

Theory of multi-point probability densities for incompressible Navier-Stokes fluids

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Abstract

An open problem arising in the statistical description of turbulence is related to the determination of the so-called multi-point velocity probability density functions (PDFs) characterizing a Navier-Stokes fluid. In this paper it will be shown that - relaying on a suitable axiomatic approach which permits to determine the *local* PDFs (i.e., before performing the ensemble-average) - as explicit solution to this problem can actually be achieved. The result is based on the so-called inverse kinetic theory (IKT), for incompressible NS fluids. More precisely, based on a suitable entropic principle, it is shown that all local multi-point PDFs are *necessarily factorized in terms of the corresponding 1-point velocity PDF* (f_1). As a consequence the multi-point PDFs usually considered for the phenomenological description of turbulence can be theoretically predicted *based on the knowledge of f_1 achieved by means of IKT*. PACS: 05.20.Jj, 05.20.Dd, 05.70.-a

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1 Introduction

In the context of the statistical description of fluids, the problem of the determination of multi-point PDFs arises in the following two circumstances:

- the first one is in the phenomenological description of turbulence (for a review see for example Monin and Yaglom [1] 1975 and Pope, 2000 [2]). In such a context, in fact, the statistical behavior of fluids is often described in

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terms of statistical frequencies [3], namely experimentally-measured probability densities, defined for multi-point velocity spatial increments (however, in principle, similar frequencies can be established also for other fluid fields, such as vorticity, scalar pressure, temperature, etc.).

- the second one occurs in the customary approach to the statistical description of turbulence, namely the so-called *statistical hydromechanics* developed originally by Hopf [4], Rosen [5] and Edwards [6] (*HRE approach*) and later investigated also by Monin and Lundgren [7, 8] (*ML approach*). In both approaches, the goal is to predict the time evolution of the ensemble-average of the 1-point PDF, to be defined in terms of a suitable ensemble-averaging operator $\langle \cdot \rangle$. As shown by Monin and Lundgren this implies the so-called Monin-Lundgren hierarchy [7, 8], in turn equivalent [9] to the Hopf ϕ functional-differential equation [4]. Such a theory should provide, in principle, a theoretical model for the phenomenological description of turbulence and, as a consequence, be able to predict also the precise form of the velocity-difference PDF observed experimentally in HIST (homogenous, isotropic and stationary turbulence).

Several open issues are related to these approaches. In particular, they concern the search of possible *exact particular solutions* of the ML hierarchy represented by a *finite set* of ensemble-averaged multi-point PDFs. It is well known that the construction of "closure conditions" of this type for the ML hierarchy (*closure problem*) remains one of the major unsolved theoretical problems in fluid dynamics. In practice, however, the program of constructing (*exact*) theories of this type or (in some sense) *approximate*, and holding for arbitrary fluid fields, is still open due to the difficulty of preserving the full consistency with the fluid equations. In fact, it is well known that many of the customary statistical models adopted in turbulence theory - which are based on closure conditions of various type - typically reproduce at most only in some approximate (i.e., asymptotic) sense the fluid equations. This leaves fundamentally unsolved the problem of the construction of a consistent theoretical model for the multi-point PDFs arising in the phenomenological description of turbulence.

The goal of this paper is *to prove that under suitable assumptions the problem can be solved*, in an equivalent way, in the framework of the so-called IKT (inverse kinetic theory [10–14]) developed for the incompressible Navier-Stokes equations (INSE, see Appendix A).

The result is reached by considering, in contrast to the prevailing literature (in particular the HRE and ML approaches), *a statistical description based on local multi-point PDFs rather than their ensemble-averages*. For this purpose, first, it is shown that all *local multi-point velocity PDFs characterizing a turbulent NS fluid are factorizable in terms of the corresponding (local) 1-point velocity PDF* (see THM.1). Second, the local 1-point velocity PDF defined in

the framework of IKT is proved to be directly determined by the corresponding 1-point PDF used in the HRE approach, the relationship between the two being provided by THM.2 (Sec.3). The result proves also the equivalence of the two approaches, yielding the same subset of fluid equations namely that both yield (see Sec.3). A fundamental application of the theory concerns the treatment of multi-point PDFs, which are uniquely determined by the local 1-point PDF determined by the IKT approach (see Sec.4). As a further consequence, also the ensemble-averaged multi-point PDFs usually considered for the phenomenological description of turbulence *can actually be theoretically predicted* in this way! In particular, in the case of local Gaussian 1-point PDF one obtains in this way an *explicit analytic representations* of the 2-point velocity PDFs usually considered for the description of HIST (see Sec.4, subsections 4.1. and 4.2).

2 Multi-point statistical models

The description of fluids, and more generally of continua, is based on the introduction of a suitable set of fluid fields $\{Z\} \equiv \{Z_i, i = 1, k\}$ satisfying a closed set of PDEs denoted as *fluid equations*. In the case of a fluid obeying INSE (*NS fluid*), a possible representation of the fluid fields is provided by the set $\{Z\} \equiv \{\rho_0, \mathbf{V}, p_1, S_T\}$, where in particular both ρ_0 (the mass density) and S_T (the thermodynamic entropy) are assumed constant in $\bar{\Omega} \times I$ [see Eqs.(49) and (52) in Appendix A]. Furthermore, \mathbf{V} and p_1 denote respectively the fluid velocity and the kinetic pressure; in particular, p_1 is defined as the strictly positive function

$$p_1(\mathbf{r}, t) = p(\mathbf{r}, t) + p_0(t) + \phi(\mathbf{r}, t), \quad (1)$$

where $p(\mathbf{r}, t)$, $p_0(t)$ and $\phi(\mathbf{r}, t)$ represent respectively the fluid pressure, the (strictly-positive) pseudo-pressure and the (possible) potential associated to the conservative volume force density acting on the fluid [see the Appendix, Eq.(60)]. Fluids, such as a NS fluid, can be *regular* or *turbulent*, i.e., described respectively by *deterministic* or *stochastic* fluid fields [13–15]. The formulation of the problem appropriate for turbulent flows arising in a NS fluid is recalled in the Appendix. This requires that, leaving unchanged the functional form of INSE and of the related initial-boundary value problem, the fluid fields and the fluid equations, as well as the related initial and boundary conditions be considered as stochastic. It follows that the fluid fields $\{\mathbf{V}, p_1\}$ together with the NS acceleration are generally stochastic functions of the form

$$Z_i = Z_i(\mathbf{r}, t, \alpha), \quad (2)$$

$$\mathbf{F}_H = \mathbf{F}_H(\mathbf{x}_1, t, \alpha), \quad (3)$$

i.e., to depend on suitable stochastic variables $\alpha \in V_\alpha \subseteq \mathbb{R}^n$ independent of (\mathbf{r}, t) . In all cases the fluid fields are, by assumption, strong solutions of

the well-posed initial-boundary value problem associated to INSE. As a basic consequence, *both for regular and turbulent flows*, the fluid fields $\{Z\}$ *uniquely prescribe the fluid state*. In particular, the stochastic functions Z_i (for $i = 1, n$) can depend either *on* (\mathbf{r}, t, α) or only (t, α) , with (\mathbf{r}, t) spanning the whole existence domain $\bar{\Omega} \times I$ (with $\bar{\Omega}$, closure of the bounded set $\Omega \subseteq \mathbb{R}^3$, the configuration domain and $I \subseteq \mathbb{R}$ the time axis).

2.1 Complete/incomplete statistical models

The *statistical description* usually adopted for turbulent flows (which may be invoked, however, to describe also regular flows) consists, instead, in the introduction of appropriate axiomatic approaches denoted *statistical models*, i.e., sets $\{f, \Gamma\}$ formed by a suitable probability density function (PDF) and a phase-space Γ (subset of \mathbb{R}^n) on which f is defined. By definition, a statistical model (SM) $\{f, \Gamma\}$ realizes a statistical description of the fluid if it is possible to define a mapping $\{f, \Gamma\} \Rightarrow \{Z\}$, which allows the representation in terms of f by means of suitable "velocity" *moments* (of f) either: A) of the *complete set* or more generally only (*type A*) B) or a *proper subset* of the *fluid fields* $\{Z\} \equiv \{Z_i, i = 1, n\}$ which define the fluid state (*type B*). Approaches fulfilling either property A or B will be denoted respectively *complete* and *incomplete SMs*.

In both cases their construction involves, besides the specification of the phase space (Γ) and the PDF f , the identification of the functional class to which f must belong, denoted as $\{f\}$. Thus, for example, $\{f, \Gamma\}$ may be identified with $\{f_N, \Gamma_N\}$, with f_N the N -point PDF (with $N \geq 1$ to be suitably prescribed) to be generally identified with a PDF of the form $f_N \equiv f_N(\mathbf{x}_1, \dots, \mathbf{x}_N, t, \alpha)$, which is defined on $\Gamma_N \times I \times V_\alpha$, with $\Gamma_N \equiv \prod_{i=1, N} \Gamma_1$ the N -point phase-space, $\Gamma_1 = \Omega \times U$, and U a suitable velocity space. In particular, f_N may be required to satisfy a normalization condition of the form $\int_{U^N} \prod_{j=1, N} d\mathbf{v}_j f_N(\mathbf{x}, t, \alpha) = 1$, i.e., to be a velocity PDF on U^N . Based on classical statistical mechanics (CSM) statistical models can be introduced for the INSE problem. For definiteness, the standard formulation appropriate to Newtonian dynamical system of N point particles (S_N) is recalled in Appendix B. Hence, thanks to Proposition 3 (see Appendix B), in the case of an incompressible NS fluid, $f_N(\mathbf{x}, t, \alpha)$ can always be identified with the corresponding *N -body velocity PDF* for S_N [see Eqs.(107)].

As a basic consequence, consistent with CSM (see Appendix B), the following axiom is imposed on the SM $\{f_N, \Gamma_N\}$:

- *Axiom #1 (fluid moments - fluid velocity)*: $f_N(\mathbf{x}_1, \dots, \mathbf{x}_N, t, \alpha)$ determines

uniquely either the complete set or a proper subset of the local fluid fields (*type A* or *B*). Thus, introducing suitable weight functions $\{G_i(\mathbf{r}_k, \mathbf{v}_k, t, \alpha), i = 1, n\}$ the local fluid fields $Z_i(\mathbf{r}_k, t, \alpha)$, all evaluated at the local position \mathbf{r}_k and time t belonging to $\bar{\Omega} \times I$, are taken of the form $\int_U d\mathbf{v}_k G_i(\mathbf{r}_k, \mathbf{v}_k, t, \alpha) f_1(\mathbf{r}_k, \mathbf{v}_k, t, \alpha) = Z_i(\mathbf{r}_k, t, \alpha)$. In particular, we shall require

$$\mathbf{V}(\mathbf{r}_1, t, \alpha) = \int_U d\mathbf{v}_1 \mathbf{v}_1 f_1(\mathbf{x}_1, t, \alpha), \quad (4)$$

$\mathbf{V}(\mathbf{r}_1, t, \alpha)$ denoting the fluid velocity. Here the fluid fields $\{Z(\mathbf{r}_k, t, \alpha)\}$ are identified with the set (or a proper subset) of the fluid fields characterizing the INSE problem, namely (55) which by assumption are strong solution of the same problem (see Appendix A).

