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Topological aspects of a long-range model

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Abstract

The mean field XY Hamiltonian, a suitable model for studying long-range interactions in extended systems, presents, amongst other interesting features, slow relaxation and formation of quasi-stationary (QS) states. It is now known that, along these QS trajectories, the system visits critical points (maxima) of the potential energy function, characterized by a large number of directions with marginal stability. This observation may provide an interpretation for the slow relaxation dynamics and the trapping in such trajectories. In this paper we present further results and discussion on topological aspects of the model.

Keywords: Long-range interactions; Quasi-stationary states

One of the simplest classical Hamiltonian models of many particles coupled with long-range interactions is the so-called *Hamiltonian mean field* (HMF) model [1]. It consists of a set of N interacting particles or rotors of unitary mass, each one confined to move around its own unitary circle. Each particle i is then mechanically described by an angle θ_i and its corresponding conjugate momentum p_i. The dynamics is ruled by the Hamiltonian:

$$H = \frac{1}{2}\sum_i p_i^2 + \frac{1}{2N}\sum_{i,j}[1-\cos(\theta_i-\theta_j)] \equiv K + V. \tag{1}$$

We can associate to each particle a two-dimensional local magnetization vector $\vec{m}_i = (\cos\theta_i, \sin\theta_i)$ and correspondingly a global order parameter $\vec{M} = (M_x, M_y) = (1/N)\sum_i \vec{m}_i$. At energies per particle above $\varepsilon = 3/4$, the equilibrium state is disordered (with $M = |\vec{M}| = 0$ in the thermodynamic limit), while the system orders below the critical energy.

Despite its simplicity, the model displays a rich variety of complex dynamical behaviors [2–5], mimicking aspects of real systems. One particular feature that is specially worth recalling here is the fact that, depending on the initial conditions, and for energies below the critical one, the system may become trapped into non-equilibrium quasi-stationary (QS) trajectories. Along these QS solutions, whose lifetimes diverge in the limit $N \to \infty$ [2], the time average of any thermodynamical quantity does not coincide with the value predicted by

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canonical thermostatistics calculations. The analysis of this complex phenomenology has deserved extensive research and healthy controversy. Particularly intriguing is the question on whether it is possible or not to construct a measure theory able to predict the stationary values of physical observables in long-standing out-of-equilibrium regimes [6].

Recently, in collaboration with other authors [7], we have shown that the slow relaxation can be understood in terms of the topology of the potential energy function: the system cannot attain true equilibrium because it gets trapped in the vicinity of critical points (CPs) of $v = V/N$. In fact, the complex non-equilibrium QS regime observed just below the critical energy, when the system is prepared in "water-bag" initial conditions (with all the rotors aligned along one axis and the momenta drawn from a uniform distribution), can be interpreted from a topological point of view. In this paper we will show complementary details related to this perspective.

Our analysis focuses on the topology of the surface defined by the potential energy in the configuration space. The HMF potential energy can be written in terms of the order parameter of the system as $V = (N/2)(1 - M^2)$. Then, it is clear that the potential energy per particle takes values in the interval $0 \leqslant v \leqslant v_c \equiv 1/2$. The lower limit corresponds to the case of the fully ordered configurations (hence $M = 1$) and the upper bound to a completely disordered configuration. Let us get some feeling on the topology of the potential energy function and on the way it is visited along the dynamics. In the case $N = 2$, the potential can be represented as a function of the two spatial coordinates in a 3D plot (Fig. 1(a)). If initially $\theta_1 = \theta_2 = 0$ and $p_1 = -p_2$, as for water-bag initial conditions, and because of momentum conservation, then $\theta_1 = \theta_2$ for all time. Therefore, the evolution will occur along the dotted line. For small energy the system will be confined in a minima while for large enough energy the movement is unbounded and the system will alternatively visit maxima and minima of the potential. In the vicinity of a maximum of the potential, the kinetic energy is minimal, then the system will move more slowly and spend more time in that neighborhood. The influence of increasing the number of particles is represented in Fig. 1(b), for $N = 10$, where the remaining $N - 2$ angles were fixed at random values in $(-\pi, \pi]$. The plot is representative of that obtained for larger N and also for other values of the fixed variables. The landscape is similar to that for $N = 2$ except that the flat valleys and cusps became curved. We will see next that for large systems, at either high energies (disordered phase) or at QS states close below the phase transition, energy valleys (corresponding to fully magnetized states) are never visited and the dynamics occurs in the vicinity of the maxima of the potential.

