Finite thermostats in classical and quantum nonequilibrium

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Abstract

Models for studying systems in stationary states but out of equilibrium have often empirical nature and very often break the fundamental time reversal symmetry. Here a formal interpretation will be discussed of the widespread idea that, in any event, the particular friction model choice should not matter physically. The proposal is, quite generally, that for the same physical system a time reversible model should be possible. Examples about the Navier-Stokes equations are given.

keywords: *Friction, Reversibility, Irreversibility, Fluctuation Theorem, Nonequilibrium Ensembles, Quantum Dissipation.*

1 Thermostats

A mechanical system, described by coordinates $x \in R^N$, moving subject to an equation $\dot{x} = F(x)$ is "I-time reversal symmetric" if there is a coordinate transfomation $x \to Ix$ with $I^2 = 1$ and such that if $x(t) \stackrel{def}{=} S_t x$ is a motion then also $Ix(-t)$ is a motion, *i.e.* $IS_t \equiv S_{-t} I$.

A mechanical system is said *subject to thermostat forces* if the equations of motion have the form $\dot{x} = h(x) + f(x) - L(x)$ where $x \in R^N$, $N \leq \infty$, $h(x)$ is a force which in absence of the other two terms would admit a conserved energy (typically $\dot{x} = h(x)$ is a Hamiltonian system), $f(x)$ is a

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"driving force" capable of performing work thus changing the energy and the equation $\dot{x} = h(x) + f(x) \equiv F(x)$ admits a time reversal symmetry I in the above sense; $L(x)$ is a dissipative force that will keep at bay the energy increase due to the work of the force f so that the motion may possibly attain a stationary (nonequilibrum) state.

Systems subject to thermostats are obtained either by introducing empirically a dissipating force characterized in terms of few parameters ("friction coefficients" or "transport coefficients") into the equations of motion (which may be either ode's or pde's) or by imagining the system in interaction with one or more "external systems" of particles, extending to infinity and asymptotically in thermal equilibrium, as envisaged in [1]. Or, also, by introducing empirically forces which in some way absorb in average the work done by the external forces.

For instance
(1) In the simple electric resistor model, in which N point particles move in a periodic box elastically colliding with fixed spherical obstacles and are subject either to a constant uniform field E (hence non conservative) and to a friction $-\nu\dot{x}_j$, which is the empirical thermostat force (forbidding energy blow up but enforcing breaking of time reversal for $I(x_j, \dot{x}_j) = (x_j, -\dot{x}_j)$ or, in "Drude's model", [2], rescaling the kinetic energy of a particle to a fixed value $\frac{3}{2}k_BT$ at each collision.
(2) In the "Lorenz96" model

$$\dot{x}_j = \; x_{j-1}(x_{j+1} - x_{j-2}) + F - \nu x_j, \qquad \nu > 0,\; j = 1, \ldots, N \tag{1.1}$$

with $x_{N+1} = x_1$, which at $F = 0, \nu = 0$ conserves $E = \sum_i x_i^2$, the (thermostat force is $-\nu x_j$, breaking the time reversal $I x_j = -x_j$) .
(3) A further example, discussed in more detail below, is provided by the Navier-Stokes equations for an incompressible velocity field $\mathbf{v}(\mathbf{x}, t)$, called here "irreversible Navier-Stokes equation" or "I-NS":

$$\partial_t \mathbf{v} = -(\vec{v} \cdot \vec{\partial})\,\mathbf{v} + \nu\,\Delta\,\mathbf{v} + F\,\mathbf{g} - \boldsymbol{\partial} p', \quad \boldsymbol{\partial} \cdot \mathbf{v} = 0, \qquad \text{[I-NS]} \tag{1.2}$$

in dimension 2 and considered, for simplicity, in a periodic container of side L, under a forcing of strength F with fixed "structure" $\mathbf{g}$, pressure p' and viscosity ν. This is an example (a pde in which $N = \infty$): here the artificial thermostatting force is represented by the viscosity stress $-\nu\Delta\mathbf{v}$. At $\nu = 0, F \geq 0$ the flow of Eq.(1.2) is time reversible, with time reversal I defined by $I\mathbf{v} = -\mathbf{v}$, and conserves $E = \int \mathbf{v}^2(\mathbf{x})d\mathbf{x}$ as well as $E_n = \int (\vec{\partial}\mathbf{v}(\mathbf{x}))^2 d\mathbf{x}$ (because dimension is 2): but the flow breaks time reversal and both conservation laws if $\nu \neq 0$.

(4) Modeling dissipation is difficult in studying nonequilibrium states of quantum systems because the dissipative forces lead to modify the Schrödinger equation of the system by the addition of non conservative forces: not a simple task since they just cannot be represented by self adjoint operators. Restricting the analysis to heat conduction problems, the simplest thermostats to consider are the infinite ones as proposed in [1]:

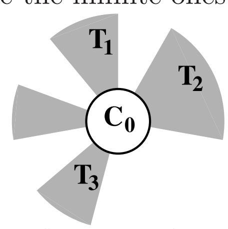

Fig.1: A finite system $\mathcal{C}_0$, called "test system", interacts with one or more "interactions sytems" supposed infinite and asymptotically in thermal equilibrium at temperatures T_j. All systems are quantum particles systems, [1].