2.2 An example: the HRE statistical model

The customary approach to the statistical description of turbulence, to be found in the literature (for a review see for example Monin and Yaglom[1] and Pope [2]) is the so-called *statistical hydromechanics* (*HRE approach*) developed originally by Hopf [4], later extended by Rosen [5] and Edwards [6] (see also Novikov [16], Kollmann [17], Pope [18], Givi [3] and Dopazo [19]). This yields a well-known example of SM *for INSE* which is consistent with Axiom #1 as well as with the applicable axioms of CSM [i.e., all Axioms indicated in Appendix B, except for CSM-#2]. The result is reached by means of an appropriate definition for $f_1(1)$, which is identified with the deterministic 1-point velocity PDF

$$f_{H1}(\mathbf{r}_1, \mathbf{u}_1, t) \equiv \delta(\mathbf{v}_1 - \mathbf{V}(\mathbf{r}_1, t, \alpha)), \quad (5)$$

(*local HRE 1-point velocity PDF*), where $\mathbf{u}_1 \equiv \mathbf{u}(\mathbf{r}_1, t) \equiv \mathbf{v}_1 - \mathbf{V}(\mathbf{r}_1, t, \alpha)$ denotes the relative kinetic velocity. It follows that $f_{H1}(1)$ obeys the Liouville equation

$$L_1(1)f_{H1}(1) = 0, \quad (6)$$

with $L_1(1)$ denoting the 1-point Liouville streaming operator

$$L_1(1) \equiv \frac{\partial}{\partial t} + \mathbf{v}_1 \cdot \frac{\partial}{\partial \mathbf{r}_1} + \frac{\partial}{\partial \mathbf{v}_1} \cdot \{\mathbf{F}(\mathbf{x}_1, t, \alpha)\} \quad (7)$$

and $\mathbf{F}(\mathbf{x}_1, t, \alpha) \equiv \mathbf{F}^{(ext)}(\mathbf{x}_1, t, \alpha) \equiv \mathbf{F}_H(\mathbf{r}_1, t, \alpha)$ the fluid acceleration at position \mathbf{r}_1 [see Eq.(59) in the Appendix A]. We remark, that in terms of $f_{H1}(1)$ the corresponding N -point velocity PDF can simply be defined as

$$f_{HN}(\mathbf{x}_1, \dots, \mathbf{x}_N, t) \equiv \prod_{i=1, N} f_{H1}(i) \quad (8)$$

(*local deterministic N-point velocity PDF*). It follows [4–6] that $f_N(1, \dots, N)$ must obey the N –point Liouville equation

$$L_N(1, \dots, N)f_{HN}(1, \dots, N) = 0 \quad (9)$$

with $L_N(1, \dots, N)$ now denoting the corresponding N –point Liouville streaming operator

$$L_N(1, \dots, N) \equiv \frac{\partial}{\partial t} + \mathbf{v}_i \cdot \frac{\partial}{\partial \mathbf{r}_i} + \frac{\partial}{\partial \mathbf{v}_i} \cdot \{\mathbf{F}(\mathbf{x}_i, t, \alpha)\}. \quad (10)$$

It is immediate to prove that in the HRE approach, denoting $\Gamma_1 = \Omega \times U$ and $\Gamma_N \equiv \Gamma_N = \Omega^N \times U^N$ respectively the 1- and N - point phase spaces, both $\{f_{H1}, \Gamma_1\}$ and $\{f_{HN}, \Gamma_N\}$ are SMs which besides fulfilling the CSM Axioms CSM-#1, #3–#5 (indicated in Appendix B), satisfy Axiom #1 but not Axiom #2–#4. Hence both are *incomplete SMs for INSE*. Nevertheless, subject to the constraints of constant mass-density [Eq.(49)], the velocity moment equations of the Liouville equation [i.e., either (6) or (9)], evaluated w.r. to the weight functions $\{G\} = \{1, \mathbf{v}_1\}$, coincide respectively with Eqs.(50) and (51) [see Appendix A].

2.3 The ensemble-averaging operator: local and ensemble-averaged PDFs

Goal of the HRE approach is actually to predict, in the presence of turbulence, the time evolution of $\langle f_1(\mathbf{x}_1, t, \alpha) \rangle \equiv \langle f_H(\mathbf{r}_1, \mathbf{u}_1, t, \alpha) \rangle$ and consequently of $\langle \mathbf{V}(\mathbf{r}_1, t, \alpha) \rangle, \langle p(\mathbf{r}_1, t, \alpha) \rangle$, where the brackets $\langle \cdot \rangle$ denote an *ensemble-averaging operator*, to be suitably prescribed, over the possible realizations of the fluid [2]. The same problem, however, can be set also for $\langle f_s(\mathbf{x}_1, \dots, \mathbf{x}_2, t, \alpha) \rangle \equiv \langle f_{Hs}(1, \dots, s, \alpha) \rangle$ (for $s = 2, N$) in terms of which correlation functions can be determined. In the remainder, we shall denote respectively $f_1(\mathbf{x}_1, t, \alpha), f_s(\mathbf{x}_1, \dots, \mathbf{x}_2, t, \alpha)$ and $\langle f_1(\mathbf{x}_1, t, \alpha) \rangle, \langle f_s(\mathbf{x}_1, \dots, \mathbf{x}_2, t, \alpha) \rangle$ as the *local* and *ensemble-averaged velocity PDFs*. In the case of so-called homogeneous, isotropic and stationary turbulence (HIST), $\langle \cdot \rangle$ by definition commutes with the [differential and integral] operators $\{Q\} \equiv \left\{ \frac{\partial}{\partial t}, \frac{\partial}{\partial \mathbf{r}_1}, \frac{\partial^2}{\partial \mathbf{r}_1 \cdot \partial \mathbf{r}_1}, \frac{\partial}{\partial \mathbf{v}_1}, \int_{\Omega} d\mathbf{r}, \int_U d\mathbf{v} \right\}$. The corresponding evolution (or transport) equation obtained in this case for $\langle f_H \rangle$ has been investigated by several authors (see for example Dopazo [19] and Pope [2]). Monin [7] and Lundgren [8] (see also Monin and Yaglom [1] and therein cited references) have shown that the construction of the ensemble-averaged PDF $\langle f_1(\mathbf{r}, \mathbf{v}, t, \alpha) \rangle$ appropriate for HIST is actually equivalent to the solution to an infinite set of PDEs denoted as ML hierarchy [7, 8].

However, more generally in the context of the statistical description of turbulence the operator $\langle \cdot \rangle$ should be understood as a mean value *in the probabilistic*

sense [20], namely a stochastic average defined in terms of a suitable stochastic probability density g_α

$$\langle \cdot \rangle = \int_{V_\alpha} d\alpha g_\alpha(\mathbf{r}, t), \quad (11)$$

where the operator $\langle \cdot \rangle$ may generally not commute with respect to the operators $\{Q\}$. In the remainder, all quantities depending locally on $(\mathbf{r}_1, t, \alpha)$, $(\mathbf{x}_1, t, \alpha)$ will be called as *local functions*, in contrast to *non-local functions*, i.e., depending more generally on $(\mathbf{r}_1, \dots, \mathbf{r}_s, t, \alpha)$, $(\mathbf{x}_1, \dots, \mathbf{x}_s, t, \alpha)$ with $s \geq 2$ or on the ensemble average (11), namely, for example, in the last case are of the form $\langle a(\mathbf{x}_1, t, \alpha) \rangle$. Finally, we shall denote as *global*, functions which are constant or depend at most only on time.

2.4 An N -point PDF statistical model for local PDFs

As indicated above, in the HRE approach both f_1 and f_N are identified with *local deterministic PDFs* which do not yield the complete set of fluid moments, to be expressed in terms of velocity moments. Let us now look for possible alternative SMs $\{f_1, \Gamma_1\}$ and $\{f_N, \Gamma_N\}$ requiring that: 1) both $f_1(1)$ and $f_N(1, \dots, N)$ are ordinary smooth functions defined and strictly positive in the domains $\Gamma_1 \times I$ and $\Gamma_N \times I$; 2) that both $\{f_1, \Gamma_1\}$ and $\{f_N, \Gamma_N\}$ are complete (i.e., of type A); 3) the velocity space U is identified with \mathbb{R}^3 . This means that all the NS fluid fields $\{\overline{Z}\}$ [see Eq.(55)] must be defined in terms of suitable moments of the corresponding PDFs. In particular we shall require that the kinetic pressure p_1 and the thermodynamic entropy S_T are respectively prescribed as follows:

- *Axiom #2 (kinetic pressure)*: consistent with CSM [21, 22], the fluid field p_1 defined by Eq.(1) is identified with the velocity moment of $\{G_i(\mathbf{r}_1, \mathbf{v}_1, t, \alpha)\} = \{\rho_o u_1^2/3\}$, namely

$$p_1(\mathbf{r}_1, t, \alpha) = \int_U d^3 \mathbf{v}_1 \rho_o \frac{u_1^2}{3} f_1(\mathbf{x}_1, t, \alpha). \quad (12)$$

- *Axiom #3 (entropy constraints)*: the thermodynamic entropy $S_T(t)$ for all $t \in I$ and $s = 1, N$ is identified with [12]

$$S_T = S(f_s) = S(f_1), \quad (13)$$

where for $s = 1, N$,

$$S(f_s) = -K_s^2 \int_{\Gamma_s} d\mathbf{x} f_s \ln f_s \quad (14)$$

and $K_1^2 = 1$. This requires for consistency that also the constraint

$$S(f_s(t)) = S(f_1(t)) \quad (15)$$

must hold identically (*entropy constraints*). Furthermore, consistent with the principle of entropy maximization (PEM [23]) holding in CSM (see Axiom CSM-#2 in Appendix B), Propositions 1 and 2 (see Appendix B) and the requirement of isentropic flow [see Eq.(52) in Appendix A] we shall require:

