{r}}, \varepsilon_{\mathbf{r}}), \\
\mu_{\mathbf{r}} &= \mu^{eq}(\rho_{\mathbf{r}}, \varepsilon_{\mathbf{r}}),
\end{aligned} \tag{40}$$

where the internal energy is $\varepsilon \equiv e - \frac{1}{2}\rho\mathbf{v}^2$. Note that the thermodynamic parameters $F_{\mathbf{r}}^m[\tilde{\alpha}]$ which are, in principle, functionals of the fields become local functions of the density variables, i.e., $F_{\mathbf{r}}^m[\tilde{\alpha}] = F^m(\tilde{\alpha}_{\mathbf{r}})$.

The reversible part $v_r^m[\tilde{\alpha}]$ of the drift term (Eq. (19)) is given by

$$\begin{aligned}\langle iL\rho_r \rangle^{\tilde{\alpha}} &= -\nabla \cdot \mathbf{g}_r, \\ \langle iL\mathbf{g}_r \rangle^{\tilde{\alpha}} &= -\nabla \cdot [\mathbf{v}_r \mathbf{v}_r \rho_r + p_r \mathbf{1}], \\ \langle iLe_r \rangle^{\tilde{\alpha}} &= -\nabla \cdot [\mathbf{v}_r(e_r + p_r)],\end{aligned}\quad (41)$$

where p_r is the equilibrium pressure evaluated at the instantaneous values of the hydrodynamic fields, i.e., $p_r = p^{eq}(\rho_r, e_r)$.

The kinetic tensor is given by Eq. (19). Note that the components corresponding to the density field vanish because this field has no projected part, i.e. $\langle iL\rho_r \rangle^{\tilde{\alpha}} = iL\rho_r$, see Eq. (41). This imply that the only components different from zero correspond to the momentum density and the energy density. The explicit forms are

$$\begin{aligned}\zeta_{rr'}^{2\beta} &= \partial_{r_\mu} \partial_{r'_\nu} \delta(\mathbf{r} - \mathbf{r}') L_r^{\alpha\mu\beta\nu}, \\ \zeta_{rr'}^{24} &= \partial_{r_\mu} \partial_{r'_\nu} \delta(\mathbf{r} - \mathbf{r}') L_r^{\alpha\mu\beta\nu} \mathbf{v}_r^\beta, \\ \zeta_{rr'}^{4\alpha} &= \partial_{r_\mu} \partial_{r'_\nu} \delta(\mathbf{r} - \mathbf{r}') L_r^{\beta\mu\alpha\nu} \mathbf{v}_r^\beta, \\ \zeta_{rr'}^{44} &= \partial_{r_\mu} \partial_{r'_\nu} \delta(\mathbf{r} - \mathbf{r}') [L_r^{\mu\nu} + L_r^{\alpha\mu\beta\nu} \mathbf{v}_r^\alpha \mathbf{v}_r^\beta],\end{aligned}\quad (42)$$

where we have introduced

$$\begin{aligned}L_r^{\mu\nu} &\equiv T(\mathbf{r})\kappa(\mathbf{r})\delta_{\mu\nu}, \\ L_r^{\alpha\beta\mu\nu} &\equiv T(\mathbf{r})\eta(\mathbf{r})g_{\alpha\beta\mu\nu} + T(\mathbf{r})\zeta(\mathbf{r})\delta_{\alpha\beta\mu\nu}, \\ g_{\alpha\beta\mu\nu} &\equiv \delta_{\alpha\mu}\delta_{\beta\nu} + \delta_{\alpha\nu}\delta_{\beta\mu} - \frac{2}{3}\delta_{\alpha\beta}\delta_{\mu\nu}, \\ \delta_{\alpha\beta\mu\nu} &\equiv \delta_{\alpha\beta}\delta_{\mu\nu},\end{aligned}\quad (43)$$

where $\eta(\mathbf{r}), \zeta(\mathbf{r})$ are the shear and bulk viscosities and $\kappa(\mathbf{r})$ is the thermal conductivity. These transport coefficients are given in terms of the usual Green–Kubo formulae where the equilibrium averages are evaluated at the instantaneous values of the temperature and chemical potential fields.