These systems are difficult to study theoretically unless the particles constituting the thermostats are free gases, [1]. And simulations are, otherwise, impossible due to the infinite size of the thermostats: infinite thermostats (either classical or quantum) cannot be simulated without approximating them by finite systems. Therefore models have been developed to build thermostat models suitable for simulations of quantum systems, hence either exactly soluble (a very rare case, as in [1, 3, 4]) or finite dimensional, *e.g.* [5, 6, 7].

In many cases several thermostat models have been introduced, or may be introduced, and the proposal here is to formulate a unification and an interpretation of the diverse theories as a generalization of the theory of ensembles of equilibrium statistical mechanics. The idea will be illustrated in detail through the examples of the irreversible 2D Navier-Stokes equation, "I-NS", and the Erehenfest model of quantum forced system, [5].

Since the founding fathers time, microscopic reversibility has been the starting point of any determinstic description (either microscopic or macroscopic) of the evolution of systems. However in more recent times progress has been achieved in the analysis of stochastic models of evolution, classical or quantum, with attention to the guiding idea that thermal noise must at all times obey the classical or quantum version of the fluctuation-dissipation theorem; and it has been observed that this implies strong constraints in models of dissipative evolutions, [8, 9]: it is proposed that the familiar consequences of the microscopic time-reversal symmetry must hold also in the approximate stochastic models for the evolutions.

In the present work thermal noise is not considered: the idea is that a large class of deterministic models can be equivalently described by different (macroscopic or not) equations whose stationary states attribute (at least in stronly chaotic regimes) the same averages, as well as same statistical fluctuations, to large classes of observables: chaotic motion is implicitly regarded as sounce of noise. And the equivalence has interesting relations with the theory of equivalent ensembles in equilibrium statistical mechanics, at least at strong chaos, thus making possible testing the fluctuation relation, *i.e.* an extension of the fluctuation-dissipation relation beyond the perturbative linear regime, [10, 11, 12, 13], via experiments on systems in which friction plays a role but is usually modeled via phenomenological constants.

2 Nonequilibrium ensembles

Consider the I-NS equation Eq.(1.2) and cast it in dimensionless form by setting $\mathbf{v}(\mathbf{x},t) = V\,\mathbf{u}(\mathbf{x}/L, t/T)$ with the rescaling parameters V, T, L so that $L = 1$, $\frac{TV}{L} = 1$ and $\frac{FT}{V} = 1$. Introducing the Reynolds number $R = (\frac{FL^3}{\nu^2})^{\frac{1}{2}}$ the dimensionless equation for $\mathbf{u}(\mathbf{x},t)$ results:

$$\partial_t\,\mathbf{u} = -(\vec{u}\cdot\vec{\partial})\,\mathbf{u} + \frac{1}{R}\,\Delta\,\mathbf{u} + \mathbf{g} - \boldsymbol{\partial} p, \quad \boldsymbol{\partial}\cdot\mathbf{u} = 0, \qquad \text{[I-NS]} \tag{2.1}$$

Fixed $\mathbf{g}$, for each R the flow generated by the above I-NS equation will define a stationary state which will be supposed, for the time being, unique for R large enough: the state will be described by a stationary probability distribution, called here $\mu_R^{mc}(d\mathbf{u})$, on the (smooth) velocity fields $\mathbf{u}$. [2]

Hence for each R the system will reach a stationary state, which will be supposed unique *for simplicity* and will be represented by an invariant probability distribution of the velocity fields a PDF denoted $\mu_R^c(d\mathbf{u})$.

As R varies a collection $\mathcal{E}^c$ of probability distributions is obtained which will be called the *"viscosity ensemble"* for I-NS.[3]

The I-NS equation is a macroscopic model of a microscopic system of interacting particles following Newton's equations subject to the condition that, by some unspecified mechanism modeled by the stress $\nu\Delta\mathbf{u}$, the work done by the external force $\mathbf{g}$ is dissipated (in average).

The same effect can be achieved in other ways: for instance consider the equation for the velocity field, conveniently represented via the Fourier's transform as $\mathbf{u}(\mathbf{x}) = \sum_{\mathbf{k}} \mathbf{u}_{\mathbf{k}} e^{2\pi i\mathbf{k}\cdot\mathbf{x}}$, $\mathbf{k}\cdot\mathbf{u}_{\mathbf{k}} = 0$ with $\mathbf{k} = (k_1, k_2)$ integers:

[2] For R small there might exist several attractors, [14], and the stationary states for the flow might be non unique so that more parameters would be needed to indicate the stationary states of the I-NS flow, [14]. But this should not happen for large R (identifying states that differ by symmetries of the equation, [15]). See below for more general cases, like small R.