- *Axiom #4 (entropic principle)*: for all for all $t \in I$ and $s = 1, N$, the s -point velocity PDF $f_s(t) \equiv f_s(1, ..s)$ satisfies PEM, i.e., for arbitrary $\delta f_s(t) = f_s(t) - f'_s(t)$, with $f_s(t), f'_s(t) \in \{f_s(t)\}$, it satisfies the variational equation

$$\delta S(f'_s(t))|_{f_s} = 0 \quad (16)$$

together with the inequality

$$\delta^2 S(f'_s(t))|_{f_s} < 0. \quad (17)$$

Let us analyze the physical interpretation of the previous assumptions. Here we remark that:

- (1) The state of the fluid is solely prescribed by the local fluid fields $\mathbf{V}(\mathbf{r}_1, t, \alpha)$, $p_1(\mathbf{r}_1, t, \alpha)$ as well as the global fluid field S_T . Hence, it cannot depend on non-local PDF, and therefore on multi-point velocity PDFs. This means that, in a complete SM it must be possible to represent all fluid fields *solely* in terms of suitable moments of the 1-point velocity PDF f_1 . This justifies Axioms #1, #2 and #3. In particular, regarding Axiom #3, Proposition 3 justifies the [equivalent] identification of the thermodynamic entropy with $S(f_1)$ and $S(f_N)$ (and hence also with $S(f_s)$ for $s = 2, N - 1$).
- (2) The entropy constraints (13) and (15) follow by noting that the thermodynamic entropy must be independent of the level of the statistical description $\{f_s, \Gamma_s\}$. In other words, the thermodynamic entropy is independent of the level adopted for the statistical description of the same fluid (i.e., the index s associated to the s -point PDF f_s).
- (3) The validity for all times $t \in I$ of the entropic principle (16), (17) is due to Proposition 3 (in Appendix B). Remarkably, its proof follows also independently from the entropic constraint (13), the condition of isentropic flow (50) as well as from the second axiom of CSM (see Axiom CSM-#2, in Appendix B).
- (4) The requirement of completeness for the SM $\{f_1, \Gamma_1\}$ demands that the local fluid fields $\mathbf{V}(\mathbf{r}_1, t, \alpha)$, $p_1(\mathbf{r}_1, t, \alpha)$ must satisfy INSE, which requires that in the set $\Omega \times I$, the following moment equations

$$\int_U d^3 \mathbf{v}_1 L_1(1) f_1(\mathbf{x}_1, t, \alpha) = \nabla \cdot \mathbf{V}(\mathbf{r}_1, t, \alpha) = 0, \quad (18)$$

$$\int_U d^3 \mathbf{v}_1 \mathbf{v}_1 L_1(1) f_1(\mathbf{x}_1, t, \alpha) = \rho(\mathbf{r}_1, t, \alpha) \frac{D}{Dt} \mathbf{V} - \rho(\mathbf{r}_1, t, \alpha) \mathbf{F}_H = 0, \quad (19)$$

must coincide respectively with the incompressibility and NS equations

[see Eqs.(50) and (51)]. Here $L_1(1)$ and $\mathbf{F}(\mathbf{x}_1, t, \alpha)$ denote respectively the 1-point Liouville operator (7) and a vector field depending only on the variables $(\mathbf{x}_1, t, \alpha)$ which must be defined, in particular, so that the constraint equation $\int_U d^3\mathbf{v}_1 \mathbf{F}(\mathbf{x}_1, t, \alpha) f_1(\mathbf{x}_1, t, \alpha) = \mathbf{F}_H$ is identically fulfilled in $\Omega \times I$.

Basic issues are related to the, possibly non-unique, determination of the appropriate SM $\{f, \Gamma\}$. These concern in particular:

(PROBLEM #1) the search of the (possible) minimum level (N) of the statistical description to be adopted for $\{f, \Gamma\}$;

(PROBLEM #2) the determination of the time-evolution of the multi-point PDFs f_N ;

(PROBLEM #3) the determination of the initial and boundary conditions for f_N .

Regarding the first problem the following remarkable result holds:

Theorem 1 - Factorization theorem for the local N -point PDF f_N .

Let us impose the Axioms of CSM [Axioms CSM-#1-#5] as well as Axioms #1-#4. Then, denoting it follows necessarily that:

1) *the variational constraint*

$$\delta \{S(f_N) - S(f_1)\} = 0 \quad (20)$$

must hold for all $t \in I$;

2) *for all $N \in \mathbb{N}_1$, the local N -point PDF $f_N(\mathbf{x}_1, \dots, \mathbf{x}_N, t, \alpha)$ is of the form:*

$$f_N(\mathbf{x}_1, \dots, \mathbf{x}_N, t, \alpha) = \prod_{i=1, N} f_1(\mathbf{x}_i, t, \alpha), \quad (21)$$

with $f_1(\mathbf{x}_1, t, \alpha)$ denoting the corresponding 1-point PDF;

3) *the constant K_N^2 entering in the in Eq.(14) reads*

$$K_N^2 = 1/N\mu(\Omega)^{N-1}. \quad (22)$$

PROOF. First we notice that the entropy constraint (15) together the entropic principle #4 [i.e., the requirement that Eqs.(16) and (17) hold for all $t \in I$] imply that, for all N and for all $t \in I$, also the variational constraint (20) must be fulfilled. To prove that the factorization property of the N -point PDF must hold for all $t \in I$, let us consider for illustration (and without

loss of generality) the case $N = 2$. Denoting $\hat{f}_2(\mathbf{x}_1, \mathbf{x}_2, t, \alpha) \equiv \hat{f}_2(1, 2)$ and $\hat{f}_1(\mathbf{x}_1, t, \alpha) \equiv \hat{f}_1(1)$, Eq.(20) delivers for arbitrary variations $\delta f_1(3)$:

$$\int_{\Gamma^3} d\mathbf{x} \delta f_1(3) \{f_2(1, 2) \ln f_2(1, 2) - f_1(1)f_1(2) [\ln f_1(1) + \ln f_1(2)]\} = 0. \quad (23)$$

This implies necessarily that the factorization condition $f_2(1, 2) = f_1(1)f_1(2)$ must hold identically in $\Gamma^2 \times I$. The proof can easily be extended to arbitrary $N > 2$, yielding Eq.(21). In turn, thanks to Eq.(21), equation (22) immediately follow from Eq.(15). Q.E.D.

We remark that in principle THM.1 can be generalized by requiring that PEM holds only at the initial time $t_o \in I$ (Axiom #5a). Nevertheless, in this case the constraint (15) only warrants that the factorization condition (??) holds at the initial time t_o , *unless* the form of the statistical (Liouville) equations holding for the s -point velocity PDFs is explicitly prescribed as done in Ref. [14]. Invoking, however, the *validity of Axiom #5b and consequently of THM.1*, the SM $\{f, \Gamma\}$ can be identified with the IKT SM for the 1-point PDF [10–13].

3 IKT statistical model - Relationship with the HRE approach

The explicit construction of a complete SM $\{f_1, \Gamma_1\}$ satisfying Axioms #1-#4, as well as the requirements set by CSM [Axioms CSM-#1-#5, in Appendix B] can be achieved following the inverse kinetic theory (IKT) developed in Ref. [10] by means of a suitable definition for the vector field $\mathbf{F}(\mathbf{x}_1, t, \alpha)$ appearing in the Liouville streaming operator $L_1(1)$. For definiteness the basic requirements of IKT are summarized in Appendix C.

In this section we intend to prove that the IKT approach is fully consistent with the customary approach to the statistical description of turbulence, namely the HRE approach.

Here, we intend to show, in particular, that IKT can be achieved in an equivalent way based on the same HRE approach. For this purpose, we pose the problem of determining the relationship between the 1-point PDF which characterizes the IKT SM $\{f_1, \Gamma_1\}$ and the PDF $f_H(t)$ associated to the statistical model $\{f_H, \Gamma_1\}$. Thus, let us denote

$$f_1 \equiv f_1(\mathbf{r}_1, \mathbf{u}_1, t, \alpha) \quad (24)$$

[with $\mathbf{u}_1 = \mathbf{v}_1 - \mathbf{V}(\mathbf{r}_1, t)$ and $\mathbf{x}_1 = (\mathbf{r}_1, \mathbf{v}_1) \in \Gamma_1$] the 1-point velocity PDF prescribed by IKT [10], namely a solution of a Liouville equation of the form (6)

with vector field $\mathbf{F}(\mathbf{x}_1, t)$, both defined according to Axioms #1-#4 and CSM (Axioms CSM-#1-#5) [see Appendix C]. Accordingly, *we intend to show that f_1 can be identified with a suitable stochastic-average of f_{H1}* [see Eq.(5)].

The result follows immediately by noting that a representation of the INSE problem is provided by the equivalent stochastic representation $\{Z_{\Delta\mathbf{V}}\}$ defined in Appendix A [Eq.(64)]. This is obtained replacing the fluid velocity $\mathbf{V}(\mathbf{r}_1, t, \alpha)$ with $\mathbf{V}'(\mathbf{r}_1, t, \alpha) = \mathbf{V}(\mathbf{r}_1, t, \alpha) + \Delta\mathbf{V}$, $\Delta\mathbf{V} \in \mathbb{R}^3$ denoting an arbitrary stochastic constant velocity fluctuation independent of $(\mathbf{r}_1, t, \alpha)$ which can be considered as stochastic. Hence, by assumption, $\Delta\mathbf{V} \equiv (\Delta V_1, \Delta V_2, \Delta V_3)$ is endowed with a stochastic PDF of the general form $g_1(\Delta\mathbf{V}, \mathbf{r}_1, t)$. Due to its arbitrariness, it can always be identified with

$$g_1(\Delta\mathbf{V}, \mathbf{r}, t, \alpha) \equiv f_1(\mathbf{r}_1, \Delta\mathbf{V}, t, \alpha), \quad (25)$$

with f_1 prescribed by Eq.(24). Thus, introducing the stochastic-averaging operator

$$\langle \cdot \rangle_{\Delta\mathbf{V}} \equiv \int_{\mathbb{R}^3} d^3\Delta\mathbf{V} g_1(\Delta\mathbf{V}, \mathbf{r}, t, \alpha) \cdot, \quad (26)$$

we can always impose, consistent with IKT (see Appendix C) that the moments of g_1 are set so that the following constraint equations

$$\langle 1 \rangle_{\Delta\mathbf{V}} \equiv \int_{\mathbb{R}^3} d^3\Delta\mathbf{V} f_1(\mathbf{r}_1, \Delta\mathbf{V}, t, \alpha), \quad (27)$$

$$\mathbf{0} = \langle \Delta\mathbf{V} \rangle_{\Delta\mathbf{V}} \equiv \int_{\mathbb{R}^3} d^3\Delta\mathbf{V} \Delta\mathbf{V} f_1(\mathbf{r}_1, \Delta\mathbf{V}, t, \alpha), \quad (28)$$