The drift term $K_r^m[\tilde{\alpha}]$ in Eq. (25) is obtained by collecting the results for the reversible part $v_r^m[\tilde{\alpha}]$ in Eq. (41), for the kinetic coefficient (Eq. (42)) and for the thermodynamic forces (Eq. (39)). We will have

$$\begin{aligned}K_r^0[\tilde{\alpha}] &= -\partial_r \cdot \mathbf{g}_r, \\ \mathbf{K}_r[\tilde{\alpha}] &= -\partial_r \cdot [\mathbf{v}_r \mathbf{v}_r \rho_r + p_r \mathbf{1} - 2\eta\dot{\gamma} - (\zeta - \frac{2}{3}\eta) \text{tr}[\dot{\gamma}]\mathbf{1}], \\ K_r^4[\tilde{\alpha}] &= -\partial_r \cdot [\mathbf{v}_r(e_r + p_r) - 2\eta\mathbf{v}_r \cdot \dot{\gamma} - (\zeta - \frac{2}{3}\eta) \text{tr}[\dot{\gamma}]\mathbf{v}_r - \kappa\nabla T_r],\end{aligned}\quad (44)$$

where $\dot{\gamma} \equiv \frac{1}{2}[\nabla\mathbf{v} + (\nabla\mathbf{v})^T]$ is the strain rate tensor.

It is shown in Ref. [28] that the term of $K_r^m[\tilde{\alpha}]$ in Eq. (25) vanishes for the case of hydrodynamic variables, i.e.,

$$\int d\mathbf{r}' \frac{\delta}{\delta \tilde{\alpha}_{r'}^{mm'}} \zeta_{rr'}^{mm'}[\tilde{\alpha}] = 0. \quad (45)$$

This is a consequence of the locality in space assumption and has the very important consequence that the Itô and Stratonovich forms of the FPE coincide [27]. In this way, the resulting SDE can be interpreted in both senses with identical results.

The diffusion matrix $D_{\mathbf{r}\mathbf{r}'}^{mm'}$ (Eq. (25)) is given by

$$\begin{aligned} D_{\mathbf{r}\mathbf{r}'}^{\alpha\beta} &= -\partial_{\mathbf{r}_\mu} \partial_{\mathbf{r}_\nu} \delta(\mathbf{r} - \mathbf{r}') G_{\mathbf{r}}^{\alpha\mu\beta\nu}, \\ D_{\mathbf{r}\mathbf{r}'}^{\alpha 4} &= -\partial_{\mathbf{r}_\mu} \partial_{\mathbf{r}_\nu} \delta(\mathbf{r} - \mathbf{r}') G_{\mathbf{r}}^{\alpha\mu\beta\nu} \mathbf{v}_{\mathbf{r}}^\beta, \\ D_{\mathbf{r}\mathbf{r}'}^{44} &= -\partial_{\mathbf{r}_\mu} \partial_{\mathbf{r}_\nu} \delta(\mathbf{r} - \mathbf{r}') [2T^2(\mathbf{r}) \kappa(\mathbf{r}) \delta_{\mu\nu} + G_{\mathbf{r}}^{\alpha\mu\beta\nu} \mathbf{v}_{\mathbf{r}}^\alpha \mathbf{v}_{\mathbf{r}}^\beta], \end{aligned} \quad (46)$$

where we have introduced

$$\begin{aligned} G_{\mathbf{r}}^{\alpha\mu\beta\nu} &\equiv L_{\mathbf{r}}^{\alpha\mu\beta\nu} + L_{\mathbf{r}}^{\beta\mu\alpha\nu} \\ &= 2T(\mathbf{r})\eta(\mathbf{r})\delta_{\alpha\beta}\delta_{\mu\nu} + T(\mathbf{r})\left(\frac{1}{3}\eta(\mathbf{r}) + \zeta(\mathbf{r})\right)[\delta_{\alpha\mu}\delta_{\beta\nu} + \delta_{\alpha\nu}\delta_{\beta\mu}] \end{aligned} \quad (47)$$

which is a tensor symmetric in α, β and μ, ν .

Now that we have the drift term $K_{\mathbf{r}}^m[\tilde{\alpha}]$ and the diffusion matrix $D_{\mathbf{r}\mathbf{r}'}^{mm'}[\tilde{\alpha}]$ we could write down the FPE (Eq. (20)) explicitly.

