Reversibility, irreversibility, friction and nonequilibrium ensembles in N–S equations

Giovanni Gallavotti

Received: 12 October 2022 / Accepted: 19 December 2022 / Published online: 18 January 2023
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Abstract
Viscosity, as a physical property of fluids, reflects an average effect over a chaotic microscopic motion described by Hamiltonian equations. It is proposed, as an example, that stationary states of an incompressible fluid subject to a constant force, can be described via several ensembles, in strict analogy with equilibrium Statistical Mechanics.

1 Regular NS evolutions

**Question:** can the phenomenological notion of fluid viscosity be represented in alternative ways?

**Related Question:** is it possible to set up a theory of statistical ensembles, and their equivalence, extending to stationary non-equilibria the ideas behind the canonical and micro-canonical ensembles [1, 2].

A guide could be provided by the existence of a fundamental symmetry like “time reversal” which cannot be “spontaneously broken”.

Therefore even the stationary states of dissipative systems ought to be describable via time reversible equations. Clearly the question is not an easy one: hence it will be better to specialize here on a paradigmatic example, namely the Navier–Stokes (NS) fluid in a $2\pi$-periodic box, in 2 or 3 dimensions (2D or 3D), viscosity $\nu$.

The $dD$ equation, $d = 2, 3$, is:

$$\dot{u}(x)_a = -((u \cdot \partial)u)_a - \partial_a p + \nu \Delta u_a + F_a = 0, \quad \partial \cdot u = 0 \quad (1.1)$$

where $u(x)$ is the velocity field that in 2D can be represented via Fourier’s series as:

$$u(x)_a = \sum_{0 \neq k \in \mathbb{Z}^d} i u_k \frac{k_a^+}{||k||} e^{-i k \cdot x} \quad (1.2)$$

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1 In the subatomic world time reversal is not a symmetry but another more fundamental symmetry, CPT, could replace it in the following discussion

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Giovanni Gallavotti
giovanni.gallavotti@roma1.infn.it
https://ipparco.roma1.infn.it

Università “La Sapienza” and INFN, Rome, Italy
and $\mathbf{F}$ is likewise represented via its Fourier’s series.

In terms of the complex scalars $u_k = \bar{u}_{-k}$ the 2D NS equation is:

$$
\dot{u}_k = - \sum_{k_1 + k_2 = k} \frac{(k_1 \cdot k_2)(k_2 \cdot k)}{|k_1||k_2||k|} u_{k_1} u_{k_2} - v k^2 u_k + F_k
$$

(1.3)

Although the 2D-NS admit general smooth solution $t \to S_t \mathbf{u}$ starting from smooth initial data $\mathbf{u}$, it is convenient (aiming to discuss also the 3D-NS) to imagine them as truncated at $|k| = \max_i |k_i| \leq N$. The ultraviolet (UV) cut-off $N$ will be temporarily fixed. The 2D-NS become $M_N = (2N + 1)^2 - 1$ dimensional ODE’s, on phase space $\mathcal{M}_N$.

In the 3D case the 3D-NS equations with UV cut-off $N$ can be likewise written on a $M_N = 2((2N + 1)^3 - 1)$ dimensional phase space $\mathcal{M}_N$.

The time reversal transformation $I \mathbf{u} = -\mathbf{u}$ does not imply $I S_t \mathbf{u} = S_{-t} I \mathbf{u}$ if $\nu > 0$: hence these are irreversible equations.

Let $\mathbf{u}$ be an initial state: then $t \to S_t \mathbf{u} \overset{\text{def}}{=} \mathbf{u}(t)$ evolves and it is easily seen that $||S_t \mathbf{u}||$ will verify an \textit{a priori} estimate on $\|\mathbf{u}(t)\|_2^2 = \sum_k |u_k(t)|^2$:

$$
\|\mathbf{u}(t)\|_2^2 \leq \left( \frac{\|\mathbf{F}\|_2}{\nu} \right)^2 +
$$

(1.4)

where the last inequality abridges stating that if $\|\mathbf{u}(0)\|_2^2$ is larger than $(\|\mathbf{F}\|_2^2)^2$ then $\|\mathbf{u}(t)\|_2^2$ will decrease until smaller than any target $\frac{\|\mathbf{F}\|_2^2}{\nu^2}$ (in a time depending on $\mathbf{u}(0)$ and on the prefixed target) to stay smaller.