$$p_1(\mathbf{r}_1, t, \alpha) = \frac{\rho_o}{3} \langle (\Delta\mathbf{V})^2 \rangle_{\Delta\mathbf{V}} \equiv \rho_o \int_{\mathbb{R}^3} d^3\Delta\mathbf{V} \frac{1}{3} (\Delta\mathbf{V})^2 f_1(\mathbf{r}_1, \Delta\mathbf{V}, t, \alpha), \quad (29)$$

and

$$S_T = - \int_{\Omega} d^3\mathbf{r}_1 \int_{\mathbb{R}^3} d^3\Delta\mathbf{V} g_1(\Delta\mathbf{V}, \mathbf{r}, t, \alpha) \ln g_1(\Delta\mathbf{V}, \mathbf{r}, t, \alpha) \equiv S(g_1) \quad (30)$$

are fulfilled identically. In particular, the third velocity moment (29) requires that, up to the constant factor, the stochastic-average of the *stochastic kinetic energy* $\frac{m}{2} (\Delta\mathbf{V})^2$, $p_1(\mathbf{r}_1, t, \alpha)$ must coincide with the corresponding *kinetic pressure*. On the other hand, since $\{Z_{\Delta\mathbf{V}}\}$ are solutions of an equivalent INSE problem [see the Appendix A, Proposition A.1], the HRE 1-point velocity PDF becomes in this case:

$$f_{H1}(\mathbf{r}_1, \mathbf{u}_1 - \Delta\mathbf{V}, t) \equiv \delta(\mathbf{v}_1 - \mathbf{V}(\mathbf{r}_1, t) - \Delta\mathbf{V}). \quad (31)$$

Therefore, since the properties of the NS flow cannot depend on $\Delta\mathbf{V}$ (see Proposition A.1 in Appendix A), it is obvious that it can be equivalently described either by $\{f_{H1}, \Gamma_1\}$ or $\{\langle f_{H1} \rangle_{\Delta\mathbf{V}}, \Gamma_1\}$, where f_{H1} and $\langle f_{H1} \rangle_{\Delta\mathbf{V}}$ are

respectively identified with the local PDF $f_{H1}(\mathbf{r}_1, \mathbf{u}_1, t)$ defined by Eq.(5) and $\langle f_{H1}(\mathbf{r}_1, \mathbf{u}_1 - \Delta \mathbf{V}, t) \rangle_{\Delta \mathbf{V}}$. Indeed thanks to the positions (27)-(30) in both cases velocity moment equations of the Liouville equation (6) evaluated w.r. to the weight functions $\{G\} = \{1, \mathbf{v}_1\}$, coincide respectively with Eqs.(50) and (51) [see Appendix A]. In fact, in this setting it follows that:

Theorem 2 - Representation of f_1 in terms of f_{H1} .

Invoking the positions (25) and (26), the stochastic average $\langle \cdot \rangle_{\Delta \mathbf{V}}$ of the HRE 1-point PDF f_{H1} , defined by Eq.(31), is provided by

$$\langle f_{H1}(\mathbf{r}_1, \mathbf{u}_1 - \Delta \mathbf{V}, t) \rangle_{\Delta \mathbf{V}} = f_1(\mathbf{r}, \mathbf{u}, t, \alpha), \quad (32)$$

with $f_1(\mathbf{r}, \mathbf{u}, t)$ denoting the 1-point velocity PDF (24) prescribed according to IKT [10]. As a consequence, it follows

$$\langle \langle f_{H1}(\mathbf{r}_1, \mathbf{u}_1 - \Delta \mathbf{V}, t) \rangle_{\Delta \mathbf{V}} \rangle = \langle f_1(\mathbf{r}, \mathbf{u}, t, \alpha) \rangle, \quad (33)$$

$\langle \cdot \rangle$ denoting the ensemble-average operator defined by Eq.(11).

PROOF. The proof of Eqs.(60) and (33) follows by noting that $\langle f_{H1} \rangle_{\Delta \mathbf{V}} \equiv \int_{\mathbb{R}^3} d^3 \Delta \mathbf{V} f_1(\mathbf{r}, \Delta \mathbf{V}, t, \alpha) \delta(\mathbf{v} - \mathbf{V}(\mathbf{r}, t, \alpha) - \Delta \mathbf{V}) = f_1(\mathbf{r}, \mathbf{u}, t, \alpha)$ is identically satisfied. Q.E.D.

As a consequence of Eq.(32) and the properties of the 1-point velocity PDF $f_1(\mathbf{r}, \mathbf{u}, t, \alpha)$ [see Appendix C, Eqs. (110),(111),(112),(113)] it follows that $\{f_1 \equiv \langle f_{H1} \rangle_{\Delta \mathbf{V}}, \Gamma_1\}$ is a complete statistical model.

In conclusion:

- the 1-point PDF of the IKT SM $\{f_1, \Gamma_1\}$ is simply defined a suitable *stochastic-average* of the PDF f_{H1} , achieved by means of the stochastic-averaging operator $\langle \cdot \rangle_{\Delta \mathbf{V}}$ defined above [Eq.(26)];
- in view of the position (29), g_1 can be interpreted as the stochastic PDF which takes into account the thermal motion of fluid particles produced in a NS fluid by the kinetic pressure $p_1(r, t)$;
- manifestly Eq.(32) does not imply any restriction on the flow dynamics, i.e., on the (strong) solutions of the INSE problem.

4 IKT for multi-point PDFs

The construction of multi-point PDFs is a problem of "practical" interest in experimental/numerical research in fluid dynamics, usually adopted for the statistical analysis of turbulent fluids. In fact, they can be experimentally measured in terms of velocity differences between different fluid elements. In the present paper, unlike elsewhere [such as the ML approach] where the ensemble-averaged PDF $\langle f_1 \rangle$ is considered, we are interested solely in the determination of the *local* 1-point velocity PDFs $f_1(\mathbf{x}_i, t, \alpha)$ and $f_s(\mathbf{x}_1, \dots, \mathbf{x}_s, t, \alpha)$ together with the related statistical equations advancing them in time. We intend to show that in the framework of the IKT approach the construction of the multi-point PDFs becomes trivial. Nonetheless, the construction method here pointed out is useful to analyze basic implications of IKT dealing with: a) the specific representation of certain "reduced" multi-point PDFs, defined in terms of the 1-point PDF; b) their dynamics, namely the statistical equations which they fulfill. Let us now identify f_1 with the 1-point PDF defined by the IKT SM [10], namely a particular solution of the Liouville equation (6) with $\mathbf{F}(i) \equiv \mathbf{F}(\mathbf{x}_i, t, \alpha; f_1)$ is the 1-point mean-field force per unit mass at (\mathbf{x}_i, t) , to be generally considered as functionally dependent on the same f_1 [10] (see also Ref.[13] for the extension to the stochastic INSE problem). Then, denoting $f_1(i) \equiv f_1(\mathbf{x}_i, t, \alpha; Z)$ (for $i = 1, s$) the 1-point velocity PDF evaluated at the states $\mathbf{x}_i \equiv (\mathbf{r}_i, \mathbf{v}_i)$ (for $i = 1, s$), the corresponding s -point velocity PDF defined in the product phase-space $\Gamma_s \equiv \prod_{i=1,s} \Gamma$ is simply defined as

$$f_s(1, 2, \dots, s) \equiv \prod_{i=1,s} f_1(i), \quad (34)$$

where f_s advances in time by means of the corresponding s -point Liouville equation, namely

$$L_s(1, \dots, s) f_s(1, 2, \dots, s) = 0, \quad (35)$$

with $L_s(1, \dots, s)$ defined by Eq.(10). As a consequence, the corresponding ensemble-averaged PDF is simply identified with

$$\langle f_s(1, 2, \dots, s) \rangle = \left\langle \prod_{i=1,s} f_1(i) \right\rangle. \quad (36)$$

Therefore the ensemble averaged PDFs $\langle f_s(1, 2, \dots, s) \rangle$ are uniquely determined! We remark that Eq.(36) generally implies the obvious consequence that $\langle f_s(1, 2, \dots, s) \rangle$ is not factorizable, i.e., $\langle f_s(1, 2, \dots, s) \rangle \neq \prod_{i=1,s} \langle f_1(i) \rangle$.

4.1 Explicit evaluation of 2-point velocity PDFs

In terms of the 2-point PDF, $f_2(1, 2)$, a number of reduced probability densities can be defined in suitable subspaces of Γ^2 . To introduce them explicitly let us first introduce the transformation to the center of mass coordinates of the two point-particles with states $(\mathbf{r}_i, \mathbf{v}_i)$ (for $i = 1, 2$)

$$\{\mathbf{r}_1, \mathbf{v}_1, \mathbf{r}_2, \mathbf{v}_2\} \rightarrow \{\mathbf{r}, \mathbf{R}, \mathbf{v}, \mathbf{V}\} \quad (37)$$

[here $\mathbf{r} = \frac{\mathbf{r}_1 + \mathbf{r}_2}{2}$, $\mathbf{R} = \frac{\mathbf{r}_1 - \mathbf{r}_2}{2}$; furthermore, \mathbf{v}, \mathbf{V} can be identified with $\mathbf{v} = \mathbf{v}_1 - \mathbf{v}_2$ and $\mathbf{V} = \mathbf{v}_1 + \mathbf{v}_2$]. Then, these are respectively:

1) the *local* (in configuration space) *velocity-difference 2-point PDF* $g_2(\mathbf{r}_1, \mathbf{r}_2, \mathbf{v}, t, \alpha)$ defined in the phase-space $\Omega^2 \times U$ and obtained integrating the 2-point velocity PDF w.r. to the mean velocity \mathbf{V}

$$\begin{aligned} g_2(\mathbf{r}_1, \mathbf{r}_2, \mathbf{v}, t, \alpha) &= \int_U d^3\mathbf{V} f_2(1, 2) \equiv \\ &\equiv \int d^3\mathbf{V} f_1(\mathbf{r}_1, \mathbf{v} + \mathbf{V}, t, \alpha) f_1(\mathbf{r}_2, \mathbf{V} - \mathbf{v}, t, \alpha; Z); \end{aligned} \quad (38)$$