6. SDE for simple fluids

The main difficulty in writing down the SDE associated to the FPE for hydrodynamic fields is that we have to compute the square root in matrix sense of the diffusion matrix D in Eq. (42). This is not trivial because this is a 5×5 matrix (rather, a 4×4 because it has the first column and first row equal to zero) that as elements has continuous matrices with indices $\mathbf{r}\mathbf{r}'$. However, one can resort to the physics of the problem to get a hint on the solution. The hint comes from Eq. (10) that states that the time derivative of conserved variables is in the form of the divergence of a flux. This suggests that if we look at the noise term in Eq. (37) it should have the form of a divergence. A little of reflection shows that we can look for a noise term of the form

$$\begin{aligned} f_{\mathbf{r}}^\alpha(t) &= \partial_{\mathbf{r}^\beta} \int d\mathbf{r}' \tilde{B}_{\mathbf{r}\mathbf{r}'}^{\alpha\beta\mu\nu}[\tilde{\alpha}(t)] \eta_{\mathbf{r}'}^{\mu\nu}(t), \\ f_{\mathbf{r}}^4(t) &= \partial_{\mathbf{r}^\alpha} \int d\mathbf{r}' \tilde{B}_{\mathbf{r}\mathbf{r}'}^{\alpha\beta} \eta_{\mathbf{r}'}^\beta(t) + \partial_{\mathbf{r}^\alpha} \int d\mathbf{r}' \mathbf{v}_{\mathbf{r}'}^\beta \tilde{B}_{\mathbf{r}\mathbf{r}'}^{\alpha\beta\mu\nu} \eta_{\mathbf{r}'}^{\mu\nu}(t). \end{aligned} \quad (48)$$

In these expressions, the white noise terms are given in terms of independent increments of the Wiener process according to Eq. (29), i.e.,

$$\begin{aligned} \eta_{\mathbf{r}}^{\mu\nu}(t) &\equiv \frac{dW_{\mathbf{r}}^{\mu\nu}(t)}{\sqrt{v_{\mathbf{r}}}dt}, \\ \eta_{\mathbf{r}}^\mu(t) &\equiv \frac{dW_{\mathbf{r}}^\mu(t)}{\sqrt{v_{\mathbf{r}}}dt}. \end{aligned} \quad (49)$$

The independent increments of the Wiener process satisfy

$$\begin{aligned}
 dW_{\mathbf{r}}^{\mu\nu}(t) &= dW_{\mathbf{r}}^{\nu\mu}(t), \\
 dW_{\mathbf{r}}^{\mu\nu}(t)dW_{\mathbf{r}'}^{\mu'\nu'}(t') &= [\delta^{\mu\mu'}\delta^{\nu\nu'} + \delta^{\nu\mu'}\delta^{\mu\nu'}]\delta_{\mathbf{r}\mathbf{r}'}dt \quad \text{if } t = t', \\
 dW_{\mathbf{r}}^{\mu\nu}(t)dW_{\mathbf{r}'}^{\mu'}(t') &= 0, \\
 dW_{\mathbf{r}}^{\mu}(t)dW_{\mathbf{r}'}^{\mu'}(t') &= \delta_{\mu\mu'}\delta_{\mathbf{r}\mathbf{r}'}dt \quad \text{if } t = t'.
 \end{aligned} \tag{50}$$

Whenever correlations of the white noise terms with other variables have to be computed, one can use the fact that in Itô sense the noise and the variables are uncorrelated at the same time allowing for a decoupling of the averages. Then one can use the following correlations for the white noise:

$$\begin{aligned}
 \langle \eta_{\mathbf{r}}^{\mu\nu}(t)\eta_{\mathbf{r}'}^{\mu'\nu'}(t') \rangle &= [\delta^{\mu\mu'}\delta^{\nu\nu'} + \delta^{\nu\mu'}\delta^{\mu\nu'}]\delta(\mathbf{r} - \mathbf{r}')\delta(t - t'), \\
 \langle \eta_{\mathbf{r}}^{\mu\nu}(t)\eta_{\mathbf{r}'}^{\mu'}(t') \rangle &= 0, \\
 \langle \eta_{\mathbf{r}}^{\mu}(t)\eta_{\mathbf{r}'}^{\mu'}(t') \rangle &= \delta_{\mu\mu'}\delta(\mathbf{r} - \mathbf{r}')\delta(t - t').
 \end{aligned} \tag{51}$$

Now, we make the ansatz that the matrices \tilde{B} in Eq. (48) are local in space:

$$\begin{aligned}
 \tilde{B}_{\mathbf{r}\mathbf{r}'}^{\alpha\beta\mu\nu} &= \tilde{B}_{\mathbf{r}}^{\alpha\beta\mu\nu}\delta(\mathbf{r} - \mathbf{r}'), \\
 \tilde{B}_{\mathbf{r}\mathbf{r}'}^{\alpha\beta} &= \tilde{B}_{\mathbf{r}}^{\alpha\beta}\delta(\mathbf{r} - \mathbf{r}').
 \end{aligned} \tag{52}$$