Definition A smooth dynamical system $S_t$ on a manifold $\mathcal{M}$ will be called \textit{regular} if in $\mathcal{M}$ there are a finite number of open sets $\mathcal{A}_i$, $i = 1, 2, \ldots, n$ which:

(1) are $S_t$-invariant,
(2) their union is $\mathcal{M}$ up to a set of zero volume,
(3) the evolution of almost all data $\mathbf{u} \in \mathcal{A}_i$ assigns an average value to the observables $O$ (i.e. to functions on $\mathcal{M}$) $\mu_i(O)$ where $\mu_i$ is an invariant distribution (hence ergodic).

The $\mu_i$ will be called “physical distributions” and if $n > 1$ the system will be said to admit $n$ phases.

The distributions are called “physical distributions” because they allow to compute the time averages of functions $O(\mathbf{u})$ on phase space: hence determine the statistical properties of almost all data (with respect to the volume).

If the motion is chaotic then it generates a “stationary state” on $\mathcal{M}_N$, i.e. a stationary probability distribution which, aside exceptions on the initial data collected in a 0-volume set in $\mathcal{M}_N$ and denoted $\mu_{\nu,i}(d\mathbf{u})$.

Stationary probability distributions generalize to the case of much more general systems, the regular ones, what in many classes of Hamiltonian systems are the equilibrium distributions studied in equilibrium statistical mechanics (SM).

Here we assume that the regularized NS equations, denoted $INS^N$, on $\mathcal{M}_N$ parameterized by the viscosity $\nu$ are regular in the above sense. And it is natural to define the collection $\mathcal{C}_{\text{viscosity}}^N$ of all physical distributions $\mu^N_{\nu,i}(d\mathbf{u})$ on $\mathcal{M}_N$. In the cases in which there are several physical distributions corresponding to the same viscosity a further label $i = 1, \ldots, n^N_\nu$ will be attached as $\mu^N_{\nu,i}$ to distinguish them.

Furthermore we fix once and for all the forcing $\mathbf{F}$, with $||\mathbf{F}||_2 = 1$, and with $|F_k| = 0$, if $|k| > k_{\text{max}}$ with $k_{\text{max}} < \infty$: physically this is read that $\mathbf{F}$ is assumed to be a large scale forcing.
2 Enstrophy ensemble

Consider the new equation [3], with UV-cut-off $N$:

\[ \dot{u}_k = - \sum_{k_1+k_2=k} \frac{(k_1^\perp \cdot k_2)(k_2 \cdot k)}{||k_1|| ||k_2|| ||k||} u_{k_1} u_{k_2} - \alpha(u) k^2 u_k + F_k, \quad |k|, |k_1|, |k_2| \leq N \]  

(2.1)

differing from the Eq. (1.3) because the multiplier $\alpha(u)$ replaces the viscosity $\nu$. The non linear term in Eq. (2.1) will be denoted $n(u, u)_k$.

The multiplier $\alpha(u)$ will be so defined that the solutions of the Eq. (2.1) will admit \( D(u) \overset{\text{def}}{=} \sum_k k^2 |u_k|^2 \), usually called enstrophy, as an exact constant of motion. From Eq. (2.1) this means that

\[ \alpha(u) = \frac{\sum_k k^2 (n(u, u)_k + F_k) u_k}{\sum_k k^1 |u_k|^2} \]  

(2.2)

(in 2D the term with $n(u, u)$ vanishes identically).

The new equation is reversible: $IS_\epsilon u = S_\epsilon, I u$ (as $\alpha(u)$ is odd) and will be called $RNS^N$. So $\alpha$ can be called a “reversible friction”.\(^2\)

The non Newtonian forces $\nu \Delta u$, $\alpha(u) \Delta u$ can be imagined to play the role of a thermostat: Ref. [4] the forcing performs work on the fluid but the fluid density remains the same. This means that the temperature must change so that the equation of state linking pressure density and temperature remains fulfilled. Heat has to be removed or inserted and both forces can be viewed as external forces allowing to achieve respect of the equation of state. Then it is natural to think that the two equations should be equivalent.