[3] Recall that after the rescaling the $\frac{1}{R}$ is identified with the viscosity ν.

$$\dot{\mathbf{u}} + (\vec{u}\cdot\vec{\partial})\mathbf{u} = -\boldsymbol{\partial} p + \mathbf{g} + \alpha(\mathbf{u})\Delta\mathbf{u}, \qquad \boldsymbol{\partial}\cdot\mathbf{u} = 0, \qquad \text{[R-NS]}$$
$$\alpha(\mathbf{u}) \stackrel{def}{=} \frac{\int_0^{2\pi} \mathbf{g}(\mathbf{x})\cdot(\Delta\mathbf{u})(\mathbf{x})d\mathbf{x}}{\int_0^{2\pi}(\Delta\mathbf{u}(\mathbf{x})^2)d\mathbf{x}} \equiv \frac{\sum_{\mathbf{k}} \mathbf{k}^2\,\mathbf{g}_{\mathbf{k}}\cdot\mathbf{u}_{-\mathbf{k}}}{\sum_{\mathbf{k}} \mathbf{k}^4|\mathbf{u}|^2}, \qquad \mathbf{k}\cdot\mathbf{u}_{\mathbf{k}} = 0 \tag{2.2}$$

in which α is so defined that the "dissipation" observable $\mathcal{D}(\mathbf{u}) = \int(\vec{\partial}\mathbf{u}(x))^2dx$ is an exact constant of motion. Eq.(2.2) will be called "R-NS", for *"reversible Navier-Stokes"*, because the transformaion $I\mathbf{u}(x) \stackrel{def}{=} -\mathbf{u}(x)$ is a time reversal for the R-NS equation above (*i.e.* it $\mathbf{u}(x,t)$ is a solution also $-\mathbf{u}(x,-t)$ is a solution).

Therefore the stationary states of the R-NS will be parameterized by the value En of $\mathcal{D}(\mathbf{u})$: it will be a PDF $\mu^{mc}_{En}(d\mathbf{u})$ on the velocity fields which will be supposed (for the time being) unique for En large.

As En varies the distributions $\mu^{mc}_{En}(d\mathbf{u})$ form a family of PDF's that will be denoted $\mathcal{E}^{mc}$, and will be called the *reversible viscosity ensemble*.

Remark that the multipler $\alpha(\mathbf{u})$ is defined no matter which flow, Eq.(2.1) or Eq.(2.2), is considered. In the flows defined by the I-NS or R-NS $\alpha(\mathbf{u})$ is a fluctuating variable, and in the R-NS flows $\mathcal{D}(\mathbf{u})$ is a constant while it fluctuates in the I-NS flows.

Assuming the "Chaotic Hypothesis", [16, 17, 18], at least for large R and large En the observable $\alpha(\mathbf{u})$ will reach an average value, *i.e.* the "running average" of α will approach a limit,

$$\frac{1}{t}\int_0^t \alpha(\mathbf{u}(t))dt \xrightarrow[t\to\infty]{} \int \mu^c_R(d\mathbf{u}) \tag{2.3}$$

(exponentially fast, taking the hypothesis literally).

The proposal is that, *although the I-NS and R-NS are very different*, the two equations should be equivalent if the interest is concentrated on the statistical fluctuations of "K-local" or "large scale" observables, meaning observables depending on the Fourier components $\mathbf{u}_{\mathbf{k}}$ with $|\mathbf{k}| < K$ if K is fixed and R or En are large enough (see, however, Sec.5 below).

More precisely the NS equations are imagined "regularized" by restricting the Fourier components to be $|\mathbf{k}_i| \le N, i = 1,2$ and the distributions μ^c_R, μ^{mc}_{En} will be imagined to be the limits of the corresponding distributions for the "regularized" equations. Then

Conjecture: *The distributions $\mu^c_R \in \mathcal{E}^c$ and μ^{mc}_{En} will assign, for R, En large enough, the same probability distribution to K-local, time reversible, observables if*

$$\mu^c_R(\mathcal{D}) = En, \qquad \text{or} \qquad \mu^{mc}_{En}(\alpha) = \frac{1}{R} \tag{2.4}$$

Remarks (1) The second in Eq.(2.4) shows that the conjecture can be interpreted as a "homogeneization property", *i.e.* in R-NS flows the fluctuating α can be replaced by its average for the purpose of studying the statistics of local observables, thus leading to the fluctuations in the I-NS flows.
(2) The R-NS equation is reversible: therefore under the chaotic hypothesis a version of the fluctuation theorem, [10, 18], should hold for the distributions in $\mathcal{E}^{mc}$. However the R-NS equation is a pde and the phase space contraction, *i.e.* the divergence of the equation $\sigma(\mathbf{u}) = \text{div}(\alpha(\mathbf{u})\Delta\mathbf{u})$, formally given by

$$\sigma(\mathbf{u}) = \alpha(\mathbf{u})\sum_{\mathbf{k}} \mathbf{k}^2 - 2\alpha(\mathbf{u})\frac{\sum_{\mathbf{k}} \mathbf{k}^6 \mathbf{g}_{-kk}\cdot\mathbf{u}_{\mathbf{k}}}{\sum_{\mathbf{k}} \mathbf{k}^4|\mathbf{u}_{\mathbf{k}}||^2} \tag{2.5}$$