In addition, the form of the matrix \tilde{B} must be simple because, roughly speaking, its square must be like the matrix G in Eq. (47) which contains only products of Kronecker deltas. Therefore, we make the further assumption that the matrices $\tilde{B}_{\mathbf{r}}^{\alpha\beta\mu\nu}$, $\tilde{B}_{\mathbf{r}}^{\alpha\beta}$ have the form

$$\begin{aligned}
 \tilde{B}_{\mathbf{r}}^{\alpha\beta\mu\nu} &= a(\mathbf{r})\delta_{\alpha\beta}\delta_{\mu\nu} + b(\mathbf{r})[\delta_{\alpha\mu}\delta_{\beta\nu} + \delta_{\alpha\nu}\delta_{\beta\mu}], \\
 \tilde{B}_{\mathbf{r}}^{\alpha\beta} &= c(\mathbf{r})\delta_{\alpha\beta},
 \end{aligned} \tag{53}$$

where $a(\mathbf{r})$, $b(\mathbf{r})$, $c(\mathbf{r})$ are functions to be specified later. These expressions have the correct symmetry properties for the matrices \tilde{B} 's. In the following, we will prove that this ansatz is correct.

If we introduce the random stress tensor $\tilde{\sigma}_{\mathbf{r}}^{\alpha\beta}(t)$ and random energy flux $\tilde{\tau}_{\mathbf{r}}^{\alpha}(t)$ in such a way that

$$\begin{aligned}
 f_{\mathbf{r}}^{\alpha}(t) &= \partial_{\mathbf{r}_{\beta}} \tilde{\sigma}_{\mathbf{r}}^{\alpha\beta}(t), \\
 f_{\mathbf{r}}^4(t) &= \partial_{\mathbf{r}_x} \tilde{\tau}_{\mathbf{r}}^{\alpha}(t),
 \end{aligned} \tag{54}$$

then we see from Eq. (48), Eq. (52), and Eq. (53) that they must have the form

$$\begin{aligned}
 \tilde{\sigma}_{\mathbf{r}}^{\alpha\beta}(t) &= a(\mathbf{r})\delta_{\alpha\beta}\text{tr}[\eta_{\mathbf{r}}] + 2b(\mathbf{r})\eta_{\mathbf{r}}^{\alpha\beta}, \\
 \tilde{\tau}_{\mathbf{r}}^{\alpha}(t) &= c(\mathbf{r})\eta_{\mathbf{r}}^{\alpha}(t) + \mathbf{v}_{\mathbf{r}}^{\beta}(t)\tilde{\sigma}_{\mathbf{r}}^{\alpha\beta}(t).
 \end{aligned} \tag{55}$$

In order to determine the functions $a(\mathbf{r}), b(\mathbf{r}), c(\mathbf{r})$ (and check that our ansatz is correct) we compute the correlation of the noises using the expressions given by Eq. (54) with the definitions (Eq. (55)) and the properties (Eq. (51)). We obtain