Integration of the equations of motion for large system size ($N = 500$) yields plots for the potential per particle v as a function of time as the one displayed in Fig. 2. It is clear that, both for QS states at $\varepsilon = 0.69$ and for equilibrium states at $\varepsilon = 5.0$ (well above the critical value), maxima of the potential are frequently visited while dynamical configurations remain far from the minima. However, for $\varepsilon = 0.69$, at equilibrium, the system does not visit the maxima and fluctuates around the canonical value.

The points in configuration space for which all the N derivatives of v vanish, i.e., $\partial v/\partial\theta_i = 0$, for $i = 1, \ldots, N$ are CPs. Writing the derivatives of the potential in terms of the two components of the order parameter,

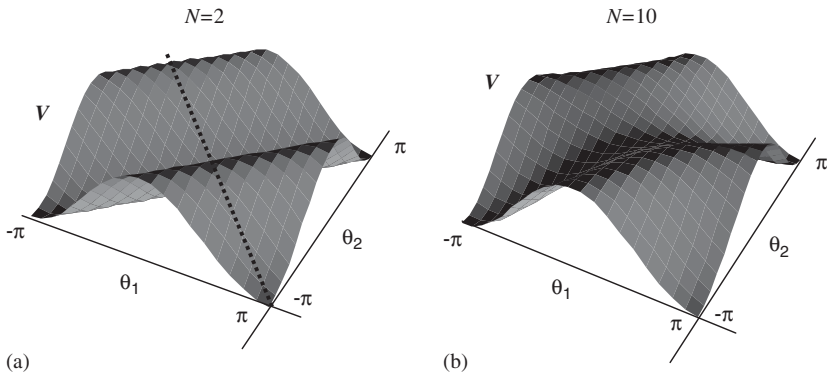

Fig. 1. Potential energy as a function of two spatial coordinates (a) for $N = 2$, and (b) for $N = 10$, in the latter case, the remaining coordinates are kept fixed at representative values.

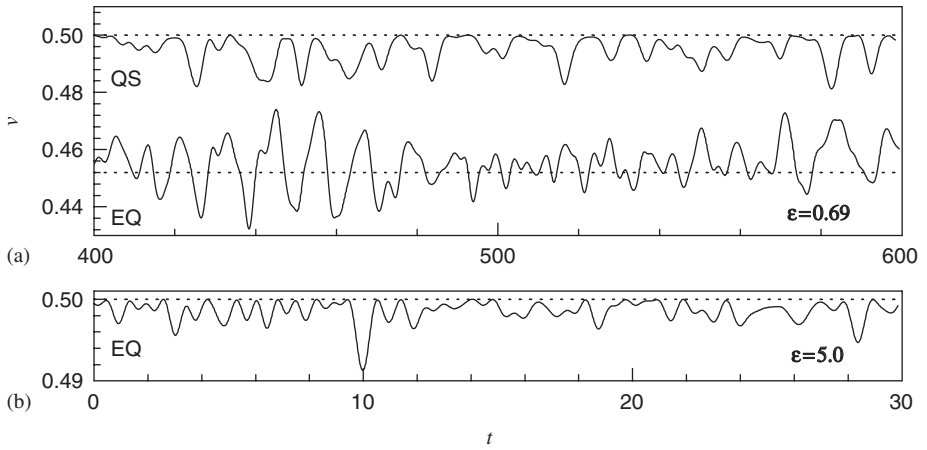

Fig. 2. Potential energy per particle v for $N = 500$ as a function of time, for energies indicated in the figure. Initial conditions are either water-bag (to yield QS), or equilibrium ones after a long transient to warrant that equilibrium (EQ) has been attained. In the time window chosen in (a) the system is in a QS state. Dotted lines correspond to values in the thermodynamic limit.

$\partial v/\partial\theta_i = (M_x \sin\theta_i - M_y \cos\theta_i)/N$, it is obvious that all the derivatives vanish for configurations with null magnetization (hence with maximal potential energy). Therefore, those configurations correspond to CPs.