2) the *velocity-difference 2-point PDF* $\hat{f}_2(\mathbf{r}, \mathbf{v}, t, \alpha)$ defined in $\Gamma_1 = \Omega \times U$ and obtained integrating also on the center-of-mass position vector \mathbf{R} . Thus denoting by

$$\langle \bullet \rangle_{\mathbf{R}, \Omega} = \frac{1}{\mu(\Omega)} \int_{\Omega} d^3\mathbf{R} \bullet \quad (39)$$

the configuration-space average operator acting on the center of mass coordinates \mathbf{R} , there it follows

$$\hat{f}_2(\mathbf{r}, \mathbf{v}, t, \alpha) = \langle g_2(\mathbf{r} + \mathbf{R}, \mathbf{R} - \mathbf{r}, \mathbf{v}, t, \alpha) \rangle_{\mathbf{R}, \Omega}. \quad (40)$$

In particular, in the case of a Gaussian PDF [see Eq.(114) in Appendix C], Eq.(38) delivers again a Gaussian-type PDF

$$g_2(\mathbf{r}_1, \mathbf{r}_2, \mathbf{v}, t, \alpha) = \frac{1}{\pi^{3/2} v_{th}^3} \exp \left\{ - \frac{\left\| \mathbf{v} - \frac{\mathbf{V}(1) - \mathbf{V}(2)}{2} \right\|^2}{v_{th}^2} \right\}, \quad (41)$$

where $\mathbf{V}(i) \equiv \mathbf{V}(\mathbf{r}_i, t)$, $v_{th,p}^2(i) = v_{th,p}^2(\mathbf{r}_i, t)$ and v_{th}^2 denotes

$$v_{th}^2 = \frac{v_{th,p}^2(1) + v_{th,p}^2(2)}{4}. \quad (42)$$

In a similar way it is possible to obtain explicit representations for the following additional 2-point PDFs:

- (1) *the velocity-difference 2-point PDF for parallel velocity increments.* Introducing the representations $\mathbf{v} = \mathbf{n}v$ and $\mathbf{r} = \mathbf{n}r$, \mathbf{n} denoting a unit vector, $\hat{f}_{2\parallel}(r, v, t)$ can be simply defined as the solid-angle average

$$\hat{f}_{2\parallel}(r, v, t, \alpha) = \int d\Omega(\mathbf{n}) \hat{f}_2(\mathbf{r} = \mathbf{n}r, \mathbf{v} = \mathbf{n}v, t, \alpha); \quad (43)$$

- (2) *the velocity-difference 2-point PDF for perpendicular velocity increments.* Introducing, instead, the representations $\mathbf{v} = \mathbf{n}v$ and $\mathbf{r} = \mathbf{n} \times \mathbf{b}r$, \mathbf{n} and \mathbf{b} denoting two independent unit vectors, $\hat{f}_{2\perp}(r, v, t)$ can be defined as the double-solid-angle average

$$\begin{aligned} \hat{f}_{2\perp}(r, v, t, \alpha) &= \int d\Omega(\mathbf{n}) \int d\Omega(\mathbf{b}) \\ &\hat{f}_2(\mathbf{r} = \mathbf{n} \times \mathbf{b}r, \mathbf{v} = \mathbf{n}v, t, \alpha). \end{aligned} \quad (44)$$

An interesting property which emerges from these results is that in all cases indicated above [i.e., Eqs.(40),(43) and (44)] the definition of g_2 given above [Eq.(38)] implies that non-Gaussian features, respectively in \hat{f}_2 , $\hat{f}_{2\parallel}$ and $\hat{f}_{2\perp}$, may arise even if the 1-point PDF is Gaussian. This occurs due to velocity and pressure fluctuations occurring between different spatial positions \mathbf{r}_1 and \mathbf{r}_2 .

4.2 Statistical evolution equation for the velocity-difference 2-point PDF

From the 2-point Liouville equation (35) it is immediate to obtain the corresponding evolution equation for the reduced PDFs indicated above. For example, the velocity-difference 2-point PDF \hat{f}_2 satisfies the equation

$$\frac{\partial \hat{f}_2}{\partial t} + \mathbf{v} \cdot \frac{\partial}{\partial \mathbf{r}} \hat{f}_2 = - \frac{\partial}{\partial \mathbf{v}} \cdot \mathbf{D} \quad (45)$$

where \mathbf{D} is the diffusion vector

$$\mathbf{D} = \frac{1}{\mu(\Omega)} \int d^3\mathbf{V} \int_{\Omega} d^3\mathbf{R} \frac{\mathbf{F}_1(1) - \mathbf{F}_2(2)}{2} f_2(1, 2). \quad (46)$$

It follows, in particular, that in the case of a Gaussian 1-point PDF this equation reduces to the Fokker-Planck equation

$$\begin{aligned} \frac{\partial \hat{f}_2}{\partial t} + \mathbf{v} \cdot \frac{\partial}{\partial \mathbf{r}} \hat{f}_2 &= - \frac{\partial}{\partial \mathbf{v}} \cdot \widehat{\mathbf{D}} \\ \mathbf{F}^{(T)} g_2(\mathbf{r} + \mathbf{R}, \mathbf{R} - \mathbf{r}, \mathbf{v}, t, \alpha), \end{aligned} \quad (47)$$

where the Fokker-Planck diffusion vector $\widehat{\mathbf{D}}$ reads

$$\widehat{\mathbf{D}} = \frac{1}{\mu(\Omega)} \int_{\Omega} d^3\mathbf{R} \mathbf{F}^{(T)} g_2(\mathbf{r} + \mathbf{R}, \mathbf{R} - \mathbf{r}, \mathbf{v}, t, \alpha) \quad (48)$$

and the vector field $\mathbf{F}_1^{(T)} \equiv \mathbf{F}_1^{(T)}(\mathbf{r}_1, \mathbf{r}_2, \mathbf{V}, t, \alpha; f_M)$ is reported in Ref. [10]. It follows that both equations are manifestly *non-Markovian* as a consequence of the non-local dependencies arising (in both cases) in the Fokker-Planck coefficients \mathbf{D} and $\widehat{\mathbf{D}}$.

We stress, that from Eqs.(45) and (47) the corresponding statistical equations advancing in time the ensemble-averaged PDF $\langle \widehat{f}_2 \rangle$ can simply be determined. Therefore, to evaluate $\langle \widehat{f}_2 \rangle$ only the knowledge of the local PDF \widehat{f}_2 , defined by Eq.(40), is required. Therefore, in turn, $\langle \widehat{f}_2 \rangle$ is uniquely prescribed by the local 1-point velocity f_1 , determined by the IKT SM $\{f_1, \Gamma_1\}$.

An interesting issue is here provided by the comparison with the statistical formulation developed by Peinke and coworkers [24–28]. Their approach, based on the statistical analysis of experimental observations, indicates that in case of stationary and homogeneous turbulence both the 2-point PDFs for parallel and velocity increments obey stationary Fokker-Planck equations. In particular, according to experimental evidence [27, 28] a reasonable agreement with a Markovian approximation for Eq.(47) - at least in some limited subset of parameter space- is suggested. Our theory implies, however, that a breakdown of the Markovian property should be expected due to non-local contributions appearing in the previous statistical equations (45) and (47).

5 Conclusions

In this paper we have shown that the multi-point PDFs used in customary phenomenological approaches to turbulence can be explicitly evaluated in terms of the local 1-point velocity PDF (f_1) determined in the framework on the IKT SM [10–14]. As a basic consequence the corresponding ensemble-averaged multipoint PDFs can be simply evaluated.

Starting points are provided by THM.1, showing that under suitable hypotheses the local multi-point PDF f_N is necessarily factorized in terms of the 1-point PDF f_1 , and THM.2, displaying the relationship between the local 1-point velocity PDFs used in the HRE and IKT approaches. The requirements here imposed include, in particular, the assumption that $\{f_1, \Gamma_1\}$ is a complete SM, i.e., that in terms of the *local* 1-point PDF the complete set of fluid fields (defining the fluid state) can be represented by means of suitable velocity and phase-space moments [see Axioms #1-#4]. Then, provided the SM satisfies the axioms of CSM (Axioms CSM-#1-#5) as well as the entropic principle (Axiom#4) the factorization condition (21) for f_N in terms of the 1-point PDF f_1 necessarily follows. As a result, in validity of the previous requirements, the SM for NS fluid can be identified with the IKT SM $\{f_1, \Gamma_1\}$

earlier developed [10–13] and based on the 1-point PDF f_1 .

Important consequences of the theory include:

- (1) arbitrary multi-point PDFs can be uniquely represented in terms of the 1-point PDF characterizing the IKT SM $\{f_1, \Gamma_1\}$;
- (2) the time evolution of the multi-point PDFs is uniquely determined by $\{f_1, \Gamma_1\}$;
- (3) the theoretical prediction of multipoint PDFs based uniquely on first principles is actually made possible;
- (4) as a particular case, the example of a Gaussian 1-point PDF has been considered;
- (5) qualitative properties of the multi-point PDFs can be investigated. In particular, this concerns the possible prediction of non-Gaussian behavior for the 2-point PDFs arising in HIST. As pointed out in Sec.4 this may arise, even in the presence of a Gaussian 1-point PDF, due to non-local velocity and pressure effects.

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6 Appendix: stochastic INSE Problem

For stochastic fluid fields of the form (2) the fluid equations for an incompressible NS fluid are the so-called incompressible Navier-Stokes equations (INSE) :

$$\rho = \rho_o, \quad (49)$$

$$\nabla \cdot \mathbf{V} = 0, \quad (50)$$

$$N\mathbf{V} = 0, \quad (51)$$

$$\frac{\partial}{\partial t} S_T = 0, \quad (52)$$

$$\{Z(\mathbf{r}, t_o, \alpha)\} = \{Z_o(\mathbf{r}, \alpha)\}, \quad (53)$$

$$\{Z(\mathbf{r}, t, \alpha)|_{\partial\Omega}\} = \{Z_w(\mathbf{r}, t, \alpha)|_{\partial\Omega}\}, \quad (54)$$

for the stochastic *NS fluid fields*

$$\{Z\} \equiv \{\rho_o, \mathbf{V}(\mathbf{r}, t, \alpha), p_1(\mathbf{r}, t, \alpha), S_T\}. \quad (55)$$

Eqs. (49)- (54) denote respectively the *uniformly (space- and time-) constant mass density, incompressibility (or isochoricity), Navier-Stokes and constant thermodynamic entropy equations* and the initial and Dirichlet boundary conditions for $\{Z\}$, with $\{Z_o(\mathbf{r}, \alpha)\}$ and $\{Z_w(\mathbf{r}, t, \alpha)|_{\partial\Omega}\}$ suitably prescribed initial and boundary-value fluid fields, defined respectively at the initial time $t = t_o$ and on the boundary $\partial\Omega$. In particular, this means that they are required to be at least continuous in all points of the closed set $\bar{\Omega} \times I$, with $\bar{\Omega}$ the closure of Ω . Due to Eq.(49), since in the domain $\bar{\Omega} \times I$, ρ is a positive constant parameter the fluid fields describing the NS fluid can be effectively reduced to the subset of *NS proper* fluid fields

$$\{Z\}_R \equiv \{\mathbf{V}(\mathbf{r}, t, \alpha), p_1(\mathbf{r}, t, \alpha), S_T\} \quad (56)$$

In the remainder we shall require that:

- (1) Ω (*configuration domain*) is a bounded subset of the Euclidean space E^3 on \mathbb{R}^3 ;
- (2) I (*time axis*) is identified, when appropriate, either with a bounded interval, *i.e.*, $I =]t_0, t_1[\subseteq \mathbb{R}$, or with the real axis \mathbb{R} ;
- (3) in the open set $\Omega \times I$ the functions $\{Z\}$, are assumed to be solutions of Eqs.(49)-(52) subject, while in $\bar{\Omega} \times I$ they satisfy the whole set of Eqs. (49)-(54). In particular: Eqs. (53)- (54) define the *initial-boundary value INSE problem*,
- (4) by assumption, the fluid fields are *strong solutions* of the fluid equations. Hence Eqs.(53)- (54) are required to define a well-posed problem with unique strong solution defined everywhere in $\Omega \times I$.