$$\begin{aligned}
 \langle f_{\mathbf{r}}^{\alpha}(t) f_{\mathbf{r}'}^{\beta}(t') \rangle &= -\delta(t-t') \left[\delta_{\alpha\beta} \nabla_{\mathbf{r}}^2 \delta(\mathbf{r}-\mathbf{r}') \langle 4b^2(\mathbf{r}) \rangle \right. \\
 &\quad \left. + \partial_{\mathbf{r}_x} \partial_{\mathbf{r}_\beta} \delta(\mathbf{r}-\mathbf{r}') \langle 4b^2(\mathbf{r}) + 8a(\mathbf{r})b(\mathbf{r}) + 6a^2(\mathbf{r}) \rangle \right], \\
 \langle f_{\mathbf{r}}^{\alpha}(t) f_{\mathbf{r}'}^4(t') \rangle &= -\delta(t-t') \left[\nabla_{\mathbf{r}}^2 \delta(\mathbf{r}-\mathbf{r}') \langle \mathbf{v}_{\mathbf{r}}^{\alpha} 4b^2(\mathbf{r}) \rangle \right. \\
 &\quad \left. + \partial_{\mathbf{r}_x} \partial_{\mathbf{r}_\beta} \delta(\mathbf{r}-\mathbf{r}') \langle \mathbf{v}_{\mathbf{r}}^{\beta} (4b^2(\mathbf{r}) + 8a(\mathbf{r})b(\mathbf{r}) + 6a^2(\mathbf{r})) \rangle \right], \\
 \langle f_{\mathbf{r}}^4(t) f_{\mathbf{r}'}^{\alpha}(t') \rangle &= \langle f_{\mathbf{r}}^{\alpha}(t) f_{\mathbf{r}'}^4(t') \rangle \\
 \langle f_{\mathbf{r}}^4(t) f_{\mathbf{r}'}^4(t') \rangle &= -\delta(t-t') \left[\nabla_{\mathbf{r}}^2 \delta(\mathbf{r}-\mathbf{r}') \langle c^2(\mathbf{r}) \rangle + \nabla_{\mathbf{r}}^2 \delta(\mathbf{r}-\mathbf{r}') \langle \mathbf{v}_{\mathbf{r}}^2 4b^2(\mathbf{r}) \rangle \right. \\
 &\quad \left. + \partial_{\mathbf{r}_x} \partial_{\mathbf{r}_\beta} \delta(\mathbf{r}-\mathbf{r}') \langle \mathbf{v}_{\mathbf{r}}^{\alpha} \mathbf{v}_{\mathbf{r}}^{\beta} (4b^2(\mathbf{r}) + 8a(\mathbf{r})b(\mathbf{r}) + 6a^2(\mathbf{r})) \rangle \right]. \tag{56}
 \end{aligned}$$

These expressions should coincide with Eq. (36) which can be rewritten as

$$\begin{aligned}
 \langle f_{\mathbf{r}}^{\alpha}(t) f_{\mathbf{r}'}^{\beta}(t') \rangle &= \delta(t-t') \langle D_{\mathbf{r}\mathbf{r}'}^{\alpha\beta} \rangle, \\
 \langle f_{\mathbf{r}}^{\alpha}(t) f_{\mathbf{r}'}^4(t') \rangle &= \delta(t-t') \langle D_{\mathbf{r}\mathbf{r}'}^{\alpha 4} \rangle, \\
 \langle f_{\mathbf{r}}^4(t) f_{\mathbf{r}'}^4(t') \rangle &= \delta(t-t') \langle D_{\mathbf{r}\mathbf{r}'}^{44} \rangle, \tag{57}
 \end{aligned}$$

where the diffusion matrix is given in Eq. (46). After substitution of Eq. (46) into Eq. (57) one obtains

$$\begin{aligned}
 \langle f_{\mathbf{r}}^{\alpha}(t) f_{\mathbf{r}'}^{\beta}(t') \rangle &= -\delta(t-t') [\delta_{\alpha\beta} \nabla_{\mathbf{r}}^2 \delta(\mathbf{r}-\mathbf{r}') \langle 2T(\mathbf{r})\eta(\mathbf{r}) \rangle \\
 &\quad + \partial_{\mathbf{r}_x} \partial_{\mathbf{r}_\beta} \delta(\mathbf{r}-\mathbf{r}') \langle 2T(\mathbf{r})(\eta(\mathbf{r})/3 + \zeta(\mathbf{r})) \rangle], \\
 \langle f_{\mathbf{r}}^{\alpha}(t) f_{\mathbf{r}'}^4(t') \rangle &= -\delta(t-t') [\nabla_{\mathbf{r}}^2 \delta(\mathbf{r}-\mathbf{r}') \langle \mathbf{v}_{\mathbf{r}}^{\alpha} 2T(\mathbf{r})\eta(\mathbf{r}) \rangle \\
 &\quad + \partial_{\mathbf{r}_x} \partial_{\mathbf{r}_\beta} \delta(\mathbf{r}-\mathbf{r}') \langle \mathbf{v}_{\mathbf{r}}^{\beta} (2T(\mathbf{r})(\eta(\mathbf{r})/3 + \zeta(\mathbf{r}))) \rangle], \\
 \langle f_{\mathbf{r}}^4(t) f_{\mathbf{r}'}^{\alpha}(t') \rangle &= \langle f_{\mathbf{r}}^{\alpha}(t) f_{\mathbf{r}'}^4(t') \rangle, \\
 \langle f_{\mathbf{r}}^4(t) f_{\mathbf{r}'}^4(t') \rangle &= -\delta(t-t') [\nabla_{\mathbf{r}}^2 \delta(\mathbf{r}-\mathbf{r}') \langle 2T(\mathbf{r})^2 \kappa(\mathbf{r}) \rangle \\
 &\quad + \nabla_{\mathbf{r}}^2 \delta(\mathbf{r}-\mathbf{r}') \langle \mathbf{v}_{\mathbf{r}}^2 2T(\mathbf{r})\eta(\mathbf{r}) \rangle + \partial_{\mathbf{r}_x} \partial_{\mathbf{r}_\beta} \delta(\mathbf{r}-\mathbf{r}') \\
 &\quad \times \langle \mathbf{v}_{\mathbf{r}}^{\alpha} \mathbf{v}_{\mathbf{r}}^{\beta} (2T(\mathbf{r})(\eta(\mathbf{r})/3 + \zeta(\mathbf{r}))) \rangle]. \tag{58}
 \end{aligned}$$