Numerical simulations for large N (typically $N \geqslant 500$) have shown the following results [7]: Both in the disordered high-energy phase (well above the critical energy $\varepsilon = 3/4$) and in QS states close below the critical energy, the system visits CPs of the potential that correspond to $v = 1/2$ (hence $M = 0$). This conclusion resulted from the measurement of $\lambda = \max_i |\partial v/\partial\theta_i|$ and the observation that $\lambda = 0$ occurs only when $M = 0$.

CPs can be classified according to the eigenvalues of the Hessian of v [8]. The CPs visited along the dynamics in the cases here considered correspond to $v = v_c$, hence they are characterized by null magnetization. Straightforwardly, the Hessian of the potential energy v, when $M = 0$, can be written as

$$\mathbf{H} = -\frac{1}{N^2}\,(\mathbf{1} + \mathbf{A}) \quad \text{where } A_{kl} = (1 - \delta_{kl})\cos(\theta_k - \theta_l). \tag{2}$$

Both in the high-energy phase and in QS states, the distribution of angles at CPs is approximately uniform [5]. For regularly distributed angles in the interval $(0, 2\pi]$, i.e., $\theta_k = 2\pi k/N$, $k = 1, \ldots, N$, yielding $M = 0$, the eigenvalues H_l, with $1 \leqslant l \leqslant N$, of the Hessian matrix are such that

$$-N^2 H_l = \begin{cases} 1 + \cos(\pi l) + 2\sum_{r=1}^{N/2} \cos(2\pi r l/N)\cos(2\pi r/N) & \text{for even } N, \\ 1 + 2\sum_{r=1}^{(N-1)/2} \cos(2\pi r l/N)\cos(2\pi r/N) & \text{for odd } N. \end{cases} \tag{3}$$

Thus, the only non-null eigenvalues are $H_1 = H_{N-1} = -1/(2N)$. This means that at these CPs there are two unstable directions and $N - 2$ marginal ones. This picture remains valid for more general configurations with vanishing magnetization. Symmetrically distributed clusters of rotors, yielding $M = 0$, also present two negative eigenvalues, while the others are null, except for the bi-cluster configuration for which there is only one (negative) non-null eigenvalue. Also randomly chosen angles in $(0, 2\pi]$ yield two eigenvalues with values close to $-1/(2N)$ and the remaining $N - 2$ vanishing ones. Some illustrative examples are given in Fig. 3 for $N = 8$.

In conclusion, we have presented additional information on topological aspects which can contribute to interpret the complex relaxational dynamics of the HMF, a paradigm of long-range couplings. From this perspective it is clear that in QS states, as well as in the high-energy phase, the system wanders visiting CPs of the potential energy function characterized by many flat directions, as arises from the linear stability analysis.

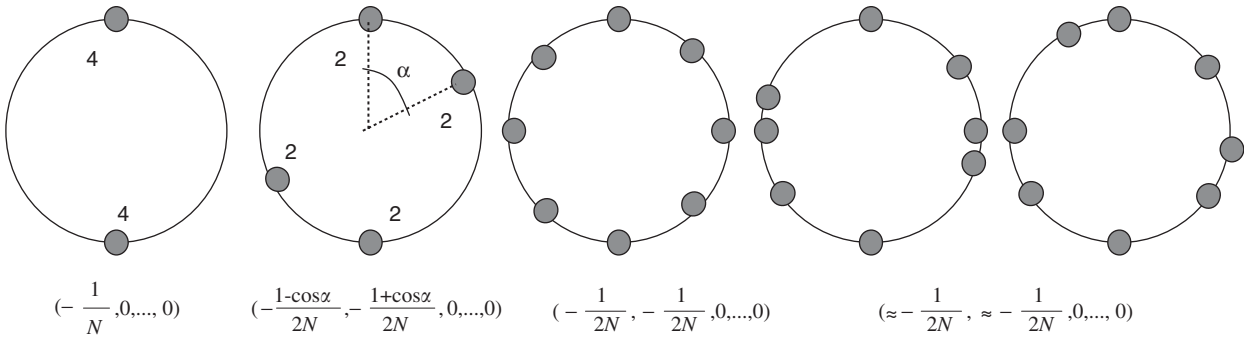

Fig. 3. Different configurations of rotors with null magnetization, for $N = 8$, and the corresponding eigenvalues of the Hessian matrix of the potential.

The flat landscape in the vicinity of CPs may justify the slow relaxation dynamics [4] observed both in QS states and in the high-energy phase.

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