Here the notation as follows. N is the *NS nonlinear operator*

$$N\mathbf{V} = \frac{D}{Dt}\mathbf{V} - \mathbf{F}_H, \quad (57)$$

with $\frac{D}{Dt}\mathbf{V}$ and \mathbf{F}_H denoting respectively the *Lagrangian fluid acceleration* and the *total force per unit mass*

$$\frac{D}{Dt}\mathbf{V} = \frac{\partial}{\partial t}\mathbf{V}(\mathbf{r}, t, \alpha) + \mathbf{V}(\mathbf{r}, t, \alpha) \cdot \nabla \mathbf{V}(\mathbf{r}, t, \alpha), \quad (58)$$

$$\mathbf{F}_H \equiv -\frac{1}{\rho_o}\nabla p(\mathbf{r}, t, \alpha) + \frac{1}{\rho_o}\mathbf{f}(\mathbf{r}, t, \alpha) + \nu \nabla^2 \mathbf{V}(\mathbf{r}, t, \alpha), \quad (59)$$

while $\rho_o > 0$ and $\nu > 0$ are the *constant mass density* and the constant *kinematic viscosity*. In particular, \mathbf{f} is the *volume force density* acting on the fluid, namely which is assumed of the form

$$\mathbf{f} = -\nabla \phi((\mathbf{r}, t, \alpha) + \mathbf{f}_R(\mathbf{r}, t, \alpha), \quad (60)$$

$\phi((\mathbf{r}, t, \alpha)$ being a suitable scalar potential, so that the first two force terms [in

Eq.(59)] can be represented as

$$-\nabla p(\mathbf{r}, t, \alpha) + \mathbf{f}(\mathbf{r}, t, \alpha) = -\nabla p_1(\mathbf{r}, t, \alpha) + \mathbf{f}_R(\mathbf{r}, t, \alpha), \quad (61)$$

with $p_1(\mathbf{r}, t, \alpha)$ defined by Eq.(1) denoting the kinetic pressure. As a consequence the fluid pressure necessarily satisfies the *Poisson equation*

$$\nabla^2 p(\mathbf{r}, t, \alpha) = S(\mathbf{r}, t, \alpha), \quad (62)$$

where the source term S reads

$$S(\mathbf{r}, t, \alpha) = -\rho_o \nabla \cdot (\mathbf{V} \cdot \nabla \mathbf{V}) + \nabla \cdot \mathbf{f}. \quad (63)$$

6.1 An equivalent form of INSE

An equivalent form for INSE follows by introducing a stochastic representation for the fluid fields $\{Z\}$.

PROPOSITION A.1 - Stochastic representation $\{Z_{\Delta \mathbf{V}}\}$

An equivalent representation for INSE is provided by the stochastic fluid fields

$$\{Z_{\Delta \mathbf{V}}\} = \{\mathbf{V}(\mathbf{r}_1, t, \alpha) + \Delta \mathbf{V}, p(\mathbf{r}_1, t, \alpha), S_T\}, \quad (64)$$

where $\{Z\}_R = \{\mathbf{V}(\mathbf{r}_1, t, \alpha), p_1(\mathbf{r}_1, t, \alpha), S_T\}$ and $\Delta \mathbf{V} \in \mathbb{R}^3$ denote respectively an arbitrary particular solution of the INSE problem [Eqs. (49)- (54)] and an arbitrary stochastic vector independent of (\mathbf{r}, t, α) . $\{Z_{\Delta \mathbf{V}}\}$ are solutions of the equivalent INSE problem in which the NS equation (51) and similarly the initial and boundary conditions (53)- (54) are replaced respectively with

$$\frac{D}{Dt} \mathbf{V}' = \mathbf{F}_H + \Delta \mathbf{F}_H, \quad (65)$$

and

$$\{Z_{\Delta \mathbf{V}}(\mathbf{r}, t_o, \alpha)\} = \{Z_{\Delta \mathbf{V}, o}(\mathbf{r}, \alpha)\}, \quad (66)$$

$$\{Z_{\Delta \mathbf{V}}(\mathbf{r}, t_o, \alpha)|_{\partial \Omega}\} = \{Z_{\Delta \mathbf{V}, \mathbf{w}}(\mathbf{r}, t, \alpha)|_{\partial \Omega}\}, \quad (67)$$

while $\Delta \mathbf{F}_H$ denotes the vector field

$$\Delta \mathbf{F}_H = \Delta \mathbf{V} \cdot \nabla \mathbf{V}(\mathbf{r}, t, \alpha). \quad (68)$$

PROOF (omitted)

7 Appendix B - Statistical mechanics of Newtonian dynamical systems

In this Appendix the basic assumptions and elementary consequences of classical statistical mechanics are recalled. Let us consider, for definiteness, a Newtonian dynamical system associated to an ensemble of N like point-particles (S_N), i.e., the flow defined for all $\mathbf{x}_o \in \Gamma_N$ and $t_o, t \in I$:

$$T_{t_o, t} : \mathbf{x}_o \rightarrow \mathbf{x}(t) = T_{t_o, t} \mathbf{x}_o \equiv \chi(\mathbf{x}_o, t_o, t) \quad (69)$$

and with inverse transformation

$$T_{t, t_o} : \mathbf{x}(t) \rightarrow \mathbf{x}_o \equiv \mathbf{x}(t_o) = T_{t, t_o} \mathbf{x}(t) \equiv \chi(\mathbf{x}(t), t, t_o), \quad (70)$$

which is generated by initial value problem

$$\begin{cases} \frac{d\mathbf{x}}{dt} = \mathbf{X}(\mathbf{x}, t), \\ \mathbf{x}(t_o) = \mathbf{x}_o, \end{cases} \quad (71)$$

with $\mathbf{X}(\mathbf{x}, t) \equiv \{\mathbf{v}, \mathbf{F}(\mathbf{x}, t)\}$,

$$\mathbf{F}(\mathbf{x}, t) \equiv (\mathbf{F}_1(\mathbf{x}, t), \dots, \mathbf{F}_N(\mathbf{x}, t)) \quad (72)$$

a suitable vector field, $\mathbf{x} = (\mathbf{r}, \mathbf{v}) = \{\mathbf{x}_1 = (\mathbf{r}_1, \mathbf{v}_1), \dots, \mathbf{x}_N = (\mathbf{r}_N, \mathbf{v}_N)\} \in \Gamma_N$ the state of S_N , each point-particle being endowed with the Newtonian state $\mathbf{x}_i = (\mathbf{r}_i, \mathbf{v}_i)$. In particular, we shall require that the vector fields \mathbf{F}_i (for $i = 1, N$) are of the form

$$\mathbf{F}_i(\mathbf{x}, t) = \frac{1}{m} \mathbf{F}^{(ext)}(\mathbf{x}_i, t) + \frac{1}{m} \sum_{\substack{j=1, N \\ j \neq i}} \mathbf{F}^{(int)}(\mathbf{x}_i, \mathbf{x}_j, t), \quad (73)$$

with $\mathbf{F}^{(ext)}(\mathbf{x}_i, t)$ and $\mathbf{F}^{(int)}(\mathbf{x}_i, \mathbf{x}_j, t)$ denoting unary and binary forces, with the latter ones satisfying the action-reaction principle

$$\mathbf{F}^{(int)}(\mathbf{x}_i, \mathbf{x}_j, t) = -\mathbf{F}^{(int)}(\mathbf{x}_j, \mathbf{x}_i, t). \quad (74)$$

Then, according to Classical Statistical Mechanics (CSM), the statistical description for the dynamical system (69) is defined by the following Axioms #1-#5:

- (1) *Axiom CSM-#1 (initial PDF - Deterministic/stochastic initial conditions -Functional setting)*: the initial state \mathbf{x}_o is a stochastic vector endowed with a probability density $p_N(t_o) \equiv p_N(\mathbf{x}_o, t_o, \alpha)$ (*initial PDF*), belonging to a suitable functional class $\{p_N(t_o)\}$. Then the initial state \mathbf{x}_o will be

denoted *deterministic* or *stochastic* on Γ_N if everywhere in Γ_N , $p_N(t_o)$ takes either the form: A) $p_N(t_o) = \delta(\mathbf{x}_o - \mathbf{x}(t_o))$ (*deterministic PDF*), yielding $\langle\langle \mathbf{x}_o \rangle\rangle = \mathbf{x}_o$ [the brackets denoting the stochastic average $\langle\langle \rangle\rangle = \int d\mathbf{x}_o p_N(t_o)$], or respectively B) $p_N(t_o)$ (*stochastic PDF*) is at least $C^{(o)}(\Gamma_N)$, which, instead, implies that almost everywhere in Γ_N , $\langle\langle \mathbf{x}_o \rangle\rangle \neq \mathbf{x}_o$.