This leads to an equivalence conjecture [5], which we formulate still making use of our knowledge of Statistical Mechanics where examples of equivalences are well known and can guide us.

The evolution with $RNS^N$ will be assumed regular in the sense of the above definition; it generates a family of stationary distributions on phase space: $\mu^N_D$ parameterized by the constant value $D$ of the enstrophy $D(u)$. Again for a given $D$ there may be $m^N_D > 1$ physical states which will be distinguished by extra label $j = 1, \ldots, m^N_D$. The collection of such distributions will form the “enstrophy ensemble”, $\mathcal{E}^N_{\text{enstrophy}}$.

To formulate the connection between the two ensembles $\mathcal{E}^N_{\text{viscosity}}, \mathcal{E}^N_{\text{enstrophy}}$, it is necessary to define the local observables $O(u)$: these are functions on phase space whose value depends on the harmonics $\mathbf{k}$ contained in a finite region $\Delta$ independent on $N$.\(^3\)

The local observables here are analogous to the SM observables on phase space depending only on the positions and velocities of particles located in finite region $\Delta$ independent on the size $V$ of the container. So once more arises a similarity between the SM of a system enclosed in a volume $V$ and of a NS fluid with UV cut-off $N$: one can say that locality in SM is in position space while in NS it is in momentum space.

With this in mind the following conjecture has been proposed to relate physical distributions $\mu^N_{\nu, \beta}, \mathcal{E}^N_{\nu, \beta}$ in $\mathcal{E}^N_{\text{viscosity}}, \mathcal{E}^N_{\text{enstrophy}}$ where $\beta = 1, \ldots, n^\nu_D$; $\beta' = 1, \ldots, m^N_D$ are labels

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\(^2\) In the 3D case the equations are very similar (for instance the $u_k$ are replaced by vectors orthogonal to $\mathbf{k}$, \ldots); the main and important difference is that the expression of $\alpha(u)$ receives a contribution from the quadratic transport term which, although present also in 2D, cancels from $\alpha$ essentially because in 2D when $\nu = 0$ the $D(u)$ is conserved.

\(^3\) Hence depend on finitely many Fourier’s harmonics of $u$, \textit{i.e.} are “large scale” observables”, but unlike the forcing, which only has the harmonics $|k| < k_{\text{max}}$ with $k_{\text{max}}$ fixed, no limit is set on the size scale.
distinguishing the physical distributions, if more then one: note however that cases in which \( n^N_N, m^N_D > 1 \) are expected to be rare. Then: Ref. \([5]\)

**Conjecture**  
Let \( \mu^N_{\nu,\beta} \in \mathcal{E}^N_{\text{viscosity}} \) and \( \rho^N_{D,\beta'} \in \mathcal{E}^N_{\text{enstrophy}} \) be physical distributions with the same enstrophy, i.e.

\[
\mu^N_{\nu,\beta}(D) = D \tag{2.3}
\]

Then if \( N \) is large enough it is \( n^N_{\nu} = m^N_D \) and for each \( \beta \) there is \( \beta' \) and:

\[
\lim_{N \to \infty} \nu^N_{\nu,\beta}(O) = \lim_{N \to \infty} \rho^N_{D,\beta'}(O) \tag{2.4}
\]

for all local observables.

So the averages of large scale observables will show the same statistical properties, as \( N \to \infty \), in \( INS^N \) and \( RNS^N \) evolutions, under the correspondence condition of equal enstrophy, Eq. \((2.3)\).

The \( \alpha(u) \) in the \( RNS^N \) evolution will fluctuate strongly in turbulence regime and it will “self-average” to a constant \( \nu \) thus “homogenizing” the equation and formally turning it into the \( INS^N \) with friction \( \nu \).

The conjecture however does not mention a condition like for \( \nu \) small enough: it should hold also at high viscosity where often \( INS^N \) exhibits periodic attractors. The reason it is proposed also in such cases is that in all cases the NS equations should be regarded as yielding macroscopic descriptions of microscopic, certainly chaotic, evolutions derived via scaling limits without modifying the microscopic equations \([6]\).