is divergent in the limit $N \to \infty$ and the fluctuation relation needs to be suitably interpreted, see Sec.5.
(3) The above conjecture holds in a sense analogous to the equivalence of descriptions of equilibria by different ensembles, like microcanonical or canonical ensembles. The superscripts c and mc are used to stress the analogy with the canonical ensemble (with R playing the role of the canonical inverse temperature) and the microcanonical ensemble (with En playing the role of microcanonical energy). In the notion of local observable the cut-off K plays the role of the finite volume V_0 inside a large container V (which has to be considered in the "thermodynamic limit $V \to \infty$") represented, in the present context, by the cut-off N.
(4) The analogy with he equivalence between equilibrium ensembles suggests intrepreting R as the inverse temperature $\mathcal{D}(\mathbf{u}) = En$ as the energy and $\alpha(\mathbf{u})$ as the kinetic energy: and this suggests the relation

$$\mu^c_R(\alpha) = \frac{1}{R} + o(\frac{1}{R}) \tag{2.6}$$

(where $o(1/R)$ tends to0 faster than $1/R$)) which is a parameterless relation that could be tested.
(5) In other words this is an instance of a general proposition "*In microscopically reversible (chaotic) systems time reversal symmetry cannot be spontaneously broken, but only phenomenologically so*",[13].
(6) A simple further remark is that En in Eq.(2.4) is exactly equal to R

times the μ^c_R-average of the *local* observable $\mathbf{g}\cdot\mathbf{u}$ and the second average in Eq.(2.4) is exactly equal to En times the μ^{mc}_{En} of the same local observable.

3 Quantum nonequilibrium ensembles

Temperature and heat, defined by the special apparata that measure them, [19], are important physical observables in *meso-physics* and *nano-physics* studies of nonequilibrium steady states, [6, 7, 20]. In simulations the use of finite thermostat, [21], as well as the connection with dynamical systems theory have been useful. Here the discussion will be restricted to problems in which there are no external forces and the energy exchanges only involve heat transfer.

The natural model above, see Figure 1, of a quantum system $\mathcal{C}_0$ coupled to quantum thermostats $\mathcal{T}_1,\mathcal{T}_2,\ldots$, was proposed in [1] where it was studied only with infinite thermostats consisting of free gases. A similar semiclassical model goes back to Ehrenfest and has been considered by many authors, see [5, 6, 7] for recent accounts, with finite thermostats as in the Ehrenfest thermostat model described as follows.

Let H be operator on $L_2(\mathcal{C}_0^{3N_0})$ acting on wave functions Ψ (symmetric or antisymmetric functions of $\vec X_0$),

$$H=-\frac{\hbar^2}{2}\Delta_{\vec X_0}+U_0(\vec X_0)+\sum_{j>0}\big(U_{0j}(\vec X_0,\vec X_j)+U_j(\vec X_j)+K_j\big)\tag{3.1}$$

where $\vec X_1,\vec X_2,\ldots,\vec X_n$ are configurations of $N_1,\ldots,N_n$ particles located in *finite* regions $\mathcal{T}_1,\ldots,\mathcal{T}_n$ external to $\mathcal{C}_0$ with densities $\delta_j=\frac{N_j}{|\mathcal{T}_j|}$.

The equations of motion of the system in $\mathcal{C}_0\cup\mathcal{T}_1\cup\ldots\cup\mathcal{T}_n$ are

$$\begin{aligned}&(1)\ \ -i\hbar\dot\Psi(\vec X_0)=\,(H(\{\vec X_j\}_{j>0})\Psi)(\vec X_0),\\ &(2)\ \ \ddot{\vec X}_j=-\Big(\partial_jU_j(\vec X_j)+\langle\,\partial_jU_j(\cdot,\vec X_j)\,\rangle_\Psi\Big)-\alpha_j\dot{\vec X}_j,\qquad j>0\end{aligned}\tag{3.2}$$

where

$$\langle\,\partial_jU_j(\cdot,\vec X_j)\,\rangle_\Psi\stackrel{def}{=}\langle\Psi|\partial_jU_j(\cdot,\vec X_j)|\Psi\rangle=\int|\Psi(X_0)|^2\partial_jU_j(\vec X_0,\vec X_j)\,dX_0\tag{3.3}$$

The Eq.(3.2) defines a *dynamical system* on the phase space consisting of the points $x=\Big(\Psi,(\{\vec X_j\},\ \{\dot{\vec X}_j\})_{j>0}\Big)$ as soon as the "thermostat force" $\alpha_i=\alpha_i(\Psi,\vec X_i,\dot{\vec X}_i)$ is specified.

A possible choice, "isokinetic thermostats", of the α_j is:

$$\alpha_j \stackrel{def}{=} \frac{\langle W_j \rangle_\Psi - \dot U_j}{2K_j}, \qquad W_j \stackrel{def}{=} -\dot{\vec X}_j \cdot \vec\partial_j U_{0j}(\vec X_0, \vec X_j) \tag{3.4}$$

and with this choice the evolution keeps $K_j \stackrel{def}{=} \frac12 \dot{\vec X}_j^2 \stackrel{def}{=} \frac32 k_B T_j N_j$ exact constants.