- (2) *Axiom CSM-#2 (PEM)*: if $\{p_N(t_o)\}$ is identified with the set of stochastic PDFs $p_N(t_o)$ which are strictly positive and admit the Boltzmann-Shannon entropy functional

$$S(p_N(t_o)) = -K_N^2 \int_{\Gamma_s} d\mathbf{x}_o p_N(t_o) \ln p_N(t_o) \quad (75)$$

(*N-body BS entropy*), with $d\mathbf{x}_o = \prod_{k=1,s} d\mathbf{r}_{ok} d\mathbf{v}_{ok}$ and K_N a suitable real constant. Then the initial PDF entering Eq.(78), $p_{No} \equiv p_{No}(\mathbf{x}_o, \alpha)$, maximizes the N-body BS-entropy $S(p'_N(t_o))$ in a suitable functional class to which it belongs $\{p_N(t_o)\}$ [principle of entropy maximization (PEM [23])]. Thus, denoting respectively with $\delta S(f'_N(t_o))$ and $\delta^2 S(f'_N(t_o))$ the first and second variations of $S(p'_N(t_o))$ evaluated for an arbitrary $p'_N(t_o) \equiv p'_N(\mathbf{x}_o, t_o, \alpha) \in \{p_N(t_o)\}$ and variation $\delta p_N(t_o) = p_{No} - p'_{No}(t_o)$, the variational equation

$$\delta S(p'_N(t_o))|_{f_{No}} = 0 \quad (76)$$

must hold for arbitrary $\delta p_N(t_o)$ and p_{No} such that

$$\delta^2 S(p'_N(t_o))|_{f_{No}} < 0. \quad (77)$$

- (3) *Axiom CSM-#3 (Liouville equation and BBGKY hierarchy)*: the probability density p_N satisfies the integral Liouville equation

$$p(\mathbf{x}, t, \alpha) = \left| \frac{\partial \mathbf{x}_o(t_o)}{\partial \mathbf{x}} \right| p_{No}(\mathbf{x}(t_o), \alpha) \quad (78)$$

with $\left| \frac{\partial \mathbf{x}_o(t_o)}{\partial \mathbf{x}} \right|$ denoting the Jacobians of the inverse transformation (70). Then, if $p_{No}(\mathbf{x}(t_o), \alpha)$ is at least $C^{(1)}(\Gamma_N)$, $p_N(\mathbf{x}, t, \alpha)$ satisfies necessarily the differential Liouville equation

$$L_N(1, \dots, N) p_N(\mathbf{x}, t, \alpha) = 0, \quad (79)$$

with $L_N(1, \dots, N)$ denoting the N-body Liouville streaming operator

$$L_N(1, \dots, N) \equiv \frac{\partial}{\partial t} + \mathbf{v} \cdot \frac{\partial}{\partial \mathbf{r}} + \frac{\partial}{\partial \mathbf{v}} \cdot \left\{ \frac{1}{m} \mathbf{F}(\mathbf{x}, t) \cdot \right\} \equiv \quad (80)$$

$$\equiv \frac{\partial}{\partial t} + \mathbf{v}_i \cdot \frac{\partial}{\partial \mathbf{r}_i} + \frac{\partial}{\partial \mathbf{v}_i} \cdot \left\{ \frac{1}{m} \mathbf{F}_i(\mathbf{x}, t) \cdot \right\} \quad (81)$$

with summation understood on repeated indexes. As a consequence, for $s = 1, N - 1$ the reduced PDFs

$$p_s(\mathbf{x}_1, \dots, \mathbf{x}_s, t, \alpha) = \int_{\Gamma_1} d^3\mathbf{x}_{s+1} p_{s+1}(\mathbf{x}_1, \dots, \mathbf{x}_{s+1}, t, \alpha), \quad (82)$$

satisfy the equations (of the BBGKY hierarchy):

$$L_s(1, \dots, s)p_s \equiv C_s(p_{s+1}), \quad (83)$$

with $C_s(p_{s+1})$ the integro-differential operator

$$C_s(p_{s+1}) = - \sum_{j=s+1, N} \frac{\partial}{\partial \mathbf{v}_i} \cdot \int_{\Gamma_1} d^3\mathbf{x}_j \frac{1}{m} \mathbf{F}^{(int)}(\mathbf{x}_i, \mathbf{x}_j, t) p_{s+1}(\mathbf{x}_1, \dots, \mathbf{x}_s, \mathbf{x}_j, t, \alpha). \quad (84)$$

- (4) *Axiom CSM-#4 (like-particles)*: In the case of an ensemble of N like particles $p_N(\mathbf{x}, t, \alpha)$ is endowed with the symmetry property

$$p_N((\mathbf{x}_1, \dots, \mathbf{x}_N), t, \alpha) = p_N((\mathbf{x}_1, \dots, \mathbf{x}_N)', t, \alpha), \quad (85)$$

$(\mathbf{x}_1, \dots, \mathbf{x}_N)'$ denoting an arbitrary permutation of $(\mathbf{x}_1, \dots, \mathbf{x}_N)$. It follows that in this case (84) becomes

$$C_s(p_{s+1}) = - \frac{\partial}{\partial \mathbf{v}_i} \cdot \mathbf{A}_s(p_{s+1}), \quad (86)$$

where $\mathbf{A}_s(p_{s+1}) \equiv (N-s) \int_{\Gamma_1} d^3\mathbf{x}_{s+1} \frac{1}{m} \mathbf{F}^{(int)}(\mathbf{x}_i, \mathbf{x}_{s+1}, t) p_{s+1}(\mathbf{x}_1, \dots, \mathbf{x}_s, \mathbf{x}_{s+1}, t, \alpha)$.

- *Axiom CSM-#5 (moments, fluid fields and fluid equations)*: Let us require that $\{p_{No}\}$ is prescribed so that:

A) the statistical entropies associated to the s -body PDFs p_s

$$S(p_s) = -K_s^2 \int_{\Gamma^s} d\mathbf{x} p_s \ln p_s \quad (87)$$

(s -body *BS entropy*) are defined for all $t \in I$ and all $s = 1, N$, with K_s denoting suitable real constants and letting $K_1^2 = 1$.

B) $p_N(\mathbf{x}, t, \alpha)$ is summable on Γ_N so that for all $(\mathbf{r}_1, t) \in \overline{\Omega} \times I$ there exist the velocity moments of the form:

$$\int_U d^3\mathbf{v}_1 G_i(\mathbf{r}_1, \mathbf{v}_1, t, \alpha) p_1(\mathbf{r}_1, \mathbf{v}_1, t, \alpha) = Z_i(\mathbf{r}_1, t, \alpha), \quad (88)$$

where for $i = 1, n$, $G_i(\mathbf{r}_1, \mathbf{v}_1, t, \alpha)$ and $Z_i(\mathbf{r}_k, t, \alpha)$ denote respectively suitable *weight functions* and *fluid fields*. Thus, in particular, we shall require that

(at least) the following velocity moments are defined

$$\left\{ \begin{array}{l} \rho(\mathbf{r}_1, t, \alpha) = mn(\mathbf{r}_1, t, \alpha) \equiv mN \int_U d^3\mathbf{v}_1 p_1(\mathbf{r}_1, \mathbf{v}_1, t, \alpha), \\ \mathbf{V}(\mathbf{r}_1, t, \alpha) = \frac{1}{n(\mathbf{r}_1, t, \alpha)} N \int_U d^3\mathbf{v}_1 p_1(\mathbf{r}_1, \mathbf{v}_1, t, \alpha), \\ P_1(\mathbf{r}_1, t, \alpha) = mN \int_U d^3\mathbf{v}_1 \frac{u_1^2}{3} p_1(\mathbf{r}_1, \mathbf{v}_1, t, \alpha), \\ \underline{\underline{\Pi}}(\mathbf{r}_1, t, \alpha) \equiv mN \int_U d^3\mathbf{v}_1 \mathbf{u}_1 \mathbf{u}_1 p_1(\mathbf{r}_1, \mathbf{v}_1, t, \alpha), \\ \mathbf{Q}(\mathbf{r}_1, t, \alpha) \equiv mN \int_U d^3\mathbf{v}_1 \mathbf{u}_1 \frac{u_1^2}{3} p_1(\mathbf{r}_1, \mathbf{v}_1, t, \alpha), \\ \mathbf{P}_L(\mathbf{r}_1, t, \alpha) \equiv mN \int_U d^3\mathbf{v}_1 \left[\frac{1}{m} \mathbf{F}^{(ext)}(\mathbf{x}_1, t) p_1(\mathbf{r}_1, \mathbf{v}_1, t, \alpha) + \mathbf{A}_s(f_{s+1}) \right], \\ Q_T(\mathbf{r}_1, t, \alpha) \equiv \frac{2}{3} mN \int_U d^3\mathbf{v}_1 \mathbf{u}_1 \cdot \left[\frac{1}{m} \mathbf{F}^{(ext)}(\mathbf{x}_1, t) p_1(\mathbf{r}_1, \mathbf{v}_1, t, \alpha) + \mathbf{A}_s(f_{s+1}) \right], \end{array} \right. \quad (89)$$

with \mathbf{u}_1 denoting the relative velocity $\mathbf{u}_1 = \mathbf{v}_1 - \mathbf{V}(\mathbf{r}_1, t, \alpha)$. Here $\rho(\mathbf{r}_1, t, \alpha)$ and $n(\mathbf{r}_1, t, \alpha)$ are respectively the mass and number densities, $\mathbf{V}(\mathbf{r}_1, t, \alpha)$ the fluid velocity, $P_1(\mathbf{r}_1, t, \alpha)$ and $\underline{\underline{\Pi}}(\mathbf{r}_1, t, \alpha)$ the scalar and tensor pressures, $\mathbf{Q}(\mathbf{r}_1, t, \alpha)$ the relative heat flux, while $\mathbf{P}_L(\mathbf{r}_1, t, \alpha)$ and $Q_T(\mathbf{r}_1, t, \alpha)$ are respectively the linear momentum and energy density exchange rates.

C) As a consequence of A, for $\{G_i(\mathbf{r}_1, \mathbf{v}_1, t, \alpha)\} = \{mN, mN\mathbf{v}_1, mN\frac{u_1^2}{3}\}$ the following moment equations

$$\frac{\partial}{\partial t} \rho + \frac{\partial}{\partial \mathbf{r}_1} \cdot [\rho \mathbf{V}] = 0, \quad (90)$$

$$\rho \left[\frac{\partial}{\partial t} \mathbf{V} + \mathbf{V} \frac{\partial}{\partial \mathbf{r}_1} \mathbf{V} \right] + \nabla \cdot \underline{\underline{\Pi}} = \mathbf{P}_L \quad (91)$$

$$\frac{\partial}{\partial t} P_1 + \frac{\partial}{\partial \mathbf{r}_1} \cdot [\mathbf{V} P_1] + \nabla \cdot \mathbf{Q} + \frac{2}{3} \nabla \mathbf{V} : \underline{\underline{\Pi}} = Q_T, \quad (92)$$

are identified with the *mass continuity*, *linear momentum* and *scalar pressure fluid equations*.

