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Out of Equilibrium Solutions in the XY-Hamiltonian Mean Field model

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Abstract. - Out of equilibrium magnetised solutions of the XY-Hamiltonian Mean Field (XY-HMF) model are build using an ensemble of integrable uncoupled pendula. Using these solutions we display an out-of equilibrium phase transition using a specific reduced set of the magnetised solutions.

Long-range interactions are such that the two-body potential decays at large distances with a power–law exponent which is smaller than the space dimension. A large number of fundamental physical systems falls in such a broad category, including for instance gravitational forces and unscreened Coulomb interactions [1], vortices in two dimensional fluid mechanics [2–4], wave-particle systems relevant to plasma physics [5, 6], Free-Electron Lasers (FELs) [7–9] and even condensed matter physics for easy-axis anti-ferromagnetic spin chains, where dipolar effects become dominant. While for short–range systems only adjacent elements are effectively coupled, long-range forces result in a global network of inter-particles connections, each element soliciting every other constitutive unit. Clearly, from such an enhanced degree of complexity stems the difficulties in addressing the fascinating realm of long-range systems, for which standard techniques in physics, notably in the framework of equilibrium statistical mechanics, proves essentially inadequate. It is in particular customarily accepted that long–range systems display universal out-of-equilibrium features: Long-lived intermediate states can in fact emerge, where the system gets, virtually indefinitely, trapped (the time of escape diverging with the number of particles), before relaxing towards its deputed thermodynamic equilibrium. These are the so–called Quasi Stationary States (QSSs) which have been shown to arise in several different physical contexts, ranging from laser physics to cosmology, via plasma applications. A surprising, though general, aspect relates to the role of initial conditions of which QSS keeps memory. More intriguingly, such a dependence can eventually materialise in a genuine out-of-equilibrium phase transition: By properly adjusting dedicated control parameters which refers to the initial state, one observes the convergence towards intimately distinct macroscopic regimes (e.g. homogeneous/non homogeneous) [10, 11]. Recently, such phase transitions for systems embedded in one spatial dimension have been re-interpreted as a topological change in the single particles orbits [12]. This conclusion is achieved by performing a stroboscopic analysis of individual trajectories, which are being sampled at a specific rate imposed by the emerging time evolution of a collective variable and consequently sensitive to the intrinsic degree of microscopic self-organisation.

QSSs out of equilibrium regimes have been explained by resorting to a maximum entropy principle inspired to the Lynden-Bell's seminal work on the so-called *violent relaxation theory*, an analytical treatment based on the Vlasov equation and originally developed for astrophysical applications [13].

In this letter we shall provide a strategy to construct a whole family of out-of-equilibrium solutions with reference to the paradigmatic XY-Hamiltonian Mean Field (XY-HMF) model [14]. This procedure exploits the analogy with an ensemble made of uncoupled pendula and

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explicitly accommodate for self-consistency as a crucial ingredient. Even more importantly, out-of equilibrium phase transitions are displayed using a reduced set of the non-homogeneous (magnetised) solutions. The proposed approach is inspired by the observation that in the continuum limit (for an infinite number of particles) the discrete set of equations describing the physical system under scrutiny, converges towards the Vlasov equation, which governs the evolution of the one-particle distribution function.

The N-body Hamiltonian for the XY-HMF model with ferromagnetic interactions writes

$$H = \sum_{i=1}^{N} \left[\frac{p_i^2}{2} + \frac{1}{2N} \sum_{j=1}^{N} 1 - \cos\left(q_i - q_j\right) \right] , \qquad (1)$$

where p_i and q_i are respectively the (canonically conjugate) momentum and position of particle (rotor) i. To monitor the time evolution of the system, one can introduce the "magnetisation" as

$$\mathbf{M} = \frac{1}{N} \left(\sum \cos q_i, \sum \sin q_i \right) = M \left(\cos\varphi, \sin\varphi \right) . \qquad (2)$$

The equations of motion for the particles can be therefore cast in the form

$$\begin{cases} \dot{p_i} &= -M \sin\left(q_i - \varphi\right) \\ \dot{q_i} &= p_i \end{cases} , \qquad (3)$$

where the dot denotes the time derivative. Notice that it is tempting to imagine equations (3) as resulting from a set of uncoupled, possibly driven, one dimensional pendula Hamiltonian. Inspired by this analogy, we here intend to shed light onto the out-of-equilibrium dynamics of the original N-body model, by investigating the equilibrium properties of an associated pendula system. More specifically, let us imagine that the system of coupled rotators has reached some equilibrium state , such that in the $N \to \infty$ limit the magnetisation M of the XY-HMF model is constant and equal to m. Equations of motion (3) implies that the system formally reduces to an infinite set of uncoupled pendula. Our strategy to construct stationary solutions for (1) is to consider a finite ensemble of N uncoupled pendula whose Hamiltonian reads

$$H = \sum_{i=1}^{N} \frac{p_i^2}{2} + m(1 - \cos q_i) , \qquad (4)$$

and compute stationary solutions in the thermodynamic limit of this $m-$pendula system [15].