Remarks: (1) The above Ehrenfest's dynamics in not a time dependent Schrödinger equation, [6], and it can be interpreted as the evolution of a quantum system interacting with n thermostats $\mathcal{T}_1, \ldots$ at temperatures $T_1, \ldots$.
(2) The divergence, *i.e.* the dissipation, of the above equations can be computed directly from the equations of motion Eq.(3.2)-(3.4); it is

$$\sigma(x) = -\sum_j \Big(\frac{Q_j}{k_B T_j} + \frac{\dot U_j}{k_B T_j}\Big) = -\Big(\sum_j \frac{Q_j}{k_B T_j}\Big) - \frac{d}{dt}\Big(\sum_j \frac{U_j}{k_B T_j}\Big) \tag{3.5}$$

where Q_j is the work per unit time performed by the test system particles (located at $\vec X_0$) on the particles of the j-th thermostat while the last term in Eq.(3.5) is a total derivative (work internal to the j-th thermostat) and, therefore, does not contribute to the long time averages of $\sigma(x(t))$.
(3) Recalling that there are no nonconservative forces acting on the system, so that its evolution physically just corresponds to a heat exchange process, the $-\sigma(x)$ is naturally interpreted as entropy creation rate
(4) *Time reversal*, *i.e.* change in sign of the velocities $\dot{\vec X}_j$ and conjugation of the wave function $\Psi(\vec X_0)$ is a *symmetry* for the above dynamics. Hence the equations are reversible and (expected to be) chaotic: then accepting the chaotic hypothesis it will follow that the stationary state $\mu^r_{T_1,\ldots,T_n(dx)}$ will be an SRB state and the fluctuations of $\sigma(x(t))$ satisfy the (stationary state) fluctuation relation, [18].

As the external temperatures $T_1, \ldots, T_n$ vary (keeping the densities δ_j fixed, for simplicity) the stationary states $\mu^r_{T_1,\ldots,T_n}(dx)$ form an ensemble $\mathcal{E}^r$ of probability distributions. The point of view leading to the conjecture discussed in the previous section about the irrelevance of the particular thermostat used can be applied here as well.

Therefore it is possible to consider several other thermostat models: for instance suppose that the external containers $\mathcal{T}_1, \ldots, \mathcal{T}_n$ are infinite containers and that the stationary state $\mu^\infty_{T_1,\ldots,T_n}$ is the stationary state reached starting from an initial state which in each container $\mathcal{T}_j$ is a typical configuration of a Gibbs' state with density δ_j and temperature T_j. As T_j vary the distributions $\mu^\infty_{T_1,\ldots,T_n}$ form a family which can be denoted $\mathcal{E}^\infty$. It is then natural to conjecture:

Conjecture 2: *Given the temperatures $T_1,\ldots,T_N$, $\mu^r_{T_1,\ldots,T_n}(dx)\in\mathcal{E}^r$ and $\mu^\infty_{T_1,\ldots,T_n}(dx)\in\mathcal{E}^\infty$ assign the same probability distribution to localized observables in the limit in which the volume of $\mathcal{C}_0$ grows (homothetically) to ∞, i.e. in the thermodynamic limit.*

If the system is in contact with a single thermostat at temperature T_1 it should be true, by consistency, that the local properties of the stationary distribution should be the same as those of the Gibbs distribution at temperature T_1 of the system enclosed in $\mathcal{C}_0$ with no external thermostat.

Even the latter simple property is not necessarily true and it would be interesting to test it, to provide some support to the more general conjecture above, [20].

Other ensembles have been introduced via suitable modifications of the Erhenfest dynamics: to some of them the conjecture can be adapted, although not always. For instance not to the studies in [22, 6]: the main difference is that the above analysis requires, in the quantum cases, a sharp separation between thermostats and test system, with the consequent dissipation taking place as a *boundary effect* whose particular properties become irrelevant in the thermodynamic limit (*i.e.* when the "test system", in the sense of [1], becomes large).

It is possible to extend the conjecture 2 to the ensembles considered in the references just quoted: however the role of the thermodynamic limit is important; and it is in this limit that conjecture 2 should hold *exactly*.[4]

The appropriate formulation of the Ehrenfest dynamics has been proposed in [7], see [23] for purely quantum evolutions. The extension considered is that the Ehrenfest dynamics is a Hamiltonian dynamics with Hamil-

[4] In the above references, among other remarks, emerges the importance of the connection of some of the ensembles with the adiabatic approximation (which means that the classical motion of the thermostat particles evolves on a time scale much slower than the quantum evolution of the system). And it is stressed that such approximation is usually not correct, for instance not in the case of the Ehrenfest dynamics: on the other hand the conjecture 2 should hold even for the Ehrenfest dynamics, provided the thermodynamic limit is taken. In other words the difficulty in obtaining agreement between the three kinds of thermostats might be due to the "test system", in the sense of [1], small size.

tonian

$$\begin{aligned} H_E =& \sum_{j=1}^{n} \frac{1}{2M_j} \vec{P}_j^2 + \int d\vec{X}_0 \overline{\Psi}(\vec{X}_0) \Big(-\frac{\hbar^2}{2m} \Delta_{\vec{X}_0} \\ &+ U_0(\vec{X}_0) + \sum_{j>0} (U_{0j}(\vec{X}_0, \vec{X}_j) + U_j(\vec{X}_j)) \Big) \Psi(\vec{X}_0) \end{aligned} \tag{3.6}$$

where $(\vec{P}_j, \vec{X}_j)$ are the canonical coordinates of the classical particles (of masses M_j) while the other canonical coordinates are the real and imaginary parts of the components $p_s + iq_s$, $s = 0, 1, \dots$ of $\Psi(\vec{X}_0)$ on a orthonormal basis (arbitrarily fixed).