Compatibility between Eq. (56) and Eq. (58) then requires that

$$\begin{aligned} 4b^2(\mathbf{r}) &= 2T(\mathbf{r})\eta(\mathbf{r}), \\ 3a^2(\mathbf{r}) + 4a(\mathbf{r})b(\mathbf{r}) + 2b^2(\mathbf{r}) &= T(\mathbf{r}) \left[\frac{1}{3}\eta(\mathbf{r}) + \zeta(\mathbf{r}) \right], \\ c^2(\mathbf{r}) &= 2T^2(\mathbf{r})\kappa(\mathbf{r}). \end{aligned} \quad (59)$$

We observe then that our ansatz for the matrices \tilde{B} is correct because this compatibility condition can be satisfied. The solution of this system of equations is

$$\begin{aligned} a(\mathbf{r}) + \frac{2}{3}b(\mathbf{r}) &= \pm \sqrt{\frac{1}{3}T(\mathbf{r})\zeta(\mathbf{r})}, \\ b(\mathbf{r}) &= \pm \sqrt{\frac{1}{2}T(\mathbf{r})\eta(\mathbf{r})}, \\ c(\mathbf{r}) &= T(\mathbf{r})\sqrt{2\kappa(\mathbf{r})}. \end{aligned} \quad (60)$$

Therefore, the random stress tensor in Eq. (55) will have the following form:

$$\begin{aligned} \tilde{\sigma}_r^{\alpha\beta}(t) &\equiv \sqrt{2T(\mathbf{r})\eta(\mathbf{r})} \left[\eta_r^{\alpha\beta}(t) - \delta^{\alpha\beta} \frac{1}{3} \sum_{\mu} \eta_r^{\mu\mu}(t) \right] \\ &\quad \pm \sqrt{3T(\mathbf{r})\zeta(\mathbf{r})} \delta^{\alpha\beta} \frac{1}{3} \sum_{\mu} \eta_r^{\mu\mu}(t). \end{aligned} \quad (61)$$

We have decomposed this tensor as a traceless part plus a diagonal part. Both components are statistically independent and therefore the sign \pm is indifferent. Actually, we can compute the correlation of the random stress tensor and the result is

$$\begin{aligned} \left\langle \tilde{\sigma}_r^{\alpha\beta}(t) \tilde{\sigma}_{r'}^{\mu\nu}(t') \right\rangle &= \delta(\mathbf{r} - \mathbf{r}') \delta(t - t') \left[\langle 2T(\mathbf{r})\eta(\mathbf{r}) \rangle [\delta^{\alpha\mu} \delta^{\beta\nu} + \delta^{\alpha\nu} \delta^{\beta\mu}] \right. \\ &\quad \left. + \langle 2T(\mathbf{r})(\zeta(\mathbf{r}) - \frac{2}{3}\eta(\mathbf{r})) \rangle \delta_{\alpha\beta} \delta_{\mu\nu} \right]. \end{aligned} \quad (62)$$

In the same fashion, we can define a random heat flux according to

$$\tilde{\mathbf{J}}_r^{\alpha} \equiv \tilde{\tau}_r^{\alpha}(t) - \tilde{\sigma}_r^{\alpha\beta}(t) \mathbf{v}_r^{\beta}(t) = T(\mathbf{r})\sqrt{2\kappa(\mathbf{r})}\eta_r^{\alpha}(t). \quad (63)$$

This random heat flux is uncorrelated with the random stress tensor and its autocorrelation is given by

$$\left\langle \tilde{\mathbf{J}}_r^{\alpha}(t) \tilde{\mathbf{J}}_{r'}^{\beta}(t') \right\rangle = \langle 2T^2(\mathbf{r})\kappa(\mathbf{r}) \rangle \delta_{\alpha\beta} \delta(\mathbf{r} - \mathbf{r}') \delta(t - t'). \quad (64)$$

The expressions in Eq. (61) and Eq. (63) of the random stress tensor and random heat flux in terms of the independent increments of the Wiener process are the main results of this paper.