It is natural to think that there should be no condition for strong chaos. The microscopic motion is always strongly chaotic and the chaoticity condition should be always fulfilled even when motion appears laminar.

The analogy with SM becomes even more clear: the \( N \to \infty \) limit corresponds to the thermodynamic limit \( V \to \infty \).

As a final remark other ensembles can be imagined: first is the “energy ensemble” formed by the physical distributions for the equation Eq. \((2.1)\) with \( \alpha \) so defined that the energy \( \|u\|^2_2 \) is an exact constant (i.e. \( \alpha \) is given, in 2D and also in 3D by Eq. \((2.2)\) replacing \( k^2 \) with 1 and \( k^4 \) with \( k^2 \)) and a similar analysis and conjecture be can be set up: for results obtained with this approach see \([7]\).

At this point it is convenient to pause and show a few results from simulations which begin to test the equivalence proposal.

### 3 Some 2D simulations

Here are collected results of the earlier (< 2018) simulations that might interest readers: skipping this part does not preclude following the final comments in Sect. 4.

There is a first obvious test suggested by a rigorous consequence of the conjecture based on the remark that the work per unit time of the forcing is a local observable, being \( W = F \cdot u = \sum_{|k| < k_{\text{max}}} F_k \tilde{u}_k \). Multiplying both sides of \( RNS^N \) or \( INS^N \) by \( \tilde{u}_k \) one finds the energy conservation identity:

\[
\alpha(u)D = F \cdot u, \quad RNS^N
\]

\(^4\) In many cases no “intermittency” is expected, i.e. \( n^N_{\nu} = m^N_D = 1 \).
\[ \nu D(u) = F \cdot u, \quad INS^N \] (3.1)

The conjecture implies that \( \rho_N^W(W) \equiv \rho_N^\nu(\alpha) D \) has to be equal in the \( \lim_{N \to \infty} \) to the average \( W \) which in the \( INS^N \) by the second line of Eq. (3.1) is \( \nu \mu_N^\nu(D) \). Hence in absence of intermittency the equivalence condition \( \mu_N^\nu(D) = D \) yields:

\[ \lim_{N \to \infty} \rho_N^\nu(\alpha) = \nu \] (3.2)

Hence a test is: i) fix \( \nu, N \) and run the \( INS^N \) evolution from a random initial \( u \) until the average enstrophy value \( D \) of the enstrophy \( D(u(t)) \) is numerically reached. Then run the

**Fig. 1 a** The running average of the reversible friction \( \frac{\alpha(u(t))}{\nu} \equiv \frac{1}{\nu} \sum_k k^2 |f_k u_k|^2 \), superposed to the conjectured value 1 and to the fluctuating values \( \frac{\alpha(u(t))}{\nu} \); Evolution is by \( RNS^N \), \( R \equiv \frac{1}{\nu} = 2048 \), 224 modes \((N = 7)\), Lyap.-max \( \simeq 2 \), x-axis unit \( 2^{19} \), forcing only on modes \( k = \pm(2, -1) \). Data are obtained via a sequence of integration steps of size \( h = 2^{-19} \) registered every \( 4h \). The plot gives 4000 successive registered results but only every 10 of them to avoid too dense a plot. The running average of the reversible friction \( \frac{\alpha(u(t))}{\nu} \), superposed to the conjectured limit value 1. **b** Same data as the Fig. 1 but for the shorter time interval \([0, 300]\) to show the initial transient.
Fig. 2  Running average of \( \frac{1}{\nu} W(u(t)) \) (dark green) in \( INS^N \); the average \( \frac{1}{\nu} D(u) \) in \( INS^N \) (straight red line) running average of \( \frac{1}{\nu} D(u(t)) \) in \( INS^N \), ‘converging’ to \( \frac{1}{\nu} D \) (very close to \( \frac{1}{\nu} D \)) large fluctuations are those of \( \frac{1}{\nu} D(u(t)) \). Data are the same in the previous figures.