The Authors refrain from investigating, in systems like quantum electrons + classical ions, how close the Ehrenfest dynamics is to the corresponding quantum electrons interacting with quantum ions. But if their formulation is applied to quantum systems in interaction with *external* classical systems (as in Sec.3) it leads naturally to the statement of conjecture 2 on independence of the particular model adopted for the external thermostats once the thermodynamic limit is added.

Furhermore the proposal in [7, Sec.5] remarkably provides stationary states for the Ehrenfest dynamics of an isolated system (given by the equidistribution on the energy surface of the Hamiltonian H_E).

In nonequilibrium cases the difficulty of proving boundedness of the region of phase space visited, so that a SRB distribution could be really defined, is still an open problem even for a system in contact with a single thermostat[5] except, perhaps, when very special thermostat models are assumed, in which the thermostat forces acts on all particles as in the classical case discussed in [26], and not just through the boundaries. For instance in [7, Sec.7] the case of an Ehrenfest dynamics with a single temperature Nosé–Hoover thermostat is treated proving the equivalence of the thermostatted stationary state with the canonical distribution for H_E (at the same temperature).[6]

There are a few cases in which an exact solution for a problem of quantum nonequilibrium is known, [4, 27, 28].

Simulations to test the conjecture seem possible and might be attempted in the future.

[5] A difficulty already present in the case of purely classical systems, [24, 25].

[6] The analogous case, [26], of a isokinetic thermostat can be possibly treated by the same method thus extending the result to Ehrenfest dynamics.

4 Reversible-irreversible equivalence for NS

Here some results that can be derived, so far, in the case of the I-NS e R-NS equations, continuing the series of simulations in [29], will be briefly presented. They are derived as a first attempt at a systematic study of the equivalence: *although preliminary* they are encouraging they will require, if confirmed, further analysis.

Several checks of the conjecture have been attempted, beginning with [30]. In the check it is important to determine first the average value of the enstrophy En in the I-RS: the average turns out to be approached quite slowly and this seems to be the main difficulty.

In the experiments (*i.e.* simulations) the I-RS and R-NS equations had to be truncated in momentum space and only with very moderate size N were considered (keep in mind that $N \to \infty$ should be taken). It is interesting to present a few recent (preliminary) results. The main difficulty is always to determine, fixed the Reynolds number R, which is the corresponding average enstrophy En in the I-NS flows.

The following picture shows, in a structured (960 Fourier modes) and turbulent ($R = 2048$) flow, the *slow approach amid strong fluctuations* of the instantaneous enstrophy to its running average:

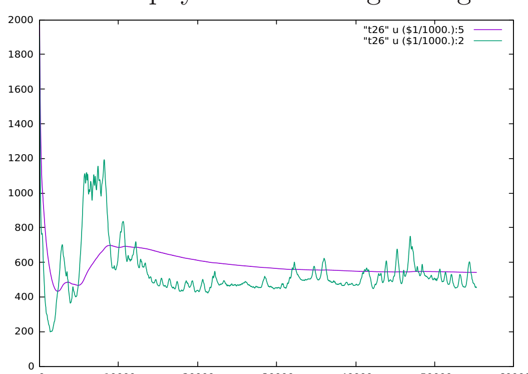

Fig.2: At 960 modes (480 independent complex components), $R = 2048$: the approach and fluctuations of enstrophy; integration step is $h = 2^{-15}$ so the time in abscissa is 1500 time units (*i.e.* $50\,10^6$ time steps). FigEn-64-26-26-4-15_11[7]

The simplest check is to test the parameterless relation, Eq.(2.6), between the running average of the reversible viscosity $\alpha(\mathbf{u})$ in the I-NS flow approaches $\frac{1}{R}$ up to $o(\frac{1}{R})$ for large R. And Fig.3 represents for $R = 2048$ the

[7] The *general* coding notation is in this case: 64 refers to the cut off size, $N = 64/4 - 1$, 26 says that the number of iterations cannot exceed 2^{26} in computing the Lyapunov exponents (not used here), the second 26 says that the number of iterations in computing the running averages cannot exceed 2^{26}, the 4 says that is the local Lyapunov exponents with $T_L = 2^4$, the 15 mens that the integration step is 2^{-15} and the 11 indicates that $R = 2^{11}$.

evolution under I-NS, the irreversible NS, of the data $\alpha(\mathbf{u}(t))$, their running average and 1./2048: the ratio of he two sides of Eq.(2.5) is 1 within a few percent.