Now, we have all the elements to write the full Langevin Eq. (30). After some rearrangement, the Langevin equations can be cast in the form

$$\begin{aligned} \partial_t \rho(\mathbf{r}, t) &= -\nabla \cdot \mathbf{v}(\mathbf{r}, t) \rho(\mathbf{r}, t), \\ \partial_t \mathbf{g}(\mathbf{r}, t) &= -\nabla \cdot [\mathbf{v}(\mathbf{r}, t) \mathbf{g}(\mathbf{r}, t) + \sigma(\mathbf{r}, t)], \\ \partial_t e(\mathbf{r}, t) &= -\nabla \cdot (\mathbf{v}(\mathbf{r}, t) e(\mathbf{r}, t) + \mathbf{v}(\mathbf{r}, t) \cdot \sigma(\mathbf{r}, t) + \mathbf{J}(\mathbf{r}, t)). \end{aligned} \quad (65)$$

The terms $\mathbf{v}\rho, \mathbf{v}\mathbf{g}, \mathbf{v}e$ represent the purely convective part of the fluxes. The total stress tensor σ and total heat flux \mathbf{J} are given by a systematic and a random part,

$$\begin{aligned}\sigma(\mathbf{r}, t) &= \bar{\sigma}(\mathbf{r}, t) + \tilde{\sigma}(\mathbf{r}, t), \\ \mathbf{J}(\mathbf{r}, t) &= \bar{\mathbf{J}}(\mathbf{r}, t) + \tilde{\mathbf{J}}(\mathbf{r}, t).\end{aligned}\quad (66)$$

The systematic parts have the form of Newton's and Fourier's constitutive equations:

$$\begin{aligned}\bar{\sigma} &= p\mathbf{1} - 2\eta(\dot{\gamma} - \frac{1}{3}\text{tr}[\dot{\gamma}]\mathbf{1}) - \zeta\text{tr}[\dot{\gamma}]\mathbf{1}, \\ \bar{\mathbf{J}} &= -\kappa\nabla T,\end{aligned}\quad (67)$$

where $\dot{\gamma} \equiv \frac{1}{2}[\nabla\mathbf{v} + (\nabla\mathbf{v})^T]$ is the strain rate tensor. The random parts are given by Eq. (61) and Eq. (63) which are the main result of this paper.

7. Discussion

The Langevin equations for non-linear hydrodynamic are the same in structure as the usual macroscopic non-linear hydrodynamic equations except that they govern the instantaneous fluctuating values of the hydrodynamic fields and they have, in addition, a random contribution to the stress tensor and heat flux. The form in which the thermal noise is described here is similar to the Landau and Lifshitz theory [22]. The differences arise on the stochastic properties of the random parts in these equations. The correlations of the random stress tensor and heat flux, Eqs. (62) and (64), are to be compared with those given by Landau and Lifshitz [22]:

$$\begin{aligned}\langle \tilde{\sigma}_{\mathbf{r}}^{\alpha\beta}(t) \tilde{\sigma}_{\mathbf{r}'}^{\mu\nu}(t') \rangle &= \delta(\mathbf{r} - \mathbf{r}') \delta(t - t') [2T_{eq}\eta_{eq}(\delta^{\alpha\mu}\delta^{\beta\nu} + \delta^{\alpha\nu}\delta^{\beta\mu}) \\ &\quad + 2T_{eq}(\zeta_{eq} - \frac{2}{3}\eta_{eq})\delta_{\alpha\beta}\delta_{\mu\nu}], \\ \langle \tilde{\mathbf{J}}_{\mathbf{r}}^{\alpha}(t) \tilde{\mathbf{J}}_{\mathbf{r}'}^{\beta}(t') \rangle &= 2T_{eq}^2\kappa_{eq}\delta_{\alpha\beta}\delta(\mathbf{r} - \mathbf{r}')\delta(t - t').\end{aligned}\quad (68)$$

Here $T_{eq}, \eta_{eq}, \zeta_{eq}, \kappa_{eq}$ are the equilibrium values of the temperature and the transport coefficients. It is apparent that the results Eqs. (62) and (64) will coincide with Eq. (68) only if the system is at equilibrium and the fluctuations can be considered small, in such a way that the decoupling approximation

$$\langle T(\mathbf{r})\eta(\mathbf{r}) \rangle = \langle T(\mathbf{r}) \rangle \langle \eta(\mathbf{r}) \rangle = T_{eq}\eta_{eq} \quad (69)$$

can be taken.