Given an initial condition each pendulum i is confined on a specific torus of the pendulum phase portrait depicted in Fig 1.

To build a stationary state we naturally consider the ergodic measure on the torus which originate from the pendulum motion and time averages. In order to proceed further in the analysis and due to integrability, we employ

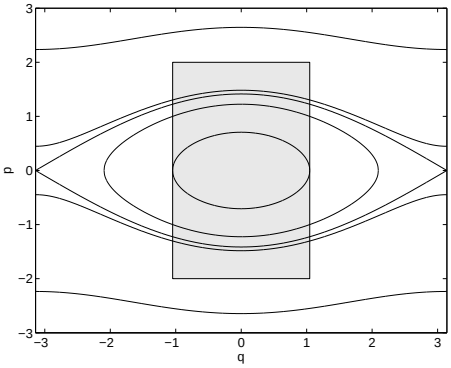

Fig. 1: Phase portrait of the pendulum for $m = 0.5$. The gray region is here used as a tool to estimate numerically the function g(I) as introduced in eq. (9). It is termed in the literature a water-bag and has no reference to the selected particles' initial condition.

the canonical transformation to the action-angle variables (I, θ) of the system (see for instance [16]). We thus obtain $H_m = H_m(I_i)$, with $\dot{\theta}_i = \partial H_m / \partial I = \omega(I_i)$, where I_i stands for the constant action, which is fixed by the initial state of the uncoupled pendulum i. For any selected initial condition, as time evolves, θ covers uniformly the circle $[-\pi, \pi[$, while the action I keeps its constant value. The ergodic measure reduces hence to $\rho_i(I, \theta) = \frac{1}{2\pi}\delta(I - I_i)$, which immediately translates in

$$\rho_E = \prod_{i=1}^{N} \rho_i , \qquad (5)$$

when considering an ensemble of N particles. Because of the above and since particles are identical and non interacting one can straightforwardly deduce the following expression for the one particle density function:

$$f(I, \theta) = \frac{g(I)}{2\pi} , \qquad (6)$$

where $g(\cdot)$ is a discrete valued function, solely determined by the selected initial conditions. In the limit $N \to \infty$, $g(\cdot)$ can change smoothly with the (continuous) action variable.

In order to get a stationary equilibrium solution of the system of pendula we can then consider a given positive and integrable function g, associate to it the function $f(I, \theta)$ according to (6). Then we perform an "inverse" transform to obtain an explicit expression for the one particle density function $\tilde{f}(p, q)$ as defined in the original phase space Γ_{pq}. This latter represents an equilibrium (time invariant) solution, and enables us to estimate any macroscopic observable, defined as a function of the sea of microscopic constituents. More concretely let us turn to consider the global magnetisation $\mathbf{M}$ as specified by eq. (2)). In the infinite N limit the time average of the magnetisation, which coincides with the ergodic-spatial aver-

age, reads:

$$\bar{\mathbf{M}} = \langle \mathbf{M} \rangle = \left(\int \tilde{f}(p,q) \cos q \, \mathrm{d}p\mathrm{d}q \, , 0 \right) \, , \qquad (7)$$

where the observation that $\tilde{f}$ is even in p and q has been used. Expressing the above in term action-angle variables, one can write

$$\bar{\mathbf{M}} = \langle \mathbf{M} \rangle = \left(\frac{1}{2\pi} \int g(I) \cos q(I,\theta) \, \mathrm{d}I \mathrm{d}\theta \, , 0 \right) \, . \qquad (8)$$