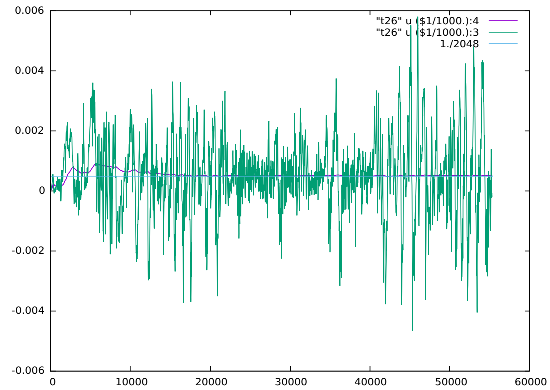

Fig.3: Fluctuations of reversible viscosity $\alpha(\mathbf{u})$ at 960 modes (480 independent complex components), shows coincidence between the running average of reversible viscosity and the asymptotically expected value $\frac{1}{R}$. The two values, $\frac{1}{R}$ and the running average of the reversible viscosity, agree at the last time within 2.5% but the running average is still slightly fluctuating, see Fig.3a below (obtained with a smaller integration step as it seems that the agreement improves if the integration step is made smaller); but more accurate study needs to be performed. (FigA2-64-26-26-4-15_11.0)

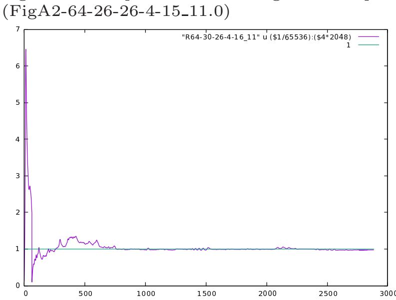

Fig.3a: This is the graph of $R\mu^c_R(\alpha)$ which according to Eq.(2.5) should tend to 1 as $R \to \infty$. The integration step is $\frac{1}{2}$ of the one in Fig.3 and the number of time units (each of 2^{16} integration steps) is ~ 2900. (FigA-64-30-26-4-16_11)

5 How general is the equivalence? Open problems

Looking at the above analysis it emerges that the conjecture should hold quite generally. It should apply to equations that describe chaotic many particles systems or to systems that model macroscopic behavior of systems microscopically subject to the time reversal symmetry, for instance to the equations described in Sec.2.

Equations $\dot{x} = h(x) + f(x), x \in R^N$ may admit a symmetry I with the property $IS_t = S_{-t}I$, like the truncated Euler equations: if a thermostat force $-\frac{1}{R}L(x)$ is introduced but N is kept fixed (so that the map I loses its fundamental physical meaning of time reversal symmetry) it is still possible to formulate equivalence statements: however the only parameter that can be varied (if N is fixed) is R and (properly formulated) equivalence can be conjectured at least asymptotically in the limit $R \to \infty$.

The question has been analyzed in few cases, *e.g.* in the Lorenz96 model: with encouraging results, [31].

(1) How important is the observable that is fixed? in the cases of Sec.2,3 the enstrophy $\mathcal{D}(\mathbf{u})$ and the kinetic energy of the thermostats have been considered. The role of the artificial thermostat force is just to provide a mechanism to keep energy away from building up due to the work of the driving forces. Therefore several choices should be possible for determining the multiplier to use to replace the empirical friction coefficients. In the NS equation discussed in Sec.2, instead of the enstrophy, the energy $\mathcal{E}(\mathbf{u}) = \int_0^{2\pi} \mathbf{u}(\mathbf{x})^2 d\mathbf{x} = \sum_{\mathbf{k}} |\mathbf{u_k}|^2$ could be used: obtaining a reversible viscosity of the form

$$\alpha_e(\mathbf{u}) = \frac{\int_0^{2\pi} \mathbf{g}(\mathbf{x}) \cdot \mathbf{u}(\mathbf{x}) d\mathbf{x}}{\int_0^{2\pi} (\vec{\partial}\mathbf{u})^2(\mathbf{x}) d\mathbf{x}} = \frac{\sum_{\mathbf{k}} \mathbf{g_k} \cdot \mathbf{u_{-k}}}{\sum_{\mathbf{k}} \mathbf{k}^2 |\mathbf{u_k}|^2} \tag{5.1}$$

For this equation, which can be called R-NSe and which maintains the total energy $\mathcal{E}(\mathbf{u})$ exactly constant,

$$\dot{\mathbf{u}} + (\vec{u} \cdot \vec{\partial})\mathbf{u} = -\boldsymbol{\partial} p + \mathbf{g} + \alpha_e(\mathbf{u}) \Delta \mathbf{u}, \qquad \boldsymbol{\partial} \cdot \mathbf{u} = 0, \qquad \text{[R-NSe]} \tag{5.2}$$

equivalence between corresponding PDF's of the I-NS and R-NSe flows should also be achieved for R large enough. The value of R beyond which a given local observable displays the same statistics in two corresponding PDF's within a prefixed precision might, however, depend on the observable and on the regularization cut-off. [8] As it is the case in equilibrium statistical mechanics equivalence may possible for certain choices of the observable kept constant and not for others: the dissipation $\mathcal{D}(\mathbf{u})$ is a natural observable to consider.