Fig. 3  Same as Fig. 1 but for \( INS^N \). The running average of the reversible friction \( \alpha(u(t)) \) in a \( N = 7 \) regularized \( INS^N \) evolution forced on the mode \( k = \pm (2, -1) \): the running average is in the large fluctuations curve.

\( RNS^N \) with initial \( u \) adjusted to have enstrophy \( D \): the result should be that if \( N \) is large enough the running average of \( \alpha \), i.e. \( \frac{1}{T} \int_0^T \frac{1}{\nu} \alpha(u(t')) dt' \rightarrow \infty \). An example is: (Fig 1)

The Fig. 2 shows the preliminary evaluation of the average enstrophy: it shows that in the case considered the average value of the enstrophy is reached quite rapidly in spite of the strong fluctuations.

It is natural to study the observable \( \alpha(u) \) as it evolves under the \( INS^N \) equation. It is not covered by the conjecture, that only implies that its average should be, under the equivalence condition, close to 1 in the \( RNS^N \) evolution. An unexpected result is that the running average of \( \frac{1}{\nu} \alpha(u(t)) \) also has running average very close to 1 as indicated by the following Fig 3.5
This is one more example of a non local observable with equal averages in corresponding physical distributions for the two evolutions considered.

The equality to $\nu$ under the equivalence condition between the average value of $\alpha(u) = \sum_k k^2 f_k \bar{\lambda}_k$ considered as an observable for both $RNS^N$ and $INS^N$ with $\nu$ is perhaps surprising. It is a theorem (consequence of the conjecture) in the $RNS^N$ evolution but it might not be even expected in the case of $INS^N$ because $\alpha(u)$ is not a local observable.

Therefore it is tempting to test possible equality of the averages of other nonlocal quantities, as such equalities are well known to hold in the thermodynamic limit for several non local observables (Fig. 4).

One such observable is the spectrum of the symmetric part of the Jacobian $J(u,t)$, the $M \times M$ matrix $J_{k,k'} = \frac{\partial u_k}{\partial u_{k'}}$, formally $\frac{\partial u}{\partial u}$. The spectrum can be called the “local Lyapunov spectrum”.

The above coincidence to some extent is due to the wide ordinate scale used. It is expected the two spectra are subject to computational errors which should be more visible near the $k$ to which correspond $\lambda_k$’s close to 0. This is clarified in (Fig. 5)

Certainly a cut-off at $N = 3$ is much too small to be of any significance (Fig. 6). In fact agreement between the $INS^N$ and $RNS^N$ is expected also at fixed $N$ and small $\nu$ [8], as a consequence of appearance of turbulence: which generates apparently random fluctuations on $\alpha$ with a corresponding homogenization phenomenon: and physically different phenomenon.

The following figure tests the equivalence in the case of a higher UV cut-off: (Fig. 7)

The latter graph shows the spectra for both $INS^N$ and $RNS^N$ cases: again they are superposed. As in the previous case the relative difference can be studied more closely:
Fig. 5 Relative difference $\frac{|\lambda_{k}^{RNS} - \lambda_{k}^{INS}|}{\max(|\lambda_{k}^{RNS}|,|\lambda_{k}^{INS}|)}$ between (local) Lyapunov exponents in the previous Fig. 3

$[(v = 2048^{-1}, N = 3\ (i.e. 48\ modes)]$

Fig. 6 Local Lyapunov spectra in a $15 \times 15$ (960 modes) truncation for $INS^{N}$ and $RNS^{N}$ (keys ending respectively in 0 or 1), with the $\lambda_k$ interpolated versus $k$ by lines, $v = \frac{1}{2048}$, forcing on the modes $k = \pm(2, -1)$. Each of the $\lambda_k(u(t))$ is evaluated every $2^{19}$ integration steps and the graf reports the average of of each $\lambda_k(u(t))$ over 2200 successive evaluations.
4 Further results and problems

(1) The question of exhibiting examples of “regular systems” in the sense of Sect. 2 has been essentially answered in the proposal by Ruelle that I interpret as saying that “generically” all systems exhibiting chaotic evolution should be “regular”.