The integration over the angle can be performed (see Appendix), yielding to the final form

$$\begin{aligned} M &= \int_0^{\frac{8}{\pi}\sqrt{m}} g(I) \left(2\frac{E(\kappa)}{K(\kappa)} - 1 \right) \mathrm{d}I \\ &+ \int_{\frac{8}{\pi}\sqrt{m}}^{\infty} g(I) \left(1 + 2\kappa^2 \left(\frac{E(\kappa^{-1})}{K(\kappa^{-1})} - 1 \right) \right) \mathrm{d}I, \quad (9) \end{aligned}$$

with $\kappa = \kappa(I) = (H(I) + m)/2m$. Notice that if we consider an initial distribution given by $\tilde{f}$, then the magnetisation (9) stays constant as, by construction $\tilde{f}$ is stationary. In order to reconcile the m-model of uncoupled pendula to the XY-HMF interacting rotors, we need to impose the condition

$$\langle \mathbf{M} \rangle = m \, . \qquad (10)$$

Should there exist an $\tilde{f}$ for which equation (10) had an $m \neq 0$ solution, then we would have obtained a stationary solution of the system of pendula, which is in turn also magnetised stationary solution of the XY-HMF model in the $N \to \infty$ limit. Indeed the equations of motion for the system of pendula write

$$\left\{ \begin{array}{lcl} \dot{p}_i &=& -m \, \sin q_i \\ \dot{q}_i &=& p_i \end{array} \right. \, , \qquad (11)$$

and given the imposed condition (10) they are formally identical to (3) with a constant $\varphi = 0$. Note that the condition of the phase $\varphi = 0$, can be modified at will by a simple shift in the m-pendula Hamiltonian.

Such an out of equilibrium solution is displayed in Fig. 2, for a specific choice of the initial condition and output magnetisation amount. One typically recognises the underlying pendulum phase portrait, with each tori being differently populated according to the function $g(I)$. The non-uniformity of $\tilde{f}(p,q)$ on each torus stems from the nonlinearity of the transformation $q = q(I,\theta)$, $p = p(I,\theta)$.

As previously mentioned out of equilibrium, phase transition have been previously reported separating macroscopically distinct QSSs phases. These findings are here revisited in the framework of the proposed approach, which holds promise to generalise the conclusion beyond the water-bag regime so far inspected via the Lynden-Bell ansatz. The water-bag regimes correspond to initially assign the particles to populate, randomly and uniformly, a bound domain $[-q_0, \, q_0] \times [-p_0, \, p_0]$ depicted

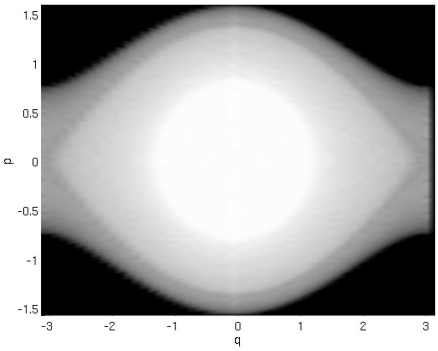

Fig. 2: Stationary out of equilibrium distribution $\tilde{f}(p,q)$ with $m = \langle M \rangle = 0.5$ obtained for $g(I)$ reconstructed from a waterbag with $q_0 = 2\pi/5$ and $p_0 = 1.37$.

in gray in Fig. 2. This latter initial condition is then univoquely specified by the magnetisation at time zero, namely $M_0 = \sin(q_0)/q_0$, and the energy per particle $U = p_0^2/6 + (1 - M_0^2)/2$. Notice that the water bag concept will be here invoked as a mere numerical strategy to calculate the needed function $g(I)$. We are hence not limiting the present analysis to a specific class of initial conditions, as e.g. done in [10], but we rather present a compelling evidence on the existence of a phase transition in a broader perspective.

Equation (10) is implicit in m parametrised through the initial conditions which enter the definition of the function g. Such an equation admits $m = 0$ as a trivial solution. One can then look for more general solutions of Eq. (10) with $m \neq 0$. Even though $\tilde{f}(p,q)$ water bag type is definitely not of, the water-bag type, as clearly depicted in Fig. 2, we have here decided to facilitate the forthcoming analysis, namely the calculation of the associated $g(I)$, by focusing on a finite portion of phase space as delimited by a water-bag window. This choice allows us to obtain a family of solutions monitored by the two same parameters, namely U and M_0. To construct $g(I)$ it is possible to analytically compute the length of the intersection of each tori with the water-bag (see Fig. 2), however we settled for a simple numerical procedure. Namely we consider a large ensemble of particles whose distribution approximates a waterbag, then for each particle and a given m we compute its corresponding action to construct an histogram of I and use it as an approximate form of $g(I)$. Finally we use this expression and check whether $m = \langle M \rangle$ and look for possible solutions. The drawback of this choice results in a dependence on the number N of particles used to construct the approximate waterbag wich may be important when we are close to the $m = \langle M \rangle = 0$ transition line. We however believe its accuracy is sufficient to present our point.