(2) In the case of the I-NS and the R-NSe some equivalence tests have been performed: with mixed results depending on the size of the truncation: equivalence has been established at large R in equations strongly truncated, [30], but it has been reported to fail at higher truncations, [32], with Fourier modes with $|\mathbf{k}| \le 10$ (hence 220 complex modes) and low $R \sim 90$. A more detailed check would be desirable in this case, for instance probing higher

[8] The pde's, like the NS equations, have to be truncated to be studied in simulations: and the truncation will also affect the size of R to realize equivalence of the distribution of the fluctuations in corresponding PDF's.

values of R and determine more accurately the averages of $\mathcal{E}(\mathbf{u})$ or $\mathcal{D}(\mathbf{u})$ corresponding to R.

(3) In the case of the I-NS equations (not truncated) conjecture 1 could possibly be extended, to state equivalence with the corresponding R-NS (not truncated) at all R (even if the stationary motion is laminar and there may be several attractors). This does not remain true if the equations are truncated at $|k_i| < N$ with N fixed: as it must be done in the simulations, and suitable consideration of the limits $R \to \infty$ may become essential.

(4) It is also possible to introduce thermostat forces which fix more than one constant of motion: a very interesting example is in the work [33] where the 3D NS equation, truncated at the Kolmogorov scale, is considered at high R. There a reversible friction acts so designed to enforce the value of the energy in *each momentum shell* to equal the value predicted by the OK $\frac{5}{3}$ law, [34]. The result is that the statistical properties of large scale observables in such reversible 3D NS are essentially the same as those in the simulations of the classical 3D NS equation truncated at the Kolmogorov scale. Actually, accepting the OK law, the Kolmogorov scale puts a natural truncation cut off (at $\sim R^{\frac{9}{4}}$ modes) and therefore the 3D NS equation is a natural arena where to formulate and test equivalence conjectures).

For instance the conjecture in Sec.2 would imply that the *single constraint* of constant total dissipation $\mathcal{D}(\mathbf{u})$ should give the same results as those of the mentioned experiment: a check would be interesting.

(5) The conjecture also suggests that the fluctuations of the phase space contraction $\sigma(\mathbf{u})$, given by the divergence of the reversible dissipation $\sigma(\mathbf{u}) = \mathrm{div}(\alpha(\mathbf{u})\Delta\mathbf{u})$ (which makes sense in any truncation of the equations), satisfies, in chaotic regimes, a fluctuation relation. If $\overline{\sigma}$ denotes the infinite time average of $\sigma(\mathbf{u})$ then the variable $p \stackrel{def}{=} \frac{1}{\tau}\int_0^\tau \frac{\sigma(\mathbf{u}(t))}{\overline{\sigma}} dt$ should have a probability density $P_\tau(p)$ verifying the property

$$\frac{1}{\tau}\log\frac{P_\tau(p)}{P_\tau(-p)} \underset{\tau\to\infty}{\sim} \kappa\, p\, \overline{\sigma} \tag{5.3}$$

where κ is a parameterless number: under strong chaoticity assumptions the above relation has been proposed in [35] for reversible systems. It is natural to ask whether the same variable $\sigma(\mathbf{u})$ follows the same (one parameter, *i.e.* κ) relation also in the I-NS.

It has been mentioned that in the case of the R-NS equations the $\sigma(\mathbf{u})$ is only formally defined: however the fluctuation relation is a property of the distribution of the running average $\frac{1}{t}\int_0^t \frac{\sigma(\mathbf{u}(t))}{\overline{\sigma}}$. And in a cut-off version

of the equation (*e.g.* setting $\mathbf{u_k}=0$ if $|\mathbf{k}|>N$ for some N as in the tests of Sec.4 above) from the expression of $\sigma(\mathbf{u})$ in R-NS, Eq.(2.6), it appears that in the ratio $\frac{\sigma(\mathbf{u})}{\overline{\sigma}}$ the divergent factors $\sum_{\mathbf{k}}\mathbf{k}^2$ *cancel* provided $\kappa\overline{\sigma}$ remains finite, so that it makes sense to check if a fluctuation relation holds.
Some checks of this property have been performed only in the case of the Lorenz96 model, [31].

(6) The very strong fluctuations of the reversible viscosity observed in the I-NS, see Fig.5 above, and the equivalence conjecture suggest that it might be of interest to establish a possible relation between the theory of the NS equation and its studies under stochastic forces: it would be interesting to study the NS equation with *fixed stirring* force $\mathbf{g}$ but with *random viscosity* with *average* $\frac{1}{R}$ and *distribution satisfying the fluctuation relation* (*e.g.* a simple Gaussian white process centered at $\frac{1}{R}$ and width determined by the fluctuation relation).

In this context it should be stressed that there is no theorem of existence and uniqueness of the R-NS equations (unlike the classical viscous NS equation, [34]) nor of stochastic NS equations with noise in the reversible viscosity (in the sense just proposed), even though here only 2D fluids are considered. The detailed work, [36], could suggest how to approach the problem.

(7) Periodic solutions to I-NS exist, as well as different chaotic stationary states that can be reached from different initial data, [37, 38, 39, 14, 40], particularly a low Reynolds numbers: in such cases the conjecture can still be formulated, see (3) above, by requiring that the extremal stationary states corresponding to a given R be in correspondence with equivalent extremal states with the same En, just as in the case of equivalent ensembles at phase transitions in statistical mechanics (cases in which it is also essential to consider the thermodynamic limit to obtain equivalence).

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