Another point of discrepancy is that the random fluxes *are not Gaussian*. What is Gaussian is the Wiener process, but not the product of the Wiener process with the temperature and the transport coefficients. This result is consistent with that of Ref. [27] where the assumption of Gaussian random fluxes lead to unphysical results. In particular, it was found that if the Einstein distribution is assumed to be the equilibrium solution, then the viscosities were inversely proportional to the temperature and that the heat conductivity was inversely proportional to the temperature squared. This dependences are not observed in real systems. Conversely, one could obtain physically

acceptable transport coefficients by relaxing the requirement that the Einstein distribution is the equilibrium distribution, which is equally unacceptable. A full discussion of this point has been made in Ref. [28].

The “size of the fluctuations” is what determines the validity of the decoupling approximation (Eq. (69)) and we comment on this point now. We note that despite of the continuum appearance of the Langevin Eq. (65) there is an implicit dependence of the random parts on the coarse graining, i.e. on the volume of the cells. This is apparent in the definition (Eq. (49)) of the noise appearing in Eqs. (61) and (63). In principle, different coarse-graining procedures (different discretization with distinct typical volumes v_r of the cells) will leave the systematic part of the equations invariant, but will change the intensity of the noise terms. The $1/\sqrt{v_r}$ dependence is consistent with the amplitude of the fluctuations encountered in equilibrium ensemble theory. Therefore, the question of whether the fluctuations are large or small is a matter of the level of description used. Fine resolutions of the hydrodynamic fields in which the coarse graining cells are small will produce large relative fluctuations in the hydrodynamic variables. The existence of characteristic length scales imposed on the fluid is what dictates the level of coarsening required. In the case of colloidal particles, it is observed experimentally that submicronic particles diffuse whereas the diffusion for larger particles is small and negligible. Therefore, in order to “resolve” submicronic particles, one needs a fine level of coarse graining such that the fluctuations are relevant.

The Landau and Lifshitz fluctuating hydrodynamics arises as the small noise expansion [33] of the SDE obtained in this paper. This can be seen by writing schematically the SDE (Eq. (30)) with Eq. (52) as

$$d\tilde{\alpha} = K[\tilde{\alpha}]dt + \varepsilon\tilde{B}[\tilde{\alpha}]dW(t), \quad (70)$$

where $\varepsilon = 1/\sqrt{v_r}$. In a perturbative expansion in ε one assumes that the solution of Eq. (70) can be written as $\tilde{\alpha}(t) = \tilde{\alpha}_0(t) + \varepsilon\tilde{\alpha}_1(t) + \varepsilon^2\tilde{\alpha}_2(t) + \dots$. By substitution in Eq. (70) and cancelling order by order one obtains

$$\begin{aligned} d\tilde{\alpha}_0(t) &= K[\tilde{\alpha}_0(t)]dt, \\ d\tilde{\alpha}_1(t) &= K'[\tilde{\alpha}_0(t)]\tilde{\alpha}_1(t)dt + \tilde{B}[\tilde{\alpha}_0(t)]dW, \\ d\tilde{\alpha}_2(t) &= [K'[\tilde{\alpha}_0(t)]\tilde{\alpha}_2(t)dt + \frac{1}{2}K''[\tilde{\alpha}_0(t)]\tilde{\alpha}_1(t)]dt \\ &\quad + \tilde{B}'[\tilde{\alpha}_0(t)]\tilde{\alpha}_1(t)dW(t), \end{aligned} \quad (71)$$

where the primes denote derivatives. The first equation for the dominant contribution $\alpha_0(t)$ to the solution of the SDE constitutes the deterministic non-linear hydrodynamic equations with fluctuations neglected. The next equation for the contribution $\alpha_1(t)$ is equivalent to linearize the equations of hydrodynamics around the deterministic solution and add a Gaussian white noise of amplitude $\tilde{B}[\tilde{\alpha}_0]$. At long times when the system has relaxed to equilibrium, these equations are the Landau and Lifshitz linear equations governing the equilibrium hydrodynamic fluctuations [22]. Higher-order contributions $\tilde{\alpha}_2, \dots$ are usually not considered, although, in principle, they can be computed systematically [33].

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