Results for different M_0 are depicted in Fig. 3. One can clearly appreciate the transition from a magnetised state to a non magnetised one, as well as a first order type of

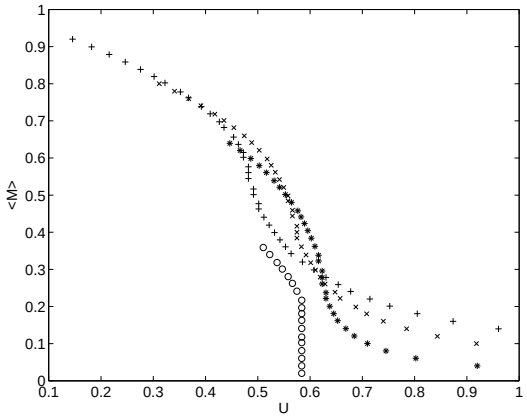

Fig. 3: Magnetisation $\langle M \rangle$ as a function of energy density U for different values of M_0. The symbols $+$, $\times$, $+$, $\circ$ correspond to non-zero solutions of the system of equations (9) and (10) computed respectively for $M_0 = 0.854, 0.637, 0.368, 0$. One can notice a dependence on M_0, as well as a first order transition for $M_0 = 0$. Computation of the function $g(I)$ is made using an approximate water-bag filled with $1.6\ 10^7$ particles. Note also that the that the transition point around $U = 0.59$ for $M_0 = 0$ is very close to that found, numerically in [10] probably because the initial condition is "closer" to a water-bag one when $M_0 = 0$.

transition for $M_0 = 0$.

A few comments are mandatory at this point. First, we insist on the fact that the phase space trajectories corresponding to derived solutions and its associated time evolution in Γ_{pq} apply to two, intrinsically different, dynamical systems, namely (1) and (4). Second, consider the average energy per particle $U = E/N$. We point out that the constants in Hamiltonians (1) and (4) are chosen in order to have 0 as a minimal value for the energy, which, in the thermodynamic limit, implies $U = 0$ for a zero temperature. Now focus on U_{HMF} for the XY-HMF model: We obtain $U_{HMF} = T/2 - M^2/2 + 1/2$, while for the pendula one gets $U_p = T/2 - M^2 + M$. Here, in both cases, $T/2$ is the average kinetic energy per particle. Different energies are thus associated to the same trajectory, depending on the dynamical system that is being chosen to generate it. In order to reconcile the two models one can infer that the chemical potential of the particle is different, yielding to $\delta\mu = \delta U = (M-1)^2/2$ for respectively the integrable uncoupled model and the globally coupled one. Moreover, solutions with constant $M = m = 0$ do correspond to a one dimensional perfect gas: the observed phase transition can hence be seen as a sort of sublimation.

In conclusion, with reference to the XY-HMF model, we have designed an analytical scheme which allows to identify all possible stationary solutions with constant magnetisation $\mathbf{M}$ using a set of integrable uncoupled pendula. This includes as a subset the celebrated QSSs, which are therefore formally understood within a consistent mathematical framework. Following these lines, it can be inferred that the out of equilibrium states predicted by the statistical mechanics scenario pioneered by Lynden-Bell [11], should belong to the class of solutions here displayed. We are then providing de facto a testbed for accuracy of the controversial Lynden-Bell theory [13]. Note though that the stability of the solutions has not been discussed, it is currently under investigation and is likely to provide further restrictions on the possible out of equilibrium stationary states.

* * *

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Appendix. – We shall here review the main mathematical tools which are employed in the above derivation. When it comes to the pendulum motion, trapped orbits (libration) are characterised by:

$$\begin{aligned} q &= 2\sin^{-1}\left[\kappa sn\left(\frac{2K(\kappa)\theta}{\pi},\kappa\right)\right] \\ I &= \frac{8}{\pi}\sqrt{m}\left[E(\kappa) - \kappa'^2 K(\kappa)\right] \\ \langle\cos q\rangle &= 2\frac{E(\kappa)}{K(\kappa)} - 1 \end{aligned}$$

while for the untrapped ones (rotation) the following relations hold:

$$\begin{aligned} q &= 2am\left(\frac{2K(1/\kappa)\theta}{\pi},\kappa^{-1}\right) \\ I &= \frac{8\kappa}{\pi}\sqrt{m}E(1/\kappa) \\ \langle\cos q\rangle &= 1 + 2\kappa^2\left(\frac{E(\kappa^{-1})}{K(\kappa^{-1})} - 1\right) \end{aligned}$$

with $\kappa^2 = (h+m)/2m$. Here $< \cdot >= \int_0^{2\pi} \cdot \mathrm{d}\theta/(2\pi)$.

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