In more mathematically oriented works the idea emerges from the theory of Anosov flows: they play the role, in chaotic dynamics, of the harmonic oscillators in ordered dynamics they are the paradigm of Chaos. This idea rests on fundamental works of Sinai (on Anosov sys.), and Ruelle, Bowen (on Axioms A systems). A strict, general, heuristic, interpretation of original ideas on turbulence phenomena [9–13], led to the [14]:

Chaotic hypothesis: A chaotic evolution takes place (generically) on a smooth surface $A$, “attracting surface”, contained in phase space, and on $A$ the maps $S$ (or the flow $S_t$) is an Anosov map (or flow).

So a regular system is a system with $n \geq 1$ attractors $A_i$ whose basins of attraction are open sets $\hat{A}_i$ whose union of the entire phase space up to a set of zero volume.

(2) The chaotic hypothesis is dismissed (by many) with arguments like (1999) More recently Gallavotti and Cohen have emphasized the “nice” properties of Anosov systems. Rather than finding realistic Anosov examples they have instead promoted their “Chaotic Hypothesis”: if a system behaved “like” a [wildly unphysical but well-understood] time reversible Anosov system there would be simple and appealing consequences, of exactly the kind mentioned above. Whether or not speculations concerning such hypothetical Anosov systems are an aid or a hindrance to understanding seems to be an aesthetic question [15].

While giving up any evaluation of the statement I stress that Statistical Mechanics, after Clausius, Boltzmann and Maxwell was a simple and appealing consequence of the “[wildly unphysical but well-understood]” periodicity of motions of atoms in a gas.

(3) The same tests mentioned here (dated up to 2018) have been made in 2D NS with up to 920 modes and in 3D NS even up to $\sim 5 \cdot 10^6$ modes [4].
(4) The 3D, @ tests have suggested that the notion of local observable should be made more strict defining \( O \) a local observable if \( O(\mathbf{u}) \) depends on finitely many harmonics \( \mathbf{k} \), as above, further verifying \( |\mathbf{k}| < cK_\nu \) where \( K_\nu = (\frac{\nu}{\nu_0})^{\frac{1}{4}} \) is Kolmogorov’s scale and \( c \) is a constant and \( \eta = \nu \langle W \rangle \) is the average work per unit time: it is believed widely the in the limit \( \nu \to 0 \) \( \eta \) should remain finite and positive [16].

Although the 3D tests seem to suggest \( c \) is of order \( O(1) \) in my view the possibility that \( c = \infty \) should still be studied with further simulations: the attempts to estimate \( c \) in [16] (remark 4 in Sect. 3) in my view should be considered only as preliminary.

(5) one of the consequences of the chaotic hypothesis is that if the system is time reversible then a general result is the “fluctuation theorem” (FT). The problem is that there is strong evidence that in the NS the asymptotic motion is attracted on a set of dimension lower than that of phase space: this is shown by the fact that as soon as \( N \) is large enough and \( \nu \) small enough the attractor has dimension less that that of phase space: this is shown by the \( > 0 \) Lyapunov exponents seem to be less than half the number of negative ones [5].

In 2D this seems to be the case with \( \nu = 1/2048 \) and \( N = 7 \) and 15. There are a few examples in which even though the attractor \( A \) has dimension lower than that of phase space the motion on \( A \) admits a symmetry \( I' : A \to A \) which has the same properties as time reversal (i.e. \( I'S_t = S_{-t}I' \)) [17]: but is is unclear that the NS admit such a symmetry. Positive results in testing validity of the FT have been found [18], in 2D in the \( RNS^N \) with \( N = 48 \), \( \nu = 1/2048 \), way too small for being really interesting, while already for the case \( N = 224 \), \( \nu = 1/2048 \) it seems that FT does not hold.

Acknowledgements This is a readacted and updated version of a talk at the DinAmici meeting on 21/Dec/2018 at the Accademia dei Lincei, Roma.

Declarations
Conflict of interest The author states that there is no conflict of interest.

Appendix: a path through the theme

(1) A first equivalence example: [2].

(2) Path to the conjecture: [5, 16, 19, 20].

(3) 3D enstrophy ensemble: [16, 21].

(4) 3D energy ensemble: [7].

(5) Shell model: [22].

(7) Stat-Mech: [12, 13, 23–25].

(8) Turbulence physics: [26–30].

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