7.1 Implications

Axioms CSM-#1-#5 imply the following elementary propositions:

PROPOSITION B.1 - PEM for $p_N(\mathbf{x}, t, \alpha)$

In validity of Axioms CSM-#1-#5 $p_N(t) \equiv p_N(\mathbf{x}, t, \alpha)$ satisfies identically PEM for all $t \in I$, i.e., $p_N(t)$ solution of the integral Liouville equation (78) maximizes the N -body BS-entropy $S(p_N(t))$, so that

$$\delta S(p'_N(t))|_{p_N(t)} = 0 \quad (93)$$

must hold for arbitrary variations $\delta p_N(t) = p_N(t) - p'_N(t)$ with $p_N(t)$ and $p'_N(t) \equiv p'_N(\mathbf{x}, t, \alpha)$ both belonging to $\{p_N(t)\}$ and $p_N(t)$ such that

$$\delta^2 S(p'_N(t)) \Big|_{p_N(t)} < 0. \quad (94)$$

PROOF

We first notice that by construction the functional class $\{p_N(t_o)\}$ prescribed in Axiom CSM-#2 must be such that the N -body BS-entropy $S(p'_N(t))$ exists $\forall t \in I$ and for $p'_N(t) = p_N(t) \equiv p_N(\mathbf{x}, t, \alpha)$ solution of Eq.(78). Then, $\{p_N(t)\}$ can be identified with the set of strictly positive real functions $p'_N(t)$ which admit the N -body BS-entropy $S(p'_N(t))$ and such that one of them coincides with $p_N(t)$ itself. Hence, introducing the functional

$$S_1(p'_N(t), \lambda(t)) = S(p'_N(t)) + \Delta S(p'_N(t)), \quad (95)$$

$$\Delta S(p'_N(t)) = \int_{\Gamma_N} d\mathbf{x} \lambda'(\mathbf{x}, t, \alpha) [p'_N(\mathbf{x}, t, \alpha) - p_N(\mathbf{x}, t, \alpha)] \quad (96)$$

to be considered variational both with respect to $p'_N(\mathbf{x}, t, \alpha)$, an arbitrary element of $\{p_N(t)\}$, and $\lambda'(\mathbf{x}, t, \alpha)$, a suitable smooth real function (Lagrange multiplier), it follows that $\Delta S(p'_N(t))$ vanishes identically for the extremal functions $p'_N(t) = p_N(t)$ and $\lambda'(\mathbf{x}, t, \alpha) = \lambda(\mathbf{x}, t, \alpha)$, with $\lambda(\mathbf{x}, t, \alpha)$ to be suitably determined. Hence, the variational equation (93) is equivalent to impose

$$\delta S(p'_N(t), \lambda'(t)) \Big|_{p_N(t), \lambda(t)} = 0,$$

which implies the Euler-Lagrange equations

$$\frac{\delta S_1(p'_N(t), \lambda(t))}{\delta \lambda(t)} = p'_N(\mathbf{x}, t, \alpha) - p_N(\mathbf{x}, t, \alpha) = 0, \quad (97)$$

$$\frac{\delta S_1(p'_N(t), \lambda(t))}{\delta p'_N(t)} = -K_N^2 [1 + \ln p'_N(\mathbf{x}, t, \alpha)] - \lambda(\mathbf{x}, t, \alpha) = 0. \quad (98)$$

Hence, since $\lambda(\mathbf{x}, t, \alpha)$ [in Eq.(98)] can always be defined consistent with Eq.(97) it follows that $p_N(\mathbf{x}, t, \alpha)$ is indeed extremal for $S(p'_N(t))$. In a similar way it is immediate to prove also the inequality (94). Q.E.D.

PROPOSITION B.2 - H-theorems for PEM for $S(p_1(t))$

Let us assume that the vector field \mathbf{F} [see Eq.(72)] is such that $\forall t \in I$

$$\frac{\partial}{\partial t} S(p_N(t)) = 0 \quad (99)$$

(constant H-theorem for $S(p_N)$). Then in validity of Axiom CSM-#5, $\forall t \in I$

$$\frac{\partial}{\partial t} S(p_1(t)) \geq 0. \quad (100)$$

In particular, if the binary forces $\mathbf{F}^{(int)}(\mathbf{x}_i, \mathbf{x}_j, t)$ vanish identically, namely $\forall(\mathbf{x}_i, \mathbf{x}_j, t)$

$$\mathbf{F}^{(int)}(\mathbf{x}_i, \mathbf{x}_j, t) = 0, \quad (101)$$

it follows that:

A) the factorization condition:

$$p_N(\mathbf{x}, t, \alpha) = \prod_{i=1, N} p_N(\mathbf{x}_i, t, \alpha); \quad (102)$$

B) the constant H-theorem for $S(p_1)$:

$$\frac{\partial}{\partial t} S(p_1(t)) \equiv 0 \quad (103)$$

both hold identically.

PROOF

The proof follows from the inequality

$$S(p_N(t)) \leq - \int_{\Gamma_N} d\mathbf{x} p_N(\mathbf{x}, t, \alpha) \ln \prod_{i=1, N} p_1(\mathbf{x}_i, t, \alpha).$$

Then, thanks to Axiom CSM-#4 and the constant H-theorem for $S(p_N)$ [Eq.(99)] it follows that

$$S(p_N(t)) \leq N S(p_1(t))$$

which implies the inequality (100). The proof of Eqs.(102) and (103) follow respectively by noting that in case of validity of Eq.(101):

- the N-body Liouville streaming operator $L_N(1, \dots, N)$ takes the form (10);
- thanks to the (99), (72), (73) and again invoking Axiom CSM-#4, since

$$\frac{\partial}{\partial t} S(p_N(t)) = -N \int_{\Gamma_1} d\mathbf{x}_1 p_1(\mathbf{x}_1, t, \alpha) \frac{\partial}{\partial \mathbf{v}_1} \cdot \mathbf{F}^{(ext)}(\mathbf{x}_1, t) \equiv 0, \quad (104)$$

it follows that

$$\frac{\partial}{\partial t} S(p_1(t)) = - \int_{\Gamma_1} d\mathbf{x}_1 p_1(\mathbf{x}_1, t, \alpha) \frac{\partial}{\partial \mathbf{v}_1} \cdot \mathbf{F}^{(ext)}(\mathbf{x}_1, t) \equiv 0 \quad (105)$$

holds identically. Q.E.D.

Finally, let us consider the case in which the mass (and number) density is constant in $\bar{\Omega} \times I$, i.e.

$$\rho(\mathbf{r}_1, t, \alpha) = mn(\mathbf{r}_1, t, \alpha) \equiv mN \int_U d^3\mathbf{v}_1 p_1(\mathbf{r}_1, \mathbf{v}_1, t, \alpha) \equiv \rho_o, \quad (106)$$

with $\rho_o \equiv mn_o > 0$. Then the following proposition holds:

PROPOSITION B.3 - Multipoint velocity PDFs f_s .

In validity of the constraint equation (106) it follows that denoting for $s = 1, N$

$$f_s(\mathbf{x}_1, \dots, \mathbf{x}_s, t, \alpha) = \frac{N}{n_o} p_s(\mathbf{x}_1, \dots, \mathbf{x}_s, t, \alpha), \quad (107)$$

$f_s(\mathbf{x}_1, \dots, \mathbf{x}_s, t, \alpha)$ are velocity PDFs, namely satisfy the normalization conditions

$$\int_U d^3\mathbf{v}_1 \dots \int_U d^3\mathbf{v}_s f_s(\mathbf{x}_1, \dots, \mathbf{x}_s, t, \alpha) = 1. \quad (108)$$

As a consequence for $s = N$, $f_N(\mathbf{x}_1, \dots, \mathbf{x}_N, t, \alpha)$ satisfies the N -body Liouville equation

$$L_N(1, \dots, N) f_N(\mathbf{x}_1, \dots, \mathbf{x}_N, t, \alpha) = 0. \quad (109)$$

PROOF (omitted)

8 Appendix C - Requirements of IKT

In this Appendix we recall the basic assumptions of IKT [10–14]:

1) the 1-point velocity PDF $f_1 \equiv f_1(\mathbf{r}_1, \mathbf{u}_1, t, \alpha)$ [with $\mathbf{u}_1 = \mathbf{v}_1 - \mathbf{V}(\mathbf{r}_1, t)$ and $\mathbf{x}_1 = (\mathbf{r}_1, \mathbf{v}_1) \in \Gamma_1$] is required to be a solution of a Liouville equation (6) with suitable vector field $\mathbf{F}(\mathbf{x}_1, t)$;

2) in agreement with Axioms #1, #2 and #3 the moments of $f_1(\mathbf{r}_1, \mathbf{u}_1, t, \alpha)$ are prescribed so that that the equations

$$\int_U d^3\mathbf{v}_1 \mathbf{v}_1 f_1(\mathbf{r}_1, \mathbf{u}_1, t, \alpha) = \mathbf{V}(\mathbf{r}, t, \alpha), \quad (110)$$

$$\rho_o \int_U d^3\mathbf{v}_1 \frac{u_1}{3} f_1(\mathbf{r}_1, \mathbf{u}_1, t, \alpha) = p_1(\mathbf{r}_1, t, \alpha) \equiv \frac{1}{2} \rho_o v_{th}^2, \quad (111)$$

$$S(f_1) \equiv - \int_{\Gamma_1} d\mathbf{x}_1 f_1(\mathbf{r}_1, \mathbf{u}_1, t, \alpha) \ln f_1(\mathbf{r}_1, \mathbf{u}_1, t, \alpha) = S_T, \quad (112)$$

hold identically in $\bar{\Omega} \times I$ [Eqs.(110) and (111)] or I [Eq.(112)];

3) the pseudo-pressure $p_o(t)$ [see Eq.(1)] is prescribed in order to satisfy identically Eq.(112) and the entropy constraint set by Axiom #3 [Eq.(13)], i.e., the requirement

$$S(f_1(t)) = S(f_1(t_o)) \quad (113)$$

to be fulfilled for all $t, t_o \in I$;

4) the vector field $\mathbf{F}(\mathbf{x}_1, t)$ in Eq. (6) is prescribed in such a way that the same equation:

a) admits as a particular solution the Gaussian kinetic equilibrium, namely the PDF

$$f_1(\mathbf{r}_1, \mathbf{u}_1, t, \alpha) = f_M(\mathbf{r}_1, \mathbf{u}_1, t, \alpha) = \frac{1}{\pi^{3/2} v_{th}^3} \exp \left\{ -\frac{u_1^2}{v_{th}^2} \right\}; \quad (114)$$

b) yields solely, by means of its velocity-moment equations for $\{G_i\} \equiv \{\rho_o, \rho_o \mathbf{v}_1, \rho_o u_1^2/3\}$, the closed set of fluid equations coinciding with the incompressibility and NS equations (50) and